On Thermal Ionization for Open Quantum Systems

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Zusammenfassung

Die vorliegende Arbeit behandelt das Phänomen der Ionisierung eines idealisierten Atoms durch ein umgebendes unendlich ausgedehntes quantisiertes elektromagnetisches Feld positiver Temperatur. Nach dem Planck'schen Strahlungsgesetz erwartet man in einer solchen Situation Photonen mit beliebig hoher Energie, die irgendwann die Ionisierungsschwelle des Atoms überwinden. Mathematisch interpretieren lässt sich dies durch die Abwesenheit von zeitlich invarianten Zuständen in einem geeigneten dynamischen System.

Derartige Probleme können mittels des selbstadjungierten Generators der Zeitentwicklung, des Liouvillians L, in eine spektraltheoretische Fragestellung überführt werden. Konkret genügt es zu zeigen, dass L keinen Eigenwert Null besitzt. Eine geläufige Technik für solche Zwecke stellt die Methode der positiven Kommutatoren dar, bei der es darum geht, einen selbstadjungierten Operator A zu finden, für den

$$\mathrm{i}[L, A] > 0$$

erfüllt ist. Mit einem geeigneten Virialtheorem lässt sich dann schließen, dass L keine Eigenwerte besitzen kann.

Das Ziel dieser Dissertation besteht im Beweis von thermischer Ionisierung für eine Klasse von konkreteren Modellen mit weniger Einschränkungen, als dies in früheren Arbeiten der Fall war. Es wird ein QED-ähnlicher Kopplungsterm mit räumlichen Abfall und ein idealisiertes Atom in Form eines Schrödinger-Operators betrachtet. Dann werden zwei verschiedene Klassen von Modellen unterschieden: zum einen Potentiale mit unendlich vielen gebundenen Zuständen, bei denen nur endlich viele in der Kopplung berücksichtigt werden, zum anderen kompakt getragene glatte Potentiale mit endlich vielen gebunden Zuständen, bei denen keine weiteren Einschränkungen in der Kopplung notwendig sind. Der Beweis im ersten Fall erfolgt ähnlich vorheriger Arbeiten mittels positiver Kommutatoren und jeweils dem Generator der Translation und der Dilatation auf dem Feld bzw. Atom. Im zweiten Fall werden als neue Methode Dilatationen im Raum der verallgemeinerten Eigenfunktionen des Schrödinger-Operators verwendet. Über eine approximative Form von Fermis Goldener Regel erhält man das Resultat in jedem beschränkten Temperaturbereich für Kopplungskonstanten unabhängig von der Temperatur.

Abstract

This thesis addresses the phenomenon of ionization of an idealized atom by a surrounding infinitely extended quantized electromagnetic field at positive temperature. According to Planck's law one expects photons with arbitrary high energy, which eventually exceed the ionization threshold of the atom. Mathematically, this can be interpreted as the absence of time-invariant normal states in a suitable dynamical system. Such problems can be converted into a spectral-theoretical question by means of the self-adjoint generator of the time evolution – the Liouvillian L. In this setting it suffices to show that zero is not an eigenvalue of L. The goal of this thesis is the proof of thermal ionization for more concrete models with less restrictions than in previous works, including a QED-like coupling term with a spatial decay and an idealized atom, given as Schrödinger operator. With respect to the atom it will be differentiated between two cases: first, potentials with infinitely many bound states, but only finitely many coupled to the field, and second, compactly supported smooth potentials. For the latter there are, apart from the spatial decay, no further artificial restrictions required in the coupling. The proof is based on positive commutators. On the field it uses the generator of translations, and for the atom the generator of dilations (first case) or the generator of dilations in the space of scattering functions (second case). By means of an approximated version of Fermi's Golden Rule one obtains a uniform result in every bounded temperature range.

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Contents

1. Introduction

This thesis is dealing with a problem within the large field of open quantum systems, that is, a 'small' quantum mechanical system interacting with its environment, modeled as a large infinitely extended heat reservoir. This is the common approach for many realistic scenarios, as in practice it is not possible to accomplish a perfect isolation of a system, and moreover, it is not feasible and also not interesting to describe its complete macroscopic dynamics. Most recently, the concept of open quantum systems seems to draw more attention due to the growing field of quantum information theory and quantum computing. There, the unavoidable perturbation of the very fragile systems leading to decoherence and relaxation is a major challenge.

We consider the model of an idealized atom being subject to radiation emitted by the environment, an electromagnetic quantized field. The latter is supposed to be in thermal equilibrium at a certain positive temperature, thus emitting photons according to Planck's probability distribution of black-body radiation. Since there is a positive probability for arbitrary high energy photons, eventually one with sufficiently high energy will show up exceeding the ionization threshold of the atom. This will cause an ionization and the corresponding phenomenon is also called *thermal ionization*.

This problem was studied in a rigorous mathematical manner by Fröhlich and Merkli in [FM04b] and in a subsequent paper [FMS04] by the same authors together with Sigal. They constructed a W^*-dynamical system describing the dynamics of the composite system in the setting of quantum statistical mechanics, and they showed under certain conditions the absence of time-invariant normal states, which can be interpreted as the actual ionization of the atom.

The basic strategy is that the time-invariant states can be shown to be in one-to-one correspondence with the elements of the kernel of the *Liouvillian*, also sometimes called *Thermal Hamiltonian*. The latter denotation already indicates that this is the operator generating the time evolution in a certain representation. This is given by the Gelfand–Naimark–Segal construction with respect to the equilibrium state of the reservoir and an arbitrary reference state of the atom. Thus, in order to show that thermal ionization occurs, one has to rule out that zero is an eigenvalue of the Liouvillian.

Therefore, the problem reduces to a spectral-theoretical question, namely proving the absence of eigenvalues embedded in the continuous spectrum of a self-adjoint operator. There are two common techniques to tackle this problem. One of them is the method of complex deformations of the operator, which bend down the continuous spectrum into the imaginary plane and reveal the eigenvalues on the real line (and the resonances in the complex plane). In the second approach one uses positive commutators, which originates from MOURRE ([Mou81]) and can be regarded as an infinitesimal version of complex deformations. The basic principle works as follows. If L is a self-adjoint operator, E is an eigenvalue of L with corresponding eigenvector ψ, and A is another self-adjoint operator (the so-called *conjugate operator*), a formal calculation neglecting any domain problems yields

$$\langle \psi, [L, A]\psi \rangle = \langle L\psi, A\psi \rangle - \langle A\psi, L\psi \rangle = E \langle \psi, A\psi \rangle - E \langle A\psi, \psi \rangle = 0.$$

This relation is in fact non-trivial for unbounded operators and is also called *virial theorem*. On the other hand, if one can show that $\mathrm{i}[L, A]$ is strictly positive, this yields a contradiction. While complex deformations often yield stronger results and enable the study of resonances, they also require stricter assumptions, in particular, analyticity of the potentials and coupling functions. In this thesis we follow [FM04b; FMS04] and use the positive commutator method.

Goal and comparison with previous results

In [FM04b] the atom was represented in an abstract way by a Hamiltonian in diagonal form with respect to the energy with a single negative eigenvalue. For the proof certain regularity assumptions on the interaction with respect to the energy were imposed. However, it was not shown how these assumptions translate to a more concrete setting, in particular, to Schrödinger operators and typical coupling functions which appear in quantum electrodynamics. As in [JP96b] they used the generator of translations with respect to the momentum in the field space as conjugate operator, and the generator of translations with respect to the energy on the atomic space. Furthermore, they developed a novel virial theorem for the positive temperature setting where L is not bounded from below.

The second paper [FMS04] covers the case of a Schrödinger operator admitting a certain class of potentials including the Coulomb potential which always yield infinitely many (or no) bound states with an accumulation at zero. However, the authors admit only finitely many modes to be coupled via the interaction. Moreover, the coupling is additionally restricted to a compact interval away from zero on the essential (positive) spectrum of the atom, that is, a cutoff is imposed for low and high energies. In the proof they utilized the same virial theorem and the same conjugate operator on the field space as in the preceding paper. However, they choose the generator of dilations in combination with a cutoff for high energies on the atomic space instead, which leads to the constraints with respect to the admissible class of potentials and the cutoff near zero.

Both results are not uniform in the temperature. More precisely, the maximal coupling strength, where the proof is still feasible, decays exponentially fast to zero when the temperature tends to zero. Furthermore, they require a special class of coupling terms which does not include couplings appearing in quantum electrodynamics.

The general goal of this thesis is to establish a similar result as in [FM04b; FMS04] for a specific model with less restrictions. It basically consists of two parts.

The first one can be regarded as partial extension of the results in [FMS04]. Most importantly, we can lift the restrictions with respect to the essential spectrum with a partially new proof for the positivity of the commutator. The basic approach, namely the choice of the conjugate operators, is essentially the same as in [FMS04]. However, a refined analysis, an additional auxiliary term on a part of the vacuum subspace and using the localization of the relevant error terms in combination with a Birman-Schwinger argument enables us to avoid the cutoff near zero. Our proof relies on rather elementary operator inequalities and does not need the Feshbach method as in [FMS04].

The physically less relevant cutoff for high energies (in this non-relativistic setting) is removed by means of a modification of the cutoff in the conjugate operator. This requires a review of the tedious verification of the conditions for the virial theorem. Finally, we get a uniform result for a bounded temperature range if we assume an approximated version of the Fermi Golden Rule condition. We also consider some more general (still linear) coupling terms, and we give an explicit example. There, one has to impose a (non-physical) spatial cutoff which arises due to the generator of translations on the field.

It should be emphasized that our approach could not remove the restriction of only finitely many coupled eigenmodes, yet. Thus, the important example of a hydrogen atom without any restrictions in the coupling remains to be an open problem. Nevertheless, the verification of the conditions of the virial theorem as well as the proof for the positivity of the commutator is presented in some generality and the requirements are stated in form of hypotheses. This could possibly facilitate further work in this direction.

The second part of this thesis corresponds to [HS20], which was joint work with David Hasler, and covers the case of potentials with finitely many bound states, which could not be treated by the former approach. More precisely, up to now we can control only compactly supported potentials which are sufficiently smooth. Here one can work with a similar proof as before and the artificial restriction to finitely many eigenmodes in the coupling can be dropped. The proof differs in the way that the generator of dilations for the atom is replaced by the generator of dilations in the scattering space, that is, where the positive part of the Hamiltonian of the atom is diagonal with respect to its generalized eigenfunctions. The difficulty lies now in the verification of the assumptions for the virial theorem. One has to compute the transformation of the coupling functions and their commutators in the scattering space, and has to prove that they are sufficiently bounded. However, the proof of positivity is similar as before. As a consequence we can present an explicit model of a toy atom with finitely many bound states and, apart from the spatial cutoff, no further unnatural restrictions in the coupling, which exhibits the behavior of thermal ionization.

For the sake of convenience we refer to the first part for potentials with infinitely many eigenvalues as the 'long-range' (LR) case and the second one with the compactly supported smooth potentials as the 'short-range' (SR) case. Note that these notions are not completely consistent with their typical use in scattering theory. Our LR case also comprises potentials decaying as $|x|^{-\mu}$, $1 < \mu < 2$ at spatial infinity, which are usually called 'short-range' in the sense of scattering theory. On the other hand, our SR case covers only a subset of all 'short-range' potentials in the sense of scattering theory.

Related work in the literature

A lot of mathematically rigorous papers about small systems interacting with an infinitely extended environment appeared in the last 20-30 years. In a large part of them the behavior of thermal relaxation or *return to equilibrium* was analyzed. This can be regarded as analog for thermal ionization in case that the small system is a confined particle or a finite-level system without any continuous spectrum. That is, the system will eventually reach an equilibrium state by permanent exchange of heat of the small system with the environment. The difference to our situation in these cases is the existence of a Gibbs state due to the absence of continuous spectrum. However, the underlying spectral problem and the appropriate technical methods are similar. Instead of proving that zero is not an eigenvalue, one has to show that the degeneracy of the eigenvalue zero is lifted if the system is coupled to the environment.

An important milestone for concrete systems was set in a series of papers [JP95; JP96a; JP96b; JP97] by Jakšić and Pillet, who considered a single spin coupled to a bosonic reservoir. They drew the connection between the dynamical properties of the system and the spectral properties of the Liouvillian and their proof established the method of translations in the glued Fock space as a new complex deformation technique.

Subsequently, Bach, Fröhlich and Sigal treated similar models in [BFS00] with fewer restrictions. In particular, they could prove return to equilibrium uniformly in the temperature. Their proof relies on complex dilations rather than translations and uses the renormalization group method of [BFS98b].

Merkli applied in [Mer01] for the first time the concept of Mourre's positive commutators in the setting of open quantum systems. Like Jakšić and Pillet he also used the generator of translations in the glued Fock space. His approach was particularly inspired by the methods in [Bac+99] for temperature zero. He could made further progress in a subsequent paper [FM04a], especially a uniform result for bounded temperatures. Another application of positive commutators in this context appeared by Dereziński and Jakšić in [DJ03; DJ01], where they used positive commutators for the reduced Liouvillian orthogonal to the vacuum and combined it with the Feshbach method.

Furthermore, Merkli studied in [Mer05] a thermal reservoir consisting of a very dense or very cold Bose gas containing a Bose-Einstein condensate. Here return to equilibrium could be proven in a rather weak sense, applying positive commutators as well. Another example, a harmonic and anharmonic oscillator as small system was considered by Könenberg in [Kön11a; Kön11b].

A similar situation as in the case of thermal ionization occurs if one considers a small finite-dimensional or confined system coupled to multiple reservoirs at different temperatures, namely, the non-existence of equilibrium and time-invariant states of the composite system. This was first investigated by Jakšić and Pillet for fermionic reservoirs in [JP02] and by Dereziński and Jakšić in [DJ03] for bosonic reservoirs. An improvement of the latter with a uniform result for low temperatures and small temperature differences of the reservoirs was given by Merkli, Mück, and Sigal in [MMS07a]. There appears the same spectral-theoretical problem as in our case, namely whether zero is an eigenvalue of the corresponding Liouvillian. Moreover, by studying the resonances of the Liouvillian (e.g. with complex deformations) it is possible to identify so-called non-equilibrium stationary states (cf. [MMS07b]), which exhibit a stability condition similar to 'return to equilibrium'.

Both thermal ionization and return to equilibrium have a zero temperature counterpart. For the latter this is the return to the ground state under emission of radiation (cf. [BFS98a; BFS99; Sig11]), where the resonances correspond so-called metastable states ([Müc04a]). For thermal ionization this is the well-known photoelectric effect as it was already predicted by Einstein ([Ein05]): An atom can only be ionized if the energy of the incoming photon exceeds the ionization threshold. A first mathematically rigorous qualitative and quantitative elaboration of this phenomenon was given in [BKZ02] by Bach, Klopp and Zenk for a very simplified model of an atom with one bound state. Their results could be extended in subsequent work by Zenk ([Zen08]) and by Zenk together with Griesemer ([GZ09]) to more realistic models including the hydrogen atom and couplings which appear in non-relativistic quantum electrodynamics.

Organization of the thesis

In Chapter 2 the open quantum system is derived in a heuristic way from a zero temperature model with general coupling terms by means of operator algebras. We construct the interacting dynamics on a von Neumann algebra of the composite system and introduce the Liouvillian. The main goal is to establish in our setting the well-known correspondence between time-invariant normal states in that algebra and zero eigenmodes of the Liouvillian.

The main results Theorem 3.5 and Theorem 3.8 are presented in Chapter 3. The technical requirements, which have to be imposed on the atom and the coupling, are stated in the same chapter at the beginning. Furthermore, some models are described where these requirements are satisfied, the most explicit one for the SR case in Corollary 3.10. At the end we discuss several open problems and possible starting points for further work. Subsequently, Chapter 4 provides a formal sketch of the proof and an orientation where its ingredients can be found. It also recalls the concept of the gluing transformation with the corresponding notation and the abstract virial theorem of [FM04b; FMS04].

Then it follows the exact specification of the conjugate operators and the first part of the proof, the verification of the assumptions of the abstract virial theorem. It is divided into the LR case in Chapter 5 and the SR case in Chapter 6. The latter is significantly more extensive due to the estimates of the interaction terms in the scattering space in Section 6.4.

The second part of the proof, the positivity and error estimates for the commutator together with the auxiliary term, is contained in Chapter 7. The last and the final part is carried out once more separately for the LR case (Section 7.3) and the SR case (Section 7.4).

Some preliminaries about Fock spaces and operator algebras and the corresponding notation, which is used throughout this thesis, are stated in Appendix A. appendix B contains some technical requirements and variations of well-known techniques like Combes Thomas estimates and Birman-Schwinger bounds, which are required in this form in some of the proofs. Additionally, basic symbols and notation which are used throughout this thesis can be found in the nomenclature at the end.

2. Description of the Model

This chapter introduces the positive temperature model of an atom represented by a Schrödinger operator interacting with a quantized bosonic field. The goal is the construction of an algebraic (W^*-dynamical) system describing the dynamics and to find its self-adjoint generator – the Liouvillian, which in particular encodes the time-invariant states of the system. This is the content of Theorem 2.15, which provides the motivation for studying the kernel of the Liouvillian in the further course of this thesis.

The setting can be derived in a heuristic way from a zero temperature model – in our case the Nelson model (first studied in [Nel64]), one of the simplest models for describing the interaction of an uncharged non-relativistic particle interacting with a relativistic spinless bosonic field, e.g. consisting of phonons. Its Hamiltonian

$$H_{\mathrm{p}} \otimes \mathrm{Id}_{\mathrm{f}} + \mathrm{Id}_{\mathrm{p}} \otimes H_{\mathrm{f}} + \lambda(a(G) + a^*(G)) \tag{2.1}$$

is defined on the Hilbert space $\mathcal{H}_{\mathrm{p}} \otimes \mathfrak{F}(L^2(\mathbb{R}^3))$, where H_{p} is a self-adjoint operator on a Hilbert space $\mathcal{H}_{\mathrm{p}}$, typically a Schrödinger operator, $H_{\mathrm{f}} := \mathsf{d}\Gamma(\omega)$, $\omega(k) := |k|$ is the field energy, and

$$G \colon \mathbb{R}^3 \longrightarrow \mathcal{L}(\mathcal{H}_{\mathrm{p}}) \tag{2.2}$$

is a measurable, square-integrable function, which describes the coupling to the field.

The strategy is as follows. First, we consider the free bosonic field in its algebraic form as Weyl C^*-algebra. Then we identify its equilibrium state at a certain inverse temperature $\beta > 0$, which can be characterized by the KMS condition. The GNS construction with respect to this state yields the so-called Araki-Woods representation of the Weyl C^*-algebra. This can be combined with the GNS construction with respect to an arbitrary reference state on the full algebra of bounded operators on the atomic space. Subsequently, we consider the weak closure of the representation to obtain a von Neumann algebra, which enables us to define the dynamics of the interacting system using the free dynamics and the interaction term in (2.1) of the zero temperature model. By means of modular theory for von Neumann algebras one can then draw the connection between time-invariant normal states and the kernel of the standard Liouvillian.

This approach can be found in different variations in the literature, however mainly for atoms with purely discrete spectrum or N-level atoms, see for instance [DJP03; JP96b; Kön11a; BFS00; Müc04b; AJP06]. Our version can be regarded as a mild modification of [FM04b; FMS04] with an extension to general types of coupling terms. Some of the presented material is also inspired by [Müc04b].

In the following we will use the notation for bosonic Fock spaces and second quantization as given in Appendix A.1. Further more elementary symbols can be found in the nomenclature.

2.1. The Algebra of the Free Field

We first describe the Weyl C^*-algebra of the free field, which implements the canonical commutation relations in exponential form for bosons with arbitrary many degrees of freedom.

Definition 2.1 (Weyl C^*-algebra)
Let $\mathfrak{h}$ be a Hilbert space. The universal C^*-algebra (cf. [Bla06, section II.8.3.1] for the notion of a universal C^*-algebra) generated by elements $W(f)$, $f \in \mathfrak{h}$, satisfying the so-called Weyl relations

$$W(-f) = W(f)^*, \qquad W(f)W(g) = e^{-\mathrm{i}\,\mathrm{Im}\langle f,g\rangle/2} W(f+g), \qquad f, g \in \mathfrak{h},$$

is called Weyl C^*-algebra $\mathfrak{W}(\mathfrak{h})$.

It is well-known that such an algebra can be constructed explicitly and it can be also generalized to symplectic spaces (cf. [Mor13, section 14.2.2]). By definition the Weyl C^*-algebra has the following universal property: If there is another C^*-algebra $\mathfrak{W}'$ with elements $W'(f)$, $f \in \mathfrak{h}$, satisfying the Weyl relations, then there is a unique injective $*$-morphism $\phi\colon \mathfrak{W}(\mathfrak{h}) \to \mathfrak{W}'$ such that $\phi(W(f)) = W'(f)$ for all $f \in \mathfrak{h}$. One can show that $\mathfrak{W}(\mathfrak{h})$ is simple (cf. [Mor13, Theorem 11.26]), that is, in particular, every non-trivial representation is faithful.

The most prominent representation of the Weyl C^*-algebra is the standard Fock representation corresponding to systems at zero temperature. For $f \in \mathfrak{h}$ we define

$$\pi_{\mathfrak{W}}(W(f)) := \widehat{W}(f) := \exp\left(\mathrm{i}\frac{1}{\sqrt{2}}\Phi(f)\right) \in \mathcal{L}(\mathfrak{F}(\mathfrak{h})),$$

where $\mathfrak{F}(\mathfrak{h})$ denotes the bosonic Fock space over $\mathfrak{h}$ (definition A.1) and Φ the field operator (A.1). By direct computation one can show that the elements $\widehat{W}(f)$, $f \in \mathfrak{h}$, satisfy the Weyl relations (cf. [RS2, Theorem X.41]). Thus, by the universal property of $\mathfrak{W}(\mathfrak{h})$, it follows that $\pi_{\mathfrak{W}}$ is a representation.

We can approximate the Segal field operators and creation and annihilation operators with elements of the Weyl algebra in an obvious manner. For $f \in \mathfrak{h}$ and $\epsilon > 0$, we set

$$\begin{aligned}\Phi_\epsilon^{\mathfrak{W}}(f) &:= \sqrt{2}\frac{W(\epsilon f) - \mathrm{Id}}{\mathrm{i}\epsilon},\\ (a^*)_\epsilon^{\mathfrak{W}}(f) &:= \frac{1}{2}(\Phi_\epsilon^{\mathfrak{W}}(f) - \mathrm{i}\Phi_\epsilon^{\mathfrak{W}}(f)),\\ a_\epsilon^{\mathfrak{W}}(f) &:= \frac{1}{2}(\Phi_\epsilon^{\mathfrak{W}}(f) + \mathrm{i}\Phi_\epsilon^{\mathfrak{W}}(f)).\end{aligned}$$

Then we have in the strong sense on $\mathfrak{F}_{\mathrm{fin}}(\mathfrak{h})$,

$$\lim_{\epsilon\to 0} \pi_{\mathfrak{W}}(\Phi_\epsilon^{\mathfrak{W}}(f)) = \Phi(f),$$

$$\lim_{\epsilon\to 0} \pi_{\mathfrak{W}}((a^*)_\epsilon^{\mathfrak{W}}(f)) = a^*(f), \tag{2.3}$$

$$\lim_{\epsilon\to 0} \pi_{\mathfrak{W}}(a_\epsilon^{\mathfrak{W}}(f)) = a(f). \tag{2.4}$$

Remark 2.2
Furthermore, using the functional calculus and the inequality $|e^{\mathrm{i}x} - 1| \leq C\,|x|$, $x \in \mathbb{R}$, for some fixed $C > 0$, one realizes that in analogy to Lemma A.3,

$$\left\|\pi_{\mathfrak{W}}(\Phi_\epsilon^{\mathfrak{W}}(f))\psi\right\| \leq C\,\|\Phi(f)\psi\|\,, \qquad \psi \in \mathcal{D}(\Phi(f)),\ \epsilon > 0.$$

We state some elementary properties of the Fock representation.

Proposition 2.3 (Fock representation)
The representation $\pi_{\mathfrak{W}}$ of $\mathfrak{W}(h)$ on $\mathfrak{F}(\mathfrak{h})$ is irreducible with cyclic vector Ω, and for all $f \in \mathfrak{h}$,

$$\langle \Omega, \pi_{\mathfrak{W}}(W(f))\Omega\rangle = e^{-\|f\|/4}. \tag{2.5}$$

Proof. The relation (2.5) follows from a direct computation on Fock space with the exponential series expansion of the Weyl operator, see for instance [AJP06, eq. (120)] for the details.

Cyclicity of Ω: Let $f_1, \dots, f_n \in \mathfrak{h}$. Then using the strong convergence of $\pi_{\mathfrak{W}}(\Phi_{\epsilon_i}^{\mathfrak{W}}(f_i)) \to \Phi(f_i)$, $i \in \{1, \dots, n\}$, as $\epsilon_i \to 0$, we find for all $\varepsilon > 0$ numbers $\epsilon_1, \dots, \epsilon_n > 0$ such that

$$\left\|\pi_{\mathfrak{W}}(\Phi_{\epsilon_n}^{\mathfrak{W}}(f_n)\dots\Phi_{\epsilon_1}^{\mathfrak{W}}(f_1))\Omega - \Phi(f_n)\dots\Phi(f_1)\Omega\right\| < \varepsilon, \tag{2.6}$$

cf. [AJP06, Theorem 2.5]. This shows that

$$\{\Phi(f_n)\dots\Phi(f_1)\Omega : f_1, \dots, f_n \in \mathfrak{h}\} \subseteq \overline{\{\pi_{\mathfrak{W}}(A)\Omega\colon A \in \mathfrak{W}(\mathfrak{h})\}}. \tag{2.7}$$

Hence, $\overline{\{\pi_{\mathfrak{W}}(A)\Omega : A \in \mathfrak{W}(\mathfrak{h})\}} = \mathfrak{F}(\mathfrak{h})$, as the left-hand side of (2.7) is dense in $\mathfrak{F}(\mathfrak{h})$ by Lemma A.2.

Irreducibility: Assume that $T \in \mathcal{L}(\mathfrak{F}(\mathfrak{h}))$ and $T\pi_{\mathfrak{W}}(A) = \pi_{\mathfrak{W}}(A)T$ for all $A \in \mathfrak{W}(\mathfrak{h})$. By Schur's Lemma (cf. [BR1, Proposition 2.3.8]) it suffices to show that $T = z\,\mathrm{Id}$ for some $z \in \mathbb{C}$. Let $f \in \mathfrak{h}$. By assumption,

$$\pi_{\mathfrak{W}}(a_\epsilon^{\mathfrak{W}}(f))T = T\pi_{\mathfrak{W}}(a_\epsilon^{\mathfrak{W}}(f)), \qquad \pi_{\mathfrak{W}}((a^*)_\epsilon^{\mathfrak{W}}(f))T = T\pi_{\mathfrak{W}}((a^*)_\epsilon^{\mathfrak{W}}(f)),$$

hold for all $\epsilon > 0$. Then taking the limit $\epsilon \to 0$ yields $T\psi \in \mathcal{D}(a(f)) \cap \mathcal{D}(a^*(f))$, and

$$a(f)T\psi = Ta(f)\psi, \qquad a^*(f)T\psi = Ta^*(f)\psi,$$

for all $\psi \in \mathfrak{F}_{\mathrm{fin}}(\mathfrak{h})$. In particular, we have $a(f)T\Omega = 0$. Thus, there exists $z \in \mathbb{C}$ such that $T\Omega = z\Omega$. Then, for all $f_1, \ldots, f_n \in \mathfrak{h}$,

$$Ta^*(f_n)\ldots a^*(f_1)\Omega = a^*(f_n)\ldots a^*(f_1)T\Omega = za^*(f_n)\ldots a^*(f_1)\Omega.$$

This implies that $T = z\,\mathrm{Id}$. □

In the following the one-particle space $\mathfrak{h}$ will be chosen as

$$L_0^2(\mathbb{R}^3) := L^2(\mathbb{R}^3, (1 + |k|^{-1})\mathrm{d}k),$$

and we write $\mathfrak{W} := \mathfrak{W}(L_0^2(\mathbb{R}^3))$. As we will see below, the restriction to the space $L_0^2(\mathbb{R}^3)$ is necessary for the definition of the equilibrium state.

On $\mathfrak{W}$, the free time evolution is given by

$$\alpha_t^{\mathfrak{W}}(W(f)) := W(e^{\mathrm{i}\omega t}f), \qquad t \in \mathbb{R},\ f \in L_0^2(\mathbb{R}^3),\ \omega(k) := |k|\,.$$

Clearly, $(\alpha_t^{\mathfrak{W}})_{t\in\mathbb{R}}$ is a group of $*$-automorphisms, that is, $\alpha_s^{\mathfrak{W}} \circ \alpha_t^{\mathfrak{W}} = \alpha_{s+t}^{\mathfrak{W}}$, $s, t \in \mathbb{R}$ and $\alpha_t^{\mathfrak{W}}$ is a $*$-automorphism for all $t \in \mathbb{R}$. However, note that the map $t \mapsto \alpha_t(W(f))$ is not continuous in norm, so in particular, $(\mathfrak{W}, (\alpha_t^{\mathfrak{W}})_{t\in\mathbb{R}})$ is not a C^*-dynamical system. The reason is that $\|W(f) - W(g)\| = 2$ for $f \neq g$, cf. [AJP06, Theorem 2.3].

Now we want to identify the thermal equilibrium state of the free non-interacting Bose gas on the Weyl algebra at inverse temperature $\beta > 0$. The standard notion of equilibrium states for systems of infinitely many degrees of freedom is the KMS condition. In this context this condition can be phrased as follows (cf. [Müc04b]).

Definition 2.4 (KMS state)
Let $\mathfrak{A}$ be a C^*-algebra, and let $(\alpha_t)_{t\in\mathbb{R}}$ be a group of $*$-isomorphisms. We call a state ω on $\mathfrak{A}$ an (α_t, β)-KMS state for some $\beta > 0$ if for all $A, B \in \mathfrak{A}$ there exists a complex function $F_{A,B}$ which is analytic on $D_\beta := \{z \in \mathbb{C} : 0 < \operatorname{Im} z < \beta\}$ and continuous and bounded on $\overline{D_\beta}$ such that for all $t \in \mathbb{R}$, we have

$$F_{A,B}(t) = \omega(A\alpha_t(B)), \qquad F_{A,B}(t + \mathrm{i}\beta) = \omega(\alpha_t(B)A).$$

The equilibrium state of the free Bose gas can be obtained as thermodynamic limit of equilibrium states on boxes Λ with finite volume. In a finite-volume system equilibrium states are exactly the Gibbs states, which can be characterized as the unique KMS states or the states minimizing the entropy of such systems. Then taking $\Lambda \to \mathbb{R}^3$ in a suitable sense and assuming a density which is not too high to avoid the regime of Bose-Einstein condensation, one arrives at (2.9). The details are omitted at this point and can be found in the literature (cf. [Müc04b], [BR2, section 5.2.5] and [Mer05]).

Let

$$\rho_\beta(u) := (e^{\beta u} - 1)^{-1}, \qquad u \in \mathbb{R} \setminus \{0\}, \tag{2.8}$$

denote PLANCK's law and write $\rho_\beta(k) := \rho_\beta(|k|)$ for $k \in \mathbb{R}^3 \setminus \{0\}$. For $f \in \mathfrak{h}$ we set

$$\omega_\beta^{\mathfrak{W}}(W(f)) := \exp\left(-\frac{1}{4}\int_{\mathbb{R}^3} (1 + 2\rho_\beta(k)) \left|f(k)\right|^2 \mathrm{d}^3 k\right), \qquad f \in L_0^2(\mathbb{R}^3). \tag{2.9}$$

At this point we do not discuss the thermodynamic limit and just show that $\omega_\beta^{\mathfrak{W}}$ is a well-defined KMS state, which is the content of the following proposition. Its GNS representation was first described by ARAKI and WOODS ([AW63]).

Proposition 2.5
The map $\omega_\beta^{\mathfrak{W}}$ given in (2.9) extends to a well-defined state on $\mathfrak{W}$, which satisfies the $(\alpha_t^{\mathfrak{W}}, \beta)$-KMS condition. Furthermore, its GNS representation $\pi_{\mathfrak{W}}^\beta$ on $\mathfrak{F}(L^2(\mathbb{R}^3)) \otimes \mathfrak{F}(L^2(\mathbb{R}^3))$ is given by

$$\pi_{\mathfrak{W}}^\beta(W(f)) := \widehat{W}\left(\sqrt{1+\rho_\beta} f\right) \otimes \widehat{W}\left(\sqrt{\rho_\beta}\overline{f}\right),$$

with cyclic vector $\Omega^{\otimes 2} := \Omega \otimes \Omega$.

Proof. First note that $0 < \rho_\beta(k) \leq (\beta\,|k|)^{-1}$ and thus the choice of the space $L_0^2(\mathbb{R}^3)$ guarantees that $\sqrt{1+\rho_\beta} f, \sqrt{\rho_\beta} f \in L^2(\mathbb{R}^3)$. From the fact that $\widehat{W}(\cdot)$ is a representation of the Weyl algebra, it follows directly that the operators $\pi_{\mathfrak{W}}^\beta(W(f))$, $f \in L_0^2(\mathbb{R}^3)$, satisfy the Weyl relations as well. Thus, $\pi_{\mathfrak{W}}^\beta$ indeed defines a representation of $\mathfrak{W}$ on $\mathfrak{F}(L^2(\mathbb{R}^3)) \otimes \mathfrak{F}(L^2(\mathbb{R}^3))$.

Now, (2.5) yields for $f \in L_0^2(\mathbb{R}^3)$,

$$\begin{aligned}\left\langle \Omega^{\otimes 2}, \pi_{\mathfrak{W}}^\beta(W(f))\Omega^{\otimes 2}\right\rangle &= \left\langle \Omega, \widehat{W}(\sqrt{1+\rho_\beta} f)\Omega\right\rangle \left\langle \Omega, \widehat{W}(\sqrt{\rho_\beta}\overline{f})\Omega\right\rangle \\ &= e^{-\frac{1}{4}(\|\sqrt{1+\rho_\beta} f\|^2 + \|\sqrt{\rho_\beta} f\|^2)} \\ &= \omega_\beta^{\mathfrak{W}}(W(f)).\end{aligned}$$

This shows that $\omega_\beta^{\mathfrak{W}}$ extends to a well-defined state on $\mathfrak{W}$.

Cyclicity of $\Omega^{\otimes 2}$: By a direct computation,

$$\lim_{\epsilon\to 0} \pi_{\mathfrak{W}}^{\beta}\left(a_\epsilon^{\mathfrak{W}}(f)\right)\psi = \left(a\left(\sqrt{1+\rho_\beta}f\right)\otimes \mathrm{Id} + \mathrm{Id}\otimes a^*\left(\sqrt{\rho_\beta}\overline{f}\right)\right)\psi$$

holds for all $\psi \in \mathfrak{F}_{\mathrm{fin}}(L^2(\mathbb{R}^3)) \mathbin{\widehat{\otimes}} \mathfrak{F}_{\mathrm{fin}}(L^2(\mathbb{R}^3))$. Let $f_1,\dots,f_n \in L_0^2(\mathbb{R}^3)$ and $\varepsilon > 0$. Then, as in (2.6), we find $\epsilon_1,\dots,\epsilon_n > 0$ such that

$$\left\|\pi_{\mathfrak{W}}^{\beta}\left(a_{\epsilon_n}^{\mathfrak{W}}(f_n)\dots a_{\epsilon_1}^{\mathfrak{W}}(f_1)\right)\Omega^{\otimes 2} - \Omega\otimes\left(a^*(\sqrt{\rho_\beta}\overline{f_n})\dots a^*(\sqrt{\rho_\beta}\overline{f_1})\Omega\right)\right\| < \varepsilon.$$

Because

$$\{\sqrt{\rho_\beta}f : f\in L_0^2(\mathbb{R}^3)\}$$

is dense in $L^2(\mathbb{R}^3)$, the set

$$\{a^*(\sqrt{\rho_\beta}\overline{f_n})\dots a^*(\sqrt{\rho_\beta}\overline{f_1})\Omega : f_1,\dots,f_n\in L_0^2(\mathbb{R}^3)\}$$

is dense in $\mathfrak{F}(L^2(\mathbb{R}^3))$ by Lemma A.2. This shows that

$$\Omega\otimes\mathfrak{F}(L^2(\mathbb{R}^3)) \subseteq \overline{\{\pi_{\mathfrak{W}}^{\beta}(A)\Omega^{\otimes 2} : A\in\mathfrak{W}\}}. \tag{2.10}$$

The right-hand side of (2.10) is invariant under the operators $\pi_{\mathfrak{W}}^{\beta}(B)$, $B\in\mathfrak{W}$, and $\pi_{\mathfrak{W}}^{\beta}(B)(\Omega\otimes\mathfrak{F}(L^2(\mathbb{R}^3))) = \widehat{W}(\sqrt{1+\rho_\beta}f)\Omega\otimes\mathfrak{F}(L^2(\mathbb{R}^3))$ for $B = W(f)$, $f\in L_0^2(\mathbb{R}^3)$. Thus, it follows

$$\mathrm{lin}\{\widehat{W}(\sqrt{\rho_\beta+1}f)\Omega : f\in L_0^2(\mathbb{R}^3)\}\otimes\mathfrak{F}(L^2(\mathbb{R}^3)) \subseteq \overline{\{\pi_{\mathfrak{W}}^{\beta}(A)\Omega^{\otimes 2} : A\in\mathfrak{W}\}}.$$

Since $(1+\rho_\beta)^{-1/2}\tilde{f}\in L_0^2(\mathbb{R}^3)$ for $\tilde{f}\in L^2(\mathbb{R}^3)$, we find

$$\mathrm{lin}\{\widehat{W}(\sqrt{\rho_\beta+1}f)\Omega : f\in L_0^2(\mathbb{R}^3)\} = \mathrm{lin}\{\widehat{W}(f)\Omega : f\in L^2(\mathbb{R}^3)\}.$$

This set is dense in $\mathfrak{F}(L^2(\mathbb{R}^3))$, as Ω is cyclic for the Fock representation. Thus, we conclude

$$\mathfrak{F}(L^2(\mathbb{R}^3))\otimes\mathfrak{F}(L^2(\mathbb{R}^3)) = \overline{\{\pi_{\mathfrak{W}}^{\beta}(A)\Omega^{\otimes 2} : A\in\mathfrak{W}\}}.$$

KMS condition: For $A, B\in\mathfrak{W}$, $t\in\mathbb{R}$ we define

$$F_{A,B}(t) := \omega_\beta^{\mathfrak{W}}(A\alpha_t(B)).$$

First, we show the KMS condition for $A = W(f)$, $B = W(g)$, $f, g \in L^2_0(\mathbb{R}^3)$. We have for $t \in \mathbb{R}$,

$$\begin{aligned}
F_{W(f),W(g)}(t) &= \omega_\beta^{\mathfrak{W}}(W(f)W(e^{\mathrm{i}t\omega}g)) \\
&= e^{-\frac{\mathrm{i}}{2}\operatorname{Im}\left\langle f, e^{\mathrm{i}t\omega}g\right\rangle}\ \omega_\beta^{\mathfrak{W}}(W(f+e^{\mathrm{i}t\omega}g)) \\
&= e^{-\frac{\mathrm{i}}{2}\operatorname{Im}\left\langle f, e^{\mathrm{i}t\omega}g\right\rangle} e^{-\frac{1}{4}\left\langle (f+e^{\mathrm{i}t\omega}g),(1+2\rho_\beta)(f+e^{\mathrm{i}t\omega}g)\right\rangle} \\
&= e^{-\frac{1}{4}\left\langle f, e^{\mathrm{i}t\omega}g\right\rangle + \frac{1}{4}\left\langle e^{\mathrm{i}t\omega}g, f\right\rangle} e^{-\frac{1}{4}\left\langle (f+e^{\mathrm{i}t\omega}g),(1+2\rho_\beta)(f+e^{\mathrm{i}t\omega}g)\right\rangle} \\
&= e^{-\frac{1}{2}\left(\left\langle f, e^{\mathrm{i}t\omega}g\right\rangle + \left\langle f, \rho_\beta e^{\mathrm{i}t\omega}g\right\rangle + \left\langle g, \rho_\beta e^{-\mathrm{i}t\omega}f\right\rangle\right) - \frac{1}{4}\left\langle f,(1+2\rho_\beta)f\right\rangle - \frac{1}{4}\left\langle g,(1+2\rho_\beta)g\right\rangle} \\
&= e^{-\frac{1}{2}\left(\left\langle f,(1+\rho_\beta)e^{\mathrm{i}t\omega}g\right\rangle + \left\langle g, \rho_\beta e^{-\mathrm{i}t\omega}f\right\rangle\right)} \omega_\beta^{\mathfrak{W}}(W(f))\omega_\beta^{\mathfrak{W}}(W(g)).
\end{aligned} \tag{2.11}$$

Notice that there is a constant C such that $\left|\rho_\beta(k)e^{-\mathrm{i}z\omega(k)}\right| \leq C\,|k|^{-1}$ for all $k \neq 0$ and $z \in D_\beta$, where

$$D_\beta := \{z \in \mathbb{C} : 0 < \operatorname{Im} z < \beta\}.$$

Thus, $t \mapsto \langle f, (1+\rho_\beta)e^{\mathrm{i}t\omega}g\rangle$ and $t \mapsto \langle g, \rho_\beta e^{-\mathrm{i}t\omega}f\rangle$ extend to analytic functions on D_β. The same applies to $F_{W(f),W(g)}$, and the analytic extension will be denoted by the same symbol. Furthermore, using the Weyl relations and (2.11), we find

$$\begin{aligned}
&\omega_\beta^{\mathfrak{W}}(W(e^{\mathrm{i}t\omega}g)W(f)) \\
&\quad = e^{-\mathrm{i}\operatorname{Im}\left\langle e^{\mathrm{i}t\omega}g, f\right\rangle}\omega_\beta^{\mathfrak{W}}(W(f)W(e^{\mathrm{i}t\omega}g)) \\
&\quad = e^{-\mathrm{i}\operatorname{Im}\left\langle e^{\mathrm{i}t\omega}g, f\right\rangle} e^{-\frac{1}{2}\left(\left\langle e^{\mathrm{i}t\omega}g,(1+\rho_\beta)f\right\rangle + \left\langle e^{-\mathrm{i}t\omega}f, \rho_\beta g\right\rangle\right)}\omega_\beta^{\mathfrak{W}}(W(f))\omega_\beta^{\mathfrak{W}}(W(g)).
\end{aligned}$$

This yields

$$\begin{aligned}
&F_{W(f),W(g)}(t+\mathrm{i}\beta) \\
&= e^{-\frac{1}{2}\left(\left\langle f,(1+\rho_\beta)e^{\mathrm{i}(t+\mathrm{i}\beta)\omega}g\right\rangle + \left\langle g,\rho_\beta e^{-\mathrm{i}(t+\mathrm{i}\beta)\omega}f\right\rangle\right)}\omega_\beta^{\mathfrak{W}}(W(f))\omega_\beta^{\mathfrak{W}}(W(g)) \\
&= e^{-\frac{1}{2}\left(\left\langle f,(1+\rho_\beta)e^{-\beta\omega}e^{\mathrm{i}t\omega}g\right\rangle + \left\langle g,\rho_\beta e^{\beta\omega}e^{-\mathrm{i}t\omega}f\right\rangle\right)}\omega_\beta^{\mathfrak{W}}(W(f))\omega_\beta^{\mathfrak{W}}(W(g)) \\
&= e^{-\frac{1}{2}\left(\left\langle f,\rho_\beta e^{\mathrm{i}t\omega}g\right\rangle + \left\langle g,(1+\rho_\beta)e^{-\mathrm{i}t\omega}f\right\rangle\right)}\omega_\beta^{\mathfrak{W}}(W(f))\omega_\beta^{\mathfrak{W}}(W(g)) \\
&= e^{\mathrm{i}\operatorname{Im}\left\langle e^{\mathrm{i}t\omega}g,f\right\rangle} e^{-\frac{1}{2}\left(\left\langle e^{\mathrm{i}t\omega}g,(1+\rho_\beta)f\right\rangle + \left\langle e^{-\mathrm{i}t\omega}f,\rho_\beta g\right\rangle\right)}\omega_\beta^{\mathfrak{W}}(W(f))\omega_\beta^{\mathfrak{W}}(W(g)) \\
&= \omega_\beta^{\mathfrak{W}}(W(e^{\mathrm{i}t\omega}g)W(f)).
\end{aligned}$$

For general $A, B \in \mathfrak{W}$ one can write $A = \sum_{n=1}^\infty \lambda_n W(f_n)$ and $B = \sum_{m=1}^\infty \mu_m W(g_m)$, with $\lambda_n, \mu_m \in \mathbb{C}$, $f_n, g_m \in L^2_0(\mathbb{R}^3)$, $n, m \in \mathbb{N}$. Note that

$$F_{A,B}(t) = \sum_{n,m=1}^\infty \lambda_n \mu_m F_{W(f_n),W(g_m)}(t), \qquad t \in \mathbb{R}.$$

Hence, $F_{A,B}$ extends to an analytic function on D_β as well, which follows from dominated convergence using (2.11) together with the observation that

$$\sup_{z\in D_\beta}\left|e^{-\frac{1}{2}\left(\left\langle f,(1+\rho_\beta)e^{\mathrm{i}z\omega}g\right\rangle+\left\langle g,\rho_\beta e^{-\mathrm{i}z\omega}f\right\rangle\right)}\right|<\infty.$$

Therefore, we have for all $t\in\mathbb{R}$,

$$\begin{aligned}F_{A,B}(t+\mathrm{i}\beta)&=\sum_{n,m=1}^{\infty}\lambda_n\mu_m F_{W(f_n),W(g_m)}(t+\mathrm{i}\beta)\\&=\sum_{n,m=1}^{\infty}\lambda_n\mu_m\omega_\beta^{\mathfrak{W}}(W(e^{\mathrm{i}t\omega}g_m)W(f_n))\\&=\omega(\alpha_t(B)A).\end{aligned}$$

□

2.2. Full System and Reference State

In this part we introduce the algebra of the atom in the bosonic field. The latter is represented by the Weyl algebra, which was studied in the previous section. For the atom we choose the full C^*-algebra

$$\mathfrak{A}_\mathrm{p}:=\mathcal{L}(\mathcal{H}_\mathrm{p}),$$

where we assume for now that $\mathcal{H}_\mathrm{p}$ is a separable Hilbert space, which we call atomic space.

Furthermore, we suppose in the following that H_p is a self-adjoint operator on $\mathcal{H}_\mathrm{p}$ – the atomic Hamiltonian. The time evolution on the algebra $\mathcal{A}_\mathrm{p}$ is given in the Heisenberg picture,

$$\alpha_t^\mathrm{p}(A):=e^{\mathrm{i}tH_\mathrm{p}}Ae^{-\mathrm{i}tH_\mathrm{p}},\qquad A\in\mathfrak{A}_\mathrm{p}.$$

The algebra of the full system is given as the spatial (or minimal) tensor product

$$\mathfrak{A}:=\mathfrak{A}_\mathrm{p}\otimes\mathfrak{W}.$$

On $\mathfrak{A}$ we define the free time evolution naturally as

$$\alpha_{t,0}:=\alpha_t^\mathrm{p}\otimes\alpha_t^{\mathfrak{W}},$$

where the tensor product of $*$-morphisms is to be understood as in Proposition A.8. The zero indicates that there is no coupling yet.

The next step will be the consideration of the dynamics in a GNS representation with respect to certain reference state. This should be a combination of the equilibrium state on $\mathfrak{W}$ with an arbitrary density matrix ρ_p on $\mathcal{H}_\mathrm{p}$. That is, we assume that $\rho_\mathrm{p} \in \mathcal{L}(\mathcal{H}_\mathrm{p})$, $\rho_\mathrm{p} \geq 0$ and $\operatorname{tr} \rho_\mathrm{p} = 1$. By the spectral theorem, one may write ρ_p as

$$\rho_\mathrm{p} = \sum_{n\in\mathbb{N}} \mu_n \langle \phi_n, \cdot \rangle \phi_n, \tag{2.12}$$

with an orthonormal basis $(\phi_n)_{n\in\mathbb{N}}$ of $\mathcal{H}_\mathrm{p}$ and eigenvalues $\mu_n \geq 0$, $n \in \mathbb{N}$. Then we define the corresponding state ω_{ρ_p} on $\mathfrak{A}_\mathrm{p}$ by

$$\omega_{\rho_\mathrm{p}}(A) := \operatorname{tr}(\rho_\mathrm{p} A).$$

The reference state on the algebra $\mathfrak{A}$ is defined as

$$\omega_{\rho_\mathrm{p},\beta} := \omega_{\rho_\mathrm{p}} \otimes \omega_\beta^{\mathfrak{W}},$$

where the tensor product is to be understood as in Corollary A.9. We can describe the trivial GNS representation with respect to ω_{ρ_p} on the space $\mathcal{H}_\mathrm{p} \otimes \mathcal{H}_\mathrm{p}^{\rho_\mathrm{p}}$, where

$$\mathcal{H}_\mathrm{p}^{\rho_\mathrm{p}} := \overline{\operatorname{ran} \rho_\mathrm{p}} = \overline{\operatorname{lin}\{\phi_n : \mu_n > 0,\ n \in \mathbb{N}\}}$$

with ϕ_n, μ_n, $n \in \mathbb{N}$ being the same as in (2.12). It is given by

$$\pi_\mathrm{p} \colon \mathfrak{A}_\mathrm{p} \longrightarrow \mathcal{L}(\mathcal{H}_\mathrm{p} \otimes \mathcal{H}_\mathrm{p}^{\rho_\mathrm{p}}),\ \pi_\mathrm{p}(A) := A \otimes \mathrm{Id}_\mathrm{p},$$

with cyclic vector

$$\Omega_\mathrm{p}^{\rho_\mathrm{p}} := \sum_{n\in\mathbb{N}} \sqrt{\mu_n} \phi_n \otimes \mathcal{C}_\mathrm{p} \phi_n,$$

where $\mathcal{C}_\mathrm{p}$ is an antilinear involution on $\mathcal{H}_\mathrm{p}$ satisfying

$$\mathcal{C}_\mathrm{p} H_\mathrm{p} \mathcal{C}_\mathrm{p} = H_\mathrm{p}. \tag{2.13}$$

In the case that H_p is a Schrödinger operator on $\mathcal{H}_\mathrm{p} = L^2(\mathbb{R}^3)$, one can choose $\mathcal{C}_\mathrm{p}\psi(x) = \overline{\psi(x)}$.

Finally, we can combine both representations on the Hilbert space

$$\mathcal{H}^{\rho_\mathrm{p}} := \mathcal{H}_\mathrm{p} \otimes \mathcal{H}_\mathrm{p}^{\rho_\mathrm{p}} \otimes \mathfrak{F}(L^2(\mathbb{R}^3)) \otimes \mathfrak{F}(L^2(\mathbb{R}^3)),$$

to

$$\pi^\beta \colon \mathfrak{A} \longrightarrow \mathcal{L}(\mathcal{H}^{\rho_\mathrm{p}}),\ \pi^\beta = \pi_\mathrm{p} \otimes \pi_\mathrm{f}^\beta,$$

and obtain the GNS representation with respect to the reference state $\omega_{\rho_\mathrm{p},\beta}$ with cyclic vector

$$\Omega^{\rho_\mathrm{p}} := \Omega_\mathrm{p}^{\rho_\mathrm{p}} \otimes \Omega^{\otimes 2}.$$

This will be summarized in the following proposition.

Proposition 2.6
The GNS representation of $\mathfrak{A}$ *with respect to* $\omega_{\rho_{\mathrm{p}},\beta}$ *on the Hilbert space* $\mathcal{H}^{\rho_{\mathrm{p}}}$ *is given by* $(\pi^\beta, \Omega^{\rho_{\mathrm{p}}})$.

Proof. It is clear that π_{p} is a representation of $\mathfrak{A}_{\mathrm{p}}$ and by direct computation one checks that for all $A \in \mathfrak{A}_{\mathrm{p}}$,

$$\omega_{\rho_{\mathrm{p}}}(A) = \operatorname{tr}(\rho_{\mathrm{p}} A) = \sum_{n=1}^{\infty} \mu_n \langle \phi_n, A\phi_n \rangle = \left\langle \Omega_{\mathrm{p}}^{\rho_{\mathrm{p}}}, \pi_{\mathrm{p}}(A)\Omega_{\mathrm{p}}^{\rho_{\mathrm{p}}} \right\rangle .$$

Furthermore, $\Omega^{\rho_{\mathrm{p}}}$ is a cyclic vector for π_{p}, since for all $m, n \in \mathbb{N}$ with $\mu_n > 0$,

$$\phi_m \otimes \mathcal{C}_{\mathrm{p}}\phi_n \in \{\pi_{\mathrm{p}}(A)\Omega_{\mathrm{p}}^{\rho_{\mathrm{p}}} : A \in \mathfrak{A}_{\mathrm{p}}\},$$

and the elements $\phi_m \otimes \mathcal{C}_{\mathrm{p}}\phi_n$, $m, n \in \mathbb{N}$ with $\mu_n > 0$, form an orthonormal basis of $\mathcal{H}_{\mathrm{p}} \otimes \mathcal{H}_{\mathrm{p}}^{\rho_{\mathrm{p}}}$. This proves that $(\pi_{\mathrm{p}}, \mathcal{H}_{\mathrm{p}} \otimes \mathcal{H}_{\mathrm{p}}^{\rho_{\mathrm{p}}})$ is the GNS construction corresponding to $\omega_{\rho_{\mathrm{p}}}$.

As $(\pi_{\mathrm{p}}, \mathcal{H}_{\mathrm{p}} \otimes \mathcal{H}_{\mathrm{p}}^{\rho_{\mathrm{p}}})$ and $(\pi_{\mathfrak{W}}^{\beta}, \Omega^{\otimes 2})$ are the GNS representations for $\omega_{\rho_{\mathrm{p}}}$ and $\omega_\beta^{\mathfrak{W}}$, respectively, it follows by Corollary A.9 that $\pi^\beta = \pi_{\mathrm{p}} \otimes \pi_{\mathfrak{W}}^{\beta}$ is the GNS representation on $\mathcal{H}^{\rho_{\mathrm{p}}}$ corresponding to $\omega_{\rho_{\mathrm{p}},\beta} := \omega_{\rho_{\mathrm{p}}} \otimes \omega_\beta^{\mathfrak{W}}$. □

Clearly, the Weyl algebra and the algebra $\mathfrak{A}$ of the composite system do not contain the (unbounded) creation and annihilation operators, though they are necessary to define the interaction. For this reason it is convenient to extend the representation π^β to those expressions and introduce a $*$-algebra of formal (unbounded) creation and annihilation operators (similar as in [BFS00]).

Let $L_0^2(\mathbb{R}^3, \mathcal{L}(\mathcal{H}_{\mathrm{p}}))$ be the $\mathcal{L}(\mathcal{H}_{\mathrm{p}})$-valued extension of the space $L_0^2(\mathbb{R}^3)$. Then let $\mathfrak{P}$ be the polynomial $*$-algebra in the symbolic expressions

$$\{\tilde{a}(F), \tilde{a}^*(G) : F, G \in L_0^2(\mathbb{R}^3, \mathcal{L}(\mathcal{H}_{\mathrm{p}}))\},$$

with the involution $(\tilde{a}(F))^* = \tilde{a}^*(F)$, and let $\mathcal{I}$ denote the ideal generated by (anti)linearity in the arguments of the creation and annihilation operators, that is, the elements

$$\tilde{a}(\lambda F + \mu G) - \overline{\lambda}\tilde{a}(F) - \overline{\mu}\tilde{a}(G), \quad \lambda, \mu \in \mathbb{C},\ F, G \in L_0^2(\mathbb{R}^3, \mathcal{L}(\mathcal{H}_{\mathrm{p}})).$$

We set $\tilde{\mathfrak{A}} := \mathfrak{P}/\mathcal{I}$.

To show the consistency of the extension of π^β, we introduce also π^∞ as the zero temperature analogue of π^β, that is,

$$\pi^\infty = \mathrm{Id}_{\mathcal{L}(\mathcal{H}_{\mathrm{p}})} \otimes \pi_{\mathfrak{W}} \colon \mathfrak{A} \longrightarrow \mathcal{L}\left(\mathcal{H}_{\mathrm{p}} \otimes \mathfrak{F}(L^2(\mathbb{R}^3))\right).$$

Now we can extend the representations π^∞ and π^β in a canonical way to $\tilde{\mathfrak{A}}$. For any $A \in \tilde{\mathfrak{A}}$ we define $\pi^\infty(A)$ and $\pi^\beta(A)$ as (unbounded) operators on $\mathfrak{F}_{\text{fin}}(\mathcal{L}(\mathcal{H}_\text{p}))$ and $\mathfrak{F}_{\text{fin}}(\mathcal{L}(\mathcal{H}_\text{p})) \widehat{\otimes} \mathfrak{F}_{\text{fin}}(\mathcal{L}(\mathcal{H}_\text{p}))$, respectively, such that for all $F \in L^2_0(\mathbb{R}^3, \mathcal{L}(\mathcal{H}_\text{p}))$,

$$\begin{aligned}
&\pi^\infty(\tilde{a}^*(F)) = a^*(F),\\
&\pi^\beta_{\mathfrak{W}}(\tilde{a}^*(F)) = a^*(\sqrt{1+\rho_\beta}F) \otimes \mathrm{Id}_{\mathfrak{F}(L^2(\mathbb{R}^3))} + \mathrm{Id}_{\mathfrak{F}(L^2(\mathbb{R}^3))} \otimes a(\sqrt{\rho_\beta}F^*).
\end{aligned}$$

The consistency with the representations of the algebra $\mathfrak{A}$ appears as follows. By definition we have in the strong sense on the respective domains,

$$\begin{aligned}
\lim_{\epsilon\to 0} \pi^\infty\left(G \otimes (a^*)^{\mathfrak{W}}_\epsilon(f)\right) &= \pi^\infty(\tilde{a}^*(fG)),\\
\lim_{\epsilon\to 0} \pi^\beta\left(G \otimes (a^*)^{\mathfrak{W}}_\epsilon(f)\right) &= \pi^\beta(\tilde{a}^*(fG)),
\end{aligned}$$

for all $G \in \mathcal{L}(\mathcal{H}_\text{p})$ and $f \in L^2_0(\mathbb{R}^3)$.

2.3. Von Neumann Algebra and Modular Structure

It turns out that the C^*-formalism is too restrictive for our needs, especially, since the time evolution $t \mapsto \alpha_{t,0}$ is not continuous on $\mathfrak{A}$. However, it is strongly continuous under the representation π^β. Therefore, it is natural to consider the von Neumann algebra generated by π^β, that is,

$$\mathfrak{M}^{\rho_\text{p}}_\beta := \pi^\beta(\mathfrak{A})'' = \mathcal{L}(\mathcal{H}_\text{p}) \otimes \mathrm{Id}_{\mathcal{H}^{\rho_\text{p}}_\text{p}} \otimes \pi^\beta_{\mathfrak{W}}(\mathfrak{W})'' \subseteq \mathcal{L}(\mathcal{H}^{\rho_\text{p}}), \tag{2.14}$$

where the tensor product denotes the standard tensor product of von Neumann algebras (cf. [KR97, section 11.2]). Notice that the definition is indeed independent of ρ_p in the sense that $\mathfrak{M}^{\rho_\text{p}}_\beta$,$\mathfrak{M}^{\rho'_\text{p}}_\beta$, operating on $\mathcal{H}^{\rho_\text{p}}$ and $\mathcal{H}^{\rho'_\text{p}}$, respectively, are $*$-isomorphic for two density matrices ρ_p, ρ'_p:

$$\mathfrak{M}^{\rho_\text{p}}_\beta \cong \mathfrak{M}^{\rho'_\text{p}}_\beta,$$

which follows from the explicit form (2.14). As we are only interested in the existence or absence of invariant states of $\mathfrak{M}_\beta$, the choice of ρ_p is not relevant. Therefore, for reasons of simplicity, we may assume in the following that

$$\rho_\text{p} > 0,$$

that is, $\mu_n > 0$ for all $n \in \mathbb{N}$. In this case, $\mathcal{H}^{\rho_\text{p}}_\text{p} = \mathcal{H}_\text{p}$. Furthermore, we set

$$\mathfrak{M}_\beta := \mathfrak{M}^{\rho_\text{p}}_\beta \subseteq \mathcal{L}(\mathcal{H}_\text{p}) \otimes \mathrm{Id}_{\mathcal{H}_\text{p}} \otimes \pi^\beta_{\mathfrak{W}}(\mathfrak{W})'' \subseteq \mathcal{L}(\widetilde{\mathcal{H}}),$$

where

$$\widetilde{\mathcal{H}} := \mathcal{H}_{\mathrm{p}} \otimes \mathcal{H}_{\mathrm{p}} \otimes \mathfrak{F}(L^2(\mathbb{R}^3)) \otimes \mathfrak{F}(L^2(\mathbb{R}^3)). \tag{2.15}$$

First, we would like to extend the free time evolution $(\alpha_t)_{t\in\mathbb{R}}$ to $\mathfrak{M}_\beta$ using its unitary implementation in the representation space. For all $t \in \mathbb{R}$, we define $\sigma_{t,0}$ on $\pi^\beta(\mathfrak{A})$ by

$$\sigma_{t,0}(\pi^\beta(A)) := \pi^\beta(\alpha_{t,0}(A)), \qquad A \in \mathfrak{A}.$$

By direct calculation we have

$$\pi_{\mathrm{p}}(\alpha_t^{\mathrm{p}}(A)) = e^{\mathrm{i}tH_{\mathrm{p}}} A e^{-\mathrm{i}tH_{\mathrm{p}}} \otimes \mathrm{Id}_{\mathrm{p}} = e^{\mathrm{i}tL_{\mathrm{p}}} \pi_{\mathrm{p}}(A) e^{-\mathrm{i}tL_{\mathrm{p}}},$$

where L_{p} is the self-adjoint operator on $\mathcal{H}_{\mathrm{p}} \otimes \mathcal{H}_{\mathrm{p}}$ given by

$$L_{\mathrm{p}} := H_{\mathrm{p}} \otimes \mathrm{Id}_{\mathrm{p}} - \mathrm{Id}_{\mathrm{p}} \otimes H_{\mathrm{p}}.$$

Furthermore, for all $f \in L_0^2(\mathbb{R}^3)$,

$$\begin{aligned}
&\pi^\beta_{\mathfrak{W}}(\alpha_t^{\mathfrak{W}}(W(f))) \\
&\quad = \exp\left(\frac{\mathrm{i}}{\sqrt{2}}\Phi(\sqrt{1+\rho_\beta}e^{\mathrm{i}t\omega} f\right) \otimes \exp\left(\frac{\mathrm{i}}{\sqrt{2}}\Phi(\sqrt{\rho_\beta}e^{-\mathrm{i}t\omega}\overline{f}\right) \\
&\quad = e^{\mathrm{i}tH_{\mathrm{f}}} \exp\left(\frac{\mathrm{i}}{\sqrt{2}}\Phi(\sqrt{1+\rho_\beta} f\right) e^{-\mathrm{i}tH_{\mathrm{f}}} \otimes e^{-\mathrm{i}tH_{\mathrm{f}}} \exp\left(\frac{\mathrm{i}}{\sqrt{2}}\Phi(\sqrt{\rho_\beta}\overline{f})\right) e^{\mathrm{i}tH_{\mathrm{f}}} \\
&\quad = e^{\mathrm{i}t\widetilde{L}_{\mathrm{f}}} \pi^\beta_{\mathfrak{W}}(W(f)) e^{-\mathrm{i}t\widetilde{L}_{\mathrm{f}}},
\end{aligned}$$

where $H_{\mathrm{f}} = \mathrm{d}\Gamma(\omega)$ denotes the field energy, and $\widetilde{L}_{\mathrm{f}}$ is the self-adjoint operator on $\mathcal{H}_{\mathrm{f}} \otimes \mathcal{H}_{\mathrm{f}}$ given by

$$\widetilde{L}_{\mathrm{f}} := H_{\mathrm{f}} \otimes \mathrm{Id}_{\mathrm{f}} - \mathrm{Id}_{\mathrm{f}} \otimes H_{\mathrm{f}}.$$

Thus, we can write

$$\sigma_{t,0}(\pi^\beta(A)) = e^{\mathrm{i}t\widetilde{L}_0} \pi^\beta(A) e^{-\mathrm{i}t\widetilde{L}_0},$$

where

$$\widetilde{L}_0 := L_{\mathrm{p}} \otimes \mathrm{Id}_{\mathrm{f}} \otimes \mathrm{Id}_{\mathrm{f}} + \mathrm{Id}_{\mathrm{p}} \otimes \mathrm{Id}_{\mathrm{p}} \otimes \widetilde{L}_{\mathrm{f}}.$$

This shows that $(\sigma_{t,0})_{t\in\mathbb{R}}$ extends to a group of $*$-automorphisms on $\mathfrak{M}_\beta$ and $t \mapsto \sigma_{t,0}(A)$ is in fact continuous in the strong operator topology for all $A \in \mathfrak{A}$.

These preparations allow us to study a modular structure on $\mathfrak{M}_\beta$. For the basic definitions and facts we refer the reader to Appendix A.2.2. The first step is to find a cyclic and separating vector on $\mathfrak{M}_\beta$.

Proposition 2.7
$\Omega_{\mathrm{p}}^{\rho_{\mathrm{p}}}$ and $\Omega^{\otimes 2}$ are cyclic and separating for $\pi_{\mathrm{p}}(\mathfrak{A}_{\mathrm{p}})'' = \mathcal{L}(\mathcal{H}_{\mathrm{p}}) \otimes \mathrm{Id}_{\mathrm{p}}$ and $\pi_{\mathfrak{W}}^{\beta}(\mathfrak{W})''$, respectively. In particular, $\Omega^{\rho_{\mathrm{p}}}$ is cyclic and separating for $\mathfrak{M}_{\beta}$.

Proof. We have already seen that both vectors emerged as cyclic GNS vectors. That $\Omega_{\mathrm{p}}^{\rho_{\mathrm{p}}}$ is separating for $\pi_{\mathrm{p}}(\mathfrak{A}_{\mathrm{p}})''$ follows by a short direct computation from the fact that ρ_{p} is strictly positive.

The separating property in the field case follows because it is a KMS state. To be more precise, consider the unitary implementation of the time evolution $(\alpha_t^{\mathfrak{W}})_{t\in\mathbb{R}}$, that is,

$$\sigma_t^{\mathrm{f}}(\pi_{\mathfrak{W}}^{\beta}(A)) := \pi_{\mathfrak{W}}^{\beta}(\alpha_t^{\mathfrak{W}}(A)) = e^{\mathrm{i}t\widetilde{L}_{\mathrm{f}}}\pi_{\mathfrak{W}}^{\beta}(A)e^{-\mathrm{i}t\widetilde{L}_{\mathrm{f}}}, \qquad t\in\mathbb{R},\ A\in\mathfrak{W},$$

as we have seen above. Also in this case $(\sigma_t^{\mathrm{f}})_{t\in\mathbb{R}}$ extends to a strongly continuous group of $*$-automorphisms on $\pi_{\mathfrak{W}}^{\beta}(\mathfrak{W})''$. Furthermore, one can extend the state $\omega_\beta^{\mathfrak{W}}$ to a (normal) state $\hat{\omega}_\beta^{\mathfrak{W}}$ on $\pi_{\mathfrak{W}}^{\beta}(\mathfrak{W})''$ via

$$\hat{\omega}_\beta^{\mathfrak{M}}(A) = \left\langle \Omega^{\otimes 2}, A\Omega^{\otimes 2}\right\rangle, \qquad A \in \pi_{\mathfrak{W}}^{\beta}(\mathfrak{W})''.$$

Then it follows from the KMS property of $\omega_\beta^{\mathfrak{M}}$ that also $\hat{\omega}_\beta^{\mathfrak{M}}$ is a $(\sigma_t^{\mathrm{f}},\beta)$-KMS state on $\pi_{\mathfrak{W}}^{\beta}(\mathfrak{W})''$ (cf. [BR2, Proposition 5.3.7]), which implies that $\Omega^{\otimes 2}$ is separating (cf. [BR2, Corollary 5.3.9]). Now it follows from [KR97, section 11.2.36] that the tensor product $\Omega^{\rho_{\mathrm{p}}} = \Omega_{\mathrm{p}}^{\rho_{\mathrm{p}}} \otimes \Omega^{\otimes 2}$ is also separating for $\mathfrak{M}_\beta$. □

Now, we can discuss the modular structure associated to $(\mathfrak{M}_\beta, \Omega^{\rho_{\mathrm{p}}})$. We define antiunitary involutions J_{p} on $\mathcal{H}_{\mathrm{p}} \otimes \mathcal{H}_{\mathrm{p}}$ and J_{f} on $\mathcal{H}_{\mathrm{f}} \otimes \mathcal{H}_{\mathrm{f}}$, respectively, by

$$\begin{aligned} J_{\mathrm{p}}(\phi\otimes\psi) &:= \mathcal{C}_{\mathrm{p}}\psi\otimes\mathcal{C}_{\mathrm{p}}\phi, \qquad \phi,\psi\in\mathcal{H}_{\mathrm{p}},\\ J_{\mathrm{f}}(\phi\otimes\psi) &:= \mathcal{C}_{\mathrm{f}}\psi\otimes\mathcal{C}_{\mathrm{f}}\phi, \qquad \phi,\psi\in\mathfrak{F}(L^2(\mathbb{R}^3)), \end{aligned}$$

where

$$\begin{aligned} (\mathcal{C}_{\mathrm{f}}\psi)_0 &:= \overline{\psi_0},\\ (\mathcal{C}_{\mathrm{f}}\psi)_n(k_1,\ldots,k_n) &:= \overline{\psi_n(k_1,\ldots,k_n)}. \end{aligned}$$

The antiunitary operators J_{p} and J_{f} can be combined to an antiunitary operator on $\widetilde{\mathcal{H}}$,

$$J := J_{\mathrm{p}} \otimes J_{\mathrm{f}},$$

which turns out to be the modular conjugation as we will see in the following proposition.

Proposition 2.8
The operator J is the modular conjugation associated to $(\mathfrak{M}_\beta, \Omega^{\rho_\mathrm{p}})$.

Proof. It suffices to show that J_p the modular conjugation corresponding to

$$(\pi_\mathrm{p}(\mathfrak{A}_\mathrm{p})'', \Omega_\mathrm{p}^{\rho_\mathrm{p}})$$

and J_f is the one corresponding to

$$(\pi_\mathrm{f}(\mathfrak{W})'', \Omega^{\otimes 2}).$$

Then the properties carry over to the tensor product (cf. [KR97, section 11.2.36]).

For the atom we proceed similarly as in [Müc04b, section 1.2.4]. Let

$$\Delta_\mathrm{p} := \rho_\mathrm{p} \otimes (\mathcal{C}_\mathrm{p}\rho_\mathrm{p}^{-1}\mathcal{C}_\mathrm{p})$$

be defined as a self-adjoint (unbounded) operator acting on the Hilbert space $\mathcal{H}_\mathrm{p} \otimes \mathcal{H}_\mathrm{p}$. We have for $A \in \mathcal{L}(\mathcal{H}_\mathrm{p})$,

$$\begin{aligned} J_\mathrm{p}\Delta_\mathrm{p}^{1/2}(A \otimes \mathrm{Id})\Omega_\mathrm{p}^{\rho_\mathrm{p}} &= \sum_{n\in\mathbb{N}} \mu_n^{1/2} J_\mathrm{p}\left(\rho_\mathrm{p}^{1/2} A\phi_n \otimes \mathcal{C}_\mathrm{p}\rho_\mathrm{p}^{-1/2}\phi_n\right) \\ &= \sum_{n\in\mathbb{N}} \phi_n \otimes \mathcal{C}_\mathrm{p}\rho_\mathrm{p}^{1/2} A\phi_n \\ &= \sum_{m,n\in\mathbb{N}} \left\langle \mathcal{C}_\mathrm{p}\phi_m, \mathcal{C}_\mathrm{p}\rho_\mathrm{p}^{1/2} A\phi_n \right\rangle \phi_n \otimes \mathcal{C}_\mathrm{p}\phi_m \\ &= \sum_{m,n\in\mathbb{N}} \left\langle \phi_n, \mu_m^{1/2} A^*\phi_m \right\rangle \phi_n \otimes \mathcal{C}_\mathrm{p}\phi_m \\ &= \sum_{m\in\mathbb{N}} \mu_m^{1/2} A^*\phi_m \otimes \mathcal{C}_\mathrm{p}\phi_m. \end{aligned}$$

Thus, $J_\mathrm{p}\Delta_\mathrm{p}^{1/2}\pi_\mathrm{p}(A)\Omega_\mathrm{p}^{\rho_\mathrm{p}} = \pi_\mathrm{p}(A)^*\Omega_\mathrm{p}^{\rho_\mathrm{p}}$, which proves that J_p is the corresponding modular conjugation.

Similarly, for the field component one chooses the operator

$$\Delta_\mathrm{f} := e^{-\beta H_\mathrm{f}} \otimes e^{\beta H_\mathrm{f}}$$

and then one needs to verify the equality

$$J_\mathrm{f}\left(e^{-\beta H_\mathrm{f}/2}\widehat{W}(\sqrt{1+\rho_\beta}f)\Omega \otimes e^{\beta H_\mathrm{f}/2}\widehat{W}(\sqrt{\rho_\beta}\overline{f})\Omega\right) = \widehat{W}(-\sqrt{1+\rho_\beta}f) \otimes \widehat{W}(-\sqrt{\rho_\beta}\overline{f}),$$

which follows from an exponential series expansion of the Weyl operators, see [Müc04b, section 1.3.5] for the details. □

Notice that J commutes by definition with the unitary group generated by $\widetilde{L}_0$. Since

$$e^{\mathrm{i}tH_\mathrm{p}}\mathcal{C}_\mathrm{p} = \mathcal{C}_\mathrm{p}e^{-\mathrm{i}tH_\mathrm{p}}, \qquad e^{\mathrm{i}tH_\mathrm{f}}\mathcal{C}_\mathrm{f} = \mathcal{C}_\mathrm{f}e^{-\mathrm{i}tH_\mathrm{f}},$$

holds due to (2.13), we accordingly have

$$e^{\mathrm{i}t\widetilde{L}_0}J = Je^{\mathrm{i}t\widetilde{L}_0} \tag{2.16}$$

for all $t \in \mathbb{R}$.

2.4. Interacting Dynamics

The next step is the inclusion of the linear interaction term, which appears in the zero temperature model (2.1),

$$W_\infty := \tilde{a}(G) + \tilde{a}^*(G) \in \tilde{\mathfrak{A}},$$

where we assume from now on that $G \in L^2_0(\mathbb{R}^3, \mathcal{H}_\mathrm{p})$.

It is well-known from quantum mechanics that the time evolution with respect to a perturbed operator $H_0 + H_I$ can be expressed in the so-called *interaction picture* as a *Dyson series*. This contains only the free time evolution, generated by H_0, of an observable and of the interaction H_I. In our case it is given by the formal expression

$$\begin{aligned}\alpha_{t,\lambda}(A) &= \alpha_{t,0}(A) \\ &+ \sum_{n=1}^{\infty}(\mathrm{i}\lambda)^n \int_0^t \dots \int_0^{t_{n-1}} [\alpha_{t_n,0}(W_\infty), [\dots[\alpha_{t_1,0}(W_\infty), \alpha_{t,0}(A)]\dots]]\mathrm{d}t_1\dots\mathrm{d}t_n,\end{aligned} \tag{2.17}$$

where $A \in \mathfrak{A}$, $t \in \mathbb{R}$, $\lambda \in \mathbb{R}$. However, two problems cause $\alpha_{t,\lambda}(A)$ to be ill-defined. First, W_∞ is not an element of the C^*-algebra and $\pi^\beta(W_\infty)$ is unbounded. Second, we have already seen above that $t \mapsto \alpha_t(A)$ is not continuous, so it is not a priori clear how to make sense of the integral at all.

To circumvent the first problem, we can approximate W_∞ by elements in $\mathfrak{A}$, which will be done in Lemma 2.9. For the second one, we define the time evolution on the von Neumann algebra $\mathfrak{M}_\beta$ in the first place. That is, we formally apply the representation π^β to the right-hand side of (2.17) and use this as the definition for the time evolution for $\pi^\beta(A)$, see (2.23).

Lemma 2.9
There exists a sequence $(W_\infty^{(M)})_{M\in\mathbb{N}}$ in $\mathfrak{A}$ satisfying

$$\pi^\beta(W_\infty^{(M)})\psi \to \pi^\beta(W_\infty)\psi, \ \ M \to \infty, \tag{2.18}$$

for all $\psi \in \mathcal{H}_\mathrm{p} \mathbin{\widehat{\otimes}} \mathcal{H}_\mathrm{p} \mathbin{\widehat{\otimes}} \mathfrak{F}_\mathrm{fin}(L^2(\mathbb{R}^3)) \mathbin{\widehat{\otimes}} \mathfrak{F}_\mathrm{fin}(L^2(\mathbb{R}^3))$.

Proof. Let $(e_m)_{m\in\mathbb{N}}$ be an orthonormal basis of $L^2_0(\mathbb{R}^3)$ and define $\langle e_m, G\rangle \in \mathcal{L}(\mathcal{H}_\mathrm{p})$ in a natural way by

$$\langle e_m, G\rangle := \int \overline{e_m(k)} G(k) \mathrm{d}k,$$

where the integral is to be understood in the strong operator topology. For $M \in \mathbb{N}$ and $\epsilon > 0$, we define an approximation of the creation and annihilation operators on the algebra $\mathfrak{A}$ by

$$a^*_{M,\epsilon}(G) := \sum_{m=1}^{M} \langle e_m, G\rangle \otimes (a^*)^{\mathfrak{W}}_\epsilon(e_m),$$

and $a_{M,\epsilon}(G) := (a^*_{M,\epsilon}(G))^*$. The approximating interaction is then defined as

$$W^{(M)}_\infty := a^*_{M,1/M}(G) + a_{M,1/M}(G), \qquad M \in \mathbb{N}.$$

First we show that

$$\lim_{M\to\infty} \pi^\beta(a^*_{M,1/M}(G))\psi = \lim_{M\to\infty} T_M\psi, \tag{2.19}$$

for all $\psi \in \mathcal{H}_\mathrm{p} \mathbin{\widehat{\otimes}} \mathcal{H}_\mathrm{p} \mathbin{\widehat{\otimes}} \mathfrak{F}_\mathrm{fin}(L^2(\mathbb{R}^3)) \mathbin{\widehat{\otimes}} \mathfrak{F}_\mathrm{fin}(L^2(\mathbb{R}^3))$, where

$$T_M := \sum_{m=1}^{M} \langle e_m, G\rangle \otimes \mathrm{Id}_\mathrm{p} \otimes \left(a^*(\sqrt{1+\rho_\beta}e_m) \otimes \mathrm{Id} - \mathrm{Id} \otimes a(\sqrt{\rho_\beta}\overline{e_m})\right).$$

By (2.3) and (2.4) we have

$$\pi^\beta_{\mathfrak{W}}((a^*)^{\mathfrak{W}}_\epsilon(e_m))\psi \to (a^*(\sqrt{1+\rho_\beta}e_m) \otimes \mathrm{Id}_\mathrm{p} - \mathrm{Id}_\mathrm{p} \otimes a(\sqrt{\rho_\beta}\overline{e_m}))\psi, \ \epsilon \to 0, \tag{2.20}$$

for all $\psi \in \mathfrak{F}_\mathrm{fin}(L^2(\mathbb{R}^3)) \mathbin{\widehat{\otimes}} \mathfrak{F}_\mathrm{fin}(L^2(\mathbb{R}^3))$ and $m \in \mathbb{N}$. By Remark 2.2 in combination with Lemma A.3, there is a constant C such that

$$\begin{aligned}\left\|\pi^\beta_{\mathfrak{W}}((a^*)^{\mathfrak{W}}_\epsilon(e_m))\psi\right\| \le C &\left(\left\|\sqrt{1+\rho_\beta}e_m\right\| + \left\|(\sqrt{\rho_\beta}e_m\right\|\right) \\ &\times \left\|(N_\mathrm{f} \otimes \mathrm{Id}_\mathrm{f} + \mathrm{Id}_\mathrm{f} \otimes N_\mathrm{f} + \mathrm{Id}_\mathrm{f} \otimes \mathrm{Id}_\mathrm{f})^{1/2}\psi\right\|\end{aligned} \tag{2.21}$$

for all $\psi \in \mathfrak{F}_\mathrm{fin}(L^2(\mathbb{R}^3)) \mathbin{\widehat{\otimes}} \mathfrak{F}_\mathrm{fin}(L^2(\mathbb{R}^3))$, $\epsilon > 0$ and $m \in \mathbb{N}$. This shows that $\pi^\beta_{\mathfrak{W}}((a^*)^{\mathfrak{W}}_\epsilon(e_m))\psi$, $m \in \mathbb{N}$, is bounded uniformly in m for every fixed ψ. Moreover, for $\phi \in \mathcal{H}_\mathrm{p}$, we have

$$\sum_{m\in\mathbb{N}} \|\langle e_m, G\rangle \phi\|^2_{\mathcal{H}_\mathrm{p}} = \|G\phi\|^2_{L^2(\mathbb{R}^3,\mathcal{H}_\mathrm{p})} < \infty, \tag{2.22}$$

which can be seen by an expansion in an orthonormal basis $(\zeta_n)_{n\in\mathbb{N}}$ of $\mathcal{H}_\mathrm{p}$,

$$\langle e_m, G\rangle\, \phi = \sum_{n\in\mathbb{N}} \langle e_m \otimes \zeta_n, G\phi\rangle_{L^2(\mathbb{R}^3,\mathcal{H}_\mathrm{p})}\, \zeta_n.$$

Then, for $\phi_\mathrm{p}, \psi_\mathrm{p} \in \mathcal{H}_\mathrm{p}$ and $\phi_\mathrm{f}, \psi_\mathrm{f} \in \mathfrak{F}_\mathrm{fin}(L^2(\mathbb{R}^3))$,

$$\begin{aligned}
&\left\| (\pi^\beta(a^*_{M,1/M}(G)) - T_M)\phi_\mathrm{p} \otimes \psi_\mathrm{p} \otimes \phi_\mathrm{f} \otimes \psi_\mathrm{f} \right\|^2 \\
&\quad \le \sum_{m=1}^\infty \|\langle e_m, G\rangle\, \phi_\mathrm{p}\|^2\, \|\psi_\mathrm{p}\|^2 \\
&\qquad \times \left\| \left(\pi^\beta_{\mathfrak{W}}((a^*)^{\mathfrak{W}}_{1/M}(e_m)) - a^*(\sqrt{1+\rho_\beta} e_m) \otimes \mathrm{Id} - \mathrm{Id} \otimes a(\sqrt{\rho_\beta}\overline{e_m}) \right) (\psi_\mathrm{f} \otimes \phi_\mathrm{f}) \right\|^2,
\end{aligned}$$

which converges to zero as $M \to \infty$ by dominated convergence using (2.20), (2.21) and (2.22). This shows (2.19). Finally, writing

$$\begin{aligned}
T_M =& a^*\left(\sqrt{1+\rho_\beta} \sum_{m=1}^M \langle e_m, G\rangle \otimes \mathrm{Id}_\mathrm{p}\, e_m \right) \otimes \mathrm{Id}_\mathrm{f} \\
&- \mathrm{Id}_\mathrm{f} \otimes a\left(\sqrt{\rho_\beta} \sum_{m=1}^M \langle \overline{e_m}, G^*\rangle \otimes \mathrm{Id}_\mathrm{p}\, \overline{e_m} \right),
\end{aligned}$$

and using that

$$\begin{aligned}
\sqrt{1+\rho_\beta} \sum_{m=1}^M \langle e_m, G\rangle\, e_m &\to \sqrt{1+\rho_\beta} G, \qquad M\to\infty, \\
\sqrt{\rho_\beta} \sum_{m=1}^M \langle \overline{e_m}, G^*\rangle\, \overline{e_m} &\to \sqrt{\rho_\beta} G^*, \qquad M \to \infty,
\end{aligned}$$

in norm in $L^2(\mathbb{R}^3, \mathcal{L}(\mathcal{H}_\mathrm{p}))$, one obtains by Lemma A.3 that

$$T_M\psi \to \left(a^*\left(\sqrt{1+\rho_\beta} G\right) \otimes \mathrm{Id} - \mathrm{Id} \otimes a\left(\sqrt{\rho_\beta} G^*\right)\right)\psi, \qquad M\to\infty,$$

for all $\psi \in \mathfrak{F}_\mathrm{fin}(L^2(\mathbb{R}^3)) \mathbin{\widehat{\otimes}} \mathfrak{F}_\mathrm{fin}(L^2(\mathbb{R}^3))$. Repeating the same procedure for the annihilation operator yields the desired result. □

Now, let $(W_\infty^{(M)})_{M\in\mathbb{N}}$ be a sequence in $\mathfrak{A}$ satisfying (2.18). We can define an approximation of the interacting dynamics on $\mathfrak{M}_\beta$ using $(W_\infty^{(M)})_{M\in\mathbb{N}}$ by

$$\begin{aligned}
\sigma_{t,\lambda}^{(M)}(A) := \sigma_{t,0}(A) + \sum_{n=1}^\infty (\mathrm{i}\lambda)^n \int_0^t \cdots \int_0^{t_{n-1}} &[\sigma_{t_n,0}(\pi^\beta(W_\infty^{(M)})), \\
&[\ldots[\sigma_{t_1,0}(\pi^\beta(W_\infty^{(M)})), \sigma_{t,0}(A)]\ldots]]\mathrm{d}t_1 \ldots \mathrm{d}t_n,
\end{aligned} \tag{2.23}$$

where $A \in \mathfrak{M}_\beta$, and the integral is to be understood in the strong operator topology.

The interacting time evolution can be represented by a unitary group as well. Let

$$L_\lambda^{(M)} := \widetilde{L}_0 + \lambda I^{(M)}, \qquad \lambda \in \mathbb{R}, M \in \mathbb{N},$$

where

$$I^{(M)} := \pi^\beta(W_\infty^{(M)}) - J\pi^\beta(W_\infty^{(M)})J.$$

The operator $L_\lambda^{(M)}$ is essentially self-adjoint on any core for $\widetilde{L}_0$, for example on

$$\widetilde{\mathcal{D}} := C_{\mathsf{c}}^\infty(\mathbb{R}^3) \mathbin{\widehat{\otimes}} C_{\mathsf{c}}^\infty(\mathbb{R}^3) \mathbin{\widehat{\otimes}} (\mathfrak{F} \cap \mathcal{D}(H_{\mathrm{f}})) \mathbin{\widehat{\otimes}} (\mathfrak{F} \cap \mathcal{D}(H_{\mathrm{f}})). \tag{2.24}$$

Remark 2.10
The additional term $J\pi^\beta(W_\infty^{(M)})J$ in the definition of $I^{(M)}$ is not necessary to obtain a self-adjoint generator of the time evolution. However, it guarantees that $L_\lambda^{(M)}$ anti-commutes with the modular conjugation J, which will be essential in the characterization of the time-invariant normal states. We call $L_\lambda^{(M)}$ the approximating Liouvillian in *standard form*.

Lemma 2.11
For all $M \in \mathbb{N}$, $t, \lambda \in \mathbb{R}$ and $A \in \mathfrak{M}_\beta$ we have

$$\sigma_{t,\lambda}^{(M)}(A) = e^{\mathrm{i}tL_\lambda^{(M)}} A e^{-\mathrm{i}tL_\lambda^{(M)}}.$$

Proof. First, we show that the additional term $J\pi^\beta(W_\infty^{(M)})J$ does not play any role for the unitary implementation of the Dyson series. As J is the modular conjugation (Proposition 2.8), the theorem of Tomita-Takesaki (Theorem A.11) yields

$$J\mathfrak{M}_\beta J = \mathfrak{M}_\beta'. \tag{2.25}$$

Furthermore, notice that due to (2.16), we have

$$\sigma_{t,0}(J\pi^\beta(A)J) = J\sigma_{t,0}(\pi^\beta(A))J$$

for all $t \in \mathbb{R}$ and $A \in \mathfrak{A}$. Therefore, we can also write

$$\begin{aligned}\sigma_{t,\lambda}^{(M)}(\pi^\beta(A)) &= \sigma_{t,0}(\pi^\beta(A)) \\ &+ \sum_{n=1}^\infty (\mathrm{i}\lambda)^n \int_0^t \cdots \int_0^{t_{n-1}} [\sigma_{t_n,0}(I^{(M)}), [\ldots[\sigma_{t_1,0}(I^{(M)}), \sigma_{t,0}(\pi^\beta(A))]\ldots]]\mathrm{d}t_1 \ldots \mathrm{d}t_n.\end{aligned} \tag{2.26}$$

By taking the first derivative one obtains that the map defined by

$$\widetilde{\sigma}_{t,\lambda}^{(M)}(A) := e^{\mathrm{i}tL_\lambda^{(M)}} A e^{-\mathrm{i}tL_\lambda^{(M)}}, \qquad A \in \mathfrak{M}_\beta,$$

satisfies the integral equation

$$\widetilde{\sigma}_{t,\lambda}^{(M)}(A) = \sigma_{t,0}(A) + \mathrm{i}\lambda \int_0^t \widetilde{\sigma}_{t_1,\lambda}^{(M)} \left(\sigma_{-t_1,0}([\sigma_{t_1,0}(I^{(M)}), \sigma_{t,0}(A)])\right) \mathrm{d}t_1.$$

Then using this recursion formula yields (2.26), cf. [BR2, Corollary 5.4.2]. □

The final step is to take the limit $M \to \infty$ of the approximating Liouvillian and the approximating interacting dynamics, and to show that they correspond to each other. First, we define the standard Liouvillian

$$\widetilde{L}_\lambda = \widetilde{L}_0 + \lambda(\pi^\beta(W_\infty) - J\pi^\beta(W_\infty)J), \tag{2.27}$$

on the space $\widetilde{\mathcal{D}}$, where

$$\begin{aligned}\pi^\beta(W_\infty) - J\pi^\beta(W_\infty)J = \Phi(\sqrt{1+\rho_\beta} G \otimes \mathrm{Id}_\mathrm{p} - \sqrt{\rho_\beta}\, \mathrm{Id}_\mathrm{p} \otimes \overline{G}^*) \otimes \mathrm{Id}_{\mathfrak{F}(\mathbb{R}^3)} \\ + \mathrm{Id}_{\mathfrak{F}(\mathbb{R}^3)} \otimes \Phi(\sqrt{\rho_\beta} G^* \otimes \mathrm{Id}_\mathrm{p} - \sqrt{1+\rho_\beta}\, \mathrm{Id}_\mathrm{p} \otimes \overline{G})),\end{aligned}$$

and the complex conjugation is to be understood with respect to $\mathcal{C}_\mathrm{p}$. In the following we assume that $\widetilde{L}_\lambda$ is in fact essentially self-adjoint on $\widetilde{\mathcal{D}}$ and we will denote its self-adjoint extension by the same symbol.

Remark 2.12
The essential self-adjointness will be verified later for the concrete assumptions we impose on the model, cf. Proposition 5.1 (under Hypotheses A-LR and B-LR) and Proposition 6.3 (under Hypotheses A-SR and B-SR) together with (4.4).

Furthermore, for all $A \in \mathfrak{A}$ and $t, \lambda \in \mathbb{R}$, let

$$\sigma_{t,\lambda}(\pi^\beta(A)) := \lim_{M\to\infty} \sigma_{t,\lambda}^{(M)}(\pi^\beta(A)),$$

and denote the (weak) extension to $\mathfrak{M}_\beta$ by the same symbol.

Proposition 2.13
For all $\lambda \in \mathbb{R}$ the following holds.

(a) For all $t \in \mathbb{R}$ the map $\sigma_{t,\lambda}$ is well-defined on $\mathfrak{M}_\beta$ and independent of the approximating sequence $(W_\infty^{(M)})_M$,

(b) $\sigma_{t,\lambda}(A) = e^{\mathrm{i}t\widetilde{L}_\lambda} A e^{-\mathrm{i}t\widetilde{L}_\lambda}$ for all $A \in \mathfrak{M}_\beta$, $t \in \mathbb{R}$,

(c) $(\mathfrak{M}_\beta, \sigma_{t,\lambda})$ *is a* W^**-dynamical system,*

(d) $e^{\mathrm{i}t\widetilde{L}_\lambda} J = J e^{\mathrm{i}t\widetilde{L}_\lambda}$ *for all* $t \in \mathbb{R}$.

Proof. Lemma 2.11 yields $\sigma^{(M)}_{t,\lambda}(A) = e^{\mathrm{i}tL^{(M)}_\lambda} A e^{-\mathrm{i}tL^{(M)}_\lambda}$, $A \in \mathfrak{M}_\beta$. By Lemma 2.9 we know that $L^{(M)}_\lambda \to \widetilde{L}_\lambda$ as $M \to \infty$, in the strong sense on $\widetilde{\mathcal{D}}$. As $\widetilde{\mathcal{D}}$ is a common core for all $L^{(M)}_\lambda$, $M \in \mathbb{N}$ and $\widetilde{L}_\lambda$, it follows that $L^{(M)}_\lambda \to \widetilde{L}_\lambda$ in the strong resolvent sense (cf. [RS1, Theorem VIII.25]), and thus, $e^{\mathrm{i}tL^{(M)}_\lambda} \to e^{\mathrm{i}t\widetilde{L}_\lambda}$ in the strong sense. This proves the first three claims.

For the last point notice that by construction of $I^{(M)}$ we have $Je^{\mathrm{i}tI^{(M)}} = e^{\mathrm{i}tI^{(M)}}J$. From $Je^{\mathrm{i}t\widetilde{L}_0} = e^{\mathrm{i}t\widetilde{L}_0}J$ and the Trotter product formula it then follows that $e^{\mathrm{i}tL^{(M)}_\lambda}J = Je^{\mathrm{i}tL^{(M)}\lambda}$. Taking the limit $M \to \infty$ yields the desired equation. □

2.5. Time-Invariant Normal States

Finally, we can prove the connection between time-invariant normal states and the kernel of the standard Liouvillian. Modular theory yields an one-to-one correspondence between normal states and unit elements of the so-called natural positive cone $\mathcal{P}$ associated to $(\mathfrak{M}_\beta, \Omega^{\rho_\mathrm{P}})$, cf. Appendix A.2.2. Recall that $\mathcal{P}$ is defined as the closure of the set

$$\{AJA\Omega^{\rho_\mathrm{P}} : A \in \mathfrak{M}_\beta\} \subseteq \widetilde{\mathcal{H}}.$$

The importance of $\mathcal{P}$ arises from the fact that the unitary group corresponding to the standard Liouvillian leaves $\mathcal{P}$ invariant, which will be shown in Lemma 2.14.

The proofs in this subsection are mainly inspired by [FM04b], where they were performed for a more particular form of the coupling terms.

Lemma 2.14
For all $t, \lambda \in \mathbb{R}$, *we have*

$$e^{\mathrm{i}t\widetilde{L}_\lambda}\mathcal{P} = \mathcal{P}.$$

Proof. It is enough to prove $e^{\mathrm{i}t\widetilde{L}_\lambda}\mathcal{P} \subseteq \mathcal{P}$ for all $t \in \mathbb{R}$, since we can apply the inverse of the unitary group to this inclusion. Furthermore, it is sufficient to show $e^{\mathrm{i}tL^{(M)}_\lambda}\mathcal{P} \subseteq \mathcal{P}$ for all $M \in \mathbb{N}$, due to the strong resolvent convergence established in the proof of Proposition 2.13. The Trotter product formula yields

$$e^{\mathrm{i}tL^{(M)}_\lambda}\xi = \lim_{n\to\infty}(e^{\mathrm{i}t/n\widetilde{L}_0}e^{\mathrm{i}t/n\lambda I^{(M)}})^n\xi$$

for all $\xi \in \widetilde{\mathcal{H}}$. Therefore, it suffices to prove

$$e^{\mathrm{i}tT}\xi \in \mathcal{P} \tag{2.28}$$

for all $\xi \in \mathcal{P}$, $T \in \{\widetilde{L}_0, I^{(M)}\}$, $M \in \mathbb{N}$ and $t \in \mathbb{R}$. Since $\mathcal{P}$ is closed, it is enough to verify (2.28) for all elements ξ whose linear hull is dense in $\mathcal{P}$, that is, $e^{\mathrm{i}tT}AJA\Omega^{\rho_\mathrm{p}} \in \mathcal{P}$ for all $A \in \mathfrak{M}_\beta$. As $BJB\mathcal{P} \subseteq \mathcal{P}$ (by (2.25)), and

$$e^{\mathrm{i}tT}AJA\Omega^{\rho_\mathrm{p}} = e^{\mathrm{i}tT}Ae^{-\mathrm{i}tT}Je^{\mathrm{i}tT}Ae^{-\mathrm{i}tT}e^{\mathrm{i}tT}\Omega^{\rho_\mathrm{p}} = BJBe^{\mathrm{i}tT}\Omega^{\rho_\mathrm{p}},$$

with $B := e^{\mathrm{i}tT}Ae^{-\mathrm{i}tT} \in \mathfrak{M}_\beta$, it is enough to prove

$$e^{\mathrm{i}tT}\Omega^{\rho_\mathrm{p}} \in \mathcal{P}. \tag{2.29}$$

First, we have

$$e^{\mathrm{i}tL_0}\Omega^{\rho_\mathrm{p}} = (e^{\mathrm{i}tH_\mathrm{p}} \otimes e^{-\mathrm{i}tH_\mathrm{p}}\Omega_\mathrm{p}^{\rho_\mathrm{p}}) \otimes \Omega^{\otimes 2} = \Big((e^{\mathrm{i}tH_\mathrm{p}} \otimes \mathrm{Id}_\mathrm{p})J_\mathrm{p}(e^{\mathrm{i}tH_\mathrm{p}} \otimes \mathrm{Id}_\mathrm{p})\Omega_\mathrm{p}^{\rho_\mathrm{p}}\Big) \otimes \Omega^{\otimes 2},$$

thus, $e^{\mathrm{i}tL_0}\Omega^{\rho_\mathrm{p}} = AJA\Omega^{\rho_\mathrm{p}} \in \mathcal{P}$ with $A = e^{\mathrm{i}tH_\mathrm{p}} \otimes \mathrm{Id}_{\mathcal{H}_\mathrm{p}\otimes\mathfrak{F}(L^2(\mathbb{R}^3))\otimes\mathfrak{F}(L^2(\mathbb{R}^3))}$. Second, since $J\pi^\beta(W_\infty^{(M)})J \in \mathfrak{M}_\beta'$, we obtain

$$e^{\mathrm{i}tI^{(M)}} = e^{\mathrm{i}t\pi^\beta(W_\infty^{(M)})}e^{-\mathrm{i}tJ\pi^\beta(W_\infty^{(M)})J} = e^{\mathrm{i}t\pi^\beta(W_\infty^{(M)})}Je^{\mathrm{i}t\pi^\beta(W_\infty^{(M)})}J,$$

where the last step follows from the exponential series expansion of $e^{-\mathrm{i}tJ\pi^\beta(W_\infty^{(M)})J}$. Hence, $e^{\mathrm{i}tI^{(M)}}\Omega^{\rho_\mathrm{p}} = AJA\Omega^{\rho_\mathrm{p}} \in \mathcal{P}$ with $A = e^{\mathrm{i}t\pi^\beta(W_\infty^{(M)})} \in \mathfrak{M}_\beta$. This shows (2.29) and finishes the proof. □

Theorem 2.15 (cf. [FM04b, Theorem 2.2])
The $\sigma_{t,\lambda}$-invariant normal states on $\mathfrak{M}_\beta$ are in one-to-one correspondence with the unit elements of $\ker \widetilde{L}_\lambda \cap \mathcal{P}$. In particular, if $\ker \widetilde{L}_\lambda = \{0\}$, there are no $\sigma_{t,\lambda}$-invariant normal states on $\mathfrak{M}_\beta$.

Proof. By Theorem A.13 the normal states on $\mathfrak{M}_\beta$ are in one-to-one correspondence with the unit elements of $\mathcal{P}$ via the map

$$\mathcal{P} \ni \xi \mapsto w_\xi, \qquad w_\xi(A) = \langle \xi, A\xi \rangle .$$

Therefore, it is sufficient to show that for all unit vectors $\xi \in \mathcal{P}$ we have $w_\xi \circ \sigma_{t,\lambda} = w_\xi$, $t \in \mathbb{R}$, if and only if $\xi \in \ker \widetilde{L}_\lambda$. So assume that for all $t \in \mathbb{R}$, $A \in \mathfrak{M}_\beta$,

$$\langle \xi, A\xi \rangle = \omega_\xi(A) = \omega_\xi(\sigma_{t,\lambda}(A)) = \left\langle e^{-\mathrm{i}t\widetilde{L}_\lambda}\xi, Ae^{-\mathrm{i}t\widetilde{L}_\lambda}\xi \right\rangle . \tag{2.30}$$

Then, by Lemma 2.14 we know that $e^{-\mathrm{i}t\widetilde{L}_\lambda}\xi \in \mathcal{P}$, and by the uniqueness property of the representing cone vectors, $\xi = e^{-\mathrm{i}t\widetilde{L}_\lambda}\xi$. As $t \in \mathbb{R}$ was arbitrary, $\xi \in \ker \widetilde{L}_\lambda$. On the other hand, if $\xi \in \ker \widetilde{L}_\lambda$, then $\xi = e^{-\mathrm{i}t\widetilde{L}_\lambda}\xi$ holds for all $t \in \mathbb{R}$, which implies (2.30). $\square$

For the proof of the main results we also need the following elementary property of $\mathcal{P}$.

Proposition 2.16
Let P_1, P_2 be orthogonal projections in $\mathcal{H}_\mathrm{p}$ such that $P_1 P_2 = 0$ and set

$$P_\mathsf{l} := P_1 \otimes P_2 \otimes \mathrm{Id}_\mathrm{f} \otimes \mathrm{Id}_\mathrm{f}, \qquad P_\mathsf{r} := P_2 \otimes P_1 \otimes \mathrm{Id}_\mathrm{f} \otimes \mathrm{Id}_\mathrm{f}\,.$$

Then we have

$$\mathrm{ran}\, P_\mathsf{l} \cap \mathcal{P} = \mathrm{ran}\, P_\mathsf{r} \cap \mathcal{P} = \{0\}.$$

Proof. By definition of J one sees $P_\mathsf{l} J = J P_\mathsf{r}$. Let $\psi \in \mathrm{ran}\, P_\mathsf{l} \cap \mathcal{P}$. Then we have $J\psi = \psi$ (which holds for all elements of $\mathcal{P}$). Therefore,

$$P_\mathsf{r}\psi = P_\mathsf{r} J\psi = J P_\mathsf{l}\psi = J\psi = \psi.$$

This implies $\psi \in \mathrm{ran}\, P_\mathsf{r} \cap \mathrm{ran}\, P_\mathsf{l} = \{0\}$. $\square$

3. Results

After the motivation for considering the standard Liouvillian $\widetilde{L}_\lambda$ was given in the previous chapter, the main results (Theorem 3.5 and Theorem 3.8) of this thesis will be presented in this part. While the formulation of them can be made very concise, there is a certain number of assumptions with respect to the potential of the atom and the interaction functions G which have to be satisfied. Furthermore, we discuss some examples of models where those rather abstract assumptions are fulfilled. In particular, Corollary 3.10 describes a quite explicit model. At the end there is a short discussion about open problems and possibilities for future work.

3.1. Conditions

The assumptions for the main result will be formulated as hypotheses. Not all of them are necessary to obtain a well-defined model, but for certain parts of the results and the proof. In the course of this thesis it will always be explicitly stated if some or all of them have to be fulfilled.

Essentially, there are to different sets of hypotheses given, one for the long-range (LR) and one for the short-range (SR) case, and we will typically assume that one of them is satisfied. There are assumptions with respect to the atom (or more precisely, with respect to the potential of the Schrödinger operator) and with respect to the interaction, both for the SR and LR case, respectively. Furthermore, there is the so-called Fermi Golden rule condition comprising both the atom and the interaction.

3.1.1. Atom

The terms 'long-range' (infinitely many bound states) and 'short-range' (finitely many bound states) refer to the potential of the Schrödinger operator describing the atom, so there is a hypothesis for each case. Each one admits *certain*, but not all potentials with infinitely or finitely many eigenvalues, respectively.

For the Hamiltonian H_p of the atom and the corresponding Hilbert space $\mathcal{H}_\mathrm{p}$, both introduced in Chapter 2, we make the following choice. We assume that H_p

is a Schrödinger operator on $\mathcal{H}_\mathrm{p} = L^2(\mathbb{R}^3)$, i.e.,

$$H_\mathrm{p} = -\Delta + V,$$

where $-\Delta \geq 0$ denotes the standard Laplacian and V the multiplication operator with a measurable function of the same name, which is subject to the following hypotheses. Note that $\hat{\mathsf{x}} = (\hat{\mathsf{x}}_1, \hat{\mathsf{x}}_2, \hat{\mathsf{x}}_3)$ denotes the vector of multiplication operators with the respective components and $\hat{\mathsf{p}} = -\mathrm{i}\nabla = (-\mathrm{i}\partial_1, -\mathrm{i}\partial_2, -\mathrm{i}\partial_3)$ the vector of momentum operators.

Hypothesis A-LR (Atom, LR case)

(1) V is an infinitely differentiable, bounded function with $V \leq 0$. Furthermore, the functions

$$x \mapsto \nabla V(x), \;\; x \mapsto \langle x \rangle \, (x\nabla)V(x) \text{ and } x \mapsto (x\nabla)^n V(x)$$

are bounded for $n \in \{2, 3\}$.

(2) There exists $\delta > 0$ such that

$$P_\mathrm{ess} \left((1-\delta)(-\Delta) - \frac{1}{2} \hat{\mathsf{x}} \nabla V \right) P_\mathrm{ess} \geq 0,$$

where P_ess denotes the projection to the essential spectrum of H_p.

This hypothesis has the following well-known consequences. In particular, note that

$$\lim_{|x| \to \infty} V(x) = 0.$$

Proposition 3.0
Assume that V satisfies Hypothesis A-LR (1). Then

(a) H_p is essentially self-adjoint on $C_\mathsf{c}^\infty(\mathbb{R}^3)$ with domain $\mathcal{D}(\Delta)$,

(b) H_p has essential spectrum $[0, \infty)$,

(c) the discrete spectrum $\sigma_\mathrm{d}(H_\mathrm{p}) \subseteq (-\infty, 0)$ can only accumulate at zero.

Proof. For a proof see for example [Tes09, section 10.1]. □

Remark 3.1
By including the case $\delta = 0$, condition (2) in Hypothesis A-LR would be an abstract generalization of the requirements for the potential in [FMS04]. The restriction to $\delta > 0$ in our setting is necessary in order to be able to treat the coupling of low energies in the essential spectrum of H_{p}, which was not considered in [FMS04].

One can see that Hypothesis A-LR (2) is satisfied for smooth attracting potentials in $O(|x|^{-\mu})$ for $|x| \to \infty$, $0 < \mu < 2$, by writing

$$
\begin{aligned}
P_{\mathrm{ess}}\left((1-\delta)(-\Delta) - \frac{1}{2}\hat{\mathsf{x}}\nabla V\right)P_{\mathrm{ess}} &= P_{\mathrm{ess}}\left((1-\delta)H_{\mathrm{p}} - (1-\delta)V - \frac{1}{2}\hat{\mathsf{x}}\nabla V\right)P_{\mathrm{ess}} \\
&\geq -P_{\mathrm{ess}}\left((1-\delta)V + \frac{1}{2}\hat{\mathsf{x}}\nabla V\right)P_{\mathrm{ess}}.
\end{aligned}
$$

For instance, potentials given by $V(x) = -C\langle x\rangle^{-\mu}$, $C > 0$, $0 < \mu < 2$, where $\langle x\rangle = (x^2+1)^{1/2}$, are admissible, see Corollary 3.13 for details. In particular, all these potentials yield infinitely many eigenvalues for H_{p}. As so-called long-range potentials in the context of scattering theory are included, that is, the case $\mu \leq 1$, we call this the 'long-range' (LR) case.

Remark 3.2
It seems to be an interesting question whether one could find potentials V such that H_{p} has at least one but at most finitely many eigenvalues and Hypothesis A-LR (2) is still satisfied. For such a proof note that one would need to take advantage of the projection P_{ess}. More precisely, it is not possible that H_{p} has at least one negative eigenvalue and

$$
(1-\delta)(-\Delta) - \frac{1}{2}\hat{\mathsf{x}}\nabla V \geq 0
$$

for some $\delta > 0$. Indeed, suppose that H_{p} has a negative eigenvalue with corresponding eigenvector ψ, and let $\mathrm{i}[H_{\mathrm{p}}, A_{\mathsf{D}}]$ be defined in form-sense (see (4.20)), where $A_{\mathsf{D}} := \frac{1}{4}(\hat{\mathsf{p}}\hat{\mathsf{x}} + \hat{\mathsf{x}}\hat{\mathsf{p}})$ is the generator of dilations. Then

$$
\left\langle \psi, \left(-\Delta - \frac{1}{2}\hat{\mathsf{x}}\nabla V\right)\psi \right\rangle = \langle \psi, \mathrm{i}[H_{\mathrm{p}}, A_{\mathsf{D}}]\psi\rangle = 0
$$

by a classical virial theorem, see [Cyc+87, Theorem 4.6]. Thus,

$$
\left\langle \psi, \left((1-\delta)(-\Delta) - \frac{1}{2}\hat{\mathsf{x}}\nabla V\right)\psi \right\rangle = -\delta\,\langle \psi, (-\Delta)\psi\rangle < 0.
$$

Hypothesis A-SR (Atom, SR case)

(1) $V \in C_{\mathsf{c}}^{\infty}(\mathbb{R}^3)$.

(2) If $\psi \in L^2(\mathbb{R}^3)$ satisfies

$$\psi(x) = -\frac{1}{4\pi}\int \frac{|V(x)|^{1/2}\,V(y)^{1/2}}{|x-y|}\psi(y)\mathrm{d}y, \qquad \text{for a.e. } x \in \mathbb{R}^3, \tag{3.1}$$

where $V^{1/2} := |V|^{1/2}\mathrm{sgn}V$, then $\psi = 0$.

Again, we state some immediate consequences of this hypothesis.

Proposition 3.2
If Hypothesis A-SR (1) holds, then

(a) H_p is essentially self-adjoint on $C_\mathrm{c}^\infty(\mathbb{R}^3)$ with domain $\mathcal{D}(\Delta)$,

(b) H_p has essential spectrum $[0,\infty)$,

(c) the discrete spectrum of H_p is finite,

(d) H_p has no positive eigenvalues,

(e) H_p has no singular spectrum.

If Hypothesis A-SR (1) and (2) hold, then

(f) zero is not an eigenvalue of H_p.

Proof. (a) and (b) follow as in Proposition 3.0. (c) follows from [RS4, Theorem XIII.6]. (d) follows from the Kato-Agmon-Simon theorem ([RS4, Theorem XIII.58]). (e) follows from [RS4, Theorem XIII.21]. (f) Suppose ϕ were an eigenvector with eigenvalue zero. Then using the integral representation of the resolvent of the Laplacian, see for example [RS2, section IX.7], we find $\phi(x) = -(4\pi)^{-1}\int_{\mathbb{R}^3}|x-y|^{-1}V(y)\phi(y)dy$. From this it is straightforward to verify that $\psi = |V|^{1/2}\phi$ would be a nonzero solution of (3.1). $\square$

Remark 3.3
One can think of Hypothesis A-SR (2) as the absence of bound states and so-called half-bound states, which are not necessarily in L^2, see [New12]. This could also be rephrased by saying that energy zero is not an exceptional point in the sense as defined in [New12].

Another characterization of Hypothesis A-SR (2) is that 1 is not an eigenvalue of the integral operator K_V, given by the integral kernel $-|V(x)|^{1/2}V^{1/2}(y)/(4\pi|x-$

$y|)$. As K_V is compact (because it is Hilbert-Schmidt by assumption) and $K_{\mu V} = \mu K_V$ for all $\mu \geq 0$, the set

$$\{\mu \in \mathbb{R} : 1 \text{ is an eigenvalue of } K_{\mu V}\}$$

is of Lebesgue measure zero and therefore, potentials, which do not satisfy Hypothesis A-SR (2), are rather rare.

Remark 3.4
For the result and our proof one actually needs just finitely many derivatives of V. Therefore, one could weaken Hypothesis A-SR (1). However it seems quite tedious in the proof to keep track to which order exactly derivatives are required.

3.1.2. Interaction

Because of the different techniques for the proof in the LR and SR case, we also postulate different conditions for the functions

$$G\colon \mathbb{R}^3 \longrightarrow \mathcal{L}(\mathcal{H}_\mathrm{p}),$$

which were already introduced in (2.2). In the SR setting we have to assume a more specific form of G with a factorization in the different cutoff functions, while this can be relaxed in the LR setting. However, this rather mild generalization does not play any role for the intended application.

In the following derivatives of an operator-valued functions are always to be understood in the strong operator topology.

Hypothesis B-LR
For all

$$X \in \{\langle\hat{\mathsf{x}}\rangle^{n_1} G(\cdot) \langle\hat{\mathsf{x}}\rangle^{n_2} : n_1 + n_2 \leq 4, n_1, n_2 \in \mathbb{N}_0\}, \tag{3.2}$$

and all

$$X \in \{\langle\hat{\mathsf{x}}\rangle^{n_1} [G(\cdot), \hat{\mathsf{p}}_j] \langle\hat{\mathsf{x}}\rangle^{n_2} : j \in \{1,2,3\}, n_1 + n_2 \leq 3, n_1, n_2 \in \mathbb{N}_0\}, \tag{3.3}$$

where the commutator $[G(\cdot), \hat{\mathsf{p}}_j]$ is to be understood in the form sense on $\mathcal{D}(\hat{\mathsf{p}}_j)$ (see also (4.20)), we have $X(\omega\Sigma) \in \mathcal{L}(\mathcal{H}_\mathrm{p})$ for all $(\omega, \Sigma) \in \mathbb{R}_+ \times \mathbb{S}^2$, and for all $m \in \{0, \ldots, 3\}$, the partial derivatives $(\omega, \Sigma) \mapsto \partial_\omega^m X(\omega\Sigma)$ exist as $\mathcal{L}(\mathcal{H}_\mathrm{p})$-valued functions on $\mathbb{R}_+ \times \mathbb{S}^2$ and are bounded on compact subsets. Furthermore, the following holds.

(I1) *Ultraviolet cutoff:* There are constants $K, C \in (0, \infty)$ and $q > \frac{7}{2}$ such that

$$\|\partial_\omega^n X(\omega\Sigma)\| \leq C\omega^{-q}, \qquad n \in \{0, \ldots, 3\},$$

for all $\omega > K$ and $\Sigma \in \mathbb{S}^2$.

(I2) *Regularity and infrared behavior:* One of the following assumptions hold.

(i) There are constants $k, C \in (0, \infty)$, $p > 2$, such that

$$\|\partial_\omega^n X(\omega\Sigma)\| \leq C\omega^{p-n}, \qquad n \in \{0, \ldots, 3\},$$

for all $\omega < k$ and $\Sigma \in \mathbb{S}^2$.

(ii) There exist $k > 0$, $J \in \mathbb{N}_0$, $N \in \mathbb{N}$, and $\lambda_i \in \mathbb{C}$, $i \in \{1, \ldots, N\}$, such that

$$X(\omega\Sigma) = \omega^{-\frac{1}{2}+J} \sum_{i=1}^{N} \lambda_i X_0^{(i)}(\omega, \Sigma)$$

for all (ω, Σ), where each $X_0^{(i)}$, $i \in \{1, \ldots, N\}$, is an $\mathcal{L}(\mathcal{H})$-valued function on $[0, k) \times \mathbb{S}^2$ such that for $n = 0, \ldots, \max\{0, 3 - J\}$ the partial derivatives $\partial_\omega^n X_0^{(i)}$ exist, are uniformly bounded, and satisfy the relation

$$\partial_\omega^n X_0^{(i)}(\omega, \Sigma)|_{\omega=0} = (-1)^{n+J+1} \partial_\omega^n X_0^{(i)}(\omega, \Sigma)^*|_{\omega=0}.$$

Remark 3.4
Notice that we have to impose a spatial decay on G, up to order 4 in (3.2) and up to order 3 in (3.3). This has its origin in the virial theorem Theorem 4.8 which requires the consideration of three-fold commutators with the dilation operator, and another weak commutator with the harmonic oscillator to verify the GJN condition. Furthermore, the three derivatives with respect to ω arise from the virial theorem as well.

Hypothesis B-SR
For $(\omega, \Sigma) \in \mathbb{R}_+ \times \mathbb{S}^2$, we define a bounded multiplication operator on $\mathcal{H}_\mathrm{p}$ by

$$G(\omega\Sigma)(x) = \kappa(\omega)\chi(x)\widetilde{G}(\omega, \Sigma)(x), \qquad x \in \mathbb{R}^3, \tag{3.4}$$

where κ is a function on $\mathbb{R}_+$ and $\chi \in \mathcal{S}(\mathbb{R}^3)$ – the space of Schwartz functions, and for each (ω, Σ), $\widetilde{G}(\omega, \Sigma)$ is a function on $\mathbb{R}^3$, satisfying the following conditions.

(1) *Spatial cutoff:* For all $n \in \{0,1,2,3\}$ and $\alpha \in \mathbb{N}_0^3$ the partial derivatives $\partial_x^\alpha \partial_\omega^n \widetilde{G}$ exist and are continuous on $\mathbb{R}_+ \times \mathbb{S}^2 \times \mathbb{R}^3$, and there exists a polynomial P and an $M \in \mathbb{N}_0$ such that for all $(\omega, \Sigma, x) \in \mathbb{R}_+ \times \mathbb{S}^2 \times \mathbb{R}^3$,

$$\left|\partial_x^\alpha \partial_\omega^n \widetilde{G}(\omega,\Sigma)(x)\right| \leq P(\omega)\langle x\rangle^M, \tag{3.5}$$

where $\langle x\rangle := (1+x^2)^{1/2}$.

(2) *UV cutoff:* κ decays faster than any polynomial, that is, for all $n \in \mathbb{N}$,

$$\sup_{\omega \geq 1} \omega^n \left|\kappa(\omega)\right| < \infty.$$

(3) *Regularity and infrared behavior:* $\kappa \in C^3(\mathbb{R}_+)$ and one of the following two properties holds:

(i) there exist $k, C \in (0,\infty)$, $p > 2$ such that

$$|\partial_\omega^n \kappa(\omega)| \leq C\omega^{p-n}, \qquad n \in \{0,\dots,3\},$$

for all $\omega \in (0,k)$,

(ii) there exist $J \in \mathbb{N}_0$ and $\kappa_0 \in C^s([0,\infty))$, with $s = \max\{0, 3-J\}$, such that

$$\kappa(\omega) = \omega^{-\frac{1}{2}+J}\kappa_0(\omega), \quad \omega > 0,$$

and there exists an extension $\tilde{G}_0$ of $\tilde{G}$ to $[0,\infty) \times \mathbb{S}^2 \times \mathbb{R}^3$ such that for all $n \in \{0,\dots,s\}$ and all $\alpha \in \mathbb{N}_0^3$ the partial derivatives $\partial_x^\alpha \partial_\omega^n \widetilde{G}_0$ exist, are continuous, satisfy (3.5) for all $(\omega, \Sigma, x) \in [0,\infty) \times \mathbb{S}^2 \times \mathbb{R}^3$, and

$$\partial_\omega^n(\kappa_0(\omega)\chi\tilde{G}_0(\omega,\Sigma))(x)|_{\omega=0} = (-1)^{n+J+1}\partial_\omega^n\overline{(\kappa_0(\omega)\chi\tilde{G}_0(\omega,\Sigma))(x)}|_{\omega=0}.$$

3.1.3. Fermi Golden Rule Condition

For the proof of our main result we require another additional assumption. We need that the instability of the eigenvalues should be visible in second order perturbation theory with respect to the coupling. The second order term is also called level shift operator and the corresponding positivity assumption *Fermi Golden Rule condition*. In Section 3.3 an example is provided where this is satisfied.

As in [FMS04] we want to allow the restriction of the interaction to a limited number of modes. Let $\mathcal{M}$ be an index set for the discrete modes of H_p, that is, the discrete eigenvalues of H_p including multiplicity. In other words, to each $m \in \mathcal{M}$

corresponds a unique eigenfunction ϕ_m such that $(\phi_m)_{m\in\mathcal{M}}$ is an orthonormal basis of $\operatorname{ran} P_{\mathrm{disc}}$, where $P_{\mathrm{disc}} := P_{\mathrm{ess}}^{\perp}$ denotes the spectral projection to the discrete spectrum of H_{p}. For $m \in \mathcal{M}$ let E_m be the corresponding eigenvalue.

Now, let $J_{\mathrm{d}} \subseteq \mathcal{M}$ and set

$$P_J := p_{J_{\mathrm{d}}} + P_{\mathrm{ess}}, \tag{3.6}$$

where $p_{J_{\mathrm{d}}}$ denotes the spectral projection to J_{d}. We assume that

$$P_J G(k) P_J = G(k) \tag{3.7}$$

holds for almost all $k \in \mathbb{R}^3$. Clearly, the trivial case $J_{\mathrm{d}} = \mathcal{M}$ (no restriction) always satisfies this condition.

For $m \in \mathcal{M}$ let p_m be the corresponding spectral projection. For all $E \in \sigma_{\mathrm{d}}(H_{\mathrm{p}})$, for which there is an $m \in J_{\mathrm{d}}$ with $E_m = E$, and $\varepsilon > 0$, let $\gamma_\beta(E, \varepsilon, J_{\mathrm{d}}) \geq 0$ be the largest number such that

$$p_{J_{\mathrm{d}}}(E)\Big(F^{(1)}_{G,\beta}(E,\varepsilon) + F^{(2)}_{G,\beta}(E,\varepsilon)\Big)p_{J_{\mathrm{d}}}(E) \geq \gamma_\beta(E,\varepsilon,J_{\mathrm{d}})p_{J_{\mathrm{d}}}(E),$$

where $p_{J_{\mathrm{d}}}(E) := \sum_{\substack{m\in J_{\mathrm{d}}:\\ E_m = E}} p_m$, and

$$F^{(1)}_{G,\beta}(E,\varepsilon) := \int_0^\infty \int_{\mathbb{S}^2} \frac{\omega^2}{e^{\beta\omega}-1} G(\omega\Sigma) \frac{P_{\mathrm{ess}}}{(H_{\mathrm{p}} - E - \omega)^2 + \varepsilon^2} G(\omega\Sigma)^* \mathrm{d}\Sigma \mathrm{d}\omega,$$
$$F^{(2)}_{G,\beta}(E,\varepsilon) := \int_0^\infty \int_{\mathbb{S}^2} \frac{\omega^2}{1-e^{-\beta\omega}} G(\omega\Sigma)^* \frac{P_{\mathrm{ess}}}{(H_{\mathrm{p}} - E + \omega)^2 + \varepsilon^2} G(\omega\Sigma) \mathrm{d}\Sigma \mathrm{d}\omega.$$

Furthermore, we set

$$\gamma_\beta(\varepsilon, J_{\mathrm{d}}) := \inf_{m\in J_{\mathrm{d}}} \gamma_\beta(E_m, \varepsilon, J_{\mathrm{d}}). \tag{3.8}$$

We say that the Fermi Golden Rule condition for $\varepsilon > 0$, $\beta > 0$ and J_{d} is satisfied if and only if

$$\gamma_\beta(E_m, \varepsilon, J_{\mathrm{d}}) > 0 \tag{3.9}$$

for all $m \in J_{\mathrm{d}}$.

Remark 3.4
Usually the term *Fermi Golden Rule condition* (e.g as in [FM04b; FMS04]) means that

$$\liminf_{\varepsilon\to 0} \varepsilon\gamma_\beta(\varepsilon, J_{\mathrm{d}}) > 0,$$

which yields the evaluation of a Dirac function. However, $\varepsilon F^{(2)}_{G,\beta}(E,\varepsilon)$ converges to zero as $\varepsilon \to 0$ and does thus not provide any positive contribution when considering the limit. In this case one can only make use of $F^{(1)}_{G,\beta}(E,\varepsilon)$, which decays exponentially to zero as $\beta \to \infty$, that is, for low temperatures. Then we get a result which is not uniform in the temperature and the lower bound γ_β does depend on β, cf. Lemma 3.12.

Therefore, we work with an approximated version of the Fermi Golden Rule condition by just considering a fixed $\varepsilon > 0$. The operator $F^{(2)}_{G,\beta}(E,\varepsilon)$ does not converge to zero as $\beta \to \infty$ and therefore, we get a result uniformly in β for $\beta \geq \beta_0 > 0$, that is, for low temperatures (cf. Corollary 3.10).

3.2. Main Theorems

The main results of this thesis are presented in the following two theorems, which address the LR and the SR case, respectively. They yield a characterization of the time-invariant states and show that thermal ionization happens in the SR case under the given abstract hypotheses. Some concrete settings where those are satisfied, will be discussed afterwards in the subsequent section.

Both theorems essentially follow from the application of the virial theorem and the positivity proof in the subsequent chapters, together with some formal arguments in the LR case. At this point, we only collect the necessary ingredients and references in the proofs.

Recall that $\widetilde{L}_\lambda$ denotes the self-adjoint extension of the operator given in (2.27). In the LR case we have to restrict the coupling to finitely many modes of H_{p} such that the uncoupled modes naturally appear in the kernel of the Liouvillian and as time-invariant normal states of the algebra $\mathfrak{M}_\beta$.

Theorem 3.5 (Long-range)
Assume that Hypotheses A-LR and B-LR are satisfied, and (3.7) holds for a finite subset $J_{\mathrm{d}} \subseteq \mathcal{M}$. Let $\beta_0 > 0$ and $\varepsilon > 0$. Then there exists a constant $C > 0$ such that for all $\beta \geq \beta_0$ and $0 < |\lambda| < C \min\{1, \gamma_\beta(\varepsilon, J_{\mathrm{d}})^2\}$, we have

$$\ker \widetilde{L}_\lambda \cap \operatorname{ran}(P_J \otimes P_J \otimes \mathrm{Id}_{\mathrm{f}} \otimes \mathrm{Id}_{\mathrm{f}}) = \{0\}. \tag{3.10}$$

In this case, the $\sigma_{t,\lambda}$-invariant normal states on $\mathfrak{M}_\beta$ are in one-to-one correspondence with the unit elements of

$$\mathcal{P} \cap \operatorname{lin}\{\phi_m \otimes \phi_n \otimes \Omega \otimes \Omega : m, n \in \mathcal{M} \setminus J_{\mathrm{d}},\ E_m = E_n\}. \tag{3.11}$$

Proof. The first statement (3.10) follows from Theorem 5.5 and Proposition 5.7 in combination with Theorem 7.10 and Proposition 7.11.

The second statement is then a simple consequence, see also [FMS04, section 5.1]. We have

$$\begin{aligned}
&\ker \widetilde{L}_\lambda \cap \operatorname{ran}(P_J{}^\perp \otimes P_J{}^\perp \otimes \mathrm{Id}_\mathrm{f} \otimes \mathrm{Id}_\mathrm{f}) \\
&\qquad = \ker \widetilde{L}_0 \cap \operatorname{ran}(P_J{}^\perp \otimes P_J{}^\perp \otimes \mathrm{Id}_\mathrm{f} \otimes \mathrm{Id}_\mathrm{f}) \\
&\qquad = \operatorname{lin}\{\phi_m \otimes \phi_n \otimes \Omega \otimes \Omega : m, n \in \mathcal{M} \setminus J_\mathrm{d},\ E_m = E_n\}.
\end{aligned}$$

Proposition 2.16 yields

$$\mathcal{P} \cap \operatorname{ran}(P_J \otimes P_J{}^\perp \otimes \mathrm{Id}_\mathrm{f} \otimes \mathrm{Id}_\mathrm{f}) = \mathcal{P} \cap \operatorname{ran}(P_J{}^\perp \otimes P_J \otimes \mathrm{Id}_\mathrm{f} \otimes \mathrm{Id}_\mathrm{f}) = \{0\}.$$

Therefore, we conclude that $\ker \widetilde{L}_\lambda \cap \mathcal{P}$ is given by (3.11). Then the statement results from Theorem 2.15. □

Remark 3.6
Theorem 3.5 can be regarded as an extension of [FMS04, Theorem 2.3] with partially weaker assumptions and for more general coupling terms. The philosophy is that an interaction restricted to finitely many modes J_d, i.e., satisfying (3.7), can be regarded as an approximation of the real interaction corresponding to $J_\mathrm{d} = \mathcal{M}$. In a formal sense, the set (3.11) also 'converges' to $\{0\}$ if J_d tends to $\mathcal{M}$. This means that thermal ionization occurs in the 'limit' when all modes are coupled.

Remark 3.7
One could rephrase Theorem 3.5 by replacing the requirement that J_d is finite with the claim that the numbers $\delta_1^{(\beta)}, \delta_2^{(\beta)}, \delta_3^{(\beta,\varepsilon)}$ in (H1)–(H3) are strictly positive, see also Remark 7.9.

Next, in the SR case the artificial restriction (3.7) is not needed anymore for the proof. Consequently, there are also no time-invariant states originating from uncoupled modes and one can show that thermal ionization actually occurs.

Theorem 3.8 (Short-range)
Assume that Hypotheses A-SR and B-SR are satisfied. Let $\beta_0 > 0$ and $\varepsilon > 0$. Then there exists a constant $C > 0$ such that for all $\beta \geq \beta_0$ and $0 < |\lambda| < C \min\{1, \gamma_\beta(\varepsilon, \mathcal{M})^2\}$, zero is not an eigenvalue of $\widetilde{L}_\lambda$. In particular, there are no $\sigma_{t,\lambda}$-invariant normal states on $\mathfrak{M}_\beta$.

Proof. This follows from Theorem 6.5 in combination with Theorem 7.14. Then the absence of time-invariant states is a consequence of Theorem 2.15. □

Remark 3.9
Notice that the Fermi Golden Rule condition (3.9) has to be satisfied in order to obtain a non-trivial statement in the Theorems 3.5 and 3.8.

3.3. Application

We provide a rather explicit example for the SR case in Corollary 3.10, where Theorem 3.8 is applicable and thermal ionization can be proven. We consider a toy atom with a compactly supported smooth potential and a linear coupling term with spatial cutoff, motivated by QED, where the conditions for the main theorem are satisfied. In particular, no additional restrictions have to be imposed on the coupling. In doing so, we present two rather simple methods to verify the Fermi Golden Rule condition (Lemmas 3.11 and 3.12). At the end, we also give an example of a potential and a similar coupling term restricted to finitely many eigenmodes, which satisfies the LR assumptions (Corollary 3.13).

Corollary 3.10
Assume that V satisfies Hypothesis A-SR. Let

$$G(k)(x) = \kappa(|k|)e^{\mathrm{i}kx}\chi(x), \qquad k, x \in \mathbb{R}^3, \tag{3.12}$$

where $\chi \in \mathcal{S}(\mathbb{R}^3)$ is nonzero, and κ is a nonzero function on $\mathbb{R}_+$ satisfying Hypothesis B-SR (2) and one of the following two conditions.

(I) Part (i) of Hypothesis B-SR (3) holds.

(II) The function χ is real-valued and there exist positive constants c and C such that

$$\kappa(\omega) = C\omega^{-\frac{1}{2}}e^{-c\omega^2} \tag{3.13}$$

for all $\omega \geq 0$.

Then for any $\beta_0 > 0$ there exists a $\lambda_0 > 0$, such that whenever $0 < |\lambda| < \lambda_0$ and $\beta \geq \beta_0$ the operator $\widetilde{L}_\lambda$, or equivalently L_λ, does not have zero as an eigenvalue.

Proof. Derivatives with respect to ω and x yield only polynomial growth in x and ω, respectively. Thus, Hypothesis B-SR (1) is satisfied. Hypothesis A-SR (1), (2) and Hypothesis B-SR (2) are satisfied by the assumptions.

If (I) holds, the same applies to Hypothesis A-SR (3) (i).

Now, assume that (II) holds. In this case, we want to verify Hypothesis B-SR (3) (ii). Note that G in (3.12) can be multiplied with any phase $e^{\mathrm{i}\varphi}$, $\varphi \in \mathbb{R}$, which just yields unitary equivalent Liouvillians by means of the unitary transformation $\mathrm{Id}_\mathrm{p} \otimes \mathrm{Id}_\mathrm{p} \otimes \Gamma(e^{\mathrm{i}\varphi})$. Therefore, without loss of generality, we can assume

$$\kappa(\omega) = \mathrm{i}C\omega^{-\frac{1}{2}}e^{-c\omega^2}$$

instead of (3.13). Hypothesis B-SR (3) (ii) is actually satisfied in this case. One has to verify

$$\partial_\omega^j(\mathrm{i}e^{-c\omega^2}\chi(x)e^{\mathrm{i}\omega\Sigma x})|_{\omega=0} = (-1)^{j+1}\partial_\omega^j\overline{\mathrm{i}e^{-c\omega^2}\chi(x)e^{\mathrm{i}\omega\Sigma x}}|_{\omega=0}$$

for all $\Sigma \in \mathbb{S}^2$, $x \in \mathbb{R}^3$ and $j = 0, \dots, 3$, which is easy to check.

It remains to verify the Fermi Golden Rule condition. This will follow from Lemma 3.11 below, since $\sigma_\mathrm{d}(H_\mathrm{p})$ is finite. □

Lemma 3.11

Suppose the assumptions of Corollary 3.10 hold, and let $E \in \sigma_\mathrm{d}(H_\mathrm{p})$. Then for any $\varepsilon > 0$ there exists a $\gamma(E) > 0$ (independent of β) such that

$$p_E F_{G,\beta}^{(2)}(E,\varepsilon)p_E \geq \gamma(E)p_E.$$

Proof. Let ϕ_E denote a normalized eigenvector of $-\Delta+V$ with eigenvalue E. First observe that

$$\begin{aligned}&\left\langle \phi_E, F_{G,\beta}^{(2)}(E,\varepsilon)\phi_E\right\rangle \\ &\quad \geq \int_0^\infty \int_{\mathbb{S}^2} \omega^2 \left\langle \phi_E, G(\omega\Sigma)^* \frac{\varepsilon P_\mathrm{ess}}{(H_\mathrm{p} - E + \omega)^2 + \varepsilon^2} G(\omega\Sigma)\phi_E \right\rangle \mathrm{d}\Sigma\mathrm{d}\omega.\end{aligned}$$

The integrand is continuous in (ω,Σ) and non-negative. Thus, it suffices to show that there exists (ω,Σ) such that

$$\left\langle G(\omega\Sigma)\phi_E, \frac{\varepsilon P_\mathrm{ess}}{(H_\mathrm{p} - E + \omega)^2 + \varepsilon^2} G(\omega\Sigma)\phi_E \right\rangle \neq 0,$$

which follows if one can show

$$P_\mathrm{ess} G(\omega\Sigma)\phi_E \neq 0. \tag{3.14}$$

Suppose there is no (ω,Σ) such that (3.14) holds, that is, $G(\omega\Sigma)\phi_E \in \operatorname{ran} P_\mathrm{disc}$ for all (ω,Σ). By the finite dimensionality of $\operatorname{ran} P_\mathrm{disc}$, the space

$$\operatorname{lin}\{G(\omega\Sigma)\phi_E : (\omega,\Sigma) \in \mathbb{R}_+ \times \mathbb{S}^2\} \tag{3.15}$$

would be finite-dimensional. But this leads to a contradiction, as we will now show.

By unique continuation of eigenfunctions ([RS4, Theorem XIII.57]) $\phi_E(x) \neq 0$ for a.e. $x \in \mathbb{R}^3$. By assumption κ does not vanish on some nonempty open interval $I \subset (0, \infty)$. Then

$$\mathrm{lin}\{e^{\mathrm{i}\omega\Sigma\hat{x}}\chi\phi_E : (\omega, \Sigma) \in I \times \mathbb{S}^2\}$$

is a subspace of (3.15) and has infinite dimension, which can be seen by means of using Wronskians as follows.

For $n \in \mathbb{N}$ let $\omega_1, \ldots, \omega_n \in I$ be pairwise distinct and let $\lambda_1, \ldots, \lambda_n \in \mathbb{C}$ such that for all $x \in \mathbb{R}^3$,

$$\sum_{m=1}^{n} \lambda_m e^{\mathrm{i}\omega_m x_1} \chi(x)\phi_E(x) = 0.$$

Note that x_1 denotes the first component of x, which results from choosing $\Sigma = (1, 0, 0)$. As χ does not vanish and $\phi_E(x) \neq 0$ for a.e. x, we conclude that there is an open set $U \subseteq \mathbb{R}^3$ such that for all $x \in U$,

$$\sum_{m=1}^{n} \lambda_m e^{\mathrm{i}\omega_m x_1} = 0.$$

By taking $(n-1)$-fold derivatives at any point in U, and using the non-degeneracy of the Vandermonde matrix corresponding to $(\omega_1, \ldots, \omega_n)$, we obtain $\lambda_1 = \cdots = \lambda_n = 0$. $\square$

It was already indicated in Remark 3.4 that instead of using $F^{(2)}_{G,\beta}(E, \varepsilon)$ one can also verify (3.9) with the first term $F^{(1)}_{G,\beta}(E, \varepsilon)$ in the limit $\varepsilon \to 0$. This does not improve the qualitative statement of Corollary 3.10 and has the drawback that $\gamma_\beta \to 0$ as $\beta \to \infty$ as in [FM04b; FMS04]. However, in certain regimes, it still might be the dominant term. For the proof we use a dipole approximation as in [GZ09], that is, a power series expansion of the coupling term.

For $k \in \mathbb{R}^3$ let $\phi(k, \cdot)$ denote the scattering state as defined in Section 6.1. In the next proposition we shall use the following notation

$$\begin{aligned}\langle \phi(k, \cdot), f \rangle &:= \mathsf{l.i.m.} \int \overline{\phi(k, x)} f(x) \mathrm{d}x, \\ \langle f, \phi(k, \cdot) \rangle &:= \overline{\langle \phi(k, \cdot), f \rangle},\end{aligned}$$

where $f \in L^2(\mathbb{R}^3)$, for the expressions occurring in Theorem 6.1.

Lemma 3.12

Assume that V satisfies Hypothesis A-SR. Let $\delta > 0$ and $\chi \in \mathcal{S}(\mathbb{R}^3)$ be constant *and positive in a ball around the origin, and let κ be a continuous and positive function satisfying Hypothesis B-SR (2) and (3). We consider for all $\alpha > 0$,*

$$G_\alpha(k)(x) = \kappa(|k|)e^{\alpha i k x}\chi(\alpha^\delta x), \qquad k, x \in \mathbb{R}^3.$$

Then we have for all $E \in \sigma_{\mathrm{d}}(H_{\mathrm{p}})$,

$$\begin{aligned}\lim_{\varepsilon\to 0}&\left\langle \phi_E, \varepsilon\pi^{-1}F^{(1)}_{G_\alpha,\beta}(E,\varepsilon)\phi_E\right\rangle \\ &= \int_{\mathbb{S}_2}\int_{\mathbb{R}^3}\frac{(k^2-E)^2}{e^{\beta(k^2-E)}-1}|\kappa(k^2-E)|^2(k^2-E)^2\alpha^2|\chi(0)|^2|\langle\phi_E, \Sigma\hat{\mathsf{x}}\phi(k,\cdot)\rangle|^2 \mathrm{d}k\mathrm{d}\Sigma \\ &\quad + O(\alpha^3). \end{aligned} \tag{3.16}$$

In particular, if V is rotationally invariant and there are only non-degenerate eigenvalues, then there exists $\alpha_0 > 0$ such that for all $0 < \alpha < \alpha_0$,

$$\liminf_{\varepsilon\to 0}\varepsilon\gamma_\beta(\varepsilon, \mathcal{M}) > 0.$$

Proof. Notice that the operators $\varepsilon\pi^{-1}F^{(1)}_{G_\alpha,\beta}(E,\varepsilon)$, $\varepsilon > 0$, form a Dirac sequence in the limit $\varepsilon \to 0$. Then using Theorem 6.1 and the fact that G_α is continuous, we obtain

$$\begin{aligned}&\left\langle \phi_E, \varepsilon\pi^{-1}F^{(1)}_{G_\alpha,\beta}(E,\varepsilon)\phi_E\right\rangle \\ &= \int_0^\infty \frac{\omega^2}{e^{\beta\omega}-1}\int_{\mathbb{S}^2}\left\| V_{\mathsf{c}}\frac{\varepsilon}{\pi((H_{\mathrm{p}}-E+\omega)^2+\varepsilon^2)^{1/2}}G(\omega\Sigma)^*\phi_E\right\|^2 \mathrm{d}\Sigma\mathrm{d}\omega \\ &= \frac{1}{(2\pi)^3}\int_0^\infty\frac{\omega^2}{e^{\beta\omega}-1}\int_{\mathbb{S}^2}\int_{\mathbb{R}^3}\frac{\varepsilon}{\pi(k^2-E-\omega)^2+\varepsilon^2}\left|\langle G(\omega\Sigma)^*\phi_E, \phi(k,\cdot)\rangle\right|^2 \mathrm{d}k\mathrm{d}\Sigma\mathrm{d}\omega \\ &\overset{\varepsilon\to 0}{\to} \frac{1}{(2\pi)^3}\int_{\mathbb{S}_2}\int_{\mathbb{R}^3}\frac{(k^2-E)^2}{e^{\beta(k^2-E)}-1}\left|\kappa(k^2-E)\right|^2\left|\langle\phi_E, e^{\mathrm{i}\alpha(k^2-E)\Sigma\hat{\mathsf{x}}}\chi(\alpha^\delta\cdot)\phi(k,\cdot)\rangle\right|^2 \mathrm{d}k\mathrm{d}\Sigma.\end{aligned}$$

Now we consider an expansion in powers of α. Let $C > 0$ large enough such that

$$\left|e^{\mathrm{i}s} - 1 - \mathrm{i}s\right| \le C|s|^2, \quad s \in \mathbb{R}.$$

Then, for all $\alpha > 0$ and $k \in \mathbb{R}^3$,

$$\begin{aligned}&\left|\left\langle \phi_E, \left(e^{\mathrm{i}\alpha(k^2-E)\Sigma\hat{\mathsf{x}}}\chi(\alpha^\delta\cdot) - \chi(\alpha^\delta\cdot) - \mathrm{i}\alpha(k^2-E)\Sigma\hat{\mathsf{x}}\chi(\alpha^\delta\cdot)\right)\phi(k,\cdot)\right\rangle\right| \\ &\quad \le C\alpha^2\|\phi(k,\cdot)\|_\infty\|\chi\|_\infty\int|\phi_E(x)|\left|(k^2-E)\Sigma x\right|^2 \mathrm{d}x.\end{aligned} \tag{3.17}$$

First, let us estimate the contribution of $\chi(\alpha^\delta \cdot)$. By assumption there exists $r > 0$ such that χ is constant on $B_r(0)$. As the eigenfunctions decay exponentially (cf. [Shn57]), we may assume there are constants $c, C > 0$ such that

$$|\phi_E(x)| \leq Ce^{-c|x|}.$$

Thus, for $n \in \{0,1\}$ and $j \in \{1,2,3\}$, there exist constants C, C' such that

$$\begin{aligned}\left|\left\langle \hat{\mathsf{x}}_j^n \phi_E, (\chi(\alpha^\delta \cdot) - \chi(0))\phi(k,\cdot)\right\rangle\right| &\leq 2\|\phi(k,\cdot)\|_\infty \|\chi\|_\infty \int_{\alpha^\delta |x|>r} |x_j|^n |\phi_E(x)| \mathrm{d}x \\ &\leq C\|\phi(k,\cdot)\|_\infty \|\chi\|_\infty \int_{\alpha^\delta \rho > r} e^{-c\rho} \mathrm{d}\rho \\ &\leq C'\|\phi(k,\cdot)\|_\infty \|\chi\|_\infty e^{-cr\alpha^{-\delta}} \end{aligned} \tag{3.18}$$

for all $\alpha > 0$ and $k \in \mathbb{R}^3$, where we used that polynomial functions are exponentially bounded. On the other hand, since the scattering functions $\phi(k,\cdot)$ are orthogonal to all eigenfunctions, we find

$$\left\langle \phi_E, \chi(\alpha^\delta \cdot)\phi(k,\cdot)\right\rangle = \left\langle \phi_E, (\chi(\alpha^\delta \cdot) - \chi(0))\phi(k,\cdot)\right\rangle. \tag{3.19}$$

Combining (3.17), (3.18) and (3.19), we arrive at

$$\begin{aligned}&\left|\langle \phi_E, e^{\mathrm{i}\alpha(k^2-E)\Sigma\hat{\mathsf{x}}} \chi(\alpha^\delta \cdot)\phi(k,\cdot)\rangle - \langle \phi_E, \mathrm{i}\alpha(k^2-E)\Sigma\hat{\mathsf{x}}\chi(0)\phi(k,\cdot)\rangle\right| \\ &\quad \leq C\alpha^2(k^2+1)\|\phi(k,\cdot)\|_\infty \|\chi\|_\infty,\end{aligned}$$

where C denotes a constant not depending on α and k. Thus in the limit $\alpha \to 0$ we determined the leading order contribution given in (3.16).

Within the explicit model, one can now verify whether the leading order term does not vanish. If V is rotationally invariant and H_p has only non-degenerate eigenvalues E with eigenvector ϕ_E, then we find $\langle \phi_E, \hat{\mathsf{x}}_j \phi_E\rangle = 0$ by symmetry. Thus, by the orthogonality relation of the scattering states,

$$(2\pi)^{-3} \int |\langle \phi_E, \hat{\mathsf{x}}_j \phi(k,\cdot)\rangle|^2 \mathrm{d}k = \|\hat{\mathsf{x}}_j \phi_E\|^2 \neq 0. \qquad \square$$

Finally, in the following corollary we give, similar as above, an example of an atom and coupling terms for the LR case with a restriction to finitely many eigenmodes.

Corollary 3.13
Let $V(x) = -C\langle x\rangle^{-\mu}$ for some constants $C > 0$ and $1 \leq \mu < 2$. Further let $J_\mathrm{d} \subseteq \mathcal{M}$ be finite and $\chi_\mathrm{ess} \in \mathcal{L}(\mathcal{H}_\mathrm{p})$ such that

$$\chi_\mathrm{ess} P_\mathrm{ess} = \chi_\mathrm{ess}$$

and the operators

$$\langle \hat{\mathsf{x}} \rangle^{\pm n} \chi_{\mathrm{ess}} \langle \hat{\mathsf{x}} \rangle^{\mp n} \quad \textit{and} \quad [\chi_{\mathrm{ess}}, \hat{\mathsf{p}}_j] \tag{3.20}$$

are bounded for all $n \in \{1,2,3,4\}$ *and* $j \in \{1,2,3\}$. *We set*

$$G(k) = (p_{J_\mathrm{d}} + \chi_{\mathrm{ess}}) \widetilde{G}(k) (p_{J_\mathrm{d}} + \chi_{\mathrm{ess}}), \qquad k \in \mathbb{R}^3, \tag{3.21}$$

where for each $k \in \mathbb{R}^3$, $\widetilde{G}(k)$ *is a multiplication operator on* $\mathcal{H}_\mathrm{p}$ *with the function*

$$\widetilde{G}(k)(x) := C\kappa(|k|) e^{\mathrm{i}kx} \chi(x), \qquad x \in \mathbb{R}^3,$$

with $C \in \mathbb{R}$ *being a constant and*

$$\kappa(\omega) = \omega^p \langle \omega \rangle^{-q}, \qquad p > 2, \; q > \frac{9}{2} + p, \tag{3.22}$$

$$\chi(x) = \langle x \rangle^{-r}, \qquad r \geq 7. \tag{3.23}$$

Let $\beta_0 > 0$ *and* $\varepsilon > 0$. *Then there exists a constant* $C > 0$ *such that for all* $\beta \geq \beta_0$ *and* $0 < |\lambda| < C \min\{1, \gamma_\beta(\varepsilon, J_\mathrm{d})^2\}$, *the* $\sigma_{t,\lambda}$*-invariant normal states on* $\mathfrak{M}_\beta$ *are in one-to-one correspondence with the unit elements of*

$$\mathcal{P} \cap \mathrm{lin}\{\phi_m \otimes \phi_n \otimes \Omega \otimes \Omega : m, n \in \mathcal{M} \setminus J_\mathrm{d} \; E_m = E_n\}.$$

Proof. The corollary follows from Theorem 3.5 if we verify the given hypotheses. Note that (3.7) holds by assumption.

Hypothesis A-LR: Condition (1) is obviously satisfied as $x \mapsto \langle x \rangle V(x)$ and ∇V are bounded functions and the application of $\hat{\mathsf{x}}\nabla$ does not change the decay behavior in spatial infinity. Condition (2) is satisfied with $\delta = 1 - \frac{\mu}{2} > 0$, since

$$-\frac{1}{2}(x\nabla)(-\langle x \rangle^{-\mu}) = -\frac{\mu}{2} \langle x \rangle^{-\mu-1} x \frac{x}{\langle x \rangle} \geq -\frac{\mu}{2} \langle x \rangle^{-\mu}$$

implies $-\frac{1}{2}(x\nabla)V \geq -\frac{\mu}{2}V$. Hence,

$$P_{\mathrm{ess}} \left(\frac{\mu}{2}(-\Delta) - \frac{1}{2}(\hat{\mathsf{x}}\nabla)V \right) P_{\mathrm{ess}} \geq \frac{\mu}{2} P_{\mathrm{ess}}(-\Delta + V) P_{\mathrm{ess}} \geq 0.$$

Hypothesis B-LR: First, we show this hypothesis for $\widetilde{G}$. We have for $n \in \{0,1,2,3\}$ and $n_1, n_2 \in \mathbb{N}_0$ with $n_1 + n_2 \leq 4$,

$$\partial_\omega^n \langle x \rangle^{n_1} \widetilde{G}(\omega\Sigma)(x) \langle x \rangle^{n_2} = \sum_{m=0}^{n} \binom{n}{m} \partial_\omega^m \kappa(\omega) (\mathrm{i}\Sigma x)^{n-m} \langle x \rangle^{n_1+n_2} \chi(x) e^{\mathrm{i}\omega\Sigma x}.$$

As $n_1 + n_2 + n \leq 7$, we obtain by (3.23),

$$\sup_{x\in\mathbb{R}^3} \left|\partial_\omega^n \langle x\rangle^{n_1} \widetilde{G}(\omega\Sigma)(x) \langle x\rangle^{n_2}\right| \leq C \sum_{m=0}^{n} |\partial_\omega^m \kappa(\omega)|$$

for a constant $C > 0$ independent of (ω, Σ). Finally, note that κ has the decay behavior which is requested in (I1) and (I2) (i) of Hypothesis B-LR. This proves Hypothesis B-LR for all elements of the set in (3.2).

The same can be shown for elements of (3.3). The operator $[\widetilde{G}(\omega\Sigma), \hat{\mathsf{p}}_j]$, $j \in \{1, 2, 3\}$, is given by multiplication with

$$x \mapsto \mathrm{i}\partial_{x_j}\widetilde{G}(\omega\Sigma)(x) = \mathrm{i}\kappa(\omega)e^{\mathrm{i}\omega\Sigma x}(\partial_{x_j}\chi(x) + \mathrm{i}\omega\Sigma_j\chi(x)).$$

The first summand can be treated as above since derivatives of χ have a faster decay than χ itself. For the second summand the same is true since by construction, $\omega \mapsto \omega\kappa(\omega)$ behaves as ω^p, $p > 3$, for $\omega \to 0$ and as ω^{-p}, $p > \frac{7}{2}$, for $\omega \to \infty$.

Finally, consider the case when J_d is finite. Then the operators $\langle\hat{\mathsf{x}}\rangle^{\pm n} p_{J_\mathrm{d}} \langle\hat{\mathsf{x}}\rangle^{\mp n}$, $n \in \mathbb{N}_0$, and $\hat{\mathsf{p}}_j p_{J_\mathrm{d}}$, $p_{J_\mathrm{d}}\hat{\mathsf{p}}_j$ (as $\operatorname{ran} p_{J_\mathrm{d}}$ is finite and $\operatorname{ran} p_{J_\mathrm{d}} \subseteq \mathcal{D}(\hat{\mathsf{p}}_j)$), are bounded. Together with the assumptions this implies that the operators

$$\langle\hat{\mathsf{x}}\rangle^{\pm n} (p_{J_\mathrm{d}} + \chi_{\mathrm{ess}}) \langle\hat{\mathsf{x}}\rangle^{\mp n}, \qquad [p_{J_\mathrm{d}} + \chi_{\mathrm{ess}}, \hat{\mathsf{p}}_j]$$

are bounded as well for all $n \in \{1, 2, 3, 4\}$ and $j \in \{1, 2, 3\}$. Thus, Hypothesis B-LR also holds for $G = (p_{J_\mathrm{d}} + \chi_{\mathrm{ess}})\widetilde{G}(p_{J_\mathrm{d}} + \chi_{\mathrm{ess}})$. □

Remark 3.14
A generic choice for χ_{ess} in Corollary 3.13, for which the given conditions are verifiable with the methods in this thesis, can be made as follows. For some $e_0 > 0$ let $\widetilde{\chi_{\mathrm{ess}}} \in C^{10}(\mathbb{R})$ such that

$$\widetilde{\chi_{\mathrm{ess}}}(e) = \begin{cases} 1 & : e > e_0, \\ 0 & : e \leq 0. \end{cases}$$

Then one can check with $\chi_{\mathrm{ess}} = \widetilde{\chi_{\mathrm{ess}}}(H_\mathrm{p})$ that the operators in (3.20) are bounded by means of Corollary B.9 and Proposition B.11.

On the other hand, in order to get a result for $\chi_{\mathrm{ess}} = P_{\mathrm{ess}}$ (no decay at zero energy in the coupling), one needs to verify that the operators

$$\langle\hat{\mathsf{x}}\rangle^{\pm n} P_{\mathrm{ess}} \langle\hat{\mathsf{x}}\rangle^{\mp n}, \qquad n \in \{1, 2, 3, 4\},$$

are bounded.

Remark 3.15
The simple method in the proof of Lemma 3.11 does not carry over immediately to the LR setting (where $\operatorname{ran} P_{\mathrm{disc}}$ is infinite-dimensional), and an enhancement would be necessary. However, one can directly use Lemma 3.12 to verify the Fermi Golden Rule condition if J_{d} consists only of non-degenerate eigenmodes.

Remark 3.16
The condition (3.22) can be replaced with

$$\kappa(\omega) = \omega^{-\frac{1}{2}} \langle\omega\rangle^{-p}, \qquad p > 4,$$

or

$$\kappa(\omega) = \omega^{\frac{1}{2}} \langle\omega\rangle^{-p}, \qquad p > 5,$$

where one has to adapt the proof in an obvious way to verify condition (I2) (ii) of Hypothesis B-LR.

3.4. Conclusion and Open Problems

In the LR case the restrictions of the coupling with respect to the essential spectrum of H_{p} as in [FMS04] could be removed. This is especially important for low energies, as the theory is not applicable for very high energies, anyway. However, the results are still not satisfactory: on the one hand only potentials with infinitely many eigenvalues are admissible, on the other hand the proof of positivity can effectively handle only finitely of them.

It is not clear whether the analysis would also work for certain potentials with finitely many eigenvalues (cf. Remark 3.1), so an example or a proof of the contrary would be very welcome. Nevertheless, the physically more interesting and probably also more difficult challenge is the treatment of a real atom like hydrogen with infinitely many eigenvalues. It seems to be in the realms of possibility that this approach can also be used in this direction. Some ideas in this context are collected in Remark 7.9.

The SR approach resolves the limitation to potentials with infinitely many eigenvalues. One can find an explicit model of a particle with a smooth compactly supported potential and a general coupling term with spatial decay but no additional artificial restrictions, where thermal ionization can be proven. Furthermore, this result can be achieved also uniformly for bounded temperatures. The major problem here remains the non-physical spatial decay in the coupling terms, which has its origin in the choice of the commutator on the field space. A possible solution seems to require a completely new strategy in this respect.

The idea of the diagonalization of the Hamiltonian with scattering functions could potentially also be applied to the abstract diagonalized representation of the model in [FM04b]. Therefore, it would be interesting to point out exactly how their assumptions with respect to the coupling terms translate into a more concrete setting, using the methods of Section 6.4.

Furthermore, there are some other points for possible improvements or weakening of the assumptions. For example one could treat all potentials which decay faster than $|x|^{-2-\epsilon}$ for $|x| \to \infty$ and some $\epsilon > 0$. It was already mentioned in Remark 3.4 that the generalization to potentials V with only finitely many derivatives of V would be possible. Probably a bit more difficult is the weakening of the assumption with respect to the compact support. Among other things one has to optimize the Klein-Zemach estimate for the remainder terms.

Finally, a physically important but formally rather bureaucratic issue seems to be the inclusion of a spin variable in the Fock space. This is necessary for treating photons and therefore real QED models. We expect that this should not change the fundamental analysis and follows by adjusting the notation.

4. Concepts of the Proof

This chapter provides an orientation for the proof of the main results Theorem 3.5 and Theorem 3.8. Before we can state the strategy, we recapitulate the so-called gluing transformation from [JP96a] and some related notation which will be used throughout the whole proof. At the end we repeat the exact statement of the virial theorem from [FM04b].

4.1. Gluing Transformation

In order to define the conjugate operator on the field and shorten some calculations it is convenient to combine the two Fock spaces which appear in the Araki-Woods representation (cf. Proposition 2.5 and (2.15)) into a single Fock space. This concept was first introduced by Jakšić and Pillet in [JP96a].

Let $\mathbb{S}^2$ be the 2–dimensional sphere. The transformation to spherical coordinates corresponds to a unitary map

$$U_1 \colon L^2(\mathbb{R}^3) \longrightarrow L^2(\mathbb{R}_+ \times \mathbb{S}^2, \mathrm{d}\omega \times \mathrm{d}\Sigma), \ (U_1 f)(\omega, \Sigma) = \omega f(\omega\Sigma).$$

Then two half-lines can be glued together by the unitary map

$$\begin{aligned} U_2 \colon L^2(\mathbb{R}_+ \times \mathbb{S}^2, \mathrm{d}\omega \times \mathrm{d}\Sigma) \oplus L^2(\mathbb{R}_+ \times \mathbb{S}^2, \mathrm{d}\omega \times \mathrm{d}\Sigma) &\longrightarrow L^2(\mathbb{R} \times \mathbb{S}^2, \mathrm{d}u \times \mathrm{d}\Sigma), \\ U_2(f \oplus g)(u, \Sigma) = \begin{cases} f(u, \Sigma) & : u > 0, \\ -g(-u, \Sigma) & : u < 0. \end{cases} \end{aligned} \tag{4.1}$$

Remark 4.1
The negative sign in front of g in (4.1) was included to obtain the same Liouvillian in the glued space as in [FMS04] and [HS20].

In the following we omit the measure $\mathrm{d}u \times \mathrm{d}\Sigma$ in the last space and just write $L^2(\mathbb{R} \times \mathbb{S}^2)$ for the space on the right-hand side. By combining U_1 and U_2 we obtain a map

$$U_2 \circ (U_1 \oplus U_1) \colon L^2(\mathbb{R}^3) \oplus L^2(\mathbb{R}^3) \longrightarrow L^2(\mathbb{R} \times \mathbb{S}^2). \tag{4.2}$$

We can now lift (4.2) to the Fock space and combine it with the unitary map U of Theorem A.6. Then we obtain the gluing isomorphism

$$U_{\mathsf{gl}} := \Gamma(U_2 \circ (U_1 \oplus U_1))U \colon \mathfrak{F}(L^2(\mathbb{R}^3)) \otimes \mathfrak{F}(L^2(\mathbb{R}^3)) \longrightarrow \mathfrak{F}(L^2(\mathbb{R} \times \mathbb{S}^2)).$$

Note that U_{gl} extends naturally to the map

$$\begin{aligned} &\widehat{U}_{\mathsf{gl}} := \mathrm{Id}_{\mathcal{H}_\mathrm{p} \otimes \mathcal{H}_\mathrm{p}} \otimes U_{\mathsf{gl}} \colon \\ &\quad \mathcal{H}_\mathrm{p} \otimes \mathcal{H}_\mathrm{p} \otimes \mathfrak{F}(L^2(\mathbb{R}^3)) \otimes \mathfrak{F}(L^2(\mathbb{R}^3)) \longrightarrow \mathcal{H}_\mathrm{p} \otimes \mathcal{H}_\mathrm{p} \otimes \mathfrak{F}(L^2(\mathbb{R} \times \mathbb{S}^2)). \end{aligned}$$

In the following proposition we apply this transformation to the Liouvillian $\widetilde{L}_\lambda$ in (2.27). To obtain the transformed interaction, we define for a Hilbert space $\mathcal{H}$ a map

$$\begin{aligned} \tau_\beta \colon L^2_0(\mathbb{R}^3, \mathcal{L}(\mathcal{H})) &\longrightarrow L^2(\mathbb{R} \times \mathbb{S}^2, \mathcal{L}(\mathcal{H})), \\ (\tau_\beta(F))(u, \Sigma) &:= \begin{cases} u\sqrt{1 + \rho_\beta(u)}F(u\Sigma) & : u > 0, \\ u\sqrt{\rho_\beta(-u)}F(-u\Sigma)^* & : u < 0, \end{cases} \end{aligned} \tag{4.3}$$

where ρ_β is defined as in (2.8). Let

$$\mathcal{D} := C^\infty_\mathsf{c}(\mathbb{R}^3) \,\widehat{\otimes}\, C^\infty_\mathsf{c}(\mathbb{R}^3) \,\widehat{\otimes}\, \mathfrak{F}_{\mathrm{fin}}(C^\infty_\mathsf{c}(\mathbb{R} \times \mathbb{S}^2)),$$

which is a dense subspace of the composite Hilbert space

$$\mathcal{H}_\mathrm{p} \otimes \mathcal{H}_\mathrm{p} \otimes \mathfrak{F},$$

where $\mathfrak{F} := \mathfrak{F}(L^2(\mathbb{R} \times \mathbb{S}^2))$. One can check that $\mathcal{D}$ is related to $\widetilde{\mathcal{D}}$ defined in (2.24) by

$$\mathcal{D} \subseteq \widehat{U}_{\mathsf{gl}} \widetilde{\mathcal{D}}. \tag{4.4}$$

Let $\hat{\mathsf{u}}$ and $\hat{\omega}$ denote the multiplication operators with the first variables in $L^2(\mathbb{R} \times \mathbb{S}^2)$ and $L^2(\mathbb{R}_+ \times \mathbb{S}^2)$, respectively.

Proposition 4.2 (Transformed Liouvillian)
We have on $\mathcal{D}$,

$$\begin{aligned} L_\lambda &:= \widehat{U}_{\mathsf{gl}} \widetilde{L}_\lambda \widehat{U}_{\mathsf{gl}}^{-1} \\ &= (H_\mathrm{p} \otimes \mathrm{Id}_\mathrm{p} - \mathrm{Id}_\mathrm{p} \otimes H_\mathrm{p}) \otimes \mathrm{Id}_\mathrm{f} + \mathrm{Id}_\mathrm{p} \otimes \mathrm{Id}_\mathrm{p} \otimes \mathsf{d}\Gamma(\hat{\mathsf{u}}) + \lambda \Phi(I), \end{aligned} \tag{4.5}$$

where

$$I(u, \Sigma) := I_\mathsf{l}(u, \Sigma) \otimes \mathrm{Id}_\mathrm{p} + \mathrm{Id}_\mathrm{p} \otimes I_\mathsf{r}(u, \Sigma), \tag{4.6}$$

$$I_\mathsf{l}(u, \Sigma) := \tau_\beta(G)(u, \Sigma), \qquad I_\mathsf{r}(u, \Sigma) := -e^{-\beta u/2} \tau_\beta(\overline{G}^*)(u, \Sigma). \tag{4.7}$$

Proof. Theorem A.6 yields on $\mathfrak{F}_{\mathrm{fin}}(L^2(\mathbb{R}\times\mathbb{S}^2))$,

$$\begin{aligned}
&U_{\mathsf{gl}}(H_{\mathrm{f}}\otimes \mathrm{Id} - \mathrm{Id}\otimes H_{\mathrm{f}})U_{\mathsf{gl}}^{-1}\\
&\quad = \Gamma(U_2)\Gamma(U_1\oplus U_1)U(H_{\mathrm{f}}\otimes \mathrm{Id} - \mathrm{Id}\otimes H_{\mathrm{f}})U^{-1}\Gamma(U_1\oplus U_1)^{-1}\Gamma(U_2)^{-1}\\
&\quad = \mathsf{d}\Gamma(U_2(\hat{\omega}\oplus(-\hat{\omega}))U_2^{-1})\\
&\quad = \mathsf{d}\Gamma(\hat{\mathsf{u}}).
\end{aligned}$$

In the following, we use the short-hand notation $G_{\mathsf{l}} := G\otimes \mathrm{Id}_{\mathrm{p}}$, $G_{\mathsf{r}} := \mathrm{Id}_{\mathrm{p}}\otimes G$ and $\Phi_{\mathsf{l}} := \Phi\otimes \mathrm{Id}_{\mathfrak{F}(L^2(\mathbb{R}^3))}$, $\Phi_{\mathsf{r}} := \mathrm{Id}_{\mathfrak{F}(L^2(\mathbb{R}^3))}\otimes\Phi$. For the first part of the interaction we obtain on $\mathcal{D}$, using the definition of τ_β (4.3) with $\mathcal{H} = \mathcal{H}_{\mathrm{p}}\otimes\mathcal{H}_{\mathrm{p}}$,

$$\begin{aligned}
&\widehat{U}_{\mathsf{gl}}(\Phi_{\mathsf{l}}(\sqrt{1+\rho_\beta}G_{\mathsf{l}}) + \Phi_{\mathsf{r}}(\sqrt{\rho_\beta}G_{\mathsf{l}}^*))\widehat{U}_{\mathsf{gl}}^{-1}\\
&\quad = \mathrm{Id}_{\mathcal{H}_{\mathrm{p}}\otimes\mathcal{H}_{\mathrm{p}}}\otimes(\Gamma(U_2)\Gamma(U_1\oplus U_1))\,\Phi\left(\sqrt{1+\rho_\beta}G_{\mathsf{l}}\oplus\sqrt{\rho_\beta}G_{\mathsf{l}}^*\right)\\
&\qquad\times \mathrm{Id}_{\mathcal{H}_{\mathrm{p}}\otimes\mathcal{H}_{\mathrm{p}}}\otimes\left(\Gamma(U_1\oplus U_1)^{-1}\Gamma(U_2)^{-1}\right)\\
&\quad = \Phi\left(\widehat{U}_2(\widehat{U}_1(\sqrt{1+\rho_\beta}G_{\mathsf{l}})\oplus\widehat{U}_1(\sqrt{\rho_\beta}G_{\mathsf{l}}^*))\right)\\
&\quad = \Phi(\tau_\beta(G_{\mathsf{l}})),
\end{aligned}$$

where $\widehat{U}_1$ and $\widehat{U}_2$, denote the canonical extensions of U_1 and U_2, respectively, to $\mathcal{L}(\mathcal{H}_{\mathrm{p}}\otimes\mathcal{H}_{\mathrm{p}})$-valued L^2-functions. Now, the relation

$$e^{\beta\omega}\rho_\beta(\omega) = \rho_\beta(\omega)+1, \qquad \omega>0,$$

along with the definition (4.3) implies that

$$e^{-\beta u/2}\tau_\beta(\overline{G}_{\mathsf{r}}^*)(u,\Sigma) = \begin{cases} u\sqrt{\rho_\beta(u)}\overline{G}_{\mathsf{r}}^*(u\Sigma) & : u>0,\\ u\sqrt{1+\rho_\beta(-u)}\overline{G}_{\mathsf{r}}(-u\Sigma) & : u<0.\end{cases}$$

Combining this with the previous calculation we obtain

$$U_{\mathsf{gl}}(\Phi_{\mathsf{l}}(\sqrt{\rho_\beta}\overline{G}_{\mathsf{r}}^*) + \Phi_{\mathsf{r}}(\sqrt{1+\rho_\beta}\overline{G}_{\mathsf{r}}))U_{\mathsf{gl}}^{-1} = \Phi_{\mathsf{r}}(e^{-\beta\hat{\mathsf{u}}/2}\tau_\beta(\overline{G}_{\mathsf{r}}^*)). \qquad \square$$

Next, we discuss the decay behavior of functions and their derivatives after the transformation with τ_β. This will play a major role in the proof when considering commutators of the generator of translations in the glued space $\mathsf{d}\Gamma(\mathrm{i}\partial_u)$ with the interaction terms I given in (4.6). We note that in the following lemma derivatives of the $\mathcal{L}(\mathcal{H})$-valued functions can be understood in the operator norm, strong operator, or weak operator topology in $\mathcal{L}(\mathcal{H})$, respectively.

Lemma 4.3
Let $\mathcal{H}$ be a Hilbert space, $F\colon \mathbb{R}^3 \to \mathcal{L}(\mathcal{H})$ a measurable function, and $m \in \mathbb{N}$. Assume that for $n = 0, \dots, m$ the partial derivatives $(\omega, \Sigma) \mapsto \partial_\omega^n F(\omega\Sigma)$ exist on $\mathbb{R}_+ \times \mathbb{S}^2$, and that they are bounded on compact subsets. Furthermore assume that there exist constants $\varepsilon > 0$ and $k, K, C_1, C_2 \in (0, \infty)$ such that for all $\Sigma \in \mathbb{S}^2$, $n = 0, \dots, m$,

(1) $\|\partial_\omega^n F(\omega\Sigma)\| \le C_1 \omega^{m-1+\varepsilon-n}$, *for* $\omega \in (0, k)$,

(2) $\|\partial_\omega^n F(\omega\Sigma)\| \le C_2 \omega^{-\frac{3}{2}-\varepsilon}$, *for* $\omega \in (K, \infty)$.

Then the weak partial derivatives $\partial_u^n \tau_\beta(F)$ exist and are in $L^2(\mathbb{R} \times \mathbb{S}^2, \mathcal{L}(\mathcal{H}))$ for $n = 0, \dots, m$. In particular, for $n = 0, 1$, there exists a constant C_3 such that for all $\beta \in (0, \infty)$,

$$\|\partial_u^n \tau_\beta(F)\|_{L^2(\mathbb{R}\times\mathbb{S}^2, \mathcal{L}(\mathcal{H}))} \le C_3(1 + \beta^{-\frac{1}{2}}). \tag{4.8}$$

The assertion also holds, if we assume instead of Condition (1):

(1') There exists a $J \in \mathbb{N}_0$ and $N \in \mathbb{N}$ such that

$$F(\omega\Sigma) = \omega^{-\frac{1}{2}+J} \sum_{i=1}^{N} \lambda_i F_0^{(i)}(\omega, \Sigma), \quad \omega \in (0, k),$$

where $\lambda_i \in \mathbb{C}$ and each $F_0^{(i)}$, $1 \le i \le N$, is an $\mathcal{L}(\mathcal{H})$-valued function on $[0, k) \times \mathbb{S}^2$ such that for $n = 0, \dots, \max\{0, m - J\}$ the partial derivatives $\partial_\omega^n F_0^{(i)}$ exist, are uniformly bounded, and satisfy the relation

$$\partial_\omega^n F_0^{(i)}(\omega, \Sigma)|_{\omega=0} = (-1)^{n+J+1} \partial_\omega^n F_0^{(i)}(\omega, \Sigma)^*|_{\omega=0}.$$

Proof. We will treat small and large $|u|$ separately. In particular, (4.8) will follow as a consequence of (4.10) and (4.13), below. Let us start using Leibniz' formula

$$\partial_u^n \tau_\beta(F)(u, \Sigma) = \begin{cases} \sum_{l=0}^n \binom{n}{l} \partial_u^l \left(u\sqrt{1 + \rho_\beta(u)}\right) \partial_u^{n-l} F(u\Sigma) & : u > 0, \\ \sum_{l=0}^n \binom{n}{l} \partial_u^l \left(u\sqrt{\rho_\beta(-u)}\right) \partial_u^{n-l} F(-u\Sigma)^* & : u < 0. \end{cases} \tag{4.9}$$

We first consider $|u|$ at infinity. The first factor in the first line in (4.9) is in $O(u)$ for $u \to \infty$, and the first factor in the second line decays faster than any polynomial. This implies with (2) that there exist constants $C_n(\beta)$, such that, for all $n = 0, \dots, m$ and all u with $|u| > K$,

$$\|\partial_u^n \tau_\beta(F)(u, \Sigma)\| \le C_n(\beta)\, |u|^{-\frac{1}{2}-\varepsilon}.$$

This and the boundedness of F and its partial derivatives on compact subsets of $\mathbb{R}_+ \times \mathbb{S}^2$ imply that

$$(u,\Sigma) \mapsto \mathbb{1}_{\mathbb{R}\setminus[-R,R]}(u)\partial_u^n \tau_\beta(F)(u,\Sigma)$$

is in $L^2(\mathbb{R}\times\mathbb{S}^2, \mathcal{L}(\mathcal{H}))$ for all $R>0$, $\Sigma\in\mathbb{S}^2$ and $n=0,\dots,m$. In particular, for $n=0,1$ we find in view of Lemma B.14 that $C_0(\beta)$ and $C_1(\beta)$ can be bounded by a constant times $1+\beta^{-1/2}$. Thus we conclude that

$$\|\mathbb{1}_{\mathbb{R}\setminus[-k,k]}(u)\partial_u^n \tau_\beta(F)\|_{L^2(\mathbb{R}\times\mathbb{S}^2,\mathcal{L}(\mathcal{H}))} \leq C(1+\beta^{-\frac{1}{2}}), \quad n\in\{0,1\}. \tag{4.10}$$

Let us now check the decay behavior near zero. First assume that (1) is satisfied. We extend $\tau_\beta(F)$ to a function on $\mathbb{R}\times\mathbb{S}^2$ by setting $\tau_\beta(F)(0,\Sigma) := 0$. The first factors in the sums in (4.9), $\partial_u^l\left(u\sqrt{1+\rho_\beta(u)}\right)$ and $\partial_u^l\left(u\sqrt{\rho_\beta(u)}\right)$, are in $O(|u|^{\frac{1}{2}-l})$ for $u\to 0$. The norms of the second factors are in $O(|u|^{m-1-(n-l)+\varepsilon})$ by Assumption (1). Hence, there exist constants $c_n(\beta)$, such that, for all $0<|u|<k$ and $\Sigma\in\mathbb{S}^2$, we have

$$\|\partial_u^n\tau_\beta(F)(u,\Sigma)\| \leq c_n(\beta)\,|u|^{-\frac{1}{2}+m-n+\varepsilon}, \quad n\in\{0,\dots,m\}. \tag{4.11}$$

We conclude from (4.11) that for each Σ the function $u\mapsto\tau_\beta(F)(u,\Sigma)$ is $m-1$ times continuously differentiable on $\mathbb{R}$ with $\partial_u^n\tau_\beta(F)(0,\Sigma)=0$ for $n=1,\dots,m-1$. Moreover, we see from (4.11) that for each Σ, the function $u\mapsto\partial_u^{m-1}\tau_\beta(F)(u,\Sigma)$ is weakly differentiable. Furthermore, we infer from (4.11)

$$(u,\Sigma)\mapsto \mathbb{1}_{[-k,k]}(u)\partial_u^n\tau_\beta(F)(u,\Sigma) \tag{4.12}$$

is in $L^2(\mathbb{R}\times\mathbb{S}^2,\mathcal{L}(\mathcal{H}))$ for all $n=0,\dots,m$. In particular, for $n=0,1$ we find in view of Lemma B.14 that we can bound $c_0(\beta)$ and $c_1(\beta)$ by a constant times $1+\beta^{-1/2}$, and so

$$\|\mathbb{1}_{[-k,k]}(u)\partial_u^n\tau_\beta(F)\|_{L^2(\mathbb{R}\times\mathbb{S}^2,\mathcal{L}(\mathcal{H}))} \leq C(1+\beta^{-\frac{1}{2}}), \quad n\in\{0,1\}. \tag{4.13}$$

Let us now assume the alternative condition (1') is satisfied and pick any $i\in\{1,\dots,N\}$. In that case we first observe that for $F^{(i)}(\omega\Sigma) := \omega^{-\frac{1}{2}+J}F_0^{(i)}(\omega,\Sigma)$ we can write for $|u|<k$,

$$\tau_\beta(F^{(i)})(u,\Sigma) = \begin{cases} u^J\sqrt{\sigma_\beta(-u)}F_0^{(i)}(u,\Sigma) & : u>0, \\ -(-u)^J\sqrt{\sigma_\beta(-u)}F_0^{(i)}(-u,\Sigma)^* & : u<0, \end{cases}$$

where we defined the function

$$\sigma_\beta\colon \mathbb{R}\longrightarrow\mathbb{R}, \quad \sigma_\beta(x) := \begin{cases} x\rho_\beta(x) & : x\neq 0, \\ \frac{1}{\beta} & : x=0. \end{cases}$$

The function σ_β is infinitely differentiable and positive, which for large $|x|$ is obvious and for small $|x| \neq 0$ can be seen from the power series expansion

$$\sigma_\beta(x) = \beta^{-1}\left(1 + \sum_{n=1}^{\infty} \frac{(\beta x)^n}{(n+1)!}\right)^{-1}.$$

It is now straightforward to verify the claimed differentiability and boundedness property if the assumed conditions are satisfied, by continuously extending the function at zero and applying the product rule. We infer from boundedness the L^2-integrability of (4.12) for $F = F^{(i)}$. In particular, for $n = 0, 1$ we again obtain a bound of the form (4.13) for $F = F^{(i)}$, by noting that $\sigma_\beta(x) = \beta^{-1}\sigma_1(\beta x)$, and so $\sigma'_\beta(x) = \sigma'_1(\beta x)$, $\sup_y |\sigma_1(y)|\langle y\rangle^{-1} < \infty$, and $\sup_y |\sigma'_1(y)| < \infty$. Finally, we conclude that the differentiability, the L^2-integrability of (4.12) and the bound (4.13) follow for $F = \sum_{i=1}^{N} \lambda_i F^{(i)}$ from the linearity of τ_β. $\square$

Remark 4.4
Let $X\colon \mathbb{R}^3 \to \mathcal{L}(\mathcal{H}_\mathrm{p})$ be an element of the sets (3.2) or (3.3) in Hypothesis B-LR. Then, we see by Lemma 4.3 that the functions

$$\mathbb{R} \times \mathbb{S}^2 \longrightarrow \mathcal{L}(\mathcal{H}_\mathrm{p}), \quad (u, \Sigma) \mapsto (u^2+1)\partial_u^n \tau_\beta(X)(u, \Sigma), \qquad n \in \{0, 1, 2, 3\},$$

belong to $L^2(\mathbb{R} \times \mathbb{S}^2, \mathcal{L}(\mathcal{H}_\mathrm{p}))$.

4.2. Overview

The basic strategy for the proof relies on global positive commutators with an additional auxiliary term. More precisely, for some self-adjoint A and self-adjoint bounded operators A_0 and C_Q we consider the operator corresponding to the (formal) sum

$$\mathrm{i}[L_\lambda, A + A_0] + C_Q.$$

By the abstract virial theorem Theorem 4.8 and by choosing an appropriate operator C_Q, it can be shown that zero is an eigenvalue of this operator if zero is also an eigenvalue of L_λ. The conjugate operator A consists of a sum of two terms, one acting only on the atomic space $\mathcal{H}_\mathrm{p}$, the other one, called A_f, on the field space $\mathfrak{F}$.

For the latter we make the same choice as established for the first time in [JP96b] and later also used by Merkli and co-authors in [Mer01; FM04b; FMS04], namely the second quantization of the generator of translations in the glued space,

$$A_\mathrm{f} = \mathsf{d}\Gamma(\mathrm{i}\partial_u).$$

Let P_Ω denote the orthogonal projection onto the subspace generated by the vacuum Ω ("vacuum subspace"). Formally, we obtain on $\mathfrak{F}$ that

$$\mathrm{i}[\mathsf{d}\Gamma(\hat{\mathsf{u}}), A_\mathrm{f}] = \mathsf{d}\Gamma(N_\mathrm{f}) \geq P_\Omega{}^\perp,$$

which yields a positive contribution on the space orthogonal to the vacuum. The composite Hilbert space

$$\mathcal{H} := \mathcal{H}_\mathrm{p} \otimes \mathcal{H}_\mathrm{p} \otimes \mathfrak{F}$$

can be further decomposed by means of the projection

$$\Pi := \mathbb{1}_{L_0=0} = \mathbb{1}_{L_\mathrm{p}=0} \otimes P_\Omega \tag{4.14}$$

as

$$\mathcal{H} = \operatorname{ran}(\mathrm{Id}_\mathrm{p} \otimes \mathrm{Id}_\mathrm{p} \otimes P_\Omega^\perp) \oplus \operatorname{ran}\Pi \oplus \operatorname{ran}(\mathbb{1}_{L_\mathrm{p}\neq 0} \otimes P_\Omega). \tag{4.15}$$

To obtain a positive operator on $\operatorname{ran}\Pi$, we consider a self-adjoint operator $A_0 \in \mathcal{L}(\mathcal{H})$, which is chosen in such a way that the Fermi Golden Rule condition (3.9) implies that

$$\mathrm{i}\Pi[L_\lambda, A_0]\Pi > 0.$$

This is the same method as in [FM04b; FMS04].

In the case of finitely many eigenvalues (or for finite J_d), this expression (or its restriction to finitely many modes) is additionally bounded from below by a positive constant, which is essential for our proof. In case of infinitely many eigenvalues with an accumulation at zero, this is not necessarily true and would require further work (cf. Remark 7.9). Notice that we have some error terms corresponding to the diagonal block of $\mathrm{i}[L_\lambda, A_0]$ with respect to the projection $\Pi^\perp$ and the remaining non-diagonal blocks. All the details can be found in Section 7.1.

Recall that P_disc denotes the spectral projection to the discrete spectrum of H_p and $P_\mathrm{ess} = P_\mathrm{disc}{}^\perp$. The third space in (4.15) can decomposed further by use of

$$\mathbb{1}_{L_\mathrm{p}\neq 0} = (P_\mathrm{ess} \otimes P_\mathrm{ess}) \oplus (P_\mathrm{ess} \otimes P_\mathrm{disc}) \oplus (P_\mathrm{disc} \otimes P_\mathrm{ess}) \oplus \mathbb{1}_{L_\mathrm{p}\neq 0}(P_\mathrm{disc} \otimes P_\mathrm{disc}). \tag{4.16}$$

On the space generated by the first projection $P_\mathrm{ess} \otimes P_\mathrm{ess}$ two different approaches are elaborated in this thesis, depending on whether we consider the LR or SR setting.

The LR case (Hypothesis A-LR) is similar to [FMS04]. Let

$$A_\mathsf{D} := \frac{1}{4}(\hat{\mathsf{p}}\hat{\mathsf{x}} + \hat{\mathsf{x}}\hat{\mathsf{p}})$$

be the generator of dilations. Furthermore, let $\chi = \tilde{\chi}(H_\mathrm{p})$ for a real-valued function $\tilde{\chi}$, such that $\chi^2 H_\mathrm{p}$ is bounded and $\tilde{\chi}$ is supported on the non-negative (essential) spectrum of H_p, i.e., $\chi^2 H_\mathrm{p} > 0$. It will be chosen as

$$\chi = (H_\mathrm{p} + C_\mathrm{p})^{-1/2} \chi_1(H_\mathrm{p}),$$

where $C_\mathrm{p} > -\inf \sigma(H_\mathrm{p})$ and χ_1 is a smooth function supported on the positive real line. Then we define analogously to [FMS04]

$$A_\mathrm{p}^\mathrm{lr} := \chi A_\mathsf{D} \chi$$

and combine this with the conjugate field operator to an operator on $\mathcal{H}$ by

$$A^\mathrm{lr} := (A_\mathrm{p}^\mathrm{lr} \otimes \mathrm{Id}_\mathrm{p} - \mathrm{Id}_\mathrm{p} \otimes A_\mathrm{p}^\mathrm{lr}) \otimes \mathrm{Id}_\mathrm{f} + \mathrm{Id}_\mathrm{p} \otimes \mathrm{Id}_\mathrm{p} \otimes A_\mathrm{f}.$$

This yields

$$\mathrm{i}[L_\lambda, A^\mathrm{lr}] = (\chi^2 H_\mathrm{p} \otimes \mathrm{Id}_\mathrm{p} + \mathrm{Id}_\mathrm{p} \otimes \chi^2 H_\mathrm{p}) \otimes \mathrm{Id}_\mathrm{f} + \widehat{N_\mathrm{f}} + \lambda W_1^\mathrm{lr},$$

where $\widehat{N_\mathrm{f}} := \mathrm{Id}_\mathrm{p} \otimes \mathrm{Id}_\mathrm{p} \otimes N_\mathrm{f}$ and $W_1^\mathrm{lr} := \mathrm{i}[W, A^\mathrm{lr}]$. For $\lambda = 0$, this operator is strictly positive on $\mathrm{ran}(P_\mathrm{ess} \otimes P_\mathrm{ess}) \otimes \mathfrak{F}$ and bounded from below by a positive constant on $\mathrm{ran}\, \widehat{N_\mathrm{f}}$. As A^lr is unbounded, it is necessary to use an appropriate virial theorem, in our case Theorem 4.8. For $\lambda \neq 0$, the commuted interaction term W_1^lr might contain a negative contribution and it has to be treated together with the other error terms (see below).

In the SR case, that is, when the potential satisfies Hypothesis A-SR, we choose a different conjugate operator. We first diagonalize the non-negative part of H_p with generalized eigenfunctions corresponding to the continuous spectrum, the *scattering functions*, which we recall in Section 6.1. This yields a unitary map V_c between the non-negative eigenspace of H_p and $L^2(\mathbb{R}^3)$, the *scattering space*. It has the property that $V_\mathsf{c}^* H_\mathrm{p} V_\mathsf{c} = \hat{\mathsf{k}}^2$, where now $\hat{\mathsf{k}} = (\hat{\mathsf{k}}_1, \hat{\mathsf{k}}_2, \hat{\mathsf{k}}_3)$ denotes the vector of multiplication operators in the scattering space. Then taking the commutator with

$$A_\mathrm{p}^\mathrm{sr} := V_\mathsf{c}^* \mathcal{F} A_\mathsf{D} \mathcal{F}^{-1} V_\mathsf{c} = V_\mathsf{c}^* (-A_\mathsf{D}) V_\mathsf{c},$$

where $\mathcal{F}$ denotes the Fourier transform, has the effect that

$$\mathrm{i}[H_\mathrm{p}, A_\mathrm{p}^\mathrm{sr}] = V_\mathsf{c}^* \hat{\mathsf{k}}^2 V_\mathsf{c} = P_\mathrm{ess} H_\mathrm{p},$$

which is strictly positive on $\mathrm{ran}\, P_\mathrm{ess}$. Once more, we combine A_f and A_p^sr to an operator on $\mathcal{H}$ by

$$A^\mathrm{sr} = (A_\mathrm{p}^\mathrm{sr} \otimes \mathrm{Id}_\mathrm{p} - \mathrm{Id}_\mathrm{p} \otimes A_\mathrm{p}^\mathrm{sr}) \otimes \mathrm{Id}_\mathrm{f} + \mathrm{Id}_\mathrm{p} \otimes \mathrm{Id}_\mathrm{p} \otimes A_\mathrm{f},$$

which yields

$$\mathrm{i}[L_\lambda, A^{\mathrm{sr}}] = (P_{\mathrm{ess}} H_{\mathrm{p}} \otimes \mathrm{Id}_{\mathrm{p}} + \mathrm{Id}_{\mathrm{p}} \otimes P_{\mathrm{ess}} H_{\mathrm{p}}) \otimes \mathrm{Id}_{\mathrm{f}} + \widehat{N}_{\mathrm{f}} + \lambda W_1^{\mathrm{sr}},$$

where $W_1^{\mathrm{sr}} := \mathrm{i}[W, A^{\mathrm{sr}}]$. For $\lambda = 0$ the operator $\mathrm{i}[L_\lambda, A^{\mathrm{sr}}]$ is again strictly positive on $\mathrm{ran}(P_{\mathrm{ess}} \otimes P_{\mathrm{ess}}) \otimes \mathfrak{F}$ and bounded from below by a positive constant on $\mathrm{ran}\, \widehat{N}_{\mathrm{f}}$. In order to be able to apply the virial theorem Theorem 4.8, it is necessary that the first and third commutators are bounded on the atomic space (cf. (4.25) and (4.26)). In contrast to the LR setting, where we introduced the energy cutoff function χ, this is not the case for the commutators with A^{sr}, as $P_{\mathrm{ess}} H_{\mathrm{p}}$ is unbounded. Thus, one has to include a regularization in $A_{\mathrm{p}}^{\mathrm{sr}}$. The exact definition of A^{sr} and of a regularized version $A^{(\epsilon)}$, as well as the verification of the conditions for the virial theorem, can be found in Section 6.3.

For the space corresponding to the last three projections in (4.16) we choose an operator Q on $\mathcal{H}_{\mathrm{p}} \otimes \mathcal{H}_{\mathrm{p}}$ given as a bounded continuous function of L_{p}, which vanishes at the origin. We add a suitable operator T depending on the interaction and λ to accomplish

$$\langle \psi, (Q \otimes P_\Omega + T)\psi \rangle = 0$$

for all $\psi \in \ker L_\lambda$. By construction, $Q \otimes P_\Omega$ is strictly positive on

$$\mathrm{ran}(\mathbb{1}_{L_{\mathrm{p}} \neq 0} \otimes P_\Omega),$$

and bounded from below by a positive constant in the case of finitely many eigenvalues. The operator T will be viewed as an error term which will be estimated by $\widehat{N}_{\mathrm{f}}$.

Finally, we have seen that there arise further error terms from the commuted interaction W_1^{lr} or W_1^{sr}, and from the remaining blocks of $\mathrm{i}[L_\lambda, A_0]$. The general idea to control them is to estimate them by a sum of $\widehat{N}_{\mathrm{f}}$ and some bounded terms on $\mathcal{H}_{\mathrm{p}} \otimes \mathcal{H}_{\mathrm{p}} \otimes \mathrm{ran}\, P_\Omega$, respectively. It is for the latter that we need the decompositions (4.15) and (4.16) as well as the corresponding positive operators mentioned. On $\mathrm{ran}(P_{\mathrm{ess}} \otimes P_{\mathrm{ess}})$ we need in addition that the error terms are sufficiently localized. In the LR case we estimate them by $\langle \hat{\mathsf{x}} \rangle^{-4}$ and prove a generalized Birman-Schwinger bound (Proposition B.13) to show that

$$(H_{\mathrm{p}} + C_{\mathrm{p}})^{-1/2}(-\Delta)(H_{\mathrm{p}} + C_{\mathrm{p}})^{-1/2} - \lambda \langle x \rangle^{-4} \geq 0$$

for $\lambda > 0$ sufficiently small. In the SR case we prove that they are bounded by $\langle \hat{\mathsf{q}} \rangle^{-2}$, where $\hat{\mathsf{q}} := \mathrm{i}\nabla_k$ in the scattering space, and then use that

$$\hat{\mathsf{k}}^2 - \lambda \hat{\mathsf{q}}^{-2} > 0$$

for $\lambda > 0$ sufficiently small (cf. [RS2, section X.2]).

4.3. Abstract Virial Theorem

In this section we recall the abstract virial theorem of [FM04b; FMS04]. It is based on Nelson's commutator theorem, which can be used for proving self-adjointness of operators which are not bounded from below. An important notion will be that of a GJN triple.

Definition 4.5 (GJN triple)
Let $\mathcal{H}$ be a Hilbert space, $\mathcal{D} \subseteq \mathcal{H}$ a core for a self-adjoint operator $Y \geq \mathrm{Id}$, and X a symmetric operator on $\mathcal{D}$. We say the triple $(X, Y, \mathcal{D})$ satisfies the Glimm-Janne-Nelson (GJN) condition, or that $(X, Y, \mathcal{D})$ is a GJN-triple, if there is a constant $C < \infty$, such that for all $\psi \in \mathcal{D}$,

$$\|X\psi\| \leq C\|Y\psi\|, \tag{4.17}$$

$$\pm \mathrm{i} \left(\langle X\psi, Y\psi \rangle - \langle Y\psi, X\psi \rangle \right) \leq C \left\langle \psi, Y\psi \right\rangle . \tag{4.18}$$

Theorem 4.6 (GJN commutator theorem, [RS2, Theorem X.37])
If $(X, Y, \mathcal{D})$ satisfies the GJN condition, then X determines a self-adjoint operator (again denoted by X), such that $\mathcal{D}(X) \supseteq \mathcal{D}(Y)$. Moreover, X is essentially self-adjoint on any core for Y, and (4.17) is valid for all $\psi \in \mathcal{D}(Y)$.

A consequence is that the unitary group generated by X leaves the domain of Y invariant. The concrete formulation is taken from [FM04b].

Theorem 4.7 (Invariance of domain, [Frö77])
Suppose $(X, Y, \mathcal{D})$ satisfies the GJN condition. Then, for all $t \in \mathbb{R}$, $e^{\mathrm{i}tX}$ leaves $\mathcal{D}(Y)$ invariant, and there is a constant $\kappa \geq 0$ such that

$$\left\| Y e^{\mathrm{i}tX} \psi \right\| \leq e^{\kappa|t|} \left\| Y\psi \right\|, \qquad \psi \in \mathcal{D}(Y). \tag{4.19}$$

For operators X, Y, Z defined on a common domain $\mathcal{D}$ and $\mathcal{D} \subseteq \mathcal{D}(X^*), \mathcal{D}(Y^*)$, we say that $Z = [X, Y]$ in the form sense if and only if

$$\langle X^*\phi, Y\psi \rangle - \langle Y^*\phi, X\psi \rangle = \langle \phi, Z\psi \rangle \tag{4.20}$$

holds for all $\phi, \psi \in \mathcal{D}$.

Based on the GJN commutator theorem, we next describe the setting for a general virial theorem. Suppose one is given a self-adjoint operator $\Lambda \geq \mathrm{Id}$ with core $\mathcal{D} \subseteq \mathcal{H}$, and operators L, A, N, D, C_n, $n \in \{0, 1, 2, 3\}$, all symmetric on $\mathcal{D}$, and satisfying

$$D = \mathrm{i}[L, N], \tag{4.21}$$

and

$$C_0 = L, \tag{4.22}$$
$$C_{n+1} = \mathrm{i}[C_n, A], \quad n \in \{0,1,2\}, \tag{4.23}$$

in the form sense on $\mathcal{D}$. Furthermore we shall assume:

(V1) $(X, \Lambda, \mathcal{D})$ satisfies the GJN condition for $X = L, N, D, C_n$, $n \in \{0,1,2,3\}$. Consequently all these operators determine self-adjoint operators, which we denote by the same letters.

(V2) A is self-adjoint, $\mathcal{D} \subseteq \mathcal{D}(A)$, and $e^{\mathrm{i}tA}$ leaves $\mathcal{D}(\Lambda)$ invariant.

Theorem 4.8 (Abstract virial theorem, [FM04b, Theorem 3.2])
Let $\Lambda \geq \mathrm{Id}$ be a self-adjoint operator in $\mathcal{H}$ with core $\mathcal{D} \subseteq \mathcal{H}$, and let L, A, N, D, C_n, $n \in \{0,1,2,3\}$, be symmetric on $\mathcal{D}$ satisfying (4.21)–(4.23). Assume (V1) and (V2) hold. Furthermore, suppose that N and $\mathrm{e}^{\mathrm{i}tA}$ commute for all $t \in \mathbb{R}$ in the strong sense on $\mathcal{D}$, and that there exist $0 \leq p < \infty$ and $C < \infty$ such that

$$\|D\psi\| \leq C \left\| N^{1/2}\psi \right\|, \tag{4.24}$$
$$\|C_1\psi\| \leq C \left\| N^{p}\psi \right\|, \tag{4.25}$$
$$\|C_3\psi\| \leq C \left\| N^{1/2}\psi \right\|, \tag{4.26}$$

for all $\psi \in \mathcal{D}$. Then, if $\psi \in \mathcal{D}(L)$ is an eigenvector of L, there is a sequence of approximating eigenvectors $(\psi_n)_{n\in\mathbb{N}}$ in $\mathcal{D}(L) \cap \mathcal{D}(C_1)$ such that $\lim_{n\to\infty} \psi_n = \psi$ in $\mathcal{H}$, and

$$\lim_{n\to\infty} \langle \psi_n, C_1\psi_n \rangle = 0.$$

5. Virial Theorem in the Long-Range Case

In this chapter we verify the conditions for the abstract virial theorem Theorem 4.8 in the case that Hypotheses A-LR and B-LR hold. For the atomic space we use the generator of dilations as conjugate operator. However, in the same way as in [FMS04], we have to include an additional cutoff χ with respect to the energy because the virial theorem requires that the commutators are bounded on the atomic space. The application of the abstract virial theorem then yields the concrete version Theorem 5.5 – the main result of this chapter. Many of the arguments here are inspired by [FMS04], but had to be adjusted for more general energy cutoff functions. In particular, we want to admit functions, which are not compactly supported but still exhibit a sufficiently strong decay behavior for high energies, such that the commutators are bounded on the atomic space.

Our proof is elaborated for a rather general cutoff function in the first section. The necessary conditions on χ, which will be used in the proof, are collected in Hypothesis C. In the second part we make a concrete choice for χ and show that Hypothesis C is indeed fulfilled. In particular, this will be used for treating atoms with only finitely many bound states.

5.1. General Cutoff Function

First we state the necessary conditions on the energy cutoff function. Then we make the choices for the operators L, A, N, D, C_n, $n \in \{0, 1, 2, 3\}$, in Section 4.3. Subsequently, we need to verify the GJN conditions for the various operators. The most tedious part will be the verification for the commutators up to third order (Proposition 5.4).

The cutoff function is given as operator $\chi \in \mathcal{L}(\mathcal{H}_\mathrm{p})$ which will be subject to the following conditions.

Hypothesis C
For all $j \in \{1, 2, 3\}$ we have that

(χ1) $\chi = f(H_\mathrm{p})$ for some continuous function f,

(χ2) χ maps $\mathcal{D}(\hat{\mathsf{p}}^2)$ to $\mathcal{D}(\hat{\mathsf{p}}^2)$, and $\operatorname{ran}\chi \subseteq \mathcal{D}(|\hat{\mathsf{p}}|)$,

(χ3) $\hat{\mathsf{p}}_j\chi$ and $\chi\hat{\mathsf{p}}_j$ (defined on $\mathcal{D}(\hat{\mathsf{p}}_j)$) are bounded,

(χ4) χ, $\hat{\mathsf{p}}_j\chi$, $\chi\hat{\mathsf{p}}_j$ map $\mathcal{D}(|\hat{\mathsf{x}}|^n)$ to $\mathcal{D}(|\hat{\mathsf{x}}|^n)$, and the operators

$$\langle\hat{\mathsf{x}}\rangle^{\pm n}\,\hat{\mathsf{p}}_j^s\chi\hat{\mathsf{p}}_j^t\,\langle\hat{\mathsf{x}}\rangle^{\mp n}, \qquad s,t\in\{0,1\},\ s+t\leq 1,$$

are bounded for all $n\in\{1,2,3,4\}$,

(χ5) the following operators on $C_{\mathsf{c}}^\infty(\mathbb{R}^3)$ are bounded:

$$[\chi,\hat{\mathsf{x}}_j],\quad [[\chi,\hat{\mathsf{x}}_j],\hat{\mathsf{x}}_j],\quad [\chi,A_{\mathsf{D}}],\quad [[\chi,A_{\mathsf{D}}],\hat{\mathsf{x}}_j],\quad [[\chi,A_{\mathsf{D}}],\chi A_{\mathsf{D}}\chi],$$
$$[\chi^2 H_{\mathrm{p}},A_{\mathsf{D}}],\quad [\chi^2 H_{\mathrm{p}},\hat{\mathsf{x}}_j].$$

Remark 5.0
In particular, (χ4) implies that the operators

$$\langle\hat{\mathsf{x}}\rangle^{-(n+1)}\,\chi A_{\mathsf{D}}\chi\,\langle\hat{\mathsf{x}}\rangle^{n},\quad \langle\hat{\mathsf{x}}\rangle^{n}\,\chi A_{\mathsf{D}}\chi\,\langle\hat{\mathsf{x}}\rangle^{-(n+1)}, \qquad n\in\{1,2,3\},$$

are bounded.

We choose the operators from Section 4.3 as follows. On the atomic space $\mathcal{H}_{\mathrm{p}}$ we define the conjugate operator with dense domain $C_{\mathsf{c}}^\infty(\mathbb{R}\times\mathbb{S}^2)$ as

$$A_{\mathrm{p}}^{\mathrm{lr}} := \chi A_{\mathsf{D}}\chi,$$

and the bounding operator with the same domain as

$$\Lambda_{\mathrm{p}}^{\mathrm{lr}} := \hat{\mathsf{p}}^2 + \hat{\mathsf{x}}^2.$$

Next, on the field space $\mathfrak{F}$ we set

$$A_{\mathrm{f}} := \mathsf{d}\Gamma(\mathrm{i}\partial_u),$$
$$\Lambda_{\mathrm{f}} := \mathrm{d}\Gamma(\hat{\mathsf{u}}^2+1),$$

with dense domain $\mathfrak{F}_{\mathrm{fin}}(C_{\mathsf{c}}^\infty(\mathbb{R}^3))$. Now, we can define on the dense subspace of the composite space $\mathcal{H}$,

$$\mathcal{D}^{\mathrm{lr}} := C_{\mathsf{c}}^\infty(\mathbb{R}^3)\,\widehat{\otimes}\,C_{\mathsf{c}}^\infty(\mathbb{R}^3)\,\widehat{\otimes}\,\mathfrak{F}_{\mathrm{fin}}(C_{\mathsf{c}}^\infty(\mathbb{R}^3)),$$

the operators

$$\begin{aligned}
\Lambda^{\mathrm{lr}} &:= (\Lambda_{\mathrm{p}}^{\mathrm{lr}} \otimes \mathrm{Id}_{\mathrm{p}} + \mathrm{Id}_{\mathrm{p}} \otimes \Lambda_{\mathrm{p}}^{\mathrm{lr}}) \otimes \mathrm{Id}_{\mathrm{f}} + \mathrm{Id}_{\mathrm{p}} \otimes \mathrm{Id}_{\mathrm{p}} \otimes \Lambda_{\mathrm{f}}, \\
A^{\mathrm{lr}} &:= (A_{\mathrm{p}}^{\mathrm{lr}} \otimes \mathrm{Id}_{\mathrm{p}} - \mathrm{Id}_{\mathrm{p}} \otimes A_{\mathrm{p}}^{\mathrm{lr}}) \otimes \mathrm{Id}_{\mathrm{f}} + \mathrm{Id}_{\mathrm{p}} \otimes \mathrm{Id}_{\mathrm{p}} \otimes A_{\mathrm{f}}, \\
L &:= L_\lambda, \\
N &:= \widehat{N}_{\mathrm{f}} + 1, \\
D &:= \mathrm{i}[L_\lambda, \widehat{N}_{\mathrm{f}}].
\end{aligned} \tag{5.1}$$

For operators X, Y in a Hilbert space $\mathcal{H}$ with a dense domain $\mathcal{D} \subseteq \mathcal{H}$ we define multiple commutators as operators $\mathrm{ad}_Y^{(n)}(X)$, $n \in \mathbb{N}_0$ on the domain $\mathcal{D}$ as follows. First, let $\mathrm{ad}_Y^{(0)}(X) := X$. Next, assume that $\mathrm{ad}_Y^{(n)}(X)$ for some $n \in \mathbb{N}_0$ is an operator on $\mathcal{D}$. If there exists an operator Z on $\mathcal{D}$ such that

$$Z = \mathrm{i}[\mathrm{ad}_Y^{(n)}(X), Y]$$

holds in the form sense on $\mathcal{D}$, that is, in the sense (4.20), it is necessarily unique and will be denoted by $\mathrm{ad}_Y^{(n+1)}(X)$. If $\mathrm{ad}_Y^{(n)}(X)$ is bounded or essentially self-adjoint, the corresponding extension will be denoted by the same symbol. Furthermore, we write $\mathrm{ad}_Y(X) := \mathrm{ad}_Y^{(1)}(X)$.

Now we set on $\mathcal{D}^{\mathrm{lr}}$ for $n \in \{1, 2, 3\}$,

$$C_n^{\mathrm{lr}} := \delta_{n,1}\widehat{N}_{\mathrm{f}} + \mathrm{ad}_{A_{\mathrm{p}}^{\mathrm{lr}}}^{(n)}(H_{\mathrm{p}}) \otimes \mathrm{Id}_{\mathrm{p}} + (-1)^{n+1} \mathrm{Id}_{\mathrm{p}} \otimes \mathrm{ad}_{A_{\mathrm{p}}^{\mathrm{lr}}}^{(n)}(H_{\mathrm{p}}) + \lambda W_n^{\mathrm{lr}},$$

where

$$W_n^{\mathrm{lr}} := \mathrm{ad}_{A^{\mathrm{lr}}}^{(n)}(\Phi(I)) = \Phi(I_n^{\mathrm{lr}}), \tag{5.2}$$

$$\begin{aligned}
I_n^{\mathrm{lr}}(u, \Sigma) := \sum_{l=0}^{n} \binom{n}{l} (-\mathrm{i}\partial_u)^l \Big(&\tau_\beta(\mathrm{ad}_{A_{\mathrm{p}}^{\mathrm{lr}}}^{(n-l)}(G))(u, \Sigma) \otimes \mathrm{Id}_{\mathrm{p}} \\
&- (-1)^{n-l} \mathrm{Id}_{\mathrm{p}} \otimes e^{-\beta u/2} \tau_\beta(\mathrm{ad}_{A_{\mathrm{p}}^{\mathrm{lr}}}^{(n-l)}(\overline{G}^*))(u, \Sigma) \Big).
\end{aligned} \tag{5.3}$$

It is not a priori clear that the multiple commutators appearing in these formulas are actually well-defined. This will be clarified in the further course of this section.

A standard tool will be the basic operator inequality

$$A^*B + B^*A \leq A^*A + B^*B. \tag{5.4}$$

Furthermore, we will use the following conventions. We say that an operator A is bounded by B (or B-bounded) on a domain $\mathcal{D}$ if there exists a constant C such that

$$\|A\psi\| \leq C(\|B\psi\| + \|\psi\|)$$

for all $\psi \in \mathcal{D}$. We say that A is form bounded by B on $\mathcal{D}$ if there exists a constant C such that

$$|\langle \psi, A\psi \rangle| \leq C \langle \psi, B\psi \rangle$$

for all $\psi \in \mathcal{D}$. For two operators A_1, A_2 we say similarly that the (formal) commutator $[A_1, A_2]$ (which does not need to exist in the strong sense) is form bounded by B if there exists a constant C such that

$$|\langle A_1^* \psi, A_2 \psi \rangle - \langle A_2^* \psi, A_1 \psi \rangle| \leq C \langle \psi, B\psi \rangle$$

for all $\psi \in \mathcal{D}$.

We start by proving the GJN conditions for the easier cases.

Proposition 5.1
The following triples are GJN:

(1) $(A_{\mathsf{D}}, \Lambda_{\mathrm{p}}^{\mathrm{lr}}, C_{\mathsf{c}}^{\infty}(\mathbb{R}^3))$,

(2) $(H_{\mathrm{p}}, \Lambda_{\mathrm{p}}^{\mathrm{lr}}, C_{\mathsf{c}}^{\infty}(\mathbb{R}^3))$,

(3) $(\widehat{N}_{\mathrm{f}}, \Lambda^{\mathrm{lr}}, \mathcal{D}^{\mathrm{lr}})$,

(4) $(L_{\lambda}, \Lambda^{\mathrm{lr}}, \mathcal{D}^{\mathrm{lr}})$,

(5) $(D, \Lambda^{\mathrm{lr}}, \mathcal{D}^{\mathrm{lr}})$.

In particular, $L = L_{\lambda}$ *is essentially self-adjoint on* $\mathcal{D}^{\mathrm{lr}}$ *for any* $\lambda \in \mathbb{R}$.

Proof. (1) There is a constant C such that for all j and all $\psi \in C_{\mathsf{c}}^{\infty}(\mathbb{R}^3)$,

$$\left\| \hat{\mathsf{p}}_j \hat{\mathsf{x}}_j \psi \right\|^2 = \left\langle \psi, \hat{\mathsf{x}}_j \hat{\mathsf{p}}_j^2 \hat{\mathsf{x}}_j \psi \right\rangle = \left\langle \psi, [\hat{\mathsf{x}}_j, \hat{\mathsf{p}}_j^2] \hat{\mathsf{x}}_j \psi \right\rangle + \left\langle \psi, \hat{\mathsf{p}}_j^2 \hat{\mathsf{x}}_j^2 \psi \right\rangle \leq C \left(\left\| \hat{\mathsf{p}}_j^2 \psi \right\|^2 + \left\| \hat{\mathsf{x}}_j^2 \psi \right\|^2 \right),$$

where we used $[\hat{\mathsf{x}}_j, \hat{\mathsf{p}}_j] = \mathrm{i}$ and Cauchy-Schwarz. As $\hat{\mathsf{x}}^2$ and $\hat{\mathsf{p}}^2$ are bounded by $\Lambda_{\mathrm{p}}^{\mathrm{lr}} = \hat{\mathsf{p}}^2 + \hat{\mathsf{x}}^2$, we conclude that $\hat{\mathsf{p}}\hat{\mathsf{x}}$ is bounded by $\Lambda_{\mathrm{p}}^{\mathrm{lr}}$ as well. Thus, the first GJN condition is satisfied. The second GJN condition follows from $\pm\mathrm{i}[A_{\mathsf{D}}, \Lambda_{\mathrm{p}}^{\mathrm{lr}}] = \pm(\hat{\mathsf{x}}^2 - \hat{\mathsf{p}}^2) \leq \Lambda_{\mathrm{p}}^{\mathrm{lr}}$ on $C_{\mathsf{c}}^{\infty}(\mathbb{R}^3)$.

(2) As the potential is assumed to be bounded, H_{p} is bounded by $\hat{\mathsf{p}}^2$, thus also by $\Lambda_{\mathrm{p}}^{\mathrm{lr}}$. For the second GJN condition we compute on $C_{\mathsf{c}}^{\infty}(\mathbb{R}^3)$,

$$[H_{\mathrm{p}}, \hat{\mathsf{p}}^2 + \hat{\mathsf{x}}^2] = [V, \hat{\mathsf{p}}^2] + [\hat{\mathsf{p}}^2, \hat{\mathsf{x}}^2].$$

For the first term, we get

$$\pm \mathrm{i}[V, \hat{\mathsf{p}}^2] = \pm \mathrm{i} \sum_j (\hat{\mathsf{p}}_j [V, \hat{\mathsf{p}}_j] + [V, \hat{\mathsf{p}}_j]\hat{\mathsf{p}}_j) \leq C(\hat{\mathsf{p}}^2 + 1)$$

for some constant C, since derivatives of V are bounded due to Hypothesis A-LR (1). The second term $[\hat{\mathsf{p}}^2, \hat{\mathsf{x}}^2]$ equals $-8\mathrm{i}A_{\mathsf{D}}$, which, as already shown in (1), is form bounded by $\Lambda_{\mathrm{p}}^{\mathrm{lr}}$.

(3) Note that it is sufficient to show that $(N_{\mathrm{f}}, \Lambda_{\mathrm{f}}, \mathfrak{F}_{\mathrm{fin}}(C_{\mathsf{c}}^\infty(\mathbb{R}^3)))$ is a GJN triple. We have $N_{\mathrm{f}} \leq \mathsf{d}\Gamma(\hat{\mathsf{u}}^2 + 1)$ on $\mathfrak{F}_{\mathrm{fin}}(C_{\mathsf{c}}^\infty(\mathbb{R}^3))$, and $[N_{\mathrm{f}}, \mathsf{d}\Gamma(\hat{\mathsf{u}}^2 + 1)] = 0$, which implies both GJN conditions.

(4) Remember the definition of L_λ on $\mathcal{D}^{\mathrm{lr}}$,

$$L_\lambda = L_0 + \lambda W, \quad L_0 = (H_{\mathrm{p}} \otimes \mathrm{Id}_{\mathrm{p}} - \mathrm{Id}_{\mathrm{p}} \otimes H_{\mathrm{p}}) \otimes \mathrm{Id}_{\mathrm{f}} + \mathrm{Id}_{\mathrm{p}} \otimes \mathrm{Id}_{\mathrm{p}} \otimes \mathsf{d}\Gamma(\hat{\mathsf{u}}).$$

Clearly, H_{p} is bounded by $\Lambda_{\mathrm{p}}^{\mathrm{lr}}$ and $\mathsf{d}\Gamma(\hat{\mathsf{u}})$ is bounded by Λ_{f}, hence L_0 is bounded by Λ^{lr}. W is bounded by $\widehat{N_{\mathrm{f}}}^{1/2}$ due to the standard estimates for creation and annihilation operators (Lemma A.3), and thus also bounded by $\Lambda_{\mathrm{f}}^{1/2}$. Therefore, the first GJN condition is satisfied.

For the second GJN condition, note that we have

$$[L_0, \Lambda^{\mathrm{lr}}] = ([H_{\mathrm{p}}, \Lambda_{\mathrm{p}}^{\mathrm{lr}}] \otimes \mathrm{Id}_{\mathrm{p}} - \mathrm{Id}_{\mathrm{p}} \otimes [H_{\mathrm{p}}, \Lambda_{\mathrm{p}}^{\mathrm{lr}}]) \otimes \mathrm{Id}_{\mathrm{f}}\,.$$

Due to (2), $[H_{\mathrm{p}}, \Lambda_{\mathrm{p}}^{\mathrm{lr}}]$ is form bounded by $\Lambda_{\mathrm{p}}^{\mathrm{lr}}$. Thus, $[L_0, \Lambda^{\mathrm{lr}}]$ is form bounded as well by Λ^{lr}.

It remains to show that the commutator $\mathrm{ad}_{\Lambda^{\mathrm{lr}}}(\Phi(I))$ is form bounded by Λ^{lr}. First note that

$$\mathrm{ad}_{\widehat{\Lambda_{\mathrm{f}}}}(\Phi(I)) = \mathrm{i}\left(a((\hat{\mathsf{u}}^2 + 1)I) - a^*((\hat{\mathsf{u}}^2 + 1)I)\right)$$

holds on $\mathcal{D}^{\mathrm{lr}}$ by Lemma A.5. By Hypothesis B-LR we know that $(u, \Sigma) \mapsto (u^2 + 1)I(u, \Sigma)$ is in $L^2(\mathbb{R} \times \mathbb{S}^2, \mathcal{L}(\mathcal{H}_{\mathrm{p}} \otimes \mathcal{H}_{\mathrm{p}}))$. Hence by Lemma A.3,

$$\pm\, \mathrm{ad}_{\widehat{\Lambda_{\mathrm{f}}}}(\Phi(I)) \leq C(\widehat{N_{\mathrm{f}}} + 1) \leq C' \Lambda^{\mathrm{lr}}$$

for some constants C, C'. By Hypothesis B-LR we know that

$$(u, \Sigma) \mapsto \tau_\beta([G, \hat{\mathsf{p}}_j])(u, \Sigma), \qquad (u, \Sigma) \mapsto \tau_\beta([G, \hat{\mathsf{x}}_j])(u, \Sigma)$$

are in $L^2(\mathbb{R}\times\mathbb{S}^2,\mathcal{L}(\mathcal{H}_\mathrm{p}))$ for all j. Hence, the same applies to the operator-valued functions

$$(u,\Sigma)\mapsto[I_\mathsf{l}(u,\Sigma),\hat{\mathsf{p}}_j],\qquad (u,\Sigma)\mapsto[I_\mathsf{l}(u,\Sigma),\hat{\mathsf{x}}_j].$$

Thus, for some constant C,

$$\pm\,\mathrm{ad}_{\Lambda_\mathrm{p}^\mathrm{lr}\otimes\mathrm{Id}_\mathrm{p}\otimes\mathrm{Id}_\mathrm{f}}(\Phi(I_\mathsf{l}\otimes\mathrm{Id}_\mathrm{p}))\le C(\widehat{N}_\mathrm{f}+\Lambda_\mathrm{p}^\mathrm{lr}\otimes\mathrm{Id}_\mathrm{p}\otimes\mathrm{Id}_\mathrm{f})\le C\Lambda^\mathrm{lr}.$$

Analogously, we can show the same for the commutator

$$\pm\,\mathrm{ad}_{\mathrm{Id}_\mathrm{p}\otimes\Lambda_\mathrm{p}^\mathrm{lr}\otimes\mathrm{Id}_\mathrm{f}}(\Phi(\mathrm{Id}_\mathrm{p}\otimes I_\mathsf{r})).$$

(5) We have

$$D=\mathrm{i}\lambda(a(I)-a^*(I)).\tag{5.5}$$

So the proof works analogously to the one of L. □

We have seen that the verification of the GJN condition for the generator of dilations A_D was quite simple. However, including the cutoff χ makes it much more difficult due to domain problems.

Lemma 5.2 (cf. [FMS04, Proposition 3.3])
$(A_\mathrm{p}^\mathrm{lr},\Lambda_\mathrm{p}^\mathrm{lr},C_\mathsf{c}^\infty(\mathbb{R}^3))$ is a GJN triple. Furthermore, there exists a constant C such that $\left\|A_\mathrm{p}^\mathrm{lr}\psi\right\|\le C\left\|\langle\hat{\mathsf{x}}\rangle\psi\right\|$ for all $\psi\in\mathcal{D}(|\hat{\mathsf{x}}|)$.

Proof. First note that $\chi\hat{\mathsf{p}}\hat{\mathsf{x}}\chi$ and $\chi\hat{\mathsf{x}}\hat{\mathsf{p}}\chi$ are well-defined on $C_\mathsf{c}^\infty(\mathbb{R}^3)$ because of the assumptions on χ. We have

$$A_\mathsf{D}=\frac{1}{4}(\hat{\mathsf{p}}\hat{\mathsf{x}}+\hat{\mathsf{x}}\hat{\mathsf{p}})=\frac{1}{4}(2\hat{\mathsf{p}}\hat{\mathsf{x}}+3\mathrm{i}).$$

Then for any j,

$$\chi\hat{\mathsf{p}}_j\hat{\mathsf{x}}_j\chi=\chi\hat{\mathsf{p}}_j\hat{\mathsf{x}}_j\chi\left\langle\hat{\mathsf{x}}\right\rangle^{-1}\left\langle\hat{\mathsf{x}}\right\rangle,$$

where $\chi\hat{\mathsf{p}}_j\hat{\mathsf{x}}_j\chi\left\langle\hat{\mathsf{x}}\right\rangle^{-1}$ is bounded, so A_p^lr is bounded by $|\hat{\mathsf{x}}|$ on $C_\mathsf{c}^\infty(\mathbb{R}^3)$ and therefore also by $\Lambda_\mathrm{p}^\mathrm{lr}$, as $\hat{\mathsf{x}}^2\le\Lambda_\mathrm{p}^\mathrm{lr}$. Thus, the first GJN condition is satisfied.

In order to check the second one, let $\psi\in C_\mathsf{c}^\infty(\mathbb{R}^3)$. Then

$$\left\langle A_\mathrm{p}^\mathrm{lr}\psi,\Lambda_\mathrm{p}^\mathrm{lr}\psi\right\rangle=\left\langle A_\mathsf{D}\chi\psi,\Lambda_\mathrm{p}^\mathrm{lr}\chi\psi\right\rangle+E_1,$$

with $E_1 := \left\langle A_{\mathsf{D}}\chi\psi, [\chi, \Lambda_{\mathrm{p}}^{\mathrm{lr}}]\psi \right\rangle$. Now, as $\chi\psi \in \mathcal{D}(\Lambda_{\mathrm{p}}^{\mathrm{lr}})$ and $\Lambda_{\mathrm{p}}^{\mathrm{lr}}$ is essentially self-adjoint on $C_{\mathsf{c}}^\infty(\mathbb{R}^3)$, we find a sequence (ϕ_n) in $C_{\mathsf{c}}^\infty(\mathbb{R}^3)$ such that $\phi_n \overset{n\to\infty}{\to} \chi\psi$ and $\Lambda_{\mathrm{p}}^{\mathrm{lr}}\phi_n \to \Lambda_{\mathrm{p}}^{\mathrm{lr}}\chi\psi$. Then we get

$$\left\langle A_{\mathsf{D}}\chi\psi, \Lambda_{\mathrm{p}}^{\mathrm{lr}}\chi\psi \right\rangle = \lim_{n\to\infty} \left\langle A_{\mathsf{D}}\chi\psi, \Lambda_{\mathrm{p}}^{\mathrm{lr}}\phi_n \right\rangle = \lim_{n\to\infty} \left\langle \Lambda_{\mathrm{p}}^{\mathrm{lr}}\chi\psi, A_{\mathsf{D}}\phi_n \right\rangle + \left\langle \chi\psi, [A_{\mathsf{D}}, \Lambda_{\mathrm{p}}^{\mathrm{lr}}]\phi_n \right\rangle .$$

A short calculation shows that

$$[A_{\mathsf{D}}, \Lambda_{\mathrm{p}}^{\mathrm{lr}}] = \frac{1}{4}[\hat{\mathsf{p}}\hat{\mathsf{x}} + \hat{\mathsf{x}}\hat{\mathsf{p}}, \hat{\mathsf{p}}^2 + \hat{\mathsf{x}}^2] = \frac{1}{2}[\hat{\mathsf{p}}\hat{\mathsf{x}}, \hat{\mathsf{p}}^2 + \hat{\mathsf{x}}^2] = \mathrm{i}(\hat{\mathsf{p}}^2 - \hat{\mathsf{x}}^2)$$

holds on $C_{\mathsf{c}}^\infty(\mathbb{R}^3)$. As $\chi\psi \in \mathcal{D}(\hat{\mathsf{p}}^2) \cap \mathcal{D}(\hat{\mathsf{x}}^2)$, we can bring $\mathrm{i}(\hat{\mathsf{p}}^2 - \hat{\mathsf{x}}^2)$ to the left of the inner product and perform the limit. This yields

$$\left\langle A_{\mathsf{D}}\chi\psi, \Lambda_{\mathrm{p}}^{\mathrm{lr}}\chi\psi \right\rangle = \lim_{n\to\infty} \left\langle \Lambda_{\mathrm{p}}^{\mathrm{lr}}\chi\psi, A_{\mathsf{D}}\phi_n \right\rangle + E_2,$$

with $E_2 := \left\langle \chi\psi, \mathrm{i}(\hat{\mathsf{p}}^2 - \hat{\mathsf{x}}^2)\chi\psi \right\rangle$. As $\mathcal{D}(A_{\mathsf{D}}) \supset \mathcal{D}(\Lambda_{\mathrm{p}}^{\mathrm{lr}})$, we have $\lim_{n\to\infty} A_{\mathsf{D}}\phi_n = A_{\mathsf{D}}\chi\psi$ and thus,

$$\left\langle A_{\mathsf{D}}\chi\psi, \Lambda_{\mathrm{p}}^{\mathrm{lr}}\chi\psi \right\rangle = \left\langle \Lambda_{\mathrm{p}}^{\mathrm{lr}}\chi\psi, A_{\mathsf{D}}\chi\psi \right\rangle + E_2 = \left\langle \Lambda_{\mathrm{p}}^{\mathrm{lr}}\psi, A_{\mathrm{p}}^{\mathrm{lr}}\psi \right\rangle - \overline{E_1} + E_2.$$

Therefore, in order to finish the proof, we have to show that there is a constant C such that

$$|E_1|, |E_2| \le C \left\langle \psi, \Lambda_{\mathrm{p}}^{\mathrm{lr}}\psi \right\rangle$$

for all $\psi \in C_{\mathsf{c}}^\infty(\mathbb{R}^3)$. The inequality for $|E_2|$ follows from the fact that $\hat{\mathsf{p}}_j\chi$, $\chi\hat{\mathsf{p}}_j$ and $[\hat{\mathsf{x}}_j, \chi]$ are bounded for all j. With regard to E_1, using (χ5), we get

$$[\chi, \Lambda_{\mathrm{p}}^{\mathrm{lr}}] = [\chi, \hat{\mathsf{p}}^2] + \sum_j (2[\chi, \hat{\mathsf{x}}_j]\hat{\mathsf{x}}_j + [\hat{\mathsf{x}}_j, [\chi, \hat{\mathsf{x}}_j]])$$

on $C_{\mathsf{c}}^\infty(\mathbb{R}^3)$, which is bounded by $(\Lambda_{\mathrm{p}}^{\mathrm{lr}})^{1/2}$, and

$$4[A_{\mathsf{D}}, \chi] = [\hat{\mathsf{p}}\hat{\mathsf{x}} + \hat{\mathsf{x}}\hat{\mathsf{p}}, \chi] = 2[\hat{\mathsf{p}}\hat{\mathsf{x}}, \chi] = 2\sum_j (\hat{\mathsf{p}}_j[\hat{\mathsf{x}}_j, \chi] + [\hat{\mathsf{p}}_j, \chi]\hat{\mathsf{x}}_j),$$

which is bounded by $(\Lambda_{\mathrm{p}}^{\mathrm{lr}})^{1/2}$, as $\hat{\mathsf{p}}_j[\hat{\mathsf{x}}_j, \chi]$ and $[\hat{\mathsf{p}}_j, \chi]$ are bounded operators. Using these bounds, and the fact that A_{D} is bounded by $(\Lambda_{\mathrm{p}}^{\mathrm{lr}})^{1/2}$, we get

$$|E_1| \le (\|\chi A_{\mathsf{D}}\psi\| + \|[A_{\mathsf{D}}, \chi]\psi\|) \left\|[\chi, \Lambda_{\mathrm{p}}^{\mathrm{lr}}]\psi\right\| \le C \left\|(\Lambda_{\mathrm{p}}^{\mathrm{lr}})^{1/2}\psi\right\|^2$$

for some constant C. □

Next, we show that the interaction terms, which appear in the field operators, are sufficiently bounded. This will be used in the subsequent proposition, which shows that the commutators up to third order satisfy the GJN condition.

Lemma 5.3
For all $n, m \in \{0,1,2,3\}$, $n \in \mathbb{N}_0$, $j \in \{1,2,3\}$, and for all (u,Σ), the operators

(1) $\partial_u^m \tau_\beta \left(\mathrm{ad}^{(n)}_{A_\mathrm{p}^{\mathrm{lr}}}(G)\right)(u,\Sigma)$

(2) $\mathrm{ad}_{\hat{\mathsf{p}}_j}\left(\partial_u^m \tau_\beta \left(\mathrm{ad}^{(n)}_{A_\mathrm{p}^{\mathrm{lr}}}(G)\right)(u,\Sigma)\right)$

(3) $\mathrm{ad}_{\hat{\mathsf{x}}_j}\left(\partial_u^m \tau_\beta \left(\mathrm{ad}^{(n)}_{A_\mathrm{p}^{\mathrm{lr}}}(G)\right)(u,\Sigma)\right)$

are well-defined, and the corresponding functions $\mathbb{R}\times\mathbb{S}^2 \to \mathcal{L}(\mathcal{H}_\mathrm{p})$ of (u,Σ) belong to $L^2(\mathbb{R}\times\mathbb{S}^2,\mathcal{L}(\mathcal{H}_\mathrm{p}))$.

Proof. First we treat the expression in (1). We can write $\mathrm{ad}^{(n)}_{A_\mathrm{p}^{\mathrm{lr}}}(G(\omega\Sigma))$ as a linear combination of terms

$$(\chi A_\mathsf{D}\chi)^{n_1} \langle\hat{\mathsf{x}}\rangle^{-n_1} \langle\hat{\mathsf{x}}\rangle^{n_1} G(\omega\Sigma) \langle\hat{\mathsf{x}}\rangle^{n_2} \langle\hat{\mathsf{x}}\rangle^{-n_2} (\chi A_\mathsf{D}\chi)^{n_2} \qquad n_1,n_2 \in \{0,1,2,3\}.$$

Now, note that $(\chi A_\mathsf{D}\chi)^{n_1} \langle\hat{\mathsf{x}}\rangle^{-n_1}$ and $\langle\hat{\mathsf{x}}\rangle^{-n_2} (\chi A_\mathsf{D}\chi)^{n_2}$ are bounded due to (χ4) (see Remark 5.0). Thus, it suffices to prove that

$$(u,\Sigma) \mapsto \tau_\beta(\langle\hat{\mathsf{x}}\rangle^{n_1} G(\cdot) \langle\hat{\mathsf{x}}\rangle^{n_2})(u,\Sigma)$$

is three times weakly differentiable with respect to u and belongs to $L^2(\mathbb{R}\times\mathbb{S}^2, L(\mathcal{H}_\mathrm{p}))$. This follows directly from Lemma 4.3 where we insert $F(\omega,\Sigma) := \langle\hat{\mathsf{x}}\rangle^{n_1} X(\omega\Sigma) \langle\hat{\mathsf{x}}\rangle^{n_2}$ and note that the conditions in Lemma 4.3 are satisfied due to Hypothesis B-LR.

Next, we obtain with the same strategy that

$$(u,\Sigma) \mapsto \partial_u^m \tau_\beta \left(\mathrm{ad}^{(n)}_{A_\mathrm{p}^{\mathrm{lr}}}(\mathrm{ad}_X(G))\right)(u,\Sigma)$$

belongs to $L^2(\mathbb{R}\times\mathbb{S}^2,\mathcal{L}(\mathcal{H}_\mathrm{p}))$ for $X \in \{\hat{\mathsf{p}}_j, \hat{\mathsf{x}}_j : j \in \{1,2,3\}\}$ and $n,m \in \{0,1,2,3\}$. Using (χ4) one sees that

$$\langle\hat{\mathsf{x}}\rangle^{-(n+1)} [(A_\mathrm{p}^{\mathrm{lr}})^n, \hat{\mathsf{p}}_j + \hat{\mathsf{x}}_j] \langle\hat{\mathsf{x}}\rangle^n, \ n \in \mathbb{N}_0,$$

is in fact bounded. Thus, we infer that

$$(u,\Sigma) \mapsto \partial_u^m \tau_\beta \left(\mathrm{ad}_X(\mathrm{ad}^{(n)}_{A_\mathrm{p}^{\mathrm{lr}}}(G))\right)(u,\Sigma)$$

belongs to $L^2(\mathbb{R}\times\mathbb{S}^2, \mathcal{L}(\mathcal{H}_\mathrm{p}))$ for $X \in \{\hat{\mathsf{p}}_j, \hat{\mathsf{x}}_j : j \in \{1,2,3\}\}$ and $n, m \in \{0,1,2,3\}$, and therefore, the same applies to the operators in (2) and (3). $\square$

Proposition 5.4
$(C_n^{\mathrm{lr}}, \Lambda, \mathcal{D}^{\mathrm{lr}})$, $n \in \{1,2,3\}$, is a GJN triple. Furthermore, the estimates (4.25) and (4.26) are satisfied.

Proof. Step 1: $\mathrm{ad}^{(n)}_{A_\mathrm{p}^{\mathrm{lr}}}(H_\mathrm{p})$, $n \in \{1,2,3\}$, is bounded.

We have

$$\mathrm{i}[H_\mathrm{p}, A_\mathsf{D}] = H_\mathrm{p} + \widetilde{V},$$

on $C_\mathsf{c}^\infty(\mathbb{R}^3)$, where

$$\widetilde{V}(x) := -\frac{1}{2} x\nabla V(x) - V(x), \qquad x \in \mathbb{R}^3. \tag{5.6}$$

By Hypothesis A-LR (1) we know that $\widetilde{V}$ is a bounded function. Then we get that

$$\mathrm{ad}_{A_\mathrm{p}^{\mathrm{lr}}}(H_\mathrm{p}) = \chi(H_\mathrm{p} + \widetilde{V})\chi$$

is bounded. Next, in the strong sense on $C_\mathsf{c}^\infty(\mathbb{R}^3)$,

$$\mathrm{ad}^{(2)}_{A_\mathrm{p}^{\mathrm{lr}}}(H_\mathrm{p}) = \mathrm{i}(\chi[\chi^2 H_\mathrm{p}, A_\mathsf{D}]\chi + [\chi\widetilde{V}\chi, A_\mathrm{p}^{\mathrm{lr}}]). \tag{5.7}$$

(χ5) yields directly that the first term is bounded. The second term in (5.7) is bounded since $\widetilde{V}\langle\hat{\mathsf{x}}\rangle$, $[\widetilde{V}, A_\mathsf{D}]$ and $[\chi, A_\mathsf{D}]$ are bounded, cf. Hypothesis A-LR (1) and (χ5), respectively. Next, we have

$$\mathrm{ad}^{(3)}_{A_\mathrm{p}^{\mathrm{lr}}}(H_\mathrm{p}) = -([\chi[H_\mathrm{p}\chi^2, A_\mathsf{D}]\chi, A_\mathrm{p}^{\mathrm{lr}}] + [[\chi\widetilde{V}\chi, A_\mathrm{p}^{\mathrm{lr}}], A_\mathrm{p}^{\mathrm{lr}}]). \tag{5.8}$$

The second term is bounded since $\widetilde{V}\langle\hat{\mathsf{x}}\rangle$, $\mathrm{ad}^{(2)}_{A_\mathsf{D}}(\widetilde{V})$ (by Hypothesis A-LR (1)) and $\mathrm{ad}^{(2)}_{A_\mathsf{D}}(\chi)$ are bounded. The first term of (5.8) can be written as

$$[H_\mathrm{p}\chi^2[\chi, A_\mathsf{D}]\chi, A_\mathrm{p}^{\mathrm{lr}}] + [\chi[\chi H_\mathrm{p}, A_\mathsf{D}]\chi^2, A_\mathrm{p}^{\mathrm{lr}}].$$

Then it is not difficult to see that these terms are bounded as well, using the same methods as above, in particular (χ5), which yields that $\mathrm{ad}^{(2)}_{A_\mathsf{D}}(\chi)$ is bounded.

Step 2: The first GJN condition is satisfied for $(C_n^{\mathrm{lr}}, \Lambda^{\mathrm{lr}}, \mathcal{D}^{\mathrm{lr}})$, $n \in \{1,2,3\}$.

Due to Lemma 5.3 we know that the expressions in the field operators indeed belong to $L^2(\mathbb{R}\times\mathbb{S}^2, L(\mathcal{H}_\mathrm{p}))$. Hence, W_n^{lr}, $n \in \{1,2,3\}$, is bounded by $N_\mathrm{f}^{1/2}$, thus also by $\Lambda_\mathrm{f}^{1/2}$.

Step 3: The commutator $\mathrm{ad}_{\Lambda^{\mathrm{lr}}}(W_n^{\mathrm{lr}})$, $n \in \{1,2,3\}$, is form bounded by Λ^{lr}.

First we have

$$\pm\,\mathrm{ad}_{\widehat{\Lambda}_{\mathrm{f}}}(\Phi(I_n^{\mathrm{lr}})) = \pm\mathrm{i}\left(a((\hat{\mathsf{u}}^2+1)I_n^{\mathrm{lr}}) - a^*((\hat{\mathsf{u}}^2+1)I_n^{\mathrm{lr}})\right),$$

where we know from Remark 4.4 that $(\hat{\mathsf{u}}^2+1)I_n^{\mathrm{lr}} \in L^2(\mathbb{R}\times\mathbb{S}^2, \mathcal{L}(\mathcal{H}_{\mathrm{p}}\otimes\mathcal{H}_{\mathrm{p}}))$. This is form bounded by $\widehat{N}_{\mathrm{f}}+1$.

Furthermore, we have to show that the commutator

$$\mathrm{ad}_{(\Lambda_{\mathrm{p}}^{\mathrm{lr}}\otimes\mathrm{Id}_{\mathrm{p}}+\mathrm{Id}_{\mathrm{p}}\otimes\Lambda_{\mathrm{p}}^{\mathrm{lr}})\otimes\mathrm{Id}_{\mathrm{f}}}(\Phi(I_n^{\mathrm{lr}}))$$

is form bounded by Λ^{lr}. It is sufficient to show that the map

$$(u,\Sigma) \mapsto \mathrm{ad}_{\hat{\mathsf{p}}_j+\hat{\mathsf{x}}_j}(I_{n,\alpha}^{\mathrm{lr}}(u,\Sigma)), \tag{5.9}$$

is in $L^2(\mathbb{R}\times\mathbb{S}^2,\mathcal{L}(\mathcal{H}_{\mathrm{p}}))$ for all $\alpha\in\{\mathsf{l},\mathsf{r}\}$, $n\in\{1,2,3\}$ and all j. This follows from Lemma 5.3.

Step 4: The second GJN condition for $(C_1^{\mathrm{lr}}, \Lambda^{\mathrm{lr}}, \mathcal{D}^{\mathrm{lr}})$ holds.

In view of the previous step it remains to show that $\mathrm{ad}_{\Lambda_{\mathrm{p}}^{\mathrm{lr}}}(\chi(H+\widetilde{V})\chi)$ is form bounded by Λ. We have

$$\begin{aligned}[\chi(H_{\mathrm{p}}+\widetilde{V})\chi, \Lambda_{\mathrm{p}}^{\mathrm{lr}}] &= [\chi^2 H_{\mathrm{p}} + \chi\widetilde{V}\chi, H_{\mathrm{p}} - V] + [\chi^2 H_{\mathrm{p}} + \chi\widetilde{V}\chi, \hat{\mathsf{x}}^2] \\ &= -[\chi^2 H_{\mathrm{p}}, V] + [\chi\widetilde{V}\chi, \hat{\mathsf{p}}^2] + [\chi^2 H_{\mathrm{p}}, \hat{\mathsf{x}}^2] + [\chi\widetilde{V}\chi, \hat{\mathsf{x}}^2].\end{aligned}$$

Since $\chi^2 H_{\mathrm{p}}$ and V are bounded, $[\chi^2 H_{\mathrm{p}}, V]$ bounded. The second one is form bounded by $\hat{\mathsf{p}}^2$, since

$$\left|\left\langle\psi, [\chi\widetilde{V}\chi, \hat{\mathsf{p}}^2]\psi\right\rangle\right| \le 2\left\langle|\hat{\mathsf{p}}|\,\chi\widetilde{V}\chi\psi, |\hat{\mathsf{p}}|\,\psi\right\rangle$$

for $\psi\in C_{\mathsf{c}}^\infty(\mathbb{R}^3)$, and $|\hat{\mathsf{p}}|\,\chi\widetilde{V}\chi$ is bounded. Next, as $[\chi^2 H_{\mathrm{p}}, \hat{\mathsf{x}}_j]$ is bounded (due to $(\chi 5)$), the operator $[\chi^2 H_{\mathrm{p}}, \hat{\mathsf{x}}^2]$ is form bounded by $\hat{\mathsf{x}}^2$. Finally,

$$\left\langle\psi, [\chi\widetilde{V}\chi, \hat{\mathsf{x}}^2]\psi\right\rangle \le 2\left|\left\langle\psi, \chi\widetilde{V}[\chi, \hat{\mathsf{x}}^2]\psi\right\rangle\right|.$$

By expanding $[\chi, \hat{\mathsf{x}}^2]$ as above and using that $[\chi, \hat{\mathsf{x}}_j]$ is bounded for all j, we see that $[\chi\widetilde{V}\chi, \hat{\mathsf{x}}^2]$ is form bounded by $\Lambda_{\mathrm{p}}^{\mathrm{lr}}$.

Step 5: The second GJN condition for $(C_2^{\mathrm{lr}}, \Lambda^{\mathrm{lr}}, \mathcal{D}^{\mathrm{lr}})$ holds.

It remains to show that $[\mathrm{ad}^{(2)}_{A_{\mathrm{p}}^{\mathrm{lr}}}(H_{\mathrm{p}}), \Lambda_{\mathrm{p}}^{\mathrm{lr}}]$ is form bounded by $\Lambda_{\mathrm{p}}^{\mathrm{lr}}$. By equation (5.7) for $\mathrm{ad}^{(2)}_{A_{\mathrm{p}}^{\mathrm{lr}}}(H_{\mathrm{p}})$, using $(\chi 5)$, we obtain that $[\mathrm{ad}^{(2)}_{A_{\mathrm{p}}^{\mathrm{lr}}}(H_{\mathrm{p}}), \hat{\mathsf{p}}_j]$ is bounded for all

j. Therefore, we can estimate the commutator with $\hat{\mathsf{p}}^2$ in the form sense by $\hat{\mathsf{p}}^2$. Similarly, for the commutator with $\hat{\mathsf{x}}^2$, it suffices to show that $[\mathrm{ad}^{(2)}_{A^{\mathrm{lr}}_{\mathrm{p}}}(H_{\mathrm{p}}), \hat{\mathsf{x}}_j]$ is bounded. Expanding the commutators in (5.7) this follows since the operators $\chi^2 H_{\mathrm{p}}$, $[\chi^2 H_{\mathrm{p}}, \hat{\mathsf{x}}_j]$, $[[\chi, A_{\mathsf{D}}], \hat{\mathsf{x}}_j]$ and $[\chi, \hat{\mathsf{x}}_j]$ are bounded by assumption.

Step 6: The second GJN condition for $(C^{\mathrm{lr}}_3, \Lambda^{\mathrm{lr}}, \mathcal{D}^{\mathrm{lr}})$ holds.

We use $\mathrm{i}[\mathrm{ad}^{(3)}_{A^{\mathrm{lr}}_{\mathrm{p}}}(H_{\mathrm{p}}), \hat{\mathsf{p}}^2] = -2\,\mathrm{Re}[\mathrm{ad}^{(2)}_{A^{\mathrm{lr}}_{\mathrm{p}}}(H_{\mathrm{p}}) A^{\mathrm{lr}}_{\mathrm{p}}, \hat{\mathsf{p}}^2]$ and get for all j,

$$[\mathrm{ad}^{(2)}_{A^{\mathrm{lr}}_{\mathrm{p}}}(H_{\mathrm{p}}) A^{\mathrm{lr}}_{\mathrm{p}}, \hat{\mathsf{p}}_j] = \mathrm{ad}^{(2)}_{A^{\mathrm{lr}}_{\mathrm{p}}}(H_{\mathrm{p}}) [A^{\mathrm{lr}}_{\mathrm{p}}, \hat{\mathsf{p}}_j] + [\mathrm{ad}^{(2)}_{A^{\mathrm{lr}}_{\mathrm{p}}}(H_{\mathrm{p}}), \hat{\mathsf{p}}_j] \chi A_{\mathsf{D}} \chi.$$

It is not difficult to check that $[A^{\mathrm{lr}}_{\mathrm{p}}, \hat{\mathsf{p}}_j] \langle \hat{\mathsf{x}} \rangle^{-1}$ is bounded due to $(\chi 4)$. Furthermore, we have seen above that $\mathrm{ad}^{(2)}_{A^{\mathrm{lr}}_{\mathrm{p}}}(H_{\mathrm{p}})$ and $[\mathrm{ad}^{(2)}_{A^{\mathrm{lr}}_{\mathrm{p}}}(H_{\mathrm{p}}), \hat{\mathsf{p}}_j]$ are bounded. Thus, $[\mathrm{ad}^{(2)}_{A^{\mathrm{lr}}_{\mathrm{p}}}(H_{\mathrm{p}}) A^{\mathrm{lr}}_{\mathrm{p}}, \hat{\mathsf{p}}_j] \langle \hat{\mathsf{x}} \rangle^{-1}$ is bounded and we get that the commutator with $\hat{\mathsf{p}}^2$ is form bounded by $\Lambda^{\mathrm{lr}}_{\mathrm{p}}$. It remains to estimate the commutator with $\hat{\mathsf{x}}^2$. We use the same trick

$$\mathrm{i}[\mathrm{ad}^{(3)}_{A^{\mathrm{lr}}_{\mathrm{p}}}(H_{\mathrm{p}}), \hat{\mathsf{x}}^2] = -2\,\mathrm{Re}[\mathrm{ad}^{(2)}_{A^{\mathrm{lr}}_{\mathrm{p}}}(H_{\mathrm{p}}) A^{\mathrm{lr}}_{\mathrm{p}}, \hat{\mathsf{x}}^2]$$

and get for all j,

$$[\mathrm{ad}^{(2)}_{A^{\mathrm{lr}}_{\mathrm{p}}}(H_{\mathrm{p}}) A^{\mathrm{lr}}_{\mathrm{p}}, \hat{\mathsf{x}}_j] = \mathrm{ad}^{(2)}_{A^{\mathrm{lr}}_{\mathrm{p}}}(H_{\mathrm{p}}) [A^{\mathrm{lr}}_{\mathrm{p}}, \hat{\mathsf{x}}_j] + [\mathrm{ad}^{(2)}_{A^{\mathrm{lr}}_{\mathrm{p}}}(H_{\mathrm{p}}), \hat{\mathsf{x}}_j] \chi A_{\mathsf{D}} \chi.$$

Again, $[A^{\mathrm{lr}}_{\mathrm{p}}, \hat{\mathsf{x}}_j] \langle \hat{\mathsf{x}} \rangle^{-1}$ is bounded because of $(\chi 4)$. Furthermore, we have seen above that $\mathrm{ad}^{(2)}_{A^{\mathrm{lr}}_{\mathrm{p}}}(H_{\mathrm{p}})$ and $[\mathrm{ad}^{(2)}_{A^{\mathrm{lr}}_{\mathrm{p}}}(H_{\mathrm{p}}), \hat{\mathsf{x}}_j]$ are bounded. Thus, the commutator with $\hat{\mathsf{x}}^2$ is form bounded by $\Lambda^{\mathrm{lr}}_{\mathrm{p}}$.

Finally, since we have shown that $\mathrm{ad}^{(n)}_{A^{\mathrm{lr}}_{\mathrm{p}}}(H_{\mathrm{p}})$, $n \in \{1, 3\}$ is bounded, and W^{lr}_n, $n \in \{1, 3\}$, is bounded by $\widehat{N_{\mathrm{f}}}^{1/2}$, (4.25) and (4.26) are satisfied. □

Now, we can apply the abstract virial theorem for our setting and obtain the following concrete version. To this end let q^{lr}_1 denote the quadratic form corresponding to C^{lr}_1 (which is bounded from below, cf. Proposition 7.8).

Theorem 5.5 (Concrete virial theorem)
Assume Hypothesis C holds for some χ and there exists $\psi \in \mathcal{D}(L_\lambda)$ with $L_\lambda \psi = 0$. Then $\psi \in \mathcal{D}(q^{\mathrm{lr}}_1)$ and $q^{\mathrm{lr}}_1(\psi) \leq 0$.

Proof. First, we apply the virial theorem Theorem 4.8 with $\Lambda = \Lambda^{\mathrm{lr}}$, $L = L_\lambda$, $N = \widehat{N_{\mathrm{f}}} + 1$, D as in (5.1), and $A = A^{\mathrm{lr}}$. We have seen in Proposition 5.1 and Proposition 5.4 that (V1) is satisfied. Furthermore, by Lemma 5.2, $(A^{\mathrm{lr}}_{\mathrm{p}}, \Lambda^{\mathrm{lr}}_{\mathrm{p}}, C^\infty_{\mathsf{c}}(\mathbb{R}^3))$ is a GJN triple. Hence Theorem 4.6 shows that $e^{\mathrm{i}tA_\mathrm{p}^\mathrm{lr}}$, $t \in \mathbb{R}$, leaves $\mathcal{D}(\Lambda_\mathrm{p}^\mathrm{lr})$ invariant. Furthermore, on $\mathfrak{F}_{\mathrm{fin}}(C_\mathsf{c}^\infty(\mathbb{R}^3))$,

$$\Lambda_\mathrm{f} e^{\mathrm{i}tA_\mathrm{f}} = e^{\mathrm{i}tA_\mathrm{f}}(\Lambda_\mathrm{f} + \mathsf{d}\Gamma(2\hat{\mathsf{u}}t + t^2)), \qquad t \in \mathbb{R}.$$

Thus, for some fixed t there is a constant C such that $\left\| \Lambda_\mathrm{f} e^{\mathrm{i}tA_\mathrm{f}} \psi \right\| \leq C \left\| \Lambda_\mathrm{f} \psi \right\|$ for all $\psi \in \mathfrak{F}_{\mathrm{fin}}(C_\mathsf{c}^\infty(\mathbb{R}^3))$. As $\mathfrak{F}_{\mathrm{fin}}(C_\mathsf{c}^\infty(\mathbb{R}^3))$ is a core for Λ_f, we find $e^{\mathrm{i}tA_\mathrm{f}}\mathcal{D}(\Lambda_\mathrm{f}) \subseteq \mathcal{D}(\Lambda_\mathrm{f})$. Hence, we conclude that $\mathcal{D}(\Lambda)$ is invariant under the unitary group associated to A^lr and therefore (V2) holds. Also, by definition of A^lr it is clear that $\widehat{N}_\mathrm{f}$ and $e^{\mathrm{i}tA^\mathrm{lr}}$, $t \in \mathbb{R}$, commute in the stronge sense on $\mathcal{D}^\mathrm{lr}$. By (5.5), one sees that D is bounded by $N_\mathrm{f}^{1/2}$, which implies (4.24). Furthermore, (4.25) and (4.26) have been verified in Proposition 5.4.

Therefore, Theorem 4.8 yields a sequence $(\psi_n)_{n\in\mathbb{N}}$ in $\mathcal{D}(C_1^\mathrm{lr}) \cap \mathcal{D}(L_\lambda)$ such that $\lim_{n\to\infty} \psi_n = \psi$ and $\lim_{n\to\infty} \left\langle \psi_n, C_1^\mathrm{lr} \psi_n \right\rangle = 0$. Now, as q_1^lr is closed, and thus continuous from below, we obtain $\psi \in \mathcal{D}(q_1^\mathrm{lr})$ and

$$q_1^\mathrm{lr}(\psi) \leq \lim_{n\to\infty} q_1^\mathrm{lr}(\psi_n) = 0. \qquad \square$$

5.2. An Explicit Cutoff Function

Now, we want to present an example for a cutoff function χ such that Hypothesis C is satisfied. This will be used for treating finitely many eigenvalues.

First, we discuss the cutoff for high energies. Let $C_\mathrm{p} > -\inf \sigma(H_\mathrm{p})$. Then we set

$$\chi_0 := (H_\mathrm{p} + C_\mathrm{p})^{-1/2}. \tag{5.10}$$

Notice that the choice is accomplished in such a way that $\chi^2 H_\mathrm{p}$ is bounded.

Lemma 5.6
The operator χ_0 given as in (5.10) satisfies the conditions given in Hypothesis C.

Proof. (χ1), (χ2) and (χ3) are easy to check: We have $\chi = f(H_\mathrm{p})$ for $f(t) = (t + C_\mathrm{p})^{-1/2}$. Furthermore, $\operatorname{ran} \chi_0 \subseteq \mathcal{D}(|\hat{\mathsf{p}}|)$, χ_0 leaves $\mathcal{D}(\hat{\mathsf{p}}^2) = \mathcal{D}(H_\mathrm{p})$ invariant, and $\chi_0 \hat{\mathsf{p}}_j$, $\hat{\mathsf{p}}_j \chi_0$ are bounded for all j. (χ4) follows directly from Proposition B.6.

To check (χ5) using (B.5), one obtains

$$\begin{aligned}[\chi_0, \hat{\mathsf{x}}_j] &= \frac{1}{\pi}\int_0^\infty \frac{1}{\sqrt{t}}[R_\mathrm{p}(t), \hat{\mathsf{x}}_j]\mathrm{d}t \\ &= \frac{1}{\pi}\int_0^\infty \frac{1}{\sqrt{t}}R_\mathrm{p}(t)[\hat{\mathsf{x}}_j, \hat{\mathsf{p}}^2]R_\mathrm{p}(t)\mathrm{d}t \\ &= \frac{2\mathrm{i}}{\pi}\int_0^\infty \frac{1}{\sqrt{t}}R_\mathrm{p}(t)\hat{\mathsf{p}}_j R_\mathrm{p}(t)\mathrm{d}t,\end{aligned}$$

showing that $[\chi_0, \hat{\mathsf{x}}_j]$ and $\hat{\mathsf{p}}_j[\chi_0, \hat{\mathsf{x}}_j]$ are bounded. Using (B.5) again yields that $[[\chi_0, \hat{\mathsf{x}}_j], \hat{\mathsf{x}}_j]$ is bounded. The same trick applies to

$$\begin{aligned}[\chi_0, A_\mathsf{D}] &= -\frac{1}{\pi}\int_0^\infty \frac{1}{\sqrt{t}}R_\mathrm{p}(t)[H_\mathrm{p}, A_\mathsf{D}]R_\mathrm{p}(t)\mathrm{d}t \\ &= \frac{\mathrm{i}}{\pi}\int_0^\infty \frac{1}{\sqrt{t}}R_\mathrm{p}(t)(H_\mathrm{p} + \widetilde{V})R_\mathrm{p}(t)\mathrm{d}t, \end{aligned} \tag{5.11}$$

which shows that $[\chi_0, A_\mathsf{D}]$ is bounded. Then, expanding $[R_\mathrm{p}(t)(H_\mathrm{p} + \widetilde{V})R_\mathrm{p}(t), \hat{\mathsf{x}}_j]$ and evaluating

$$[R_\mathrm{p}(t), \hat{\mathsf{x}}_j] = 2\mathrm{i}R_\mathrm{p}(t)\hat{\mathsf{p}}_j R_\mathrm{p}(t), \qquad [H_\mathrm{p} + \widetilde{V}, \hat{\mathsf{x}}_j] = -2\mathrm{i}\hat{\mathsf{p}}_j,$$

yields that $[[\chi_0, A_\mathsf{D}], \hat{\mathsf{x}}_j]$ is bounded as well. Furthermore, $[[\chi_0, A_\mathsf{D}], \chi_0 A_\mathsf{D}\chi_0]$ is bounded because of (5.11) and the fact that the commutators of $\chi_0 A_\mathsf{D}\chi_0$ with $R_\mathrm{p}(t)$, H_p and $\widetilde{V}$, respectively, are bounded. For the latter recall that $\widetilde{V}\langle\hat{\mathsf{x}}\rangle$ is bounded. Finally,

$$\chi_0^2 H_\mathrm{p} = \mathrm{Id}_\mathrm{p} - C_\mathrm{p} R_\mathrm{p} \tag{5.12}$$

and the preceding results imply that $[\chi_0^2 H_\mathrm{p}, A_\mathsf{D}]$ and $\langle\hat{\mathsf{x}}\rangle\chi_0^2 H_\mathrm{p}\langle\hat{\mathsf{x}}\rangle^{-1}$ are bounded as well. □

Next, we have add a cutoff for the negative energy to χ_0.

Proposition 5.7
Let $\tilde{\chi}_1 \in C^{10}(\mathbb{R})$ be a function such that

$$\tilde{\chi}_1(e) = \begin{cases} 0 & : e \leq e_1, \\ 1 & : e \geq 0, \end{cases}$$

where $e_1 < 0$. Then $\chi = \chi_0\chi_1$, where $\chi_1 := \tilde{\chi}_1(H_\mathrm{p})$, satisfies the conditions given in Hypothesis C.

Proof. Let $\tilde{\chi}_2 := (1-\tilde{\chi}_1)\varphi \in C_{\mathsf{c}}^{10}(\mathbb{R})$, where $\varphi \in C_{\mathsf{c}}^{\infty}(\mathbb{R})$ such that $\varphi|_{[\inf\sigma(H_{\mathrm{p}}),0)} \equiv 1$. We write $\chi_2 := \tilde{\chi}_2(H_{\mathrm{p}})$ and note that $\chi_2 = \mathrm{Id}_{\mathrm{p}} - \chi_1$. By Lemma 5.6 and because the conditions (χ1), (χ2), (χ3), (χ4) and the first four commutators in (χ5) are linear in χ, it suffices to verify all conditions except the last two commutators in (χ5) for $\chi_0\chi_2$.

The conditions (χ1), (χ2) and (χ3) are satisfied by definition and the fact that $\tilde{\chi}_2$ is compactly supported. (χ4) follows from Corollary B.9.

It remains to verify (χ5). For all j, $[\chi_2, \hat{\mathsf{x}}_j]$ is bounded due to Proposition B.11 with $M = 1$ and $Y = \hat{\mathsf{p}}^2 + \hat{\mathsf{x}}^2$, therefore also $[\chi_0\chi_2, \hat{\mathsf{x}}_j]$ by Lemma 5.6.

Next, we show that $[[\chi_2, \hat{\mathsf{x}}_j], \hat{\mathsf{x}}_j]$ (and therefore $[[\chi_0\chi_2, \hat{\mathsf{x}}_j], \hat{\mathsf{x}}_j]$) is bounded. This follows by a similar commutator expansion argument. Set $\tilde{\chi}_3(s) := (s + C_{\mathrm{p}})^2\tilde{\chi}_2(s)$ and $\chi_3 := \tilde{\chi}_3(H_{\mathrm{p}})$. Then we have $\tilde{\chi}_3 \in C_{\mathsf{c}}^{10}(\mathbb{R})$ as well, so

$$[\chi_2, \hat{\mathsf{x}}_j] = [R_{\mathrm{p}}\chi_3 R_{\mathrm{p}}, \hat{\mathsf{x}}_j]$$

can be written as a sum of $R_{\mathrm{p}}[\chi_3, \hat{\mathsf{x}}_j]R_{\mathrm{p}}$ and some bounded operators. Now, also the second commutator with $\hat{\mathsf{x}}_j$ can be expressed as a sum of bounded operators plus

$$R_{\mathrm{p}}[[\chi_3, \hat{\mathsf{x}}_j], \hat{\mathsf{x}}_j]R_{\mathrm{p}}. \tag{5.13}$$

Using the commutator expansions of Theorem B.10 and Proposition B.11, on easily checks that (5.13) is bounded as well.

$[\chi_2, A_{\mathsf{D}}]$ is bounded due to Proposition B.11 with $M = 1$ and $Y = \hat{\mathsf{p}}^2 + \hat{\mathsf{x}}^2$, and so is $[\chi_0\chi_2, A_{\mathsf{D}}]$.

We now consider $[[\chi_2, A_{\mathsf{D}}], \hat{\mathsf{x}}_j]$. Set $\tilde{\chi}_4(s) := (s + C_{\mathrm{p}})\tilde{\chi}_2(s)$ and $\chi_4 := \tilde{\chi}_4(H_{\mathrm{p}})$. Then

$$\begin{aligned}[\chi_2, A_{\mathsf{D}}] &= [R_{\mathrm{p}}, A_{\mathsf{D}}]\chi_4 + R_{\mathrm{p}}[\chi_4, A_{\mathsf{D}}] \\ &= R_{\mathrm{p}}(H_{\mathrm{p}} + \widetilde{V})R_{\mathrm{p}}\chi_4 + R_{\mathrm{p}}[\chi_4, A_{\mathsf{D}}].\end{aligned}$$

The commutator of the first operator with $\hat{\mathsf{x}}_j$ is bounded, which follows from a short computation and the previous arguments. For the second operator we use the commutator expansion

$$R_{\mathrm{p}}[\chi_4, A_{\mathsf{D}}] = (2\pi)^{-1/2}\int \tilde{\chi}_4(s)\int_0^s e^{-\mathrm{i}(s-s_1)H_{\mathrm{p}}}R_{\mathrm{p}}(H_{\mathrm{p}} + \widetilde{V})e^{\mathrm{i}s_1 H_{\mathrm{p}}}\mathrm{d}s_1\mathrm{d}s,$$

and then realize that the commutator of $\hat{\mathsf{x}}_j$ with the integrand is bounded.

The same is true if we take the commutator of the integrand with $\chi A_{\mathsf{D}}\chi$.

It remains to show that $[\chi^2 H_{\mathrm{p}}, A_{\mathsf{D}}]$ and $[\chi^2 H_{\mathrm{p}}, \hat{\mathsf{x}}_j]$ are bounded. By (5.12), we have $\chi^2 H_{\mathrm{p}} = (\mathrm{Id}_{\mathrm{p}} - C_{\mathrm{p}}R_{\mathrm{p}})\chi_1^2$. Then it follows from the fact that $[\chi_1, A_{\mathsf{D}}]$ and $[\chi_1, \hat{\mathsf{x}}_j]$ are bounded, as we have already seen. □

Remark 5.8 (A sharp cutoff function)
Alternatively to the choice of a smooth function in Proposition 5.7, one could also consider a sharp cutoff at zero for negative energy. Let

$$\chi = (\mathrm{Id}_{\mathrm{p}} - p_{J_{\mathrm{d}}})\chi_0.$$

Then one can conclude from Lemma 5.6 that χ satisfies Hypothesis C provided that $p_{J_{\mathrm{d}}}$ maps $\mathcal{D}(|\hat{\mathsf{x}}|^n)$ to $\mathcal{D}(|\hat{\mathsf{x}}|^n)$ for all $n \in \mathbb{N}$, and the operators

$$\langle \hat{\mathsf{x}} \rangle^n \, p_{J_{\mathrm{d}}} \, \langle \hat{\mathsf{x}} \rangle^{-n},$$

and

$$[\chi, p_{J_{\mathrm{d}}}], \quad [\hat{\mathsf{x}}_j, [\hat{\mathsf{x}}_j, p_{J_{\mathrm{d}}}]], \quad [p_{J_{\mathrm{d}}}, A_{\mathrm{p}}], \quad [[p_{J_{\mathrm{d}}}, A_{\mathrm{p}}], \hat{\mathsf{x}}_j], \quad [[p_{J_{\mathrm{d}}}, A_{\mathrm{p}}], \chi A_{\mathrm{p}} \chi],$$

are bounded. This is obviously the case if $p_{J_{\mathrm{d}}}$ is a finite-dimensional projection, that is, if J_{d} is finite.

6. Virial Theorem in the Short-Range Case

In the same way as in the previous chapter we have to choose the commutators and verify the assumptions of Theorem 4.8, this time in the SR case. First, we repeat the definition of scattering states (Section 6.1) and use those for the concrete choice of the commutators (Section 6.2). The major difficulty in the verification of the assumptions (Section 6.3) is to check that the commutators with the interaction terms are bounded. This is much more complicated than in the LR case and requires several bounds involving the scattering functions (see Section 6.4). Like in the LR case, the application of the virial theorem then yields the concrete version Theorem 6.5, which is the main result of this chapter.

6.1. Scattering States

In this part we recall the theory of generalized eigenstates (scattering states) and the corresponding spectral decomposition.

We assume to have a potential V satisfying Hypothesis A-SR. The scattering states $\phi(k,\cdot)$, $k \in \mathbb{R}^3$, are defined as generalized eigenvectors of the Schrödinger operator,

$$(-\Delta + V)\phi(k,\cdot) = k^2\phi(k,\cdot),$$

or as solutions of the so-called Lippmann-Schwinger equation,

$$\phi(k,x) = e^{\mathrm{i}kx} - \frac{1}{4\pi}\int_{\mathbb{R}^3} \frac{e^{\mathrm{i}|k||x-y|}}{|x-y|} V(y)\phi(k,y)\mathrm{d}y. \tag{6.1}$$

We discuss their properties in the following proposition which is basically a combination of [RS3, Theorem XI.41] with the theory given in [Ike60] and [New12]. The scattering functions can be used for the spectral decomposition of the continuous spectrum of H_p, which in our case coincides with the essential spectrum, see Proposition 3.2. Denote by ϕ_n, $n = 1, \ldots, N$, the eigenvectors of H_p and recall that P_ess is the projection to the essential spectrum $[0, \infty)$ of H_p.

Theorem 6.1 (cf. [RS3, Theorem XI.41] and [Ike60; New12])
Let $f \in L^2(\mathbb{R}^3)$.

(a) *For all $k \in \mathbb{R}^3$ there exists a unique solution $\phi(k,\cdot)$ of (6.1) which obeys $|V|^{1/2}\phi(k,\cdot) \in L^2(\mathbb{R}^3)$. Moreover, for every $k \in \mathbb{R}^3$ the function $x \mapsto \phi(k,x)$ is continuous.*

(b) *The generalized Fourier transform*

$$(V_{\mathsf{c}}f)(k) := (2\pi)^{-3/2}\mathsf{l.i.m.}\int \overline{\phi(k,x)}f(x)\mathrm{d}x,$$

where $\mathsf{l.i.m.}\int g(x)\mathrm{d}x := L^2\text{-}\lim_{R\to\infty}\int_{|x|<R} g(x)\mathrm{d}x$, *exists.*

(c) *We have* $\operatorname{ran} V_{\mathsf{c}} = L^2(\mathbb{R}^3)$ *and*

$$\|V_c f\| = \|P_{\mathrm{ess}} f\|\,.$$

In particular, V_{c} is a partial isometry, $V_{\mathsf{c}}|_{\operatorname{ran} P_{\mathrm{ess}}} \colon \operatorname{ran} P_{\mathrm{ess}} \to L^2(\mathbb{R}^3)$ is a unitary operator, and $V_{\mathsf{c}}V_{\mathsf{c}}^* = \mathrm{Id}$.

(d) *We have the spectral decomposition*

$$(P_{\mathrm{ess}}f)(x) = \mathsf{l.i.m.}(2\pi)^{-3/2}\int (V_{\mathsf{c}}f)(k)\phi(k,x)\mathrm{d}k.$$

(e) *If $f \in \mathcal{D}(H_{\mathrm{p}})$, then*

$$(V_{\mathsf{c}}H_{\mathrm{p}}f)(k) = k^2 V_{\mathsf{c}}f(k),$$

in other words, $V_{\mathsf{c}}H_{\mathrm{p}}V_{\mathsf{c}}^* = \hat{\mathsf{k}}^2$.

The basic strategy for the proof of the theorem is to introduce the method of modified square integrable scattering functions, which can be found in [Ike60; RS3], originally developed by Rollnik. In particular, one introduces the so-called modified Lippmann-Schwinger equation

$$\widetilde{\phi}(k,x) = |V(x)|^{1/2}\,\mathrm{e}^{\mathrm{i}kx} + (L_{|k|}\widetilde{\phi}(k,\cdot))(x), \quad k,x \in \mathbb{R}^3, \tag{6.2}$$

where

$$L_\kappa\psi(x) := -\frac{1}{4\pi}\int \frac{|V(x)|^{1/2}\,\mathrm{e}^{\mathrm{i}\kappa|x-y|}V(y)^{1/2}}{|x-y|}\psi(y)\mathrm{d}y, \quad \kappa \geq 0, \tag{6.3}$$

and $V(y)^{1/2} := |V(y)|^{1/2}\operatorname{sgn}V(y)$. It is elementary to see that Hypothesis A-SR (1) implies that V is in the Rollnik class (cf. [Sim15, Theorem 1.22]), that is,

$$\int_{\mathbb{R}^3\times\mathbb{R}^3} \frac{|V(x)V(y)|}{|x-y|^2}\mathrm{d}(x,y) < \infty,$$

and therefore the operator L_κ is a Hilbert-Schmidt operator. If for fixed $k \in \mathbb{R}^3$ the function $\phi(k,\cdot)$ obeys (6.1) and $\tilde{\phi}(k,\cdot) := |V|^{1/2}\phi(k,\cdot)$ is an L^2-function, then $\tilde{\phi}(k,\cdot)$ obeys (6.2), provided Hypothesis A-SR (1) holds (in fact it holds for a larger class of potentials, see [RS3, section XI.6]). On the other hand, if the modified Lippmann-Schwinger equation (6.2) has a unique L^2-solution $\tilde{\phi}(k,\cdot)$, then, as outlined in [RS3, section XI.6], the original Lippmann-Schwinger equation (6.1) has a unique solution $\phi(k,\cdot)$ satisfying $|V|^{1/2}\phi(k,\cdot) \in L^2(\mathbb{R}^3)$. It is given by

$$\phi(k,x) = e^{\mathrm{i}kx} - \frac{1}{4\pi}\int \frac{e^{\mathrm{i}|k||x-y|}}{|x-y|}V(y)^{1/2}\tilde{\phi}(k,y)\mathrm{d}y. \tag{6.4}$$

Proof of Theorem 6.1. By the assumptions on the potential the operator L_κ defined as in (6.3) is a Hilbert-Schmidt operator for all $\kappa \geq 0$. Let

$$\mathcal{E} := \{\kappa \in (0,\infty) : \exists 0 \neq \tilde{\phi} \in L^2(\mathbb{R}^3) \colon \tilde{\phi} = L_\kappa\tilde{\phi}\}.$$

We claim that $\mathcal{E} = \emptyset$. To this end, let $\kappa > 0$ and assume $\tilde{\phi} = L_\kappa\tilde{\phi}$ for some $\tilde{\phi} \in L^2(\mathbb{R}^3)$. Now consider

$$\phi(x) := -\frac{1}{4\pi}\int \frac{e^{\mathrm{i}\kappa|x-y|}}{|x-y|}V(y)^{1/2}\tilde{\phi}(y)\mathrm{d}y = -\frac{1}{4\pi}\int \frac{e^{\mathrm{i}\kappa|x-y|}}{|x-y|}V(y)\phi(y)\mathrm{d}y.$$

It follows that $\phi(x) = o(|x|^{-1})$ as $|x| \to \infty$, and that $-\Delta\phi + V\phi = \kappa^2\phi$. According to [Kat59] this implies that ϕ vanishes identically outside a sufficiently large sphere. Hence by the unique continuation theorem it follows that $\phi = 0$ and $\tilde{\phi} = |V|^{1/2}\phi = 0$. This is a contradiction, and we conclude that the set $\mathcal{E}$ is empty for potentials which we consider. Thus by the Fredholm alternative, whenever $k \neq 0$, there is a unique L^2 solution $\tilde{\phi}$ of the modified Lippmann-Schwinger equation (6.2). As mentioned above it follows that the original Lippmann-Schwinger equation (6.1) has a unique solution ϕ satisfying $|V|^{1/2}\phi \in L^2(\mathbb{R}^3)$ given by (6.4). In the case $k = 0$ we argue analogously using Hypothesis A-SR (2). This shows the first part of (a). The continuity follows in view of (6.1) from dominated convergence. (b)–(e) now result from [RS3, Theorem XI.41], where we have seen in Proposition 3.2 that the essential and the absolutely continuous spectrum of H_{p} coincide. □

Furthermore, we can extend V_{c} to a unitary operator by including the eigenfunctions into consideration. We define

$$V_{\mathsf{d}} \colon L^2(\mathbb{R}^3) \longrightarrow \ell^2(N), \qquad (V_{\mathsf{d}}\psi)_n := \langle \phi_n, \psi \rangle.$$

Obviously $V_{\mathsf{d}}|_{\operatorname{ran} P_{\mathrm{disc}}} \colon \operatorname{ran} P_{\mathrm{disc}} \to \ell^2(N)$ is a unitary operator and $V_{\mathsf{d}}|_{\operatorname{ran} P_{\mathrm{ess}}} = 0$. Thus,

$$\mathcal{V} := V_{\mathsf{d}} \oplus V_{\mathsf{c}} \colon L^2(\mathbb{R}^3) \longrightarrow \ell^2(N) \oplus L^2(\mathbb{R}^3) \tag{6.5}$$

is unitary.

6.2. Setup for the Virial Theorem

In the following we will assume that Hypotheses A-SR and B-SR hold.

First, we describe the setting on the atomic space $\mathcal{H}_{\mathrm{p}}$. We consider a dense subspace given by

$$\mathcal{D}_{\mathrm{p}}^{\mathrm{sr}} := V_{\mathsf{c}}^* C_{\mathsf{c}}^\infty(\mathbb{R}^3) \oplus \operatorname{ran} P_{\mathrm{disc}}.$$

Note that $\mathcal{D}_{\mathrm{p}}^{\mathrm{sr}}$ is dense since $V_{\mathsf{c}}^* C_{\mathsf{c}}^\infty(\mathbb{R}^3) \subseteq \operatorname{ran} P_{\mathrm{ess}}$ is dense in $\operatorname{ran} P_{\mathrm{ess}}$. Now, based on the definition of the generator of dilations in the Fourier space,

$$\mathcal{F} A_{\mathsf{D}} \mathcal{F}^{-1} = \frac{1}{4}(\hat{\mathsf{k}}\hat{\mathsf{q}} + \hat{\mathsf{q}}\hat{\mathsf{k}}) = -A_{\mathsf{D}},$$

where $\hat{\mathsf{q}} := \mathrm{i}\nabla_k = (\mathrm{i}\partial_1, \mathrm{i}\partial_2, \mathrm{i}\partial_3)$, we define on $\mathcal{D}_{\mathrm{p}}^{\mathrm{sr}}$ the conjugate operator $A_{\mathrm{p}}^{\mathrm{sr}}$ and a regularized version $A_{\mathrm{p}}^{(\epsilon)}$, $\epsilon \geq 0$,

$$A_{\mathrm{p}}^{\mathrm{sr}} := V_{\mathsf{c}}^*(-A_{\mathsf{D}})V_{\mathsf{c}}, \qquad A_{\mathrm{p}}^{(\epsilon)} := V_{\mathsf{c}}^* \eta_\epsilon(-A_{\mathsf{D}})\eta_\epsilon V_{\mathsf{c}},$$

where

$$\eta_\epsilon(k) := e^{-\epsilon k^2}.$$

Note that $\eta_0 \equiv 1$ and $A_{\mathrm{p}}^{\mathrm{sr}} = A_{\mathrm{p}}^{(0)}$. It is clear that both H_{p} and $A_{\mathrm{p}}^{(\epsilon)}$, $\epsilon \geq 0$, leave $\mathcal{D}_{\mathrm{p}}^{\mathrm{sr}}$ invariant. Thus we can define $\mathrm{ad}_{A_{\mathrm{p}}^{(\epsilon)}}^{(n)}(H_{\mathrm{p}})$ on $\mathcal{D}_{\mathrm{p}}^{\mathrm{sr}}$ for all $n \in \mathbb{N}$. Furthermore, the bounding operator is chosen as

$$\Lambda_{\mathrm{p}}^{\mathrm{sr}} := V_{\mathsf{c}}^*(\hat{\mathsf{k}}^2 + \hat{\mathsf{q}}^2)V_{\mathsf{c}} + \mathrm{Id}_{\mathrm{p}}\,.$$

Next, on the field space we set

$$\begin{aligned} A_{\mathrm{f}} &:= \mathsf{d}\Gamma(\mathrm{i}\partial_u), \\ \Lambda_{\mathrm{f}} &:= \mathsf{d}\Gamma(\hat{\mathsf{u}}^2 + 1). \end{aligned}$$

Now, we can define on the dense subspace of $\mathcal{H}$,

$$\mathcal{D}^{\mathrm{sr}} = \mathcal{D}_{\mathrm{p}}^{\mathrm{sr}} \,\widehat{\otimes}\, \mathcal{D}_{\mathrm{p}}^{\mathrm{sr}} \,\widehat{\otimes}\, \mathfrak{F}_{\mathrm{fin}}(C_{\mathsf{c}}^\infty(\mathbb{R}^3)), \tag{6.6}$$

the operators

$$\begin{aligned} \Lambda^{\mathrm{sr}} &= \Lambda_{\mathrm{p}}^{\mathrm{sr}} \otimes \mathrm{Id}_{\mathrm{p}} \otimes \mathrm{Id}_{\mathrm{f}} + \mathrm{Id}_{\mathrm{p}} \otimes \Lambda_{\mathrm{p}}^{\mathrm{sr}} \otimes \mathrm{Id}_{\mathrm{f}} + \mathrm{Id}_{\mathrm{p}} \otimes \mathrm{Id}_{\mathrm{p}} \otimes \Lambda_{\mathrm{f}}, \\ A^{(\epsilon)} &= (A_{\mathrm{p}}^{(\epsilon)} \otimes \mathrm{Id}_{\mathrm{p}} - \mathrm{Id}_{\mathrm{p}} \otimes A_{\mathrm{p}}^{(\epsilon)}) \otimes \mathrm{Id}_{\mathrm{f}} + \mathrm{Id}_{\mathrm{p}} \otimes \mathrm{Id}_{\mathrm{p}} \otimes A_{\mathrm{f}}, \qquad \epsilon \geq 0, \\ D &= \mathrm{i}[L_\lambda, \widehat{N}_{\mathrm{f}}], \end{aligned} \tag{6.7}$$

and write $A^{\mathrm{sr}} := A^{(0)}$. Furthermore, we set for $n \in \{1,2,3\}$, $\epsilon \geq 0$,

$$\begin{aligned} C_n^{(\epsilon)} &:= \mathrm{ad}^{(n)}_{A^{(\epsilon)}}(L_\lambda) && (6.8)\\ &= \delta_{n,1}\widehat{N}_{\mathrm{f}} + \Big(\mathrm{ad}^{(n)}_{A_{\mathrm{p}}^{(\epsilon)}}(H_{\mathrm{p}}) \otimes \mathrm{Id}_{\mathrm{p}} + (-1)^{n+1}\,\mathrm{Id}_{\mathrm{p}} \otimes \mathrm{ad}^{(n)}_{A_{\mathrm{p}}^{(\epsilon)}}(H_{\mathrm{p}})\Big) \otimes \mathrm{Id}_{\mathrm{f}} + \lambda W_n^{(\epsilon)},\\ C_n^{(\mathrm{f})} &:= \mathrm{ad}^{(n)}_{\mathrm{Id}_{\mathrm{p}}\otimes \mathrm{Id}_{\mathrm{p}}\otimes A_{\mathrm{f}}}(L_\lambda)\\ &= \delta_{n,1}\widehat{N}_{\mathrm{f}} + \lambda W_n^{(\mathrm{f})}, && (6.9) \end{aligned}$$

where

$$W_n^{(\epsilon)} := \mathrm{ad}^{(n)}_{A^{(\epsilon)}}(\Phi(I)) = \Phi(I_n^{(\epsilon)}(u,\Sigma)), \tag{6.10}$$

$$W_n^{(\mathrm{f})} := \mathrm{ad}^{(n)}_{\mathrm{Id}_{\mathrm{p}}\otimes \mathrm{Id}_{\mathrm{p}}\otimes A_{\mathrm{f}}}(\Phi(I)) = \Phi(I_n^{(\mathrm{f})}(u,\Sigma)), \tag{6.11}$$

with

$$\begin{aligned} I_n^{(\epsilon)}(u,\Sigma) &:= \sum_{k=0}^{n} \binom{n}{k} \Big((-\mathrm{i}\partial_u)^k \tau_\beta(\mathrm{ad}^{(n-k)}_{A_{\mathrm{p}}^{(\epsilon)}}(G))(u,\Sigma) \otimes \mathrm{Id}_{\mathrm{p}}\\ &\qquad - (-1)^{n-k}(-\mathrm{i}\partial_u)^k e^{-\beta u/2}\,\mathrm{Id}_{\mathrm{p}} \otimes \tau_\beta(\mathrm{ad}^{(n-k)}_{A_{\mathrm{p}}^{(\epsilon)}}(\overline{G}^*))(u,\Sigma)\Big),\\ I_n^{(\mathrm{f})}(u,\Sigma) &:= (-\mathrm{i}\partial_u)^n I(u,\Sigma), \end{aligned}$$

and we use the shorthand notation $W_n^{\mathrm{sr}} := W_n^{(0)}$, $C_1^{\mathrm{sr}} := C_1^{(0)}$.

Note that the above identites follow from a straightforward calculation. We will see in Proposition 6.2 and Proposition 6.3 that the expressions in the field operators in (6.10) and (6.11) are well-defined and belong to $L^2(\mathbb{R}\times\mathbb{S}^2, \mathcal{L}(\mathcal{H}_{\mathrm{p}}))$. Furthermore, it will be proven in Proposition 6.3, that $C_n^{(\epsilon)}$ and $C_n^{(\mathrm{f})}$, $n \in \{1,2,3\}$, are indeed essentially self-adjoint on $\mathcal{D}^{\mathrm{sr}}$. We will denote their self-adjoint extensions by the same symbols. Moreover, it will be shown below in (6.20) that C_1^{sr} and $C_n^{(\epsilon)}$, $\epsilon > 0$, are actually bounded from below. Thus, we can assign to these operators quadratic forms q_1^{sr} and $q_1^{(\epsilon)}$, respectively.

6.3. Verification of the Assumptions of the Virial Theorem

In the given setting just described we can now start to prove the assumptions of the virial theorem Theorem 4.8. Above all, we have to check the GJN condition for the different commutators. The most difficult part will be the discussion of the interaction terms $W_n^{(\mathrm{f})}$ and $W_n^{(\epsilon)}$, $n \in \{1,2,3\}$, $\epsilon > 0$, and W_1^{sr}. Here, the expressions in the field operators need to be sufficiently bounded. These bounds will be collected in the following proposition which is the main result of Section 6.4.

Proposition 6.2
Let ∂_u denote the weak derivative of a $\mathcal{L}(\mathcal{H}_{\mathrm{p}})$-valued function in the sense of the strong operator topology. For all $m \in \{0,1,2,3\}$, $n \in \mathbb{N}_0$, $j \in \{1,2,3\}$, and for all (u,Σ), $\epsilon \geq 0$, the operators

(1) $\partial_u^m \operatorname{ad}^{(n)}_{A_{\mathrm{p}}^{(\epsilon)}}(\tau_\beta(G)(u,\Sigma))$,

(2) $\partial_u^m \operatorname{ad}_{V_{\mathsf{c}}^* \hat{\mathsf{k}}_j V_{\mathsf{c}}}(\operatorname{ad}^{(n)}_{A_{\mathrm{p}}^{(\epsilon)}}(\tau_\beta(G)(u,\Sigma)))$,

(3) $\partial_u^m \operatorname{ad}_{V_{\mathsf{c}}^* \hat{\mathsf{q}}_j V_{\mathsf{c}}}(\operatorname{ad}^{(n)}_{A_{\mathrm{p}}^{(\epsilon)}}(\tau_\beta(G)(u,\Sigma)))$,

(4) $\partial_u^m V_{\mathsf{c}}^* \hat{\mathsf{q}}_j V_{\mathsf{c}} \operatorname{ad}^{(n)}_{A_{\mathrm{p}}^{\mathrm{sr}}}(\tau_\beta(G)(u,\Sigma))$,

are well-defined, and the corresponding functions $\mathbb{R} \times \mathbb{S}^2 \to \mathcal{L}(\mathcal{H}_{\mathrm{p}})$ of (u,Σ) belong to $L^2(\mathbb{R} \times \mathbb{S}^2, \mathcal{L}(\mathcal{H}_{\mathrm{p}}))$. Moreover, there exists a constant C independent of β such that for $n,m,s \in \{0,1\}$,

$$\left\| \partial_u^m (V_{\mathsf{c}}^* \hat{\mathsf{q}}_j V_{\mathsf{c}})^s \operatorname{ad}^{(n)}_{A_{\mathrm{p}}^{\mathrm{sr}}}(\tau_\beta(G)) \right\|_{L^2(\mathbb{R}\times\mathbb{S}^2, \mathcal{L}(\mathcal{H}_{\mathrm{p}}))} \leq C(1+\beta^{-\frac{1}{2}}). \tag{6.12}$$

The result also holds true if we replace G by G^*.

By means of Proposition 6.2 we can now verify the necessary GJN conditions.

Proposition 6.3
The following triples are GJN:

(1) $(A_{\mathrm{p}}^{\mathrm{sr}}, \Lambda_{\mathrm{p}}^{\mathrm{sr}}, \mathcal{D}_{\mathrm{p}}^{\mathrm{sr}})$,

(2) $(A_{\mathrm{p}}^{(\epsilon)}, \Lambda_{\mathrm{p}}^{\mathrm{sr}}, \mathcal{D}_{\mathrm{p}}^{\mathrm{sr}})$, $\epsilon > 0$,

(3) $(H_{\mathrm{p}}, \Lambda_{\mathrm{p}}^{\mathrm{sr}}, \mathcal{D}_{\mathrm{p}}^{\mathrm{sr}})$,

(4) $(L_\lambda, \Lambda^{\mathrm{sr}}, \mathcal{D}^{\mathrm{sr}})$, $\lambda \in \mathbb{R}$,

(5) $(\widehat{N}_{\mathrm{f}}, \Lambda^{\mathrm{sr}}, \mathcal{D}^{\mathrm{sr}})$,

(6) $(D, \Lambda^{\mathrm{sr}}, \mathcal{D}^{\mathrm{sr}})$,

(7) $(C_i^{(\epsilon)}, \Lambda^{\mathrm{sr}}, \mathcal{D}^{\mathrm{sr}})$, $\epsilon > 0$, $i \in \{1,2,3\}$,

(8) $(C_i^{(\mathrm{f})}, \Lambda^{\mathrm{sr}}, \mathcal{D}^{\mathrm{sr}})$, $i \in \{1,2,3\}$,

(9) $(C_1^{\mathrm{sr}}, \Lambda^{\mathrm{sr}}, \mathcal{D}^{\mathrm{sr}})$.

In particular, L_λ is essentially self-adjoint on $\mathcal{D}^{\mathrm{sr}}$ for any $\lambda \in \mathbb{R}$ due to (4). Moreover, $D, C_1^{(\epsilon)}, C_3^{(\epsilon)}$, $\epsilon > 0$, and $C_1^{(\mathrm{f})}, C_3^{(\mathrm{f})}$ are bounded by $\widehat{N_{\mathrm{f}}}^{1/2}$.

Proof. (1) Using that $(A_{\mathsf{D}}, \hat{\mathsf{k}}^2 + \hat{\mathsf{q}}^2, C_{\mathsf{c}}^\infty(\mathbb{R}^3))$ is a GJN triple (see Proposition 5.1) and V_{c}^* is an isometry, we have, for $\psi \in \mathcal{D}_{\mathrm{p}}^{\mathrm{sr}}$,

$$\left\| A_{\mathrm{p}}^{\mathrm{sr}} \psi \right\| = \| V_{\mathsf{c}}^* A_{\mathsf{D}} V_{\mathsf{c}} \psi \| = \| A_{\mathsf{D}} V_{\mathsf{c}} \psi \| \le C \left\| (\hat{\mathsf{k}}^2 + \hat{\mathsf{q}}^2) V_{\mathsf{c}} \psi \right\| \le C' \left\| \Lambda_{\mathrm{p}} \psi \right\|,$$

and

$$\begin{aligned} &\pm \mathrm{i} \left(\left\langle A_{\mathrm{p}}^{\mathrm{sr}} \psi, \Lambda_{\mathrm{p}}^{\mathrm{sr}} \psi \right\rangle - \left\langle \Lambda_{\mathrm{p}}^{\mathrm{sr}} \psi, A_{\mathrm{p}}^{\mathrm{sr}} \psi \right\rangle \right) \\ &\quad = \pm \mathrm{i} \left(\left\langle -A_{\mathsf{D}} V_{\mathsf{c}} \psi, (\hat{\mathsf{k}}^2 + \hat{\mathsf{q}}^2) V_{\mathsf{c}} \psi \right\rangle - \left\langle (\hat{\mathsf{k}}^2 + \hat{\mathsf{q}}^2) V_{\mathsf{c}} \psi, -A_{\mathsf{D}} V_{\mathsf{c}} \psi \right\rangle \right) \\ &\quad \le C \left\langle V_{\mathsf{c}} \psi, (\hat{\mathsf{k}}^2 + \hat{\mathsf{q}}^2) V_{\mathsf{c}} \psi \right\rangle \\ &\quad \le C \left\langle \psi, \Lambda_{\mathrm{p}}^{\mathrm{sr}} \psi \right\rangle \end{aligned}$$

where C, C' denote constants independent of ψ.

(2) On $\mathcal{D}_{\mathrm{p}}^{\mathrm{sr}}$ we have

$$A_{\mathrm{p}}^{(\epsilon)} = V_{\mathsf{c}}^* \eta_\epsilon (-A_{\mathsf{D}}) \eta_\epsilon V_{\mathsf{c}} = V_{\mathsf{c}}^* \eta_\epsilon^2 (-A_{\mathsf{D}}) V_{\mathsf{c}} + V_{\mathsf{c}}^* \eta_\epsilon [-A_{\mathsf{D}}, \eta_\epsilon] V_{\mathsf{c}}.$$

The operator $V_{\mathsf{c}}^* \eta_\epsilon^2 (-A_{\mathsf{D}}) V_{\mathsf{c}}$ is bounded by $V_{\mathsf{c}}^* (-A_{\mathsf{D}}) V_{\mathsf{c}}$, and thus also by $(\hat{\mathsf{k}}^2 + \hat{\mathsf{q}}^2) V_{\mathsf{c}}$ as we have already seen in the proof of (1). Furthermore, as derivatives of η_ϵ are bounded as well, the operator

$$[-A_{\mathsf{D}}, \eta_\epsilon] = \frac{1}{2} \sum_j [\hat{\mathsf{q}}_j, \eta_\epsilon] \hat{\mathsf{k}}_j$$

is bounded by $|\hat{\mathsf{k}}|$, and thus $\eta_\epsilon [-A_{\mathsf{D}}, \eta_\epsilon] V_{\mathsf{c}}$ is also bounded by $(\hat{\mathsf{k}}^2 + \hat{\mathsf{q}}^2) V_{\mathsf{c}}$. This shows the first GJN condition.

For the second one, we compute

$$\pm \mathrm{i} \left(\left\langle \Lambda_{\mathrm{p}}^{\mathrm{sr}} \psi, A_{\mathrm{p}}^{(\epsilon)} \psi \right\rangle - \left\langle A_{\mathrm{p}}^{(\epsilon)} \psi, \Lambda_{\mathrm{p}}^{\mathrm{sr}} \psi \right\rangle \right) = \pm \left\langle V_{\mathsf{c}} \psi, \mathrm{i} [\hat{\mathsf{k}}^2 + \hat{\mathsf{q}}^2, \eta_\epsilon (-A_{\mathsf{D}}) \eta_\epsilon] V_{\mathsf{c}} \psi \right\rangle.$$

Thus, it suffices to show $\pm \mathrm{i} [\hat{\mathsf{k}}^2 + \hat{\mathsf{q}}^2, \eta_\epsilon (-A_{\mathsf{D}}) \eta_\epsilon] \le C (\hat{\mathsf{k}}^2 + \hat{\mathsf{q}}^2)$ for some constant C on $C_{\mathsf{c}}^\infty(\mathbb{R}^3)$. First,

$$[\hat{\mathsf{k}}^2, \eta_\epsilon (-A_{\mathsf{D}}) \eta_\epsilon] = \eta_\epsilon [\hat{\mathsf{k}}^2, -A_{\mathsf{D}}] \eta_\epsilon = \sum_j \eta_\epsilon \hat{\mathsf{k}}_j [\hat{\mathsf{k}}_j, \hat{\mathsf{q}}_j] \hat{\mathsf{k}}_j \eta_\epsilon = -\mathrm{i} \eta_\epsilon \hat{\mathsf{k}}^2 \eta_\epsilon.$$

Second, in order to obtain $\pm\mathrm{i}[\hat{\mathsf{q}}^2, \eta_\epsilon(-A_{\mathsf{D}})\eta_\epsilon] \leq C(\hat{\mathsf{k}}^2 + \hat{\mathsf{q}}^2)$, we use the basic operator inequality (5.4) and it suffices to show that

$$[\hat{\mathsf{q}}_j, \eta_\epsilon(-A_{\mathsf{D}})\eta_\epsilon] = \eta_\epsilon[\hat{\mathsf{q}}_j, -A_{\mathsf{D}}]\eta_\epsilon + [\hat{\mathsf{q}}_j, \eta_\epsilon](-A_{\mathsf{D}})\eta_\epsilon + \eta_\epsilon(-A_{\mathsf{D}})[\hat{\mathsf{q}}_j, \eta_\epsilon], \tag{6.13}$$

is bounded by $|\hat{\mathsf{q}}|$. The first term in (6.13) is clearly bounded as $\eta_\epsilon[\hat{\mathsf{q}}_j, -A_{\mathsf{D}}]\eta_\epsilon = \frac{\mathrm{i}}{2}\eta_\epsilon^2\hat{\mathsf{k}}_j$, and for the two remaining ones it follows by shifting the $\hat{\mathsf{q}}_j$ operators in $-A_{\mathsf{D}}$ to the right and noting that any derivatives of η_ϵ are bounded.

(3) We have with regard to the first GJN condition for all $\psi \in \mathcal{D}_{\mathrm{p}}^{\mathrm{sr}}$,

$$\|H_{\mathrm{p}}\psi\| = \left\|V_{\mathsf{c}}^*\hat{\mathsf{k}}^2 V_{\mathsf{c}}\psi + H_{\mathrm{p}}P_{\mathrm{disc}}\psi\right\| \leq C\left\|V_{\mathsf{c}}^*(\hat{\mathsf{k}}^2 + \hat{\mathsf{q}}^2)V_{\mathsf{c}}\psi\right\| + \sup_{\lambda\in\sigma_{\mathrm{d}}(H_{\mathrm{p}})} |\lambda|\, \|\psi\|\,,$$

as $\hat{\mathsf{k}}^2$ is bounded by $\hat{\mathsf{q}}^2 + \hat{\mathsf{k}}^2$, where C is a constant independent of ψ. Furthermore,

$$\begin{aligned}&\left\langle H_{\mathrm{p}}\psi, \Lambda_{\mathrm{p}}^{\mathrm{sr}}\psi\right\rangle - \left\langle \Lambda_{\mathrm{p}}^{\mathrm{sr}}\psi, H_{\mathrm{p}}\psi\right\rangle \\ &= \left\langle V_{\mathsf{c}}^*\hat{\mathsf{k}}^2 V_{\mathsf{c}}\psi, V_{\mathsf{c}}^*(\hat{\mathsf{q}}^2 + \hat{\mathsf{k}}^2)V_{\mathsf{c}}\psi\right\rangle - \left\langle V_{\mathsf{c}}^*(\hat{\mathsf{q}}^2 + \hat{\mathsf{k}}^2)V_{\mathsf{c}}\psi, V_{\mathsf{c}}^*\hat{\mathsf{k}}^2 V_{\mathsf{c}}\psi\right\rangle \\ &= \left\langle \hat{\mathsf{k}}^2 V_{\mathsf{c}}\psi, \hat{\mathsf{q}}^2 V_{\mathsf{c}}\psi\right\rangle - \left\langle \hat{\mathsf{q}}^2 V_{\mathsf{c}}\psi, \hat{\mathsf{k}}^2 V_{\mathsf{c}}\psi\right\rangle.\end{aligned}$$

Using now that $\pm\mathrm{i}[\hat{\mathsf{q}}^2, \hat{\mathsf{k}}^2] \leq C(\hat{\mathsf{k}}^2 + \hat{\mathsf{q}}^2)$ for some constant C, we get also the second GJN condition.

(4) As H_{p} is bounded by $\Lambda_{\mathrm{p}}^{\mathrm{sr}}$ (by the previous argument) and $\mathsf{d}\Gamma(\hat{\mathsf{u}})$ is bounded by Λ_{f},

$$L_0 = (H_{\mathrm{p}} \otimes \mathrm{Id}_{\mathrm{p}} - \mathrm{Id}_{\mathrm{p}} \otimes H_{\mathrm{p}}) \otimes \mathrm{Id}_{\mathrm{f}} + \mathrm{Id}_{\mathrm{p}} \otimes \mathrm{Id}_{\mathrm{p}} \otimes \mathsf{d}\Gamma(\hat{\mathsf{u}})$$

is bounded by Λ^{sr}. Furthermore, by Hypothesis B-SR and Lemma 4.3, we know that the interaction terms $I \in L^2(\mathbb{R} \times \mathbb{S}^2, \mathcal{L}(\mathcal{H}_{\mathrm{p}} \otimes \mathcal{H}_{\mathrm{p}}))$. Hence, W is bounded by $\widehat{N}_{\mathrm{f}}^{1/2}$ and thus bounded by $\mathrm{Id}_{\mathrm{p}} \otimes \mathrm{Id}_{\mathrm{p}} \otimes \Lambda_{\mathrm{f}}^{1/2}$. Therefore, the first GJN condition is satisfied.

Next, as $(H_{\mathrm{p}}, \Lambda_{\mathrm{p}}^{\mathrm{sr}}, \mathcal{D}_{\mathrm{p}}^{\mathrm{sr}})$ is a GJN triple and $\mathsf{d}\Gamma(u)$ commutes with Λ_{f}, we get a constant C, such that

$$\pm\mathrm{i}(\langle L_0\psi, \Lambda^{\mathrm{sr}}\psi\rangle - \langle \Lambda^{\mathrm{sr}}\psi, L_0\psi\rangle) \leq C\,\langle \psi, \Lambda^{\mathrm{sr}}\psi\rangle$$

for all $\psi \in \mathcal{D}^{\mathrm{sr}}$, which yields the second GJN condition for L_0.

Again by Hypothesis B-SR and Lemma 4.3 we know that $(u,\Sigma) \mapsto (u^2 + 1)I(u,\Sigma)$ is in $L^2(\mathbb{R}\times\mathbb{S}^2, \mathcal{L}(\mathcal{H}_\mathrm{p}\otimes\mathcal{H}_\mathrm{p}))$. We have

$$\begin{aligned}
&|\langle \Phi(I)\psi, \mathrm{Id}_\mathrm{p}\otimes\mathrm{Id}_\mathrm{p}\otimes\Lambda_\mathrm{f}\psi\rangle - \langle \mathrm{Id}_\mathrm{p}\otimes\mathrm{Id}_\mathrm{p}\otimes\Lambda_\mathrm{f}\psi, \Phi(I)\psi\rangle| \\
&\quad= \left|\left\langle \psi, \left(a((\hat{\mathsf{u}}^2+1)I) - a^*((\hat{\mathsf{u}}^2+1)I)\right)\psi\right\rangle\right| \\
&\quad\le C\left\|(\widehat{N}_\mathrm{f}+1)^{1/2}\psi\right\|\|\psi\| \\
&\quad\le C'\langle\psi, \Lambda^{\mathrm{sr}}\psi\rangle
\end{aligned}$$

for some constants C, C'.

It remains to consider the commutator of W with the $\Lambda_\mathrm{p}^{\mathrm{sr}}$ terms. One has to show that the commutators

$$[\Phi(I_\alpha), V_\mathsf{c}^*(\hat{\mathsf{q}}^2 + \hat{\mathsf{k}}^2)V_\mathsf{c}\otimes\mathrm{Id}_\mathrm{f}], \qquad \alpha = \mathsf{l},\mathsf{r},$$

which have to be understood in the form sense, are form bounded by $\Lambda_\mathrm{p}^{\mathrm{sr}}\otimes\mathrm{Id}_\mathrm{f} + \mathrm{Id}_\mathrm{p}\otimes\Lambda_\mathrm{f}$. We can write on $\mathcal{D}_\mathrm{p}^{\mathrm{sr}}\mathbin{\hat\otimes}\mathfrak{F}_{\mathrm{fin}}(C_\mathsf{c}^\infty(\mathbb{R}^3))$, again in the form sense,

$$[\Phi(I_\alpha), X^2\otimes\mathrm{Id}_\mathrm{f}] = \sum_j \Phi([I_\alpha, X])(X\otimes\mathrm{Id}_\mathrm{f}) + (X\otimes\mathrm{Id}_\mathrm{f})\Phi([I_\alpha,X])$$

for $X\in\{V_\mathsf{c}^*\hat{\mathsf{q}}_jV_\mathsf{c}, V_\mathsf{c}^*\hat{\mathsf{k}}_jV_\mathsf{c} : j\in\{1,2,3\}\}$, and then use that $[I_\alpha, X]\in L^2(\mathbb{R}\times\mathbb{S}^2, \mathcal{L}(\mathcal{H}_\mathrm{p}))$ by Proposition 6.2.

(5) Clearly, $\|N_\mathrm{f}\psi\| = \|\mathsf{d}\Gamma(\mathrm{Id}_\mathrm{f})\psi\| \le \left\|\mathsf{d}\Gamma(\hat{\mathsf{u}}^2+1)\psi\right\|$ for any $\psi\in\mathfrak{F}_{\mathrm{fin}}(C_\mathsf{c}^\infty(\mathbb{R}^3))$, which shows that $\widehat{N}_\mathrm{f}$ is bounded by Λ^{sr} on $\mathcal{D}^{\mathrm{sr}}$. Furthermore, $[\widehat{N}_\mathrm{f}, \Lambda] = 0$ on $\mathcal{D}^{\mathrm{sr}}$, which implies the second GJN condition.

(6) We have

$$D = \mathrm{i}\lambda(a(I) - a^*(I)).$$

Thus, one can proceed similarly as in the proof for L_λ.

(7) We first consider the atomic space. One can show by induction that for all $n\in\mathbb{N}$ there exists $f\in\mathcal{S}(\mathbb{R}^3)$ such that

$$\mathrm{ad}^{(n)}_{A_\mathrm{p}^{(\epsilon)}}(H_\mathrm{p}) = V_\mathsf{c}^* f(\hat{\mathsf{k}})V_\mathsf{c}. \tag{6.14}$$

Clearly, for $n=1$,

$$\mathrm{ad}_{A_\mathrm{p}^{(\epsilon)}}(H_\mathrm{p}) = \mathrm{i}V_\mathsf{c}^*[\hat{\mathsf{k}}^2, \eta_\epsilon(-A_\mathsf{D})\eta_\epsilon]V_\mathsf{c} = \mathrm{i}V_\mathsf{c}^*\eta_\epsilon[\hat{\mathsf{k}}^2, -A_\mathsf{D}]\eta_\epsilon V_\mathsf{c} = V_\mathsf{c}^*\eta_\epsilon\hat{\mathsf{k}}^2\eta_\epsilon V_\mathsf{c}, \tag{6.15}$$

which has the form (6.14). Next, as $[f(\hat{\mathsf{k}}), \hat{\mathsf{q}}_j] = -\mathrm{i}\partial_j f(\hat{\mathsf{k}})$,

$$[V_{\mathsf{c}}^* f(\hat{\mathsf{k}}) V_{\mathsf{c}}, A_{\mathrm{p}}^{\mathrm{sr}}] = V_{\mathsf{c}}^* \eta_\epsilon [f(\hat{\mathsf{k}}), -A_{\mathsf{D}}] \eta_\epsilon V_{\mathsf{c}} = \frac{1}{2} \sum_j V_{\mathsf{c}}^* \eta_\epsilon [f(\hat{\mathsf{k}}), \hat{\mathsf{q}}_j] \hat{\mathsf{k}}_j \eta_\epsilon V_{\mathsf{c}}$$

yields again the form (6.14).

In particular, (6.14) implies that for each $n \in \mathbb{N}$, $\mathrm{ad}^{(n)}_{A_{\mathrm{p}}^{\mathrm{sr}}}(H_{\mathrm{p}})$ is bounded and there is a constant C such that

$$\pm\mathrm{i}[\mathrm{ad}^{(n)}_{A_{\mathrm{p}}^{\mathrm{sr}}}(H_{\mathrm{p}}), \Lambda_{\mathrm{p}}] \leq C\Lambda_{\mathrm{p}}$$

on $\mathcal{D}_{\mathrm{p}}^{\mathrm{sr}}$, since

$$\pm\mathrm{i}[f(\hat{\mathsf{k}}), \hat{\mathsf{k}}^2 + \hat{\mathsf{q}}^2] = \pm\mathrm{i}[f(\hat{\mathsf{k}}), \hat{\mathsf{q}}^2] \leq C(\hat{\mathsf{k}}^2 + \hat{\mathsf{q}}^2),$$

because $[f(\hat{\mathsf{k}}), \hat{\mathsf{q}}_j]$, $j \in \{1, 2, 3\}$, is bounded.

This, together with the fact that $(\mathsf{d}\Gamma(\hat{\mathsf{u}}), \Lambda_{\mathrm{f}}, \mathfrak{F}_{\mathrm{fin}}(C_{\mathsf{c}}^\infty(\mathbb{R}^3)))$ is a GJN triple (see the proof of (4)), implies that $(\mathrm{ad}^{(n)}_{A^{(\epsilon)}}(L_0), \Lambda^{\mathrm{sr}}, \mathcal{D}^{\mathrm{sr}})$, $n \in \{1, 2, 3\}$, are GJN triples.

It remains to verify the GJN conditions for $(W_n^{(\epsilon)}, \Lambda^{\mathrm{sr}}, \mathcal{D}^{\mathrm{sr}})$, $n \in \{1, 2, 3\}$. Analogously to the proof (4) for the GJN condition of L_λ we have to show that the expressions in the field operators and the commutators with $V_{\mathsf{c}}^* \hat{\mathsf{k}}_j V_{\mathsf{c}}$ and $V_{\mathsf{c}}^* \hat{\mathsf{q}}_j V_{\mathsf{c}}$, $j \in \{1, 2, 3\}$ are integrable. That is, we have to show that the operator-valued functions

$$(u, \Sigma) \mapsto \partial_u^m \tau_\beta(\mathrm{ad}^{(n-m)}_{A_{\mathrm{p}}^{(\epsilon)}}(G))(u, \Sigma),$$
$$(u, \Sigma) \mapsto \partial_u^m [\tau_\beta(\mathrm{ad}^{(n-m)}_{A_{\mathrm{p}}^{(\epsilon)}}(G))(u, \Sigma), X],$$

$X \in \{V_{\mathsf{c}}^* \hat{\mathsf{k}}_j V_{\mathsf{c}}, V_{\mathsf{c}}^* \hat{\mathsf{q}}_j V_{\mathsf{c}} : j \in \{1, 2, 3\}\}$, $n \in \{1, 2, 3\}$, $m \in \{0, \ldots, n\}$, are in $L^2(\mathbb{R} \times \mathbb{S}^2, \mathcal{L}(\mathcal{H}_{\mathrm{p}}))$. This follows from Proposition 6.2.

(8) Analogously to the proof of (7) it suffices to show that the operator-valued functions

$$(u, \Sigma) \mapsto \partial_u^n \tau_\beta(G)(u, \Sigma),$$
$$(u, \Sigma) \mapsto \partial_u^n [\tau_\beta(G)(u, \Sigma), X],$$

$X \in \{V_{\mathsf{c}}^* \hat{\mathsf{k}}_j V_{\mathsf{c}}, V_{\mathsf{c}}^* \hat{\mathsf{q}}_j V_{\mathsf{c}} : j \in \{1, 2, 3\}\}$, $n \in \{1, 2, 3\}$, are in $L^2(\mathbb{R} \times \mathbb{S}^2, \mathcal{L}(\mathcal{H}_{\mathrm{p}}))$. This follows again from Proposition 6.2.

(9) We first consider again the free part. We have on $\mathcal{D}_{\mathrm{p}}^{\mathrm{sr}}$,

$$\mathrm{i}[H_{\mathrm{p}}, A_{\mathrm{p}}^{\mathrm{sr}}] = \mathrm{i}[V_{\mathsf{c}}^{*}\hat{\mathsf{k}}^{2}V_{\mathsf{c}}, A_{\mathrm{p}}^{\mathrm{sr}}] = \mathrm{i}V_{\mathsf{c}}^{*}[\hat{\mathsf{k}}^{2}, -A_{\mathsf{D}}]V_{\mathsf{c}} = V_{\mathsf{c}}^{*}\hat{\mathsf{k}}^{2}V_{\mathsf{c}}.$$

Then we can see as in the proof of (3) that also $(\mathrm{ad}_{A_{\mathrm{p}}^{\mathrm{sr}}}(H_{\mathrm{p}}), \Lambda_{\mathrm{p}}^{\mathrm{sr}}, \mathcal{D}_{\mathrm{p}}^{\mathrm{sr}})$ is a GJN triple and so is $(\mathrm{ad}_{A^{\mathrm{sr}}}(L_0), \Lambda^{\mathrm{sr}}, \mathcal{D}^{\mathrm{sr}})$.

It remains to verify the GJN conditions for $(W_1^{\mathrm{sr}}, \Lambda^{\mathrm{sr}}, \mathcal{D}^{\mathrm{sr}})$. As in (7) and (8) one has to show that the operator-valued functions

$$\begin{aligned}
&(u,\Sigma) \mapsto \partial_u^n \tau_\beta(\mathrm{ad}_{A_{\mathrm{p}}^{\mathrm{sr}}}^{(1-n)}(G))(u,\Sigma),\\
&(u,\Sigma) \mapsto \partial_u^n [\tau_\beta(\mathrm{ad}_{A_{\mathrm{p}}^{\mathrm{sr}}}^{(1-n)}(G))(u,\Sigma), X],
\end{aligned}$$

$X \in \{V_{\mathsf{c}}^{*}\hat{\mathsf{k}}_j V_{\mathsf{c}}, V_{\mathsf{c}}^{*}\hat{\mathsf{q}}_j V_{\mathsf{c}} : j \in \{1,2,3\}\}$, $n \in \{0,1\}$, are in $L^2(\mathbb{R}\times\mathbb{S}^2, \mathcal{L}(\mathcal{H}_{\mathrm{p}}))$, which follows again from Proposition 6.2. $\square$

The statements of Proposition 6.3 allow the application of the virial theorem Theorem 4.8 for the regularized conjugate operator $A^{(\epsilon)}$, $\epsilon > 0$. In order to remove the regularization and transfer the result to C_1^{sr}, one has to consider the limit $\epsilon \to 0$ for the corresponding quadratic forms $q_1^{(\epsilon)}$ of $C_1^{(\epsilon)}$. This is the content of the following lemma.

Lemma 6.4
Assume that $\psi \in \mathcal{D}(\widehat{N}_{\mathrm{f}}^{1/2})$ and $q_1^{(\epsilon)}(\psi) \le 0$ for all $\epsilon \in (0,1)$. Then $\psi \in \mathcal{D}(q_1^{\mathrm{sr}})$, and

$$q_1^{\mathrm{sr}}(\psi) = \lim_{\epsilon\to 0} q_1^{(\epsilon)}(\psi). \tag{6.16}$$

Proof. Let us recall that by definition

$$C_1^{(\epsilon)} = \widehat{N}_{\mathrm{f}} + (\mathrm{ad}_{A_{\mathrm{p}}^{(\epsilon)}}(H_{\mathrm{p}}) \otimes \mathrm{Id}_{\mathrm{p}} + \mathrm{Id}_{\mathrm{p}} \otimes \mathrm{ad}_{A_{\mathrm{p}}^{(\epsilon)}}(H_{\mathrm{p}})) \otimes \mathrm{Id}_{\mathrm{f}} + \lambda W_1^{(\epsilon)}. \tag{6.17}$$

First, we show that

$$\psi \in \mathcal{D}\left((V_{\mathsf{c}}^{*}|\hat{\mathsf{k}}|V_{\mathsf{c}} \otimes \mathrm{Id}_{\mathrm{p}} + \mathrm{Id}_{\mathrm{p}} \otimes V_{\mathsf{c}}^{*}|\hat{\mathsf{k}}|V_{\mathsf{c}}) \otimes \mathrm{Id}_{\mathrm{f}} + \widehat{N}_{\mathrm{f}}^{1/2}\right) \subseteq \mathcal{D}(q_1^{\mathrm{sr}}), \tag{6.18}$$

which will follow once we have established that

$$\left\langle \psi, (V_{\mathsf{c}}^{*}\eta_\epsilon\hat{\mathsf{k}}^{2}\eta_\epsilon V_{\mathsf{c}} \otimes \mathrm{Id}_{\mathrm{p}} + \mathrm{Id}_{\mathrm{p}} \otimes V_{\mathsf{c}}^{*}\eta_\epsilon\hat{\mathsf{k}}^{2}\eta_\epsilon V_{\mathsf{c}}) \otimes \mathrm{Id}_{\mathrm{f}}\, \psi \right\rangle \le C \tag{6.19}$$

for a constant C independent of $\epsilon \in (0,1)$. To this end, we use that by standard estimates for creation and annihilation operators, we obtain for any $\delta > 0$,

$$\pm \mathrm{i} W_1^{(\epsilon)} \leq \frac{1}{\delta} \widehat{N}_{\mathrm{f}} + \delta w_1^{(\epsilon)} \otimes \mathrm{Id}_{\mathrm{f}} \tag{6.20}$$

in the form sense on $\mathcal{D}(\widehat{N}_{\mathrm{f}}^{1/2})$, where we introduced the follwoing bounded operators on $\mathcal{H}_{\mathrm{p}} \otimes \mathcal{H}_{\mathrm{p}}$,

$$w_1^{(\epsilon)} := \int I_1^{(\epsilon)}(u,\Sigma)^* I_1^{(\epsilon)}(u,\Sigma) \mathrm{d}(u,\Sigma), \qquad \epsilon \geq 0.$$

To estimate this expression we use that

$$\int \mathrm{ad}_{A_{\mathrm{p}}^{(\epsilon)}}(\tau_\beta(G)(u,\Sigma))^* \, \mathrm{ad}_{A_{\mathrm{p}}^{(\epsilon)}}(\tau_\beta(G)(u,\Sigma)) \mathrm{d}(u,\Sigma) \leq C(V_{\mathsf{c}}^* \eta_\epsilon \hat{\mathsf{k}}^2 \eta_\epsilon V_{\mathsf{c}} + \mathrm{Id}_{\mathrm{p}}),$$

in the form sense for some constant C independent of ϵ, where we multiplied out the commutators, used (5.4) and the fact that the functions $(u,\Sigma) \mapsto \partial_u \tau_\beta(G)(u,\Sigma)$ and $(u,\Sigma) \mapsto V_{\mathsf{c}}^* \hat{\mathsf{q}}_j V_{\mathsf{c}} \tau_\beta(G)$ belong to $L^2(\mathbb{R} \times \mathbb{S}^2, \mathcal{L}(\mathcal{H}_{\mathrm{p}}))$ due to Proposition 6.2. This yields

$$w_1^{(\epsilon)} \leq C(V_{\mathsf{c}}^* \eta_\epsilon \hat{\mathsf{k}}^2 \eta_\epsilon V_{\mathsf{c}} \otimes \mathrm{Id}_{\mathrm{p}} + \mathrm{Id}_{\mathrm{p}} \otimes V_{\mathsf{c}}^* \eta_\epsilon \hat{\mathsf{k}}^2 \eta_\epsilon V_{\mathsf{c}} + \mathrm{Id}_{\mathrm{p}} \otimes \mathrm{Id}_{\mathrm{p}}). \tag{6.21}$$

Now using (6.15) and (6.20) to estimate (6.17) we obtain in the form sense on $\mathcal{D}(\widehat{N}_{\mathrm{f}}^{1/2})$ for any $\epsilon > 0$,

$$\begin{aligned} C_1^{(\epsilon)} \geq{}& (1 - C\,|\lambda|\,\delta)(V_{\mathsf{c}}^* \eta_\epsilon \hat{\mathsf{k}}^2 \eta_\epsilon V_{\mathsf{c}} \otimes \mathrm{Id}_{\mathrm{p}} + \mathrm{Id}_{\mathrm{p}} \otimes V_{\mathsf{c}}^* \eta_\epsilon \hat{\mathsf{k}}^2 \eta_\epsilon V_{\mathsf{c}} + \mathrm{Id}_{\mathrm{p}} \otimes \mathrm{Id}_{\mathrm{p}}) \otimes \mathrm{Id}_{\mathrm{f}} \\ &+ \left(1 - \frac{|\lambda|}{\delta}\right) \widehat{N}_{\mathrm{f}}. \end{aligned}$$

Making $\delta > 0$ sufficently small such that $C\,|\lambda|\,\delta < 1$ and using that by assumption $q_1^{(\epsilon)}(\psi) \leq 0$ and $\psi \in \mathcal{D}(\widehat{N}_{\mathrm{f}}^{1/2})$, we arrive at (6.19).

Now, it remains to prove (6.16). First observe, that by dominated convergence, we have for all $\phi \in \mathcal{D}(V_{\mathsf{c}}^* |\hat{\mathsf{k}}| V_{\mathsf{c}})$,

$$\left\| |\hat{\mathsf{k}}| \eta_\epsilon V_{\mathsf{c}} \phi \right\| \longrightarrow \left\| |\hat{\mathsf{k}}| V_{\mathsf{c}} \phi \right\|, \ \epsilon \to 0.$$

Thus (6.16) will follow once we have shown that

$$\left\langle \psi, W_1^{(\epsilon)} \psi \right\rangle \to \langle \psi, W_1 \psi \rangle \,. \tag{6.22}$$

Thus we have to show the convergence of the field operator of a commutator. To this end, we note that from Proposition 6.2 we know that the operator-valued functions

$$(u,\Sigma)\mapsto V_{\mathsf{c}}^{*}\hat{\mathsf{q}}_j V_{\mathsf{c}} H(u,\Sigma),$$

for $H\in\{\tau_\beta(G),\partial_u\tau_\beta(G)\}$, are in $L^2(\mathbb{R}\times\mathbb{S}^2,\mathcal{L}(\mathcal{H}_{\mathrm{p}}))$. Now,

$$\begin{aligned}
A_{\mathrm{p}}^{(\epsilon)}H(u,\Sigma) &= V_{\mathsf{c}}^{*}\eta_\epsilon A_{\mathsf{D}}\eta_\epsilon V_{\mathsf{c}}H(u,\Sigma)\\
&= V_{\mathsf{c}}^{*}\eta_\epsilon\frac{1}{4}(3\mathrm{i}+2\hat{\mathsf{k}}\hat{\mathsf{q}})\eta_\epsilon V_{\mathsf{c}}H(u,\Sigma)\\
&= V_{\mathsf{c}}^{*}\eta_\epsilon\frac{1}{4}\left(3\mathrm{i}\eta_\epsilon+2\sum_{j=1}^{3}\hat{\mathsf{k}}_j(\mathrm{i}(\partial_{k_j}\eta_\epsilon)+\eta_\epsilon\hat{\mathsf{q}}_j)\right)V_{\mathsf{c}}H(u,\Sigma). \qquad (6.23)
\end{aligned}$$

Observe that η_ϵ and $\partial_{k_j}\eta_\epsilon$ are bounded uniformly in $\epsilon\in(0,1)$. From (6.23) we see for $\phi\in\mathcal{D}(\mathrm{Id}_{\mathrm{p}}\otimes N_{\mathrm{f}})$ that

$$\begin{aligned}
&\left\langle\phi, a^*(A_{\mathrm{p}}^{(\epsilon)}H)\phi\right\rangle\\
&=\frac{3}{4}\left\langle V_{\mathsf{c}}^{*}\eta_\epsilon^2 V_{\mathsf{c}}\otimes\mathrm{Id}_{\mathrm{f}}\,\phi, a^*(\mathrm{i}H)\phi\right\rangle+\frac{1}{2}\sum_{j=1}^{3}\left\langle V_{\mathsf{c}}^{*}(\partial_{k_j}\eta_\epsilon)\hat{\mathsf{k}}_j\eta_\epsilon V_{\mathsf{c}}\otimes\mathrm{Id}_{\mathrm{f}}\,\phi, a^*(\mathrm{i}H)\phi\right\rangle\\
&\quad+\frac{1}{2}\sum_{j=1}^{3}\left\langle V_{\mathsf{c}}^{*}\eta_\epsilon\hat{\mathsf{k}}_j\eta_\epsilon V_{\mathsf{c}}\otimes\mathrm{Id}_{\mathrm{f}}\,\phi, a^*(V_{\mathsf{c}}^{*}\hat{\mathsf{q}}_j V_{\mathsf{c}}H)\phi\right\rangle\\
&\to\frac{3}{4}\left\langle V_{\mathsf{c}}^{*}V_{\mathsf{c}}\otimes\mathrm{Id}_{\mathrm{f}}\,\phi, a^*(\mathrm{i}H)\phi\right\rangle+\frac{1}{2}\sum_{j=1}^{3}\left\langle V_{\mathsf{c}}^{*}\hat{\mathsf{k}}_j V_{\mathsf{c}}\otimes\mathrm{Id}_{\mathrm{f}}\,\phi, a^*(V_{\mathsf{c}}^{*}\hat{\mathsf{q}}_j V_{\mathsf{c}}H)\phi\right\rangle,
\end{aligned}$$

where for the limit we used that $\partial_{k_j}\eta_\epsilon$ tends to zero as $\epsilon\downarrow 0$, (6.18), and dominated convergence. Similarly, we find

$$\begin{aligned}
&\left\langle\phi, a^*(HA_{\mathrm{p}}^{(\epsilon)})\phi\right\rangle\\
&\to\frac{3}{4}\left\langle a(\mathrm{i}H)\phi, V_{\mathsf{c}}^{*}V_{\mathsf{c}}\otimes\mathrm{Id}_{\mathrm{f}}\,\phi\right\rangle+\frac{1}{2}\sum_{j=1}^{3}\left\langle a(HV_{\mathsf{c}}^{*}\hat{\mathsf{q}}_j V_{\mathsf{c}})\phi, V_{\mathsf{c}}^{*}\hat{\mathsf{k}}_j V_{\mathsf{c}}\otimes\mathrm{Id}_{\mathrm{f}}\,\phi\right\rangle.
\end{aligned}$$

Thus, we infer

$$\begin{aligned}
&\mathrm{i}\left\langle\phi, a^*(\mathrm{ad}_{A_{\mathrm{p}}^{(\epsilon)}}(H))\phi\right\rangle\\
&\to\frac{3}{4}\left\langle V_{\mathsf{c}}^{*}V_{\mathsf{c}}\otimes\mathrm{Id}_{\mathrm{f}}\,\phi, a^*(\mathrm{i}H)\phi\right\rangle+\frac{1}{2}\sum_{j=1}^{3}\left\langle V_{\mathsf{c}}^{*}\hat{\mathsf{k}}_j V_{\mathsf{c}}\otimes\mathrm{Id}_{\mathrm{f}}\,\phi, a^*(V_{\mathsf{c}}^{*}\hat{\mathsf{q}}_j V_{\mathsf{c}}H)\phi\right\rangle\\
&\quad-\frac{3}{4}\left\langle a(\mathrm{i}H)\phi, V_{\mathsf{c}}^{*}V_{\mathsf{c}}\otimes\mathrm{Id}_{\mathrm{f}}\,\phi\right\rangle-\frac{1}{2}\sum_{j=1}^{3}\left\langle a(HV_{\mathsf{c}}^{*}\hat{\mathsf{q}}_j V_{\mathsf{c}})\phi, V_{\mathsf{c}}^{*}\hat{\mathsf{k}}_j V_{\mathsf{c}}\otimes\mathrm{Id}_{\mathrm{f}}\,\phi\right\rangle\\
&\quad=\mathrm{i}\left\langle\phi, a^*(\mathrm{ad}_{A_{\mathrm{p}}^{\mathrm{sr}}}(H(u,\Sigma)))\phi\right\rangle,
\end{aligned}$$

where the last equality follows by verifying the identiy on the dense space $\mathcal{D}_\mathrm{p}^\mathrm{sr}$, defined in (6.6), using a straightforward calculation, and then extending it to ϕ using Proposition 6.2. This shows (6.22) in view of the definition of $W_1^{(\epsilon)}$ and W_1, see (5.2). $\square$

Now we can prove the main result of this section, the concrete virial theorem in our setting. Recall that q_1^sr is the quadratic form corresponding to C_1^sr.

Theorem 6.5 (Concrete virial theorem)
Assume there exists $\psi \in \mathcal{D}(L_\lambda)$ with $L_\lambda\psi = 0$. Then $\psi \in \mathcal{D}(q_1^\mathrm{sr})$ and $q_1^\mathrm{sr}(\psi) \leq 0$.

Proof. First, we apply the virial theorem Theorem 4.8 with $\Lambda = \Lambda^\mathrm{sr}$, $L = L_\lambda$, $N = \widehat{N}_\mathrm{f} + 1$, D as in (6.7), and $A = \mathrm{Id}_\mathrm{p} \otimes \mathrm{Id}_\mathrm{p} \otimes A_\mathrm{f}$. We have seen in Proposition 6.3 that (V1) is satisfied. Furthermore, on $\mathfrak{F}_\mathrm{fin}(C_\mathsf{c}^\infty(\mathbb{R}^3))$,

$$\Lambda_\mathrm{f} e^{\mathrm{i}tA_\mathrm{f}} = e^{\mathrm{i}tA_\mathrm{f}}(\Lambda_\mathrm{f} + \mathsf{d}\Gamma(2\hat{u}t + t^2)), \qquad t \in \mathbb{R}.$$

Thus, for some fixed t there is a constant C such that $\left\| \Lambda_\mathrm{f} e^{\mathrm{i}tA_\mathrm{f}}\psi \right\| \leq C \left\| \Lambda_\mathrm{f}\psi \right\|$ for all $\psi \in \mathfrak{F}_\mathrm{fin}(C_\mathsf{c}^\infty(\mathbb{R}^3))$. As $\mathfrak{F}_\mathrm{fin}(C_\mathsf{c}^\infty(\mathbb{R}^3))$ is a core for Λ_f, we find $e^{\mathrm{i}tA_\mathrm{f}}\mathcal{D}(\Lambda_\mathrm{f}) \subseteq \mathcal{D}(\Lambda_\mathrm{f})$. Hence, we conclude that $\mathcal{D}(\Lambda)$ is invariant under the unitary group associated to A and hence (V2) holds. Furthermore, (4.24)–(4.26) are satisfied since D, $C_1^{(\mathrm{f})}$ and $C_3^{(\mathrm{f})}$ are bounded by $N_\mathrm{f}^{1/2}$ (by Proposition 6.3).

Therefore, one finds a sequence (ψ_n) in $\mathcal{D}(L_\lambda) \cap \mathcal{D}(C_1^{(\mathrm{f})})$ such that $\psi_n \to \psi$ and

$$\lim_{n\to\infty} \left\langle \psi_n, C_1^{(\mathrm{f})}\psi_n \right\rangle = 0.$$

Then, it follows from semi-continuity of closed quadratic forms that ψ is in the form domain of $C_1^{(\mathrm{f})}$. As $W_1^{(\mathrm{f})}$ is bounded by $\widehat{N}_\mathrm{f}^{1/2}$ (as shown in the proof of Proposition 6.3 (8)), $\psi \in \mathcal{D}(N_\mathrm{f}^{1/2})$.

Next, we apply the virial theorem Theorem 4.8 once more with Λ, D, L, and N as before, but $A = A^{(\epsilon)}$, $\epsilon > 0$. Again, by Proposition 6.3, (V1) and (4.24)–(4.26) are satisfied. Furthermore, Proposition 6.3 yields that $(A_\mathrm{p}^{(\epsilon)}, \Lambda_\mathrm{p}^\mathrm{sr}, \mathcal{D}_\mathrm{p}^\mathrm{sr})$ is a GJN triple. Hence Theorem 4.6 shows that $e^{\mathrm{i}tA_\mathrm{p}^{(\epsilon)}}$, $t \in \mathbb{R}$, leaves $\mathcal{D}(\Lambda_\mathrm{p})$ invariant. This and the invariance for the unitary group corresponding to A_f (as already seen above) again imply (V2).

Therefore, we find a sequence $(\psi_n)_{n\in\mathbb{N}}$ in $\mathcal{D}(C_1^{(\epsilon)}) \cap \mathcal{D}(L_\lambda)$ such that $\psi_n \to \psi$, $n \to \infty$, and $\lim_{n\to\infty} \left\langle \psi_n, C_1^{(\epsilon)}\psi_n \right\rangle = 0$. Now, as $q_1^{(\epsilon)}$ is closed, thus continuous from below, we obtain $\psi \in \mathcal{D}(q_1^{(\epsilon)})$ and

$$q_1^{(\epsilon)}(\psi) \leq \lim_{n\to\infty} q_1^{(\epsilon)}(\psi_n) = 0.$$

Then Lemma 6.4 finishes the proof. $\square$

6.4. Estimates on the Scattering Functions

The aim of this section is to prove that the commutators of the interaction with the dilation operator in scattering space are sufficiently bounded. To achieve this, we use the Born series expansion of the scattering functions, that is, we expand them using the recursion formula of the Lippmann-Schwinger equation (6.1). Then we get the Born series terms, and a remainder term since we perform only finitely many recursion steps. The idea is that the remainder term decays fast enough for the momentum $|k| \to \infty$ for sufficiently many recursion steps.

6.4.1. Born Series Expansion and Technical Preparations

First we show that that the scattering functions as well as their derivatives with respect to the wave vector k are bounded. For this purpose we use the method of modified square integrable scattering functions as described in Section 6.1. Remember that $\phi(k,\cdot)$, $k \in \mathbb{R}^3$, denote the continuous scattering functions on $\mathbb{R}^3$ and V a potential satisfying Hypothesis A-SR. As V is compactly supported we may assume that $\operatorname{supp} V$ is contained in a ball around the origin of radius R.

Recall that the modified scattering functions were given by $\widetilde{\phi}(k,x) := |V(x)|^{1/2}\phi(k,x)$. Then $\widetilde{\phi}(k,\cdot) \in L^2(\mathbb{R}^3)$ for all k, and the function satisfies the modified Lippmann-Schwinger equation (6.2). Furthermore, it was discussed in Section 6.1 that we can recover the original scattering function from the modified one by

$$\phi(k,x) = e^{ikx} - \frac{1}{4\pi}\int \frac{e^{\mathrm{i}|k||x-y|}}{|x-y|} V(y)^{1/2}\widetilde{\phi}(k,y)\mathrm{d}y. \tag{6.24}$$

Now we extend the results of boundedness of the first derivative of the scattering functions in [New12, Lemma 1.1.3] to derivatives of arbitrary order.

Proposition 6.6
Let $\hat{D}_k = \frac{\hat{\mathsf{k}}}{|\hat{\mathsf{k}}|}\nabla_k$ be the radial derivative and let ∂_{k_j} be the derivative with respect to the j-th component of k. For all $n \in \mathbb{N}_0$ and $m \in \{0,1\}$ there is a polynomial P such that for all x and $k \neq 0$,

$$\left|\partial_{k_j}^m \hat{D}_k^n \varphi(k,x)\right| \leq P(|x|).$$

Proof. We get by the modified Lippmann-Schwinger equation

$$\widetilde{\phi}(k,\cdot) = (\mathrm{Id} - L_{|k|})^{-1}(|V|^{1/2} e_k),$$

where $e_k(x) := e^{ikx}$. First we claim that $(\mathrm{Id} - L_{|k|})^{-1}$ is uniformly bounded in $k \in \mathbb{R}^3$. Note that $\kappa \mapsto L_\kappa$ is continuous on $[0,\infty)$, which is easy to see, cf.

[Sim15, Theorem 1.22]. Moreover, $\lim_{\kappa\to 0}\|L_\kappa\| \to 0$ is proven in [Sim15, Theorem 1.23] by a variant of the Klein-Zemach method. Since L_κ is Hilbert-Schmidt and hence compact, it follows from the Fredholm alternative that $\mathrm{Id} - L_\kappa$ is invertible, provided $\psi = L_\kappa\psi$ has no non-trivial solutions in L^2. But as in the proof of Theorem 6.1, such non-trivial solutions are ruled out for all $\kappa \geq 0$. Since the inverse is a continuous map on the space of bounded invertible operators, the claim about the bounded resolvent now follows.

Observe that $\hat{D}_k|k| = 1$ and $\hat{D}_k(k/|k|) = 0$. Thus, for any $n \in \mathbb{N}_0$, the operator $\hat{D}_k^n(\mathrm{Id} - L_{|k|})^{-1}$ is again uniformly bounded in $k \neq 0$, since differentiation with $\hat{D}_k$ yields just higher powers of $(\mathrm{Id} - L_{|k|})^{-1}$ and radial derivatives of $L_{|k|}$, which are again bounded operators since V decays fast enough. Similarly one sees that $\partial_{k_j}\hat{D}_k^n(\mathrm{Id} - L_{|k|})^{-1}$ is uniformly bounded in $k \neq 0$. Note that the expression is not differentiable at the origin. Furthermore, for any $n \in \mathbb{N}$,

$$\sup_{k\neq 0}\left\|\hat{D}_k^n(|V|^{1/2}e_k)\right\|_2 < \infty$$

as V is compactly supported. Thus, we have shown, for all $n \in \mathbb{N}_0$,

$$\sup_{k\neq 0}\left\|\hat{D}_k^n\tilde{\phi}(k,\cdot)\right\|_2 < \infty.$$

Now we can differentiate (6.24), estimate the integral with Cauchy-Schwarz, and use that

$$\int \frac{|V(y)|}{|x-y|^2}\mathrm{d}y \leq \|V\|_\infty \int_{B_R(x)} \frac{\mathrm{d}y}{y^2} \leq \|V\|_\infty \left(\int_{B_{3R}(0)} \frac{\mathrm{d}y}{y^2} + \frac{|B_R(0)|}{R^2}\right) < \infty \tag{6.25}$$

is bounded uniformly in x, where the second inequality can be seen by considering the cases $|x| < 2R$ and $|x| \geq 2R$. □

Next, we perform the Born series expansion. Similar to [Ike60] it is convenient to introduce a symbol for the integral operator in the Lippmann-Schwinger equation. We consider a slightly bigger class of operators to cover also derivatives with respect to k. Let $C_{\mathsf{b}}(\mathbb{R}^3)$ denote the bounded continuous functions on $\mathbb{R}^3$ and $C_{\mathsf{poly}}(\mathbb{R}^3)$ the polynomially bounded continuous functions, that is,

$$C_{\mathsf{poly}}(\mathbb{R}^3) := \{\psi \in C(\mathbb{R}^3) : \exists n \in \mathbb{N}_0\colon \exists C > 0\colon \forall x \in \mathbb{R}^3\colon\ |\psi(x)| \leq C(1+|x|)^n\}.$$

Definition 6.7
For $W \in C_{\mathsf{c}}^\infty(\mathbb{R}^3)$, $\kappa \geq 0$, $\psi \in C_{\mathsf{poly}}(\mathbb{R}^3)$ and $n \in \mathbb{N}_0$, we define

$$T_{W,\kappa}^{(n)}\psi(x) := \int \frac{e^{\mathrm{i}\kappa|x-y|}}{|x-y|^{1-n}}W(y)\psi(y)\mathrm{d}y = \int \frac{e^{\mathrm{i}\kappa|v|}}{|v|^{1-n}}W(v+x)\psi(v+x)\mathrm{d}v.$$

Furthermore, we write $T_{W,\kappa} := T^{(0)}_{W,\kappa}$. They have the following elementary properties.

Proposition 6.8
Let $W \in C_{\mathsf{c}}^\infty(\mathbb{R}^3)$ and assume $\operatorname{supp} W \subseteq B_{R'}(0)$ *for some $R' \geq 0$.*

(a) For all $\kappa \geq 0$, $T_{W,\kappa}$, $T^{(-1)}_{W,\kappa}$ are bounded operators from $C_{\mathsf{b}}(\mathbb{R}^3)$ to $C_{\mathsf{b}}(\mathbb{R}^3)$,

(b) For all $\kappa \geq 0$ and for all $n \in \mathbb{N}_0$, $T^{(n)}_{W,\kappa}$ maps $C_{\mathsf{poly}}(\mathbb{R}^3)$ to $C_{\mathsf{poly}}(\mathbb{R}^3)$. Furthermore for all $n \in \mathbb{N}_0$, there exists a polynomial P such that

$$\left|T^{(n)}_{W,\kappa}(x)\right| \leq P(|x|) \left\|\mathbb{1}_{B_{R'}(0)}\psi\right\|_\infty$$

holds for all $\kappa \geq 0$, $\psi \in C_{\mathsf{poly}}(\mathbb{R}^3)$ and $x \in \mathbb{R}^3$.

Proof. (a) It follows that for $\psi \in C_{\mathsf{b}}(\mathbb{R}^3)$, $x \in \mathbb{R}^3$, $\kappa \geq 0$,

$$\left|T^{-1}_{W,\kappa}\psi(x)\right| \leq \|\psi\|_\infty \int \frac{|W(y)|}{|x-y|^2}\mathrm{d}y \leq \|W\|_\infty \|\psi\|_\infty \int_{B_{R'}(0)} \frac{1}{|x-y|^2}\mathrm{d}y,$$
$$|T_{W,\kappa}\psi(x)| \leq \|\psi\|_\infty \int \frac{|W(y)|}{|x-y|}\mathrm{d}y \leq \|W\|_2 \|\psi\|_\infty \left(\int_{B_{R'}(0)} \frac{1}{|x-y|^2}\mathrm{d}y\right)^{1/2}.$$

The integral is bounded independent of x, see (6.25).

(b) There exists a constant $C > 0$ such that for all $x \in \mathbb{R}^3$, $n \in \mathbb{N}_0$, $\kappa \geq 0$,

$$\begin{aligned}\left|T^{(n)}_{W,\kappa}\psi(x)\right| &\leq C \int_{B_{R'}(0)} \frac{|W(y)|}{|x-y|^{1-n}} |\psi(y)| \,\mathrm{d}y \\ &\leq C \left\|\mathbb{1}_{B_{R'}(0)}\psi\right\|_\infty \|W\|_2 \left(\int_{B_{R'}(x)} |y|^{2n-2} \,\mathrm{d}y\right)^{1/2}.\end{aligned}$$

The last integral can be estimated by

$$\int_{r=0}^{R'+|x|} r^{2n}\mathrm{d}r,$$

which is bounded by a polynomial in $|x|$. □

Using the previous notation and iterating the Lippmann-Schwinger equation (6.1) we arrive at the following.

Proposition 6.9
For all $N \in \mathbb{N}_0$, $k, x \in \mathbb{R}^3$, *we have*

$$\phi(k,x) = \sum_{n=0}^{N} \phi_0^{(n)}(k,x) + \phi_{\mathsf{R}}^{(N+1)}(k,x),$$

where, for $n \in \mathbb{N}_0$,

$$\begin{aligned}\phi_0^{(n)}(k,x) &:= (-4\pi)^{-n} T_{V,|k|}^{n} e_k(x),\\ \phi_{\mathsf{R}}^{(n)}(k,x) &:= (-4\pi)^{-n} T_{V,|k|}^{n} \phi(k,\cdot)(x),\end{aligned}$$

and $e_k(x) := e^{\mathrm{i}kx}$.

As an immediate consequence of an iterated application of the first and second identity in definition 6.7 we find the following lemma, which we will use.

Lemma 6.10
Let $V_1, \ldots, V_p \in C_{\mathsf{c}}^{\infty}(\mathbb{R}^3)$, $n_1, \ldots, n_p \in \mathbb{N}_0$, *and* $\psi \in C_{\mathsf{poly}}(\mathbb{R}^3)$. *Then for all* $k, x \in \mathbb{R}^3$, *we have*

$$\begin{aligned}&(T_{V_1,|k|}^{(n_1)} \cdots T_{V_p,|k|}^{(n_p)} \psi)(x_0)\\ &\quad= \int \left\{ \prod_{l=1}^{p} \frac{e^{\mathrm{i}|k||x_{l-1}-x_l|}}{|x_{l-1}-x_l|^{1-n_l}} V_l(x_l) \right\} \psi(x_p) \mathrm{d}(x_1, \ldots, x_p), &(6.26)\\ &\quad= \int \left\{ \prod_{l=1}^{p} \frac{e^{\mathrm{i}|k||u_l|}}{|u_l|^{1-n_l}} V_l\left(x_0 + \sum_{s=1}^{l} u_s\right) \right\} \psi\left(x_0 + \sum_{s=1}^{p} u_s\right) \mathrm{d}(u_1, \ldots, u_p), &(6.27)\end{aligned}$$

and the special case

$$(T_{V_1,|k|}^{(n_1)} \cdots T_{V_p,|k|}^{(n_p)} e_k)(x) = e^{\mathrm{i}kx} \int \left\{ \prod_{l=1}^{p} \frac{e^{\mathrm{i}(|k||u_l|+ku_l)}}{|u_l|^{1-n_l}} V_l\left(x + \sum_{s=1}^{l} u_s\right) \right\} \mathrm{d}(u_1, \ldots, u_p). \tag{6.28}$$

6.4.2. Estimates of the Terms of the Born Series

In this subsection we prove decay estimates for the inner products of an abstract coupling function $\chi \in \mathcal{S}(\mathbb{R}^3)$ with (derivatives with respect to k of) the functions $\phi_0^{(n)}(k,\cdot)$, $k \in \mathbb{R}^3$, $n \in \mathbb{N}_0$, which will be collected in Proposition 6.14 and Proposition 6.15. One can actually show an arbitrary fast decay for *any* $n \in \mathbb{N}$. The main tool will be a standard stationary phase argument as given in the following lemma.

Lemma 6.11 (Stationary phase)
For any $n \in \mathbb{N}$ there exists a constant C such that for all $g \in C_\mathsf{c}^\infty(\mathbb{R}^3)$ and $k \in \mathbb{R}^3$, we have

$$\left| \int e^{\mathrm{i}xk} g(x) \mathrm{d}x \right| \leq \frac{C}{\langle k \rangle^n} \sup_{|\alpha| \leq n} \|\partial^\alpha g\|_1 .$$

Proof. For all $k \in \mathbb{R}^3$ and $j \in \{1, 2, 3\}$,

$$\begin{aligned} \mathrm{i}k_j \int e^{\mathrm{i}xk} g(x) \mathrm{d}x &= \int \partial_j e^{\mathrm{i}xk} g(x) \mathrm{d}x \\ &= \lim_{R \to \infty} \int_{S_R(0)} e^{\mathrm{i}xk} g(x) \mathrm{d}x - \int e^{\mathrm{i}xk} \partial_j g(x) \mathrm{d}x. \end{aligned}$$

The first term clearly vanishes. Now we can repeat this procedure n times. □

We proceed by computing the derivatives as well as the effect of multiple applications of the dilation operator in the variable k acting on the terms of the Born series. The idea is that the application of $\hat{\mathsf{k}}\nabla_k$ or ∇_k on terms of the form

$$T_{V_1,|k|} \cdots T_{V_p,|k|} e_k, \qquad V_1, \ldots, V_p \in C_\mathsf{c}^\infty(\mathbb{R}^3),\ p \in \mathbb{N}, \tag{6.29}$$

yields again a linear combination of such terms multiplied with polynomials in x and k (see Lemma 6.12 and Lemma 6.13). We want to remember that the Born series terms can be written in the form (6.29). This procedure can be repeated multiple times and the resulting expressions can then be estimated with the stationary phase argument.

Lemma 6.12
Assume $V_1, \ldots, V_p \in C_\mathsf{c}^\infty(\mathbb{R}^3)$. Then we can write for all $k \in \mathbb{R}^3$,

$$k\nabla_k \left(T_{V_1,|k|} \cdots T_{V_p,|k|} e_k \right)$$

as a sum of

$$\mathrm{i}(k\hat{\mathsf{x}}) T_{V_1,|k|} \cdots T_{V_p,|k|} e_k, \tag{6.30}$$

where $\hat{\mathsf{x}}$ denotes the multiplication in x, and terms of the form

$$\sum_{l=1}^{p} Q T_{W_1,|k|} \cdots T_{W_l,|k|} e_k, \tag{6.31}$$

where Q denotes the multiplication in x with a polynomial of maximal degree one, and $W_l \in C_\mathsf{c}^\infty(\mathbb{R}^3)$, $l = 1, \ldots, p$.

Proof. Recall the formula (6.28) in Lemma 6.10,

$$(T_{V_1,|k|}\cdots T_{V_p,|k|}e_k)(x) = e^{\mathrm{i}kx}\int\left\{\prod_{l=1}^{p}\frac{e^{\mathrm{i}(|k||u_l|+ku_l)}}{|u_l|}V_l\left(x+\sum_{s=1}^{l}u_s\right)\right\}\mathrm{d}(u_1,\dots,u_p).$$

Differentiation with respect to the first factor on the right-hand side yields (6.30). Under the integral we use

$$\begin{aligned}k\nabla_k\prod_{l=1}^{p}\frac{e^{\mathrm{i}(ku_l+|k||u_l|)}}{|u_l|} &= \mathrm{i}\sum_{l'=1}^{p}(ku_{l'}+|k|\,|u_{l'}|)\prod_{l=1}^{p}\frac{e^{\mathrm{i}(ku_l+|k||u_l|)}}{|u_l|}\\ &= \sum_{l'=1}^{p}(u_{l'}\nabla_{u_{l'}}+1)\prod_{l=1}^{p}\frac{e^{\mathrm{i}(ku_l+|k||u_l|)}}{|u_l|}.\end{aligned}\tag{6.32}$$

We can now do integration by parts in (6.28) to shift the derivatives to the V_l terms. Any boundary terms vanish as we consider compactly supported functions. Thus, we arrive at

$$\begin{aligned}&k\nabla_k\int\left\{\prod_{l=1}^{p}\frac{e^{\mathrm{i}(|k||u_l|+ku_l)}}{|u_l|}V_l\left(x+\sum_{s=1}^{l}u_s\right)\right\}\mathrm{d}(u_1,\dots,u_p)\\ &= -\int\left\{\prod_{l=1}^{p}\frac{e^{\mathrm{i}(|k||u_l|+ku_l)}}{|u_l|}\right\}\sum_{l'=1}^{p}(u_{l'}\nabla_{u_{l'}}+2)\prod_{l=1}^{p}V_l\left(x+\sum_{s=1}^{l}u_s\right)\mathrm{d}(u_1,\dots,u_p)\\ &= -\int\left\{\prod_{l=1}^{p}\frac{e^{\mathrm{i}(|k||u_l|+ku_l)}}{|u_l|}\right\}\sum_{l'=1}^{p}\left\{\prod_{\substack{l=1\\ l\neq l'}}^{p}V_l\left(x+\sum_{s=1}^{l}u_s\right)\right\}\\ &\qquad\left(\sum_{s=1}^{l'}u_s\nabla+2\right)V_{l'}\left(x+\sum_{s=1}^{l'}u_s\right)\mathrm{d}(u_1,\dots,u_p),\end{aligned}$$

where the last equality follows by calculating the derivatives by means of the product and chain rule and by reordering the summation. Then we can write, with $W_{l'}(y) := y\nabla V_{l'}(y)$,

$$\left(\sum_{s=1}^{l'}u_s\nabla\right)V_{l'}\left(x+\sum_{s=1}^{l'}u_s\right) = W_{l'}\left(x+\sum_{s=1}^{l}u_s\right) - x\nabla V_{l'}\left(x+\sum_{s=1}^{l}u_s\right).$$

Since $W_{l'}$ and the derivatives of $V_{l'}$ are again in $C_{\mathrm{c}}^{\infty}(\mathbb{R}^3)$ for all l', we obtain expressions of the form (6.31). □

Lemma 6.13
Let $p \in \mathbb{N}$. Assume that $V_1, \dots, V_p \in C_{\mathsf{c}}^\infty(\mathbb{R}^3)$, $n_1, \dots, n_p \in \mathbb{N}_0$. Then for $j \in \{1,2,3\}$, $k \neq 0$,

$$\partial_{k_j}\left(T_{V_1,|k|}^{(n_1)} \cdots T_{V_p,|k|}^{(n_p)} e_k\right) = \mathrm{i} T_{V_1,|k|}^{(n_1)} \cdots T_{\hat{\mathsf{x}}_j V_p,|k|}^{(n_p)} e_k + \mathrm{i}\frac{k_j}{|k|}\sum_{i=1}^p X_1^{(i)} \cdots X_p^{(i)} e_k,$$

$$\hat{D}_k\left(T_{V_1,|k|}^{(n_1)} \cdots T_{V_p,|k|}^{(n_p)} e_k\right) = \mathrm{i} T_{V_1,|k|}^{(n_1)} \cdots T_{\frac{k\hat{\mathsf{x}}}{|k|} V_p,|k|}^{(n_p)} e_k + \mathrm{i}\sum_{i=1}^p X_1^{(i)} \cdots X_p^{(i)} e_k,$$

and

$$X_l^{(i)} := \begin{cases} T_{V_l,|k|}^{(n_l)}, & i \neq l, \\ T_{V_l,|k|}^{(n_l+1)}, & i = l. \end{cases}$$

Proof. This follows by direct computation of the derivative by means of the product rule of the expression (6.28). □

Finally, we use the previous estimates for the following two propositions. Note that we generalize the notation of the inner product on $L^2(\mathbb{R}^3)$ by setting $\langle f, g\rangle := \int_{\mathbb{R}^3} \overline{f(x)} g(x) \mathrm{d}x$ if f and g are measurable functions and $fg \in L^1(\mathbb{R}^3)$.

Proposition 6.14
For all $s \in \mathbb{N}_0$, $p, m, n \in \mathbb{N}$, $X \in \{\mathrm{Id}, \nabla_k, \nabla_{k'}\}$, $Y \in \{\hat{\mathsf{k}}\nabla_k + \hat{\mathsf{k}}'\nabla_k', \eta(\hat{\mathsf{k}})\hat{\mathsf{k}}\nabla_k\}$, where $\eta \in \mathcal{S}(\mathbb{R}^3)$, there are constants $n_1, n_2 \in \mathbb{N}$, C, such that for all $k, k' \neq 0$, $\chi \in \mathcal{S}(\mathbb{R}^3)$,

$$\left|XY^s\left\langle \phi_0^{(p)}(k,\cdot), \chi\phi_0^{(m)}(k',\cdot)\right\rangle\right| \leq \frac{C}{1+|k-k'|^n} \sup_{|\alpha|\leq n_1} \left\|\langle\cdot\rangle^{n_2} \partial_x^\alpha \chi\right\|_1.$$

Proof. First, let $Y = \hat{\mathsf{k}}\nabla_k + \hat{\mathsf{k}}'\nabla_k'$. Using an induction argument in s we obtain from Lemma 6.12 that we can write

$$(\hat{\mathsf{k}}\nabla_k + \hat{\mathsf{k}}'\nabla_k')^s \left\langle \phi_0^{(p)}(k,\cdot), \chi\phi_0^{(m)}(k',\cdot)\right\rangle$$

as linear combination of terms of the form

$$(k-k')^\alpha \left\langle T_{V_1,|k|} \cdots T_{V_p,|k|} e_k, P\chi T_{W_1,|k'|} \cdots T_{W_m,|k'|} e_{k'}\right\rangle, \tag{6.33}$$

for some polynomial P, multi-index α, $V_1, \dots, V_p$, $W_1, \dots, W_m \in C_{\mathsf{c}}^\infty(\mathbb{R}^3)$. Then we obtain the desired estimate for $X = \mathrm{Id}$ by the stationary phase argument of Lemma 6.11, which can be seen using (6.28) and observing that χ is a Schwartz function and that the potential V has compact support. For $X \in \{\nabla_k, \nabla_{k'}\}$ we apply Lemma 6.13 to the expressions in (6.33), with the result that we can write

$$X(\hat{\mathsf{k}}\nabla_k + \hat{\mathsf{k}}'\nabla'_k)^s \left\langle \phi_0^{(p)}(k,\cdot), \chi\phi_0^{(m)}(k',\cdot)\right\rangle$$

for $k, k' \neq 0$ as linear combinations of terms

$$(k-k')^\alpha f(k,k') \left\langle T^{(n_1)}_{V_1,|k|}\cdots T^{(n_p)}_{V_p,|k|}e_k, P\chi T^{(n'_1)}_{W_1,|k'|}\cdots T^{(n'_m)}_{W_m,|k'|}e_{k'}\right\rangle,$$

with a bounded function f on $\mathbb{R}^3\times\mathbb{R}^3$ and $n_1+\ldots+n_p, n'_1+\ldots+n'_m \in \{0,1\}$. The desired estimate in this case follows now from the same stationary phase argument using (6.28) as before. Finally, for $Y = \eta(\hat{\mathsf{k}})\hat{\mathsf{k}}\nabla_k$ one proceeds similarly but now using only Lemma 6.13. □

Proposition 6.15
For all $s \in \mathbb{N}_0$, $p, n \in \mathbb{N}$, there exist constants $n_1, n_2 \in \mathbb{N}$, C, such that for all k, $X \in \{\mathrm{Id}, \nabla_k\}$, and $\chi \in \mathcal{S}(\mathbb{R}^3)$ we have

$$\left|X(\hat{\mathsf{k}}\nabla_k)^s \left\langle \phi_0^{(p)}(k,\cdot), \chi\right\rangle\right| \leq \frac{C}{1+|k|^n} \sup_{|\alpha|\leq n_1} \left\|\langle\cdot\rangle^{n_2}\,\partial_x^\alpha\chi\right\|_1.$$

Proof. Analogously to the proof of Proposition 6.14 the inductive application of Lemma 6.12 yields that

$$(\hat{\mathsf{k}}\nabla_k)^s \left\langle \phi_0^{(p)}(k,\cdot), \chi\right\rangle$$

can be written as

$$k^\alpha \left\langle T_{V_1,|k|}\cdots T_{V_p,|k|}e_k, P\chi\right\rangle, \tag{6.34}$$

for some polynomial P, multi-index α, $V_1, \ldots, V_p \in C_{\mathsf{c}}^\infty(\mathbb{R}^3)$. Then after inserting (6.28) and using Lemma 6.13 with $X = \nabla_k$, the stationary phase argument again yields the desired estimate. □

6.4.3. Estimates of the Remainder Terms

Now we prove arbitrarily fast polynomial decay for the remainder terms of sufficiently high order. We obtain results for remainder terms in Proposition 6.18 and scalar products of Born series terms with remainder terms in Proposition 6.20. The main tool will be the following lemma, where the basic idea is due to Klein and Zemach (cf. [ZK58]). It essentially follows from a stationary phase argument together with a suitable coordinate transformation.

Lemma 6.16
For $W \in C_c^\infty(\mathbb{R}^3)$, $n_1, n_2 \in \mathbb{N}_0$, such that $\operatorname{supp} W \subseteq B_R(0)$, there exists a constant C such that for all $\kappa \geq 0$,

$$\sup_{|x|,|x'|\leq R} \left| \int \frac{e^{\mathrm{i}\kappa|x-y|}}{|x-y|^{1-n_1}} W(y) \frac{e^{\mathrm{i}\kappa|x'-y|}}{|x'-y|^{1-n_2}} \mathrm{d}y \right| \leq \frac{C}{1+\kappa}. \tag{6.35}$$

Proof. For the proof we use Prolate Spheroidal coordinates, see [ZK58, appendix] and [MF53, p. 661]. By continuity it suffices to consider the case $x \neq x'$.

Let $D = \frac{1}{2}|x - x'|$. For

$$\xi \in [D, \infty), \qquad \eta \in [-1, 1], \qquad \varphi \in [0, 2\pi)$$

we set

$$\Phi(\xi, \eta, \varphi) := \frac{1}{2}(x + x') + \mathcal{R} \begin{pmatrix} \sqrt{(\xi^2 - D^2)(1-\eta^2)} \cos\varphi \\ \sqrt{(\xi^2 - D^2)(1-\eta^2)} \sin\varphi \\ \xi\eta \end{pmatrix},$$

where $\mathcal{R}$ is the rotation matrix transforming e_3 into $\frac{x-x'}{|x-x'|}$. A straightforward computation then shows that

$$\begin{aligned} \xi &= \frac{1}{2}\left(|x - \Phi(\xi,\eta,\varphi)| + |x' - \Phi(\xi,\eta,\varphi)|\right), \\ \eta &= \frac{1}{2D}\left(|x - \Phi(\xi,\eta,\varphi)| - |x' - \Phi(\xi,\eta,\varphi)|\right), \\ &\det \Phi(\xi,\eta,\varphi) = (\xi + D\eta)(\xi - D\eta). \end{aligned}$$

Thus, by change of coordinates,

$$\begin{aligned} \int \frac{e^{\mathrm{i}\kappa|x-y|} W(y) e^{\mathrm{i}\kappa|x'-y|}}{|x-y|^{1-n_1} |x'-y|^{1-n_2}} \mathrm{d}y &= \int e^{2\mathrm{i}\kappa\xi} W(\Phi(\xi,\eta,\varphi))(\xi + D\eta)^{n_1}(\xi - D\eta)^{n_2} \mathrm{d}(\xi,\eta,\varphi) \\ &= \int_D^\infty e^{2\mathrm{i}\kappa\xi} h(\xi) \mathrm{d}\xi, \end{aligned}$$

where $h(\xi) := \int W(\Phi(\xi,\eta,\varphi))(\xi + D\eta)^{n_1}(\xi - D\eta)^{n_2} \mathrm{d}(\eta,\varphi)$. Let $E := \frac{1}{2}|x + x'|$. Notice that by direct computation, for $\xi \geq D + E$,

$$|\Phi(\xi,\eta,\varphi)| \geq \xi - D - E.$$

Thus, we get that $h(\xi) = 0$ for $\xi \geq R + D + E$. Then, by integration by parts,

$$\begin{aligned} \int_D^\infty e^{2\mathrm{i}\kappa\xi} h(\xi) \mathrm{d}\xi &= \frac{1}{2\mathrm{i}\kappa} \int_D^{R+D+E} \partial_\xi \left(e^{2\mathrm{i}\kappa\xi}\right) h(\xi) \mathrm{d}\xi \\ &= \frac{1}{2\mathrm{i}\kappa} \bigg(- h(D) e^{2\mathrm{i}\kappa D} - \int_D^{R+D+E} e^{2\mathrm{i}\kappa\xi} \partial_\xi h(\xi) \mathrm{d}\xi \bigg). \end{aligned}$$

As $D, E \leq R$ are bounded, so is the first term. For the second one notice that

$$\partial_\xi h(\xi) = \int \langle \nabla W(\Phi(\xi,\eta,\varphi)), \partial_\xi \Phi(\xi,\eta,\varphi)\rangle (\xi + D\eta)^{n_1}(\xi - D\eta)^{n_2} \mathrm{d}(\eta,\varphi) \tag{6.36}$$

$$+ \int W(\Phi(\xi,\eta,\varphi))\partial_\xi((\xi + D\eta)^{n_1}(\xi - D\eta)^{n_2})\mathrm{d}(\eta,\varphi). \tag{6.37}$$

The term (6.37) is clearly bounded by a constant depending only on R. The term (6.36) is bounded up to a constant by

$$\sup_{\eta,\varphi} |\partial_\xi \Phi(\xi,\eta,\varphi)| \leq C\left(1 + \frac{\xi}{\sqrt{\xi^2 - D^2}}\right),$$

for some $C > 0$. This is integrable and the integral is also bounded by a constant only depending on R:

$$\int_D^{R+D+E} \frac{\xi}{\sqrt{\xi^2 - D^2}}\mathrm{d}\xi = \sqrt{(R + D + E)^2 - D^2}. \qquad \square$$

The Klein-Zemach method of Lemma 6.16 shows that compositions of sufficiently many operators $T^{(n)}_{V,|k|}$, $n \geq 0$, exhibit an arbitrary large decay in k, see the following lemma. This will be used in Proposition 6.18 to prove the decay in k for the remainder terms.

Lemma 6.17
Let $p \in \mathbb{N}$, $V_1, \ldots, V_p \in C^\infty_{\mathsf{c}}(\mathbb{R}^3)$ and $n_1, \ldots, n_p \in \mathbb{N}_0$. Then there exists a constant C such that for all $k, x \in \mathbb{R}^3$ and $\psi \in C_{\mathsf{b}}(\mathbb{R}^3)$,

$$\left|(T^{(n_1)}_{V_1,|k|} \cdots T^{(n_p)}_{V_p,|k|}\psi)(x)\right| \leq \frac{C(1 + \langle x\rangle^{n_1 - 1})\,\|\psi\|_\infty}{1 + |k|^{\lfloor \frac{p-1}{2}\rfloor}}.$$

Proof. First we assume that $p = 2p^* + 1$. Then by Lemma 6.10

$$(T^{(n_1)}_{V_1,|k|} \cdots T^{(n_p)}_{V_p,|k|}\psi)(x)$$

$$= \int \frac{e^{\mathrm{i}|k||x-y_1|}}{|x - y_1|^{1-n_1}} V_1(y_1) \tag{6.38}$$

$$\left\{\prod_{l=1}^{p^*} \frac{e^{\mathrm{i}|k||y_{2l-1}-y_{2l}|}}{|y_{2l-1} - y_{2l}|^{1-n_{2l}}} V_{2l}(y_{2l}) \frac{e^{\mathrm{i}|k||y_{2l}-y_{2l+1}|}}{|y_{2l} - y_{2l+1}|^{1-n_{2l+1}}} V_{2l+1}(y_{2l+1})\right\} \tag{6.39}$$

$$\psi(y_p)\mathrm{d}(y_1, y_2, y_3, \ldots, y_p).$$

In the following let C denote different constants depending only on V_l and n_l, $l = 1, \dots, p$. We estimate the terms in (6.39) for $l = 1, \dots, p^*$ by

$$\left| \int \frac{e^{\mathrm{i}|k||y_{2l-1}-y_{2l}|}}{|y_{2l-1} - y_{2l}|^{1-n_{2l}}} V_{2l}(y_{2l}) \frac{e^{\mathrm{i}|k||y_{2l}-y_{2l+1}|}}{|y_{2l} - y_{2l+1}|^{1-n_{2l+1}}} \mathrm{d}y_{2l} \right| \leq \frac{C}{1 + |k|}$$

using Lemma 6.16, the term (6.38) by

$$\left| \int \frac{e^{\mathrm{i}|k||x-y_1|}}{|x - y_1|^{1-n_1}} V_1(y_1) \mathrm{d}y_1 \right| \leq C(1 + \langle x \rangle^{n_1-1}),$$

and thus we find

$$\begin{aligned} &\left|(T^{(n_1)}_{V_1,|k|} \cdots T^{(n_p)}_{V_p,|k|} \psi)(x)\right| \\ &\quad \leq \frac{C(1 + \langle x \rangle^{n_1-1})}{(1 + |k|)^{p^*}} \int \left\{ \prod_{l=0}^{p^*-1} |V_{2l+2}(y_{2l+2})| \right\} \psi(y_p) \mathrm{d}(y_2, y_4, \dots, y_p) \\ &\quad \leq \frac{C(1 + \langle x \rangle^{n_1-1}) \, \|\psi\|_\infty}{(1 + |k|)^{p^*}}. \end{aligned}$$

In case p is even, we estimate the first $p - 1$ factors as in the odd case and the remaining expression we estimate using Proposition 6.8, which implies that there is a constant C independent of k such that $\| \mathbb{1}_{\operatorname{supp} V_{p-1}} T^{(n_p)}_{V_p,|k|} \psi \|_\infty \leq C \|\psi\|_\infty$. □

Proposition 6.18
Let $n \in \mathbb{N}_0$, $m \in \{0, 1\}$ and $j \in \{1, 2, 3\}$.

(a) For all $k \neq 0$, the expression

$$\partial^m_{k_j} \hat{D}^n_k T_{V,|k|} \cdots T_{V,|k|} \phi(k, \cdot)$$

can be written as linear combination of terms

$$f(k) T^{(n_1)}_{V,|k|} \cdots T^{(n_p)}_{V,|k|} \partial^{m'}_{k_j} \hat{D}^{n'}_k \phi(k, \cdot), \tag{6.40}$$

where f is a bounded function on $\mathbb{R}^3 \setminus \{0\}$, $0 \leq n' \leq n$, $0 \leq m' \leq m$, and $n_1 + \cdots + n_p + m' + n' = m + n$.

(b) For any $p \in \mathbb{N}$, there exists a constant C such that we have for all $k \neq 0$ and $x \in \mathbb{R}^3$,

$$\left| \partial^m_{k_j} \hat{D}^n_k \phi^{(p)}_{\mathsf{R}}(k, x) \right| \leq \frac{C(1 + \langle x \rangle^{n+m-1})}{1 + |k|^{\lfloor \frac{p-1}{2} \rfloor}}.$$

Proof. Part (a) follows by the product rule from Lemma 6.10. Part (b) is a result of (a), Lemma 6.17, Proposition 6.6, and the fact that V has compact support. □

When the Born series expansion is applied in products of the interaction with scattering functions, one faces mixed terms of possibly lower-order Born series terms with remainder terms of arbitrary high order. In this case one cannot only use Proposition 6.18. However, one can shift the decay of the higher-order terms to the lower-order terms by means of integration by parts. This is the idea behind the following lemma.

Lemma 6.19
"ca *Let $p, m, r \in \mathbb{N}$ with $m \geq 3r+1$, $V_1, \dots, V_p$, $W_1, \dots, W_m \in C_{\mathsf{c}}^\infty(\mathbb{R}^3)$, and $n_1, \dots, n_p$, $n'_1, \dots, n'_m \in \mathbb{N}_0$. Suppose that $\operatorname{supp} V_l \subseteq B_R(0)$ and $\operatorname{supp} W_l \subseteq B_R(0)$ for all l. Then there exists a constant C, $n_0 \in \mathbb{N}_0$, such that for all k, k', $\psi \in C_{\mathsf{poly}}(\mathbb{R}^3)$ and $\chi \in \mathcal{S}(\mathbb{R}^3)$,*

$$\begin{aligned} &\left|\left\langle T^{(n_1)}_{V_1,|k|} \cdots T^{(n_p)}_{V_p,|k|} e_k, \chi T^{(n'_1)}_{W_1,|k'|} \cdots T^{(n'_m)}_{W_m,|k'|} \psi \right\rangle\right| \\ &\qquad \leq \frac{C \sup_{|\alpha| \leq r} \|(1+\langle\cdot\rangle^{n_0})\partial^\alpha \chi\|_1 \left\|\mathbb{1}_{B_R(0)}\psi\right\|_\infty}{(1+|k|^{\lfloor \frac{p-1}{2}\rfloor + r})(1+|k'|^{\lfloor \frac{m-1-r}{2}\rfloor - r})}. \end{aligned} \tag{6.41}$$

Proof. We will show that for all $n \in \mathbb{N}_0$ and $j \in \{1,2,3\}$,

$$k_j^n \left\langle T^{(n_1)}_{V_1,|k|} \cdots T^{(n_p)}_{V_p,|k|} e_k, \chi T^{(n'_1)}_{W_1,|k'|} \cdots T^{(n'_m)}_{W_m,|k'|} \psi \right\rangle \tag{6.42}$$

can be written as a linear combination of terms

$$|k'|^s \left\langle T^{(n_1)}_{\widetilde{V}_1,|k|} \cdots T^{(n_p)}_{\widetilde{V}_p,|k|} e_k, \partial^\alpha \chi T^{(n'_1)}_{\widetilde{W}_1,|k'|} \cdots T^{(n'_{m-n})}_{\widetilde{W}_{m-n},|k'|} \widetilde{\psi} \right\rangle, \tag{6.43}$$

where $0 \leq s \leq n$, $|\alpha| \leq n$, $\widetilde{V}_1, \dots, \widetilde{V}_p$, $\widetilde{W}_1, \dots, \widetilde{W}_m \in C_{\mathsf{c}}^\infty(\mathbb{R}^3)$ and $\widetilde{\psi} \in C_{\mathsf{poly}}(\mathbb{R}^3)$, which satisfies $\left|\widetilde{\psi}(x)\right| \leq P(|x|) \left\|\mathbb{1}_{B_R(0)}\psi\right\|_\infty$, $x \in \mathbb{R}^3$, for some polynomial P not depending on k, k', ψ, χ. Then the desired estimate (6.41) immediately follows from Lemma 6.17.

Now, we prove that (6.42) can be written as linear combination of terms of the form (6.43) by induction over n. For $n = 0$ this is clear, and for the induction step it suffices to show the claim for $n = 1$.

We have

$$
\begin{aligned}
&k\left\langle T^{(n_1)}_{V_1,|k|}\cdots T^{(n_p)}_{V_p,|k|}e_k, \chi T^{(n_1')}_{W_1,|k'|}\cdots T^{(n_m')}_{W_m,|k'|}\psi\right\rangle\\
&= \int \frac{e^{-\mathrm{i}|k||v_1|}}{|v_1|^{1-n_1}}V_1(v_1+x)\frac{e^{-\mathrm{i}|k||v_2|}}{|v_2|^{1-n_2}}V_2(v_2+v_1+x)\ldots\frac{e^{-\mathrm{i}|k||v_p|}}{|v_p|^{1-n_p}}V_p\left(\sum_{l=1}^p v_l+x\right)\\
&\qquad e^{-\mathrm{i}k\sum_{l=1}^p v_l}(\mathrm{i}\nabla_x e^{-\mathrm{i}kx})\chi(x)\frac{e^{\mathrm{i}|k'||x-x_1|}}{|x-x_1|^{1-n_1'}}W_1(x_1)\frac{e^{\mathrm{i}|k'||x_1-x_2|}}{|x_1-x_2|^{1-n_2'}}W_2(x_2)\\
&\qquad\ldots\frac{e^{\mathrm{i}|k'||x_{m-1}-x_m|}}{|x_{m-1}-x_m|^{1-n_m'}}W_m(x_m)\psi(x_m)\mathrm{d}(v_1,\ldots,v_p,x,x_1,\ldots,x_m).
\end{aligned}
$$

We now use integration by parts with respect to x. By the product rule, we have a linear combination of several different terms. The ones with derivatives of the potentials $V_1,\ldots,V_p$ and χ yield terms of the form (6.43) with $s=0$, $m=0$ and $\widetilde{\psi}=\psi$. For the last term containing x we have

$$\nabla_x\frac{e^{\mathrm{i}|k'||x-x_1|}}{|x-x_1|^{1-n_1'}} = \nabla_{x_1}\frac{e^{\mathrm{i}|k'||x-x_1|}}{|x-x_1|^{1-n_1'}}.$$

Then we use again partial integration and get a term involving ∇W_1, which can be written as the former terms involving the derivatives of the V's, and

$$\nabla_{x_1}\frac{e^{\mathrm{i}|k'||x_1-x_2|}}{|x_1-x_2|^{1-n_2'}}.$$

Repeating this trick we obtain expressions with derivatives of the W's and finally the term where we take the derivative of the last fraction,

$$\nabla_{x_{m-1}}\frac{e^{\mathrm{i}|k'||x_{m-1}-x_m|}}{|x_{m-1}-x_m|^{1-n_m'}} = K(x_{m-1},x_m)\frac{x_{m-1}-x_m}{|x_{m-1}-x_m|},$$

where

$$K(x_{m-1},x_m) := \frac{e^{\mathrm{i}|k'||x_{m-1}-x_m|}}{|x_{m-1}-x_m|^{1-n_m'}}\left(\mathrm{i}\,|k'|+\frac{n_m'-1}{|x_{m-1}-x_m|}\right).$$

The integral operator corresponding to $(x_{m-1},x_m)\mapsto K(x_{m-1},x_m)W_m(x_m)$ can be expressed as

$$\mathrm{i}\,|k'|\,T_{W_m,|k'|}+(n_m'-1)T^{(n_m'-1)}_{W_m,|k'|}.$$

Accordingly, consider $\widetilde{\psi}_1 := T_{W_m,|k'|}\psi$ and $\widetilde{\psi}_2 := T^{(n_m'-1)}_{W_m,|k'|}\psi$. Then for $i=1,2$, $\widetilde{\psi}_i\in C_{\mathsf{poly}}(\mathbb{R}^3)$ and there is a polynomial P independent of ψ and k,k' such that $\left|\widetilde{\psi}_i(x)\right|\le P(|x|)\left\|\mathbb{1}_{B_R(0)}\psi\right\|_\infty$ holds for all $x\in\mathbb{R}^3$ due to Proposition 6.8. This shows the induction hypothesis for $n=1$ and finishes the proof. $\square$

Proposition 6.20
Let $s \in \mathbb{N}_0$, $n \in \mathbb{N}$, $\eta \in \mathcal{S}(\mathbb{R}^3)$, $X \in \{\mathrm{Id}, \nabla_k, \nabla_{k'}\}$, $Y \in \{\hat{\mathsf{k}}\nabla_k + \hat{\mathsf{k}}'\nabla'_k, \eta(\hat{\mathsf{k}})\hat{\mathsf{k}}\nabla_k\}$. Then there exists a constant $m_0 \in \mathbb{N}$, such for all $m \geq m_0$ and $p \in \mathbb{N}$, there are $n_1, n_2 \in \mathbb{N}$, C, such that for all $\chi \in \mathcal{S}(\mathbb{R}^3)$, $k, k' \neq 0$,

$$\left|XY^s \left\langle \phi_0^{(p)}(k,\cdot), \chi\phi_{\mathsf{R}}^{(m)}(k',\cdot)\right\rangle\right| \leq \frac{C \sup_{|\alpha|\leq n_1} \left\| \langle\cdot\rangle^{n_2} \partial^\alpha \chi \right\|_1}{(1+|k|^n)(1+|k'|^n)}.$$

Proof. By applying Lemma 6.13 and (6.40) for the left and right part of the inner product, respectively, we can write

$$XY^s \left\langle \phi_0^{(p)}(k,\cdot), \chi\phi_{\mathsf{R}}^{(m)}(k',\cdot)\right\rangle$$

for all given X, Y and s as a linear combination of expressions

$$k^\alpha (k')^\beta f(k,k') \left\langle T^{(n_1)}_{V_1,|k|} \cdots T^{(n_p)}_{V_p,|k|} e_k, \chi T^{(n'_1)}_{W_1,|k'|} \cdots T^{(n'_m)}_{W_m,|k'|} \phi(k',\cdot)\right\rangle,$$

where α, β are multi-indices with $|\alpha|, |\beta| \leq s$, f is a bounded function on $\mathbb{R}^3 \times \mathbb{R}^3$, $V_1, \ldots, V_p$, $W_1, \ldots, W_m \in C^\infty_{\mathsf{c}}(\mathbb{R}^3)$, and $n_1, \ldots, n_p$, $n'_1, \ldots, n'_m \in \mathbb{N}_0$. Now we can estimate these expressions with Lemma 6.19. $\square$

6.4.4. Commutator with the Interaction

This part provides the key for the proof of Proposition 6.2. In the following we omit for the moment the regularity function κ of the coupling and work with multiplication operators $H(\omega, \Sigma)$, $(\omega, \Sigma) \in \mathbb{R}_+ \times \mathbb{S}^2$. Throughout this section we shall always assume

$$H(\omega,\Sigma)(x) = \chi(x)\tilde{H}(\omega,\Sigma)(x) \tag{6.44}$$

where $\chi \in \mathcal{S}(\mathbb{R}^3)$ and $\tilde{H}$ is a function on $I \times \mathbb{S}^2 \times \mathbb{R}^3$, with $I = (0,\infty)$ or $I = [0,\infty)$, such that for some $s \in \mathbb{N}_0$ the following holds.

(J_s) For all $n \in \{0, \ldots, s\}$ and $\alpha \in \mathbb{N}_0^3$ the partial derivatives $\partial_x^\alpha \partial_\omega^n \tilde{H}$ exist and are continuous on $I \times \mathbb{S}^2 \times \mathbb{R}^3$, and there exists a polynomial P and $M \in \mathbb{N}_0$ such that

$$\left|\partial_x^\alpha \partial_\omega^n \tilde{H}(\omega,\Sigma)(x)\right| \leq P(\omega)\langle x\rangle^M, \qquad (\omega,\Sigma,x) \in I \times \mathbb{S}^2 \times \mathbb{R}^3.$$

To show that a commutator $[T, A_{\mathrm{p}}^{(\epsilon)}]$, for a bounded operator T on $L^2(\mathbb{R}^3)$, is bounded, we shall make of use the following decomposition on $\ell^2(N) \oplus L^2(\mathbb{R}^3)$,

$$\mathcal{V}[T, A_{\mathrm{p}}^{(\epsilon)}]\mathcal{V}^* = \begin{pmatrix} 0 & V_{\mathsf{d}} T V_{\mathsf{c}}^* \eta_\epsilon(-A_{\mathsf{D}})\eta_\epsilon \\ -\eta_\epsilon(-A_{\mathsf{D}})\eta_\epsilon V_{\mathsf{c}} T V_{\mathsf{d}}^* & [V_{\mathsf{c}} T V_{\mathsf{c}}^*, \eta_\epsilon(-A_{\mathsf{D}})\eta_\epsilon] \end{pmatrix},$$

where $\mathcal{V}$ is the unitary operator defined in (6.5) and $N \in \mathbb{N}$ is the number of linearly independent eigenfunctions of H_{p}. We treat the off-diagonal terms in Proposition 6.21 and the term on the diagonal in Lemma 6.24.

Proposition 6.21
Suppose $\tilde{H}$ satisfies (J₀). Then for all $n \in \mathbb{N}_0$, $j \in \{1,2,3\}$, (ω, Σ), the operators

(1) $(-A_{\mathsf{D}})^n V_{\mathsf{c}} H(\omega, \Sigma) P_{\mathrm{disc}}$,

(2) $\hat{\mathsf{k}}_j (-A_{\mathsf{D}})^n V_{\mathsf{c}} H(\omega, \Sigma) P_{\mathrm{disc}}$,

(3) $\hat{\mathsf{q}}_j (-A_{\mathsf{D}})^n V_{\mathsf{c}} H(\omega, \Sigma) P_{\mathrm{disc}}$,

are well-defined, their norms can be estimated uniformly in Σ by a polynomial in ω, and they are continuous in (ω, Σ). Furthermore, if $\tilde{H}$ satisfies (J_s), then (1)–(3) are s times continuously differentiable with respect to ω in the operator norm topology and

$$\begin{aligned}
\partial_\omega^s (-A_{\mathsf{D}})^n V_{\mathsf{c}} H(\omega, \Sigma) P_{\mathrm{disc}} &= (-A_{\mathsf{D}})^n V_{\mathsf{c}} \partial_\omega^s H(\omega, \Sigma) P_{\mathrm{disc}}, \\
\partial_\omega^s \hat{\mathsf{k}}_j (-A_{\mathsf{D}})^n V_{\mathsf{c}} H(\omega, \Sigma) P_{\mathrm{disc}} &= \hat{\mathsf{k}}_j (-A_{\mathsf{D}})^n V_{\mathsf{c}} \partial_\omega^s H(\omega, \Sigma) P_{\mathrm{disc}}, \\
\partial_\omega^s \hat{\mathsf{q}}_j (-A_{\mathsf{D}})^n V_{\mathsf{c}} H(\omega, \Sigma) P_{\mathrm{disc}} &= \hat{\mathsf{q}}_j (-A_{\mathsf{D}})^n V_{\mathsf{c}} \partial_\omega^s H(\omega, \Sigma) P_{\mathrm{disc}}.
\end{aligned}$$

Proof. Let $m \in \{0,1\}$ and $n \in \mathbb{N}_0$. Choose N big enough so that we find by means of Proposition 6.18 a constant C and an $n_0 \in \mathbb{N}_0$ such that

$$\left| \int \partial_{k_j}^m \hat{D}_k^n \phi_{\mathsf{R}}^{(N)}(k,x) f(x) \psi_{\mathrm{d}}(x) \mathrm{d}x \right| \le \frac{C \|\langle\cdot\rangle^{n_0} f\| \, \|\psi_{\mathrm{d}}\|}{1 + |k|^6} \tag{6.45}$$

for all $f \in \mathcal{S}(\mathbb{R}^3)$, $\psi_{\mathrm{d}} \in \operatorname{ran} P_{\mathrm{disc}}$ and $k \neq 0$. Expanding $\phi(k,x)$ using Proposition 6.9 we obtain for $\psi_{\mathrm{d}} \in \operatorname{ran} P_{\mathrm{disc}}$, $k \neq 0$,

$$\begin{aligned}
V_{\mathsf{c}} H(\omega, \Sigma) \psi_{\mathrm{d}}(k) &= (2\pi)^{-3/2} \int \overline{\phi(k,x)} H(\omega, \Sigma)(x) \psi_{\mathrm{d}}(x) \mathrm{d}x \\
&= T_0(\omega, \Sigma, k) + T_{\mathsf{R}}(\omega, \Sigma, k),
\end{aligned} \tag{6.46}$$

where

$$T_0(\omega,\Sigma;k) := (2\pi)^{-3/2}\sum_{l=0}^{N-1}\int \overline{\phi_0^{(l)}(k,x)}H(\omega,\Sigma)(x)\psi_{\mathrm{d}}(x)\mathrm{d}x, \tag{6.47}$$

$$T_{\mathsf{R}}(\omega,\Sigma;k) := (2\pi)^{-3/2}\int \overline{\phi_{\mathsf{R}}^{(N)}(k,x)}H(\omega,\Sigma)(x)\psi_{\mathrm{d}}(x)\mathrm{d}x. \tag{6.48}$$

The terms which appear if we apply $(-A_{\mathsf{D}})^n$, $\hat{\mathsf{k}}_j$, $\hat{\mathsf{q}}_j$, $n\in\mathbb{N}_0$, $j\in\{1,2,3\}$ to (6.47) can be estimated by means of Proposition 6.15 with the result that for some constant C and $n_1,n_2\in\mathbb{N}_0$,

$$\begin{aligned}&|(-A_{\mathsf{D}})^nT_0(\omega,\Sigma;k)|,\ |\hat{\mathsf{k}}_j(-A_{\mathsf{D}})^nT_0(\omega,\Sigma;k)|,\ |\hat{\mathsf{q}}_j(-A_{\mathsf{D}})^nT_0(\omega,\Sigma;k)|\\ &\quad\leq \frac{C\sup_{|\alpha|\leq n_1}\|\langle\cdot\rangle^{n_2}\,\partial_x^\alpha(H(\omega,\Sigma)\psi_{\mathrm{d}})\|_1}{1+|k|^2}\end{aligned} \tag{6.49}$$

for all (ω,Σ), $k\neq 0$, and $\psi_{\mathrm{d}}\in\operatorname{ran}P_{\mathrm{disc}}$. The terms coming from (6.48) can be estimated using (6.45) such that for some constant C and $n_1\in\mathbb{N}_0$,

$$\begin{aligned}&|(-A_{\mathsf{D}})^nT_{\mathsf{R}}(\omega,\Sigma;k)|,\ |\hat{\mathsf{k}}_j(-A_{\mathsf{D}})^nT_{\mathsf{R}}(\omega,\Sigma;k)|,\ |\hat{\mathsf{q}}_j(-A_{\mathsf{D}})^nT_{\mathsf{R}}(\omega,\Sigma;k)|\\ &\quad\leq \frac{C\|\,\langle\cdot\rangle^{n_1}\,H(\omega,\Sigma)\|\,\|\psi_{\mathrm{d}}\|}{1+|k|^2}\end{aligned} \tag{6.50}$$

for all (ω,Σ), $k\neq 0$, and $\psi_{\mathrm{d}}\in\operatorname{ran}P_{\mathrm{disc}}$. Now observe that by elliptic regularity (cf. [RS2, section IX.6]) we have $\psi_{\mathrm{d}}\in C^\infty(\mathbb{R}^3)$ and $\partial^\alpha\psi_{\mathrm{d}}\in L^2(\mathbb{R}^3)$ for all $\alpha\in\mathbb{N}_0^3$. Thus, as $\tilde{H}$ satisfies (J_0), it follows that for fixed ψ_{d} and H there exists a polynomial P and $n_1,n_2\in\mathbb{N}_0$ such that for all (ω,Σ),

$$\sup_{|\alpha|\leq n_1}\|\langle\cdot\rangle^{n_2}\,\partial_x^\alpha(H(\omega,\Sigma)\psi_{\mathrm{d}})\|_1\,,\ \|\langle\cdot\rangle^r H(\omega,\Sigma)\|\leq P(\omega),$$

using Cauchy-Schwarz and standard estimates involving Schwartz functions. Collecting esimates and using that the discrete spectrum is finite we see that the operators (1), (2) and (3) are well-defined and their norms can be estimated by a polynomial in ω. Continuity in (ω,Σ) with respect to the operator norm topology now follows from linearity, the bounds (6.49) and (6.50), and the fact that $\tilde{H}$ satisfies (J_0) (and again standard estimates involving Schwartz functions). If $s=1$, an analogous argument implies differentiability in ω with the derivative given by replacing H by $\partial_\omega H$. Now the claim for arbitrary s follows by induction. □

Lemma 6.22
Suppose $\tilde{H}$ satisfies (J_0). For all (ω,Σ) and $k,k'\in\mathbb{R}^3$, let

$$K_{\omega,\Sigma}[H](k,k') := \int\overline{\phi(k,x)}H(\omega,\Sigma)(x)\phi(k',x)\mathrm{d}x. \tag{6.51}$$

Then for all $Z \in \{\hat{\mathsf{k}}\nabla_k + \hat{\mathsf{k}}'\nabla'_k, \eta_1(\hat{\mathsf{k}})\hat{\mathsf{k}}\nabla_k + \eta_2(\hat{\mathsf{k}}) + \eta_1(\hat{\mathsf{k}}')\hat{\mathsf{k}}'\nabla_{\hat{\mathsf{k}}'} + \eta_2(\hat{\mathsf{k}}')\}$*, where* $\eta_1, \eta_2 \in \mathcal{S}(\mathbb{R}^3)$*,* $j \in \{1,2,3\}$*, and* $s \in \mathbb{N}_0$*, there exists a polynomial* P *such that the absolute values of*

(1) $Z^s K_{\omega,\Sigma}[H](k,k')$*,*

(2) $\partial_{k_j} Z^s K_{\omega,\Sigma}[H](k,k')$*,* $\partial_{k'_j} Z^s K_{\omega,\Sigma}[H](k,k')$*,*

(3) $(k_j - k'_j) Z^s K_{\omega,\Sigma}[H](k,k')$*,*

are bounded from above by

$$P(\omega)\left(\frac{1}{(1+|k|^2)(1+|k'|^2)} + \frac{1}{1+|k-k'|^4}\right) \tag{6.52}$$

for all (ω,Σ)*,* $k, k' \neq 0$ *. Furthermore the following is satisfied.*

(a) For fixed $k, k' \neq 0$*, the functions* $\mathbb{R}_+ \times \mathbb{S}^2 \to \mathbb{C}$ *mapping* (ω,Σ) *to the expressions (1)–(3), are continuous. If* $\tilde{H}$ *satisfies* (J_s)*, these functions are* s *times continuously differentiable in* ω *and the* s*-th partial derivative with respect to* ω *is obtained by replacing* H *by* $\partial_\omega^s H$*.*

(b) The integral kernels (1)–(3) define bounded operators in $L^2(\mathbb{R}^3)$ *whose norms are uniformly bounded in* Σ *by a polynomial in* ω*. With respect to the operator norm toplogy the following holds. These operators depend continuously on* (ω,Σ)*. If* $\tilde{H}$ *satisfies* (J_s)*, these operators are* s *times continuously differentiable in* ω *and the* s*-th partial derivative with respect to* ω *is obtained by replacing* H *by* $\partial_\omega^s H$*.*

Proof. Let $X \in \{\mathrm{Id}, \partial_{k_j}, \partial_{k'_j}, \hat{\mathsf{k}}_j - \hat{\mathsf{k}}'_j\}$. Assume first that

$$Y \in \{\hat{\mathsf{k}}\nabla_k + \hat{\mathsf{k}}'\nabla'_k, \eta_1(\hat{\mathsf{k}})\hat{\mathsf{k}}\nabla_k\}.$$

Fix $s \in \mathbb{N}_0$. Using Proposition 6.9 we write for $N \in \mathbb{N}$,

$$\begin{aligned}
K_{\omega,\Sigma}[H](k,k') &= \int \overline{\phi(k,x)} H(\omega,\Sigma)(x)\phi(k',x)\mathrm{d}x && (6.53)\\
&= \sum_{l,l'=0}^{N-1} \int \overline{\phi_0^{(l')}(k,x)} H(\omega,\Sigma)(x)\phi_0^{(l)}(k',x)\mathrm{d}x && (6.54)\\
&\quad + \sum_{l=0}^{N-1} \int \overline{\phi_{\mathsf{R}}^{(N)}(k,x)} H(\omega,\Sigma)(x)\phi_0^{(l)}(k',x)\mathrm{d}x && (6.55)\\
&\quad + \sum_{l=0}^{N-1} \int \overline{\phi_0^{(l)}(k,x)} H(\omega,\Sigma)(x)\phi_{\mathsf{R}}^{(N)}(k',x)\mathrm{d}x && (6.56)\\
&\quad + \int \overline{\phi_{\mathsf{R}}^{(N)}(k,x)} H(\omega,\Sigma)(x)\phi_{\mathsf{R}}^{(N)}(k',x)\mathrm{d}x. && (6.57)
\end{aligned}$$

By Proposition 6.20 we can choose N large enough such that there exist constants $n_1, n_2 \in \mathbb{N}$, C, such that for all $f \in \mathcal{S}(\mathbb{R}^3)$ and $k, k' \neq 0$, and $p = 1, \dots, N$,

$$\left| XY^s \left\langle \phi_0^{(p)}(k,\cdot), f\phi_{\mathsf{R}}^{(N)}(k',\cdot) \right\rangle \right| \leq \frac{C \sup_{|\alpha| \leq n_1} \|\langle\cdot\rangle^{n_2} \partial^\alpha f\|_1}{(1+|k|^2)(1+|k'|^2)}, \tag{6.58}$$

which implies that for all (ω, Σ),

$$|XY^s(6.55)|,\ |XY^s(6.56)| \leq \frac{C \sup_{|\alpha| \leq n_1} \|\langle\cdot\rangle^{n_2} \partial^\alpha H(\omega,\Sigma)\|_1}{(1+|k|^2)(1+|k'|^2)}. \tag{6.59}$$

Moreover, by Proposition 6.14 there are constants $n_1, n_2 \in \mathbb{N}$, C, such that for all $k, k' \neq 0$,

$$|XY^s(6.54)| \leq \frac{C \sup_{|\alpha| \leq n_1} \|\langle\cdot\rangle^{n_2} \partial_x^\alpha H(\omega,\Sigma)\|_1}{1+|k-k'|^4}. \tag{6.60}$$

Finally, using Proposition 6.18 we see, by possibly making N larger, that there exist constants $n_1 \in \mathbb{N}$ and C such that

$$|XY^s(6.57)| \ \leq \frac{C\|\langle\cdot\rangle^{n_1} H(\omega,\Sigma)\|_1}{(1+|k|^2)(1+|k'|^2)}. \tag{6.61}$$

On the other hand since $\tilde{H}$ satisfies (J_0) and $H = \chi\tilde{H}$, there exists for each $n_1 \in \mathbb{N}_0$ and $\alpha \in \mathbb{N}_0^3$ a polynomial P such that

$$\|\langle\cdot\rangle^{n_1} \partial_x^\alpha H(\omega,\Sigma))\|_1 \leq P(\omega), \qquad (\omega,\Sigma) \in \mathbb{R}_+ \times \mathbb{S}^2. \tag{6.62}$$

It follows as a consequence of (6.58)–(6.62) that

$$|XY^s K_{\omega,\Sigma}[H](k,k')| \leq \ \text{r.h.s. of } (6.52)\ . \tag{6.63}$$

This shows (1)–(3) in case $Z = \hat{\mathsf{k}}\nabla_k + \hat{\mathsf{k}}'\nabla_{k'}$. We note that $Y = \eta_1(\hat{\mathsf{k}})\hat{\mathsf{k}}\nabla_k$ will be used below.

Let us now assume

$$Z = \eta_1(\hat{\mathsf{k}})\hat{\mathsf{k}}\nabla_k + \eta_2(\hat{\mathsf{k}}) + \eta_1(\hat{\mathsf{k}}')\hat{\mathsf{k}}'\nabla_{k'} + \eta_2(\hat{\mathsf{k}}'). \tag{6.64}$$

To estimate derivatives acting on both sides of (6.53) we use Proposition 6.6, with the result that for all $r, r' \in \{0,1\}$ and $s, s' \in \mathbb{N}_0$ there exist $n_1 \in \mathbb{N}_0$ and C such that for all nonzero k, k',

$$|\partial_{k_j}^r (\hat{\mathsf{k}}\nabla_k)^s \partial_{k_j'}^{r'} (\hat{\mathsf{k}}'\nabla_{k'})^{s'} K_{\omega,\Sigma}[H](k,k')| \leq C\|\langle\cdot\rangle^{n_1} H(\omega,\Sigma)\|_1 \langle k\rangle^s \langle k'\rangle^{s'}. \tag{6.65}$$

To estimate the norm occurring on the right-hand side we shall use that for $\tilde{H}$ satisfying (J$_0$) and $n_1 \in \mathbb{N}_0$ there exists a polynomial P such that

$$\|\langle\cdot\rangle^{n_1} H(\omega,\Sigma)\|_1 \leq P(\omega). \tag{6.66}$$

Let $W(\hat{\mathsf{k}}) = \eta_1(\hat{\mathsf{k}})\hat{\mathsf{k}}\nabla_k + \eta_2(\hat{\mathsf{k}})$. Then by the binomial theorem

$$Z^n K_{\omega,\Sigma}[H](k,k') = \sum_{l=0}^{n} \binom{n}{l} W(k)^l W(k')^{n-l} K_{\omega,\Sigma}[H](k,k'). \tag{6.67}$$

We see, after commuting Schwartz functions to the left, that for each $l \geq 1$ there exist functions $\eta^{(l,s)}, \tilde{\eta}^{(l,s)} \in \mathcal{S}(\mathbb{R}^3)$, $0 \leq s \leq l$, such that

$$W(\hat{\mathsf{k}})^l = \sum_{s=0}^{l} \eta^{(l,s)}(\eta(\hat{\mathsf{k}})\hat{\mathsf{k}}\nabla_k)^s = \sum_{s=0}^{l} \tilde{\eta}^{(l,s)}(\hat{\mathsf{k}}\nabla_k)^s. \tag{6.68}$$

Let us first consider the terms in (6.67) for $l = 0$ and $l = n$. Using the first equality in (6.68) and (6.63) (as well as its adjoint) for $Y = \eta_1(\hat{\mathsf{k}})\hat{\mathsf{k}}\nabla_k$, we find

$$|XW^n(\hat{\mathsf{k}})K_{\omega,\Sigma}[H](k,k')|,\ |XW^n(\hat{\mathsf{k}}')K_{\omega,\Sigma}[H](k,k')| \leq \text{ r.h.s. of (6.52)} . \tag{6.69}$$

The terms in (6.67) for $l \in \{1,\dots,n-1\}$ are estimated using (6.65), the second equality in (6.68) controlling the growth in k and k', and finally (6.66). Thus we find with (6.69)

$$|XZ^n K_{\omega,\Sigma}[H](k,k')| \leq \text{ r.h.s. of (6.52)} .$$

This shows (1)–(3) in the case (6.64). It remains to prove (a) and (b).

(a) The continuity property in (ω,Σ) for fixed nonzero k, k' can be seen from the integral (6.53), using dominated convergence with the property that $\tilde{H}$ satisfies (J$_0$). For this purpose we note that the integrand contains a Schwartz function and that the derivatives of the scattering functions are bounded by polynomials, as shown in Proposition 6.6. If $s = 1$, we conclude analogously differentiability in ω, and furthermore, that the derivative is given by replacing H with $\partial_\omega H$. For arbitrary s the claim then follows by induction.

(b) We first note that operators with integral kernels satisfying the bound (6.52) are bounded by $P(\omega)$. To this end, observe that an integral operator T with integral kernel

$$t\colon \quad (k,k') \mapsto \frac{1}{(1+|k|^2)(1+|k'|^2)}$$

is Hilbert-Schmidt and its norm can be estimated by $\|T\| \leq \|t\|_2$, and that an operator S with integral kernel

$$(k, k') \mapsto \frac{1}{1 + |k - k'|^4} =: s(k - k')$$

is bounded by Young's inequality for convolutions: $\|S\psi\|_2 = \|s * \psi\|_2 \leq \|s\|_1 \|\psi\|_2$, $s \in L^1(\mathbb{R}^3)$, $\psi \in L^2(\mathbb{R}^3)$. In view of this, continuity in (ω, Σ) with respect to the operator norm topology now follows from linearity, the bounds (6.59)–(6.61) as well as (6.66), and the fact that $\tilde{H}$ satisfies (J_0) (and a standard estimate involving Schwartz functions). If $s = 1$, we analogously conclude differentiability in ω, and that the derivative is given by replacing H with $\partial_\omega H$. For arbitrary s the claim then follows by induction. □

Remark 6.23
We note that for the proof of the main theorem we will only use Part (b) of Lemma 6.22 and Part (a) will not be needed. We nevertheless included Part (a) in Lemma 6.22, since in principle we could work with a weaker topology.

In the following lemma we estimate the coupling functions first in scattering space.

Lemma 6.24
Suppose $\tilde{H}$ satisfies (J_0). Then for all $\epsilon \geq 0$, $n \in \mathbb{N}_0$, $j \in \{1, 2, 3\}$, (ω, Σ),

(1) $\mathrm{ad}^{(n)}_{\eta_\epsilon(-A_{\mathsf{D}})\eta_\epsilon}(V_{\mathsf{c}} H(\omega, \Sigma) V_{\mathsf{c}}^*)$,

(2) $\mathrm{ad}_{\hat{\mathsf{k}}_j}\left(\mathrm{ad}^{(n)}_{\eta_\epsilon(-A_{\mathsf{D}})\eta_\epsilon}(V_{\mathsf{c}} H(\omega, \Sigma) V_{\mathsf{c}}^*)\right)$,

(3) $\mathrm{ad}_{\hat{\mathsf{q}}_j}\left(\mathrm{ad}^{(n)}_{\eta_\epsilon(-A_{\mathsf{D}})\eta_\epsilon}(V_{\mathsf{c}} H(\omega, \Sigma) V_{\mathsf{c}}^*)\right)$,

(4) $\hat{\mathsf{q}}_j\, \mathrm{ad}^{(n)}_{-A_{\mathsf{D}}}(V_{\mathsf{c}} H(\omega, \Sigma) V_{\mathsf{c}}^*)$,

are well-defined bounded operators in $L^2(\mathbb{R}^3)$ and we can estimate their norms uniformly in Σ by a polynomial in ω. With respect to the operator norm topology the following holds. (1)–(4) are continuous $\mathcal{L}(L^2(\mathbb{R}^3))$-valued functions of (ω, Σ). Moreover if $\tilde{H}$ satisfies (J_s), then the functions (1)–(4) are s times continuously differentiable with respect to ω and the s-th partial derivative of (1)–(4) with respect to ω is obtained by replacing H by $\partial_\omega^s H$.

Proof. From Theorem 6.1 we see that for all (ω, Σ),

$$V_{\mathsf{c}} H(\omega, \Sigma) V_{\mathsf{c}}^* \psi(k) = (2\pi)^{-3} \int K_{\omega,\Sigma}[H](k, k')\psi(k')\mathrm{d}k',$$

with $K_{\omega,\Sigma}$ defined in (6.51). Thus the lemma follows directly from Lemma 6.22, observing that $\eta_\epsilon(-A_{\mathsf{D}})\eta_\epsilon = \frac{\mathrm{i}\eta_\epsilon^2(\hat{\mathsf{k}})}{2}\hat{\mathsf{k}}\nabla_k + \frac{\mathrm{i}\eta_\epsilon(\hat{\mathsf{k}})}{4}(2\hat{\mathsf{k}}\nabla_k\eta_\epsilon(\hat{\mathsf{k}}) + 3\eta_\epsilon(\hat{\mathsf{k}}))$. □

Let us now prove the central proposition of this section, which can be thought of as a preliminary version of Proposition 6.2 but without the cutoff function κ. For the proof we need the following auxiliary lemma.

Lemma 6.25
Let $\mathcal{H}_0$ and $\mathcal{H}_1$ be Hilbert spaces. Let B be a bounded operator in $\mathcal{H}_0$ and let $V_0\colon \mathcal{H}_0 \to \mathcal{H}_1$ be a partial isometry with $\operatorname{ran} V_0 = \mathcal{H}_1$. Let P be the orthogonal projection onto the kernel of V_0. Suppose A is a self-adjoint operator in $\mathcal{H}_1$ such that for all $j = 1, \dots, n$ the set $\operatorname{ran} V_0(V_0^* A V_0)^{j-1} BP$ is contained in the domain of A and the operators $\operatorname{ad}_A^{(j)}(V_0 B V_0^*)$ and $(V_0^* A V_0)^j BP$ are bounded. Then $\operatorname{ad}^{(n)}_{V_0^* A V_0}(B)$ is a bounded operator on $\mathcal{H}_0$ and

$$\operatorname{ad}^{(n)}_{V_0^* A V_0}(B) = V_0^* \operatorname{ad}_A^{(n)}(V_0 B V_0^*) V_0 + (\mathrm{i} V_0^* A V_0)^n BP + PB(-\mathrm{i} V_0^* A V_0)^n.$$

Proof. This follows by induction in n and a straightforward calculation. □

Proposition 6.26
Suppose $\tilde{H}$ satisfies (J_s). Then for all $\epsilon \geq 0$, $n \in \mathbb{N}_0$, $j \in \{1, 2, 3\}$, (ω, Σ) and $r = 0, \dots, s$ the operators

(1) $\partial_\omega^r \operatorname{ad}^{(n)}_{A_{\mathrm{p}}^{(\epsilon)}}(H(\omega, \Sigma))$,

(2) $\partial_\omega^r \operatorname{ad}_{V_{\mathsf{c}}^* \hat{\mathsf{k}}_j V_{\mathsf{c}}}\left(\operatorname{ad}^{(n)}_{A_{\mathrm{p}}^{(\epsilon)}}(H(\omega, \Sigma))\right)$,

(3) $\partial_\omega^r \operatorname{ad}_{V_{\mathsf{c}}^* \hat{\mathsf{q}}_j V_{\mathsf{c}}}\left(\operatorname{ad}^{(n)}_{A_{\mathrm{p}}^{(\epsilon)}}(H(\omega, \Sigma))\right)$,

(4) $\partial_\omega^r V_{\mathsf{c}}^* \hat{\mathsf{q}}_j V_{\mathsf{c}} \operatorname{ad}^{(n)}_{A_{\mathrm{p}}^{\mathrm{sr}}}(H(\omega, \Sigma))$ *and* $\partial_\omega^r \operatorname{ad}^{(n)}_{A_{\mathrm{p}}^{\mathrm{sr}}}(H(\omega, \Sigma)) V_{\mathsf{c}}^* \hat{\mathsf{q}}_j V_{\mathsf{c}}$,

where the derivative ∂_ω is understood with respect to the operator norm topology, are well-defined, bounded, and we can estimate their norms uniformly in Σ by a polynomial in ω. The operators (1)–(4) depend continuously on (ω, Σ) with respect to the operator norm topology.

Proof. Follows directly from Proposition 6.21, Lemma 6.24 and an application of Lemma 6.25, with $V_0 = V_{\mathrm{c}}$, $P = P_{\mathrm{disc}}$, $A = -A_{\mathsf{D}}$, and $B = H(\omega, \Sigma)$. □

Proof of Proposition 6.2. To show the proposition we will use Proposition 6.26 and Lemma 4.3. First we consider the case where (i) of Hypothesis B-SR (3) holds. Let $F, \tilde{F} \colon \mathbb{R}^3 \to \mathcal{L}(\mathcal{H}_{\mathrm{p}})$, where $F(\omega\Sigma) = \kappa(\omega)\tilde{F}(\omega\Sigma)$ and $\tilde{F}$ is one of the functions

$$\begin{aligned}&\mathrm{ad}^{(n)}_{A_{\mathrm{p}}^{(\epsilon)}}(\chi\tilde{G}(\cdot)),\ \mathrm{ad}_{V_{\mathsf{c}}^*\hat{\mathsf{k}}_j V_{\mathsf{c}}}\left(\mathrm{ad}^{(n)}_{A_{\mathrm{p}}^{(\epsilon)}}(\chi\tilde{G}(\cdot))\right),\ \mathrm{ad}_{V_{\mathsf{c}}^*\hat{\mathsf{q}}_j V_{\mathsf{c}}}\left(\mathrm{ad}^{(n)}_{A_{\mathrm{p}}^{(\epsilon)}}(\chi\tilde{G}(\cdot))\right),\\ &V_{\mathsf{c}}^*\hat{\mathsf{q}}_j V_{\mathsf{c}}\,\mathrm{ad}^{(n)}_{A_{\mathrm{p}}^{\mathrm{sr}}}(\chi\tilde{G}(\cdot)),\end{aligned} \tag{6.70}$$

for $j \in \{1,2,3\}$. Since Hypothesis B-SR (1) implies that $\tilde{G}$ satisfies (J_3) we find that the $\mathcal{L}(\mathcal{H}_{\mathrm{p}})$-valued functions (6.70) are well-defined by Proposition 6.26 as well as their first three partial derivatives with respect to $\omega \in \mathbb{R}_+$. From Leibniz' rule we find for $m \leq 3$,

$$\partial_\omega^m F(\omega\Sigma) = \sum_{l=0}^{m} \binom{m}{l} \partial_\omega^l \kappa(\omega)\partial_\omega^{m-l}\tilde{F}(\omega\Sigma). \tag{6.71}$$

By Proposition 6.26 there exists a polynomial P such that for all $l = 0, \dots, m$ and (ω, Σ),

$$\left\|\partial_\omega^{m-l}\tilde{F}(\omega\Sigma)\right\| \leq P(\omega). \tag{6.72}$$

Now Condition (2) of Lemma 4.3 holds for F by (6.72), (6.71) and Hypothesis B-SR (2). Condition (1) of Lemma 4.3 is seen to hold by (6.72), (6.71) and (i) of Hypothesis B-SR (3). Thus, by Lemma 4.3, the function $(u,\Sigma) \mapsto \partial_u^m \tau_\beta(F)(u,\Sigma)$ belongs to $L^2(\mathbb{R}\times\mathbb{S}^2, \mathcal{L}(\mathcal{H}_{\mathrm{p}}))$ for all $0 \leq m \leq 3$, and moreover (6.12) holds. Hence we have shown Proposition 6.2 in case (i) of Hypothesis B-SR (3) holds.

Let us now assume the case where (ii) of Hypothesis B-SR (3) holds. To this end, let $F_0 \colon \mathbb{R}^3 \longrightarrow \mathcal{L}(\mathcal{H}_{\mathrm{p}})$ and $\tilde{F}_0 \colon [0,\infty)\times\mathbb{S}^2 \to \mathcal{L}(\mathcal{H}_{\mathrm{p}})$ be measurable functions, where $F_0(\omega\Sigma) = \kappa_0(\omega)\tilde{F}_0(\omega,\Sigma)$ and $\tilde{F}_0$ is one of the functions

$$\begin{aligned}&\mathrm{ad}^{(n)}_{A_{\mathrm{p}}^{(\epsilon)}}(\chi\tilde{G}_0(\cdot)),\ \mathrm{ad}_{V_{\mathsf{c}}^*\hat{\mathsf{k}}_j V_{\mathsf{c}}}\left(\mathrm{ad}^{(n)}_{A_{\mathrm{p}}^{(\epsilon)}}(\chi\tilde{G}_0(\cdot))\right),\ \mathrm{ad}_{V_{\mathsf{c}}^*\hat{\mathsf{q}}_j V_{\mathsf{c}}}\left(\mathrm{ad}^{(n)}_{A_{\mathrm{p}}^{(\epsilon)}}(\chi\tilde{G}_0(\cdot))\right),\\ &V_{\mathsf{c}}^*\hat{\mathsf{q}}_j V_{\mathsf{c}}\,\mathrm{ad}^{(n)}_{A_{\mathrm{p}}^{\mathrm{sr}}}(\chi\tilde{G}_0(\cdot)) + \mathrm{ad}^{(n)}_{A_{\mathrm{p}}^{\mathrm{sr}}}(\chi\tilde{G}_0(\cdot))V_{\mathsf{c}}^*\hat{\mathsf{q}}_j V_{\mathsf{c}}\end{aligned} \tag{6.73}$$

for $j \in \{1,2,3\}$. The verification of Assumption (2) of Lemma 4.3 for F_0 is analogous to the first case. Now (ii) of Hypothesis B-SR (3) implies that $\tilde{G}_0$ satisfies (J_s) where $s = \max\{0, 3-J\}$, and we find that the $\mathcal{L}(\mathcal{H}_{\mathrm{p}})$-valued functions (6.70) are well-defined and continuous by Proposition 6.26 as well as their first s partial derivatives with respect to $\omega \in [0,\infty)$. By assumption (ii) of Hypothesis B-SR (3) it is straightforward to verify that F_0 satisfies the Assumption (1') of Lemma 4.3, noting that the adjoints are obtained by replacing $\kappa_0\chi\tilde{G}_0$ by $\overline{\kappa_0\chi\tilde{G}_0}$.

Thus Proposition 6.2 now follows from Lemma 4.3, observing that for (4) we use the identity

$$
\begin{aligned}
&V_{\mathsf{c}}^{*}\hat{\mathsf{q}}_j V_{\mathsf{c}}\, \mathrm{ad}_{A_{\mathrm{p}}^{\mathrm{sr}}}^{(n)}(\tau_\beta(G)) \\
&\quad = \frac{1}{2}\Big(V_{\mathsf{c}}^{*}\hat{\mathsf{q}}_j V_{\mathsf{c}}\, \mathrm{ad}_{A_{\mathrm{p}}^{\mathrm{sr}}}^{(n)}(\tau_\beta(G)) + \mathrm{ad}_{A_{\mathrm{p}}^{\mathrm{sr}}}^{(n)}(\tau_\beta(G)) V_{\mathsf{c}}^{*}\hat{\mathsf{q}}_j V_{\mathsf{c}} - \mathrm{i}\, \mathrm{ad}_{V_{\mathsf{c}}^{*}\hat{\mathsf{q}}_j V_{\mathsf{c}}}(\mathrm{ad}_{A_{\mathrm{p}}^{\mathrm{sr}}}^{(n)}(\tau_\beta(G)))\Big)\,.
\end{aligned}
$$

Finally, note that the proposition still holds true if we replace G by G^* since the conditions (1)–(3) in Hypothesis B-SR are obviously invariant under taking the adjoint of G. $\square$

7. Positivity and Error Estimates

In this chapter the second important ingredient for the proof of the main result is provided, namely that the sum of $C_1^{\#}$, together with two supplementary terms already mentioned in Section 4.2, is in fact positive. In the first two subsections we treat the LR and SR case parallelly. For the LR case we assume that Hypotheses A-LR and B-LR hold and that χ is a cutoff function satisfying Hypothesis C, and in the SR case that Hypotheses A-SR and B-SR hold. All statements containing the symbol # are to be understood in the sense that they are satisfied for all $\# \in \{\mathrm{lr}, \mathrm{sr}\}$.

First, we fix some notation and outline how Theorem 3.5 and Theorem 3.8 will be proven. In Section 7.1 a self-adjoint $A_0 \in \mathcal{L}(\mathcal{H})$ is introduced with $\operatorname{ran} A_0 \subseteq \mathcal{D}(L_\lambda)$ such that the commutator $[L_\lambda, A_0]$ is well-defined on $\mathcal{D}(L_\lambda)$. Subsequently, in Section 7.2 a second self-adjoint operator $C_Q \in \mathcal{L}(\mathcal{H})$ with the property that

$$\langle \psi, C_Q \psi \rangle = 0, \qquad \psi \in \ker(L_\lambda),$$

is constructed. The formal sum

$$C_1^{\#} + \mathrm{i}\theta[L_\lambda, A_0] + C_Q, \qquad \theta > 0,$$

can be rigorously defined as a quadratic form. Recall that $q_1^{\#}$ denotes the quadratic form corresponding to $C_1^{\#}$ and P_J the restriction of the discrete spectrum to the set of modes J_{d}, see (3.6). We set

$$\widehat{P}_J := P_J \otimes P_J \otimes \mathrm{Id}_{\mathrm{f}},$$

and we have $\widehat{P}_J = \mathrm{Id}$ in the SR case. For $\psi \in \mathcal{D}(q_1^{\#}) \cap \mathcal{D}(L_\lambda)$, and some $\theta > 0$, which will be specified later, we write

$$q_{\mathrm{tot}}^{\#}(\psi) := q_1^{\#}(\psi) + \theta \langle \psi, \mathrm{i}[L_\lambda, A_0]\psi \rangle + \langle \psi, C_Q \psi \rangle . \tag{7.1}$$

Clearly, if one could show that $q_{\mathrm{tot}}^{\#}|_{\operatorname{ran} \widehat{P}_J} \geq 0$, the virial theorems for $C_1^{\#}$ and the construction of A_0 and C_Q will imply that $q_{\mathrm{tot}}^{\#}$ vanishes on $\ker L_\lambda \cap \operatorname{ran} \widehat{P}_J$: Let $\psi \in \ker L_\lambda \cap \operatorname{ran} \widehat{P}_J$. From Theorem 5.5 and Theorem 6.5 it follows under the given hypotheses that $\psi \in \mathcal{D}(q_1^{\#})$, and

$$q_1^{\#}(\psi) \leq 0.$$

Furthermore, $\langle \psi, \mathrm{i}[L_\lambda, A_0]\psi\rangle = 0$ holds trivially, and $\langle \psi, C_Q \psi\rangle = 0$. This implies

$$0 \leq q_{\mathrm{tot}}^{\#}(\psi) = q_1^{\#}(\psi) \leq 0,$$

hence

$$q_1^{\#}(\psi) = 0. \tag{7.2}$$

Therefore, in order to complete the proof of the main result we need to show that $q_{\mathrm{tot}}^{\#}(\psi) > 0$ for all $0 \neq \psi \in \ker L_\lambda \cap \operatorname{ran} \widehat{P}_J$. This will be done in Section 7.3 for the LR and in Section 7.4 for the SR case.

For the further estimates it is convenient to introduce some notation with respect to the interaction and the commuted interaction. We separate them into parts which act on the left and right factor of the atomic space tensor product, respectively,

$$\begin{aligned}
I_1^{\#}(u,\Sigma) &:= I_{1,\mathsf{l}}^{\#}(u,\Sigma) \otimes \mathrm{Id}_{\mathrm{p}} + \mathrm{Id}_{\mathrm{p}} \otimes I_{1,\mathsf{r}}^{\#}(u,\Sigma),\\
I_{1,\mathsf{l}}^{\#}(u,\Sigma) &:= (-\mathrm{i}\partial_u)\tau_\beta(G)(u,\Sigma) + \tau_\beta(\mathrm{ad}_{A_{\mathrm{p}}^{\#}}(G))(u,\Sigma),\\
I_{1,\mathsf{r}}^{\#}(u,\Sigma) &:= (-\mathrm{i}\partial_u)e^{-\beta u/2}\tau_\beta(\overline{G}^*)(u,\Sigma) - e^{-\beta u/2}\tau_\beta(\mathrm{ad}_{A_{\mathrm{p}}^{\#}}(\overline{G}^*))(u,\Sigma).
\end{aligned}$$

Note that $W_1^{\#} = \Phi(I_1^{\#})$ holds by construction. Further, we introduce integrated versions

$$\begin{aligned}
w &:= \int I(u,\Sigma)^* I(u,\Sigma)\mathrm{d}(u,\Sigma),\\
w_1^{\#} &:= \int I_1^{\#}(u,\Sigma)^* I_1^{\#}(u,\Sigma)\mathrm{d}(u,\Sigma),
\end{aligned}$$

and the left and right parts, for $\alpha = \mathsf{l}, \mathsf{r}$,

$$\begin{aligned}
w_\alpha &:= \int I_\alpha(u,\Sigma)^* I_\alpha(u,\Sigma)\mathrm{d}(u,\Sigma),\\
w_{1,\alpha}^{\#} &:= \int I_{1,\alpha}^{\#}(u,\Sigma)^* I_{1,\alpha}^{\#}(u,\Sigma)\mathrm{d}(u,\Sigma).
\end{aligned}$$

Note that all these interaction terms depend on the inverse temperature β.

7.1. Fermi Golden Rule Term

On the space $\operatorname{ran}\Pi$ we use the Fermi Golden Rule and introduce an appropriate conjugate operator A_0. It yields a positive expression on $\operatorname{ran}\Pi$ as a commutator with L_λ. The operator A_0 was first introduced for zero temperature systems in

[Bac+99] and was later adapted to the positive temperature case in [Mer01]. It is given as a bounded self-adjoint operator on $\mathcal{H}$ by

$$A_0 := \mathrm{i}\lambda(\Pi W R_\varepsilon^2 \Pi^\perp - \Pi^\perp R_\varepsilon^2 W \Pi), \tag{7.3}$$

where $\varepsilon > 0$ and $R_\varepsilon^2 := (L_0^2 + \varepsilon^2)^{-1}$. Recall that $W = \Phi(I)$. Hence,

$$W\Pi = a^*(I)\mathbb{1}_{L_\mathrm{p}=0} \otimes P_\Omega,$$

which is bounded, so both summands in (7.3) extend from $\mathcal{D}(\widehat{N_\mathrm{f}})$ to bounded operators. Furthermore, as the range of the first summand of (7.3) equals $\operatorname{ran}\Pi$ and the range of the second one equals $\mathcal{D}(L_0^2) \cap \mathfrak{F}_{\mathrm{fin}}$, we conclude that $\operatorname{ran} A_0 \subseteq \mathcal{D}(L_\lambda)$.

The commutator can be computed explicitly as follows. We have

$$\mathrm{i}[L_\lambda, A_0] = -\lambda[L_\lambda, \Pi W R_\varepsilon^2 \Pi^\perp - \Pi^\perp R_\varepsilon^2 W \Pi].$$

With respect to the different subspaces, a short computation yields

$$\Pi \mathrm{i}[L_\lambda, A_0]\Pi = 2\lambda^2 \Pi W R_\varepsilon^2 W \Pi, \tag{7.4}$$

$$\Pi^\perp \mathrm{i}[L_\lambda, A_0]\Pi^\perp = -\lambda^2(\Pi^\perp W \Pi W R_\varepsilon^2 \Pi^\perp + \Pi^\perp R_\varepsilon^2 W \Pi W \Pi^\perp), \tag{7.5}$$

$$\Pi \mathrm{i}[L_\lambda, A_0]\Pi^\perp = \lambda \Pi W R_\varepsilon^2 \Pi^\perp L_\lambda \Pi^\perp. \tag{7.6}$$

First, we show that the Fermi Golden Rule condition implies strict positivity of the first term (7.4) by generalizing [FMS04, Proposition 3.2] to our type of coupling term. The proof is completely analogous.

Proposition 7.1
For all $\varepsilon > 0$,

$$\widehat{P}_J \Pi W R_\varepsilon^2 W \Pi \widehat{P}_J \geq \gamma_\beta(\varepsilon, J_\mathrm{d})\Pi \widehat{P}_J.$$

Proof. First notice that $\Pi = \mathbb{1}_{L_\mathrm{p}=0} \otimes P_\Omega = \sum_{E \in \sigma_\mathrm{d}(H_\mathrm{p})} p_E \otimes p_E \otimes P_\Omega$. Then we compute

$$\begin{aligned}
\Pi W R_\varepsilon^2 W \Pi &\geq \Pi W R_\varepsilon^2 (P_\mathrm{ess} \otimes P_\mathrm{disc} \otimes \mathrm{Id}_\mathrm{f}) W \Pi \\
&= \Pi \left(a(\tau_\beta(G \otimes \mathrm{Id}_\mathrm{p})) - a(e^{-\beta \hat{\mathrm{u}}/2}\tau_\beta(\mathrm{Id}_\mathrm{p} \otimes \overline{G}^*)) \right) \frac{P_\mathrm{ess} \otimes P_\mathrm{disc} \otimes \mathrm{Id}_\mathrm{f}}{L_0^2 + \varepsilon^2} \\
&\qquad \times \left(a^*(\tau_\beta(G \otimes \mathrm{Id}_\mathrm{p})) - a^*(e^{-\beta \hat{\mathrm{u}}/2}\tau_\beta(\mathrm{Id}_\mathrm{p} \otimes \overline{G}^*)) \right) \Pi \\
&= \Pi a(\tau_\beta(G \otimes \mathrm{Id}_\mathrm{p})) \frac{P_\mathrm{ess} \otimes P_\mathrm{disc} \otimes \mathrm{Id}_\mathrm{f}}{L_0^2 + \varepsilon^2} a^*(\tau_\beta(G \otimes \mathrm{Id}_\mathrm{p}))\Pi \\
&= \sum_{E \in \sigma_\mathrm{d}(H_\mathrm{p})} \Pi a(\tau_\beta(G \otimes \mathrm{Id}_\mathrm{p})) \frac{P_\mathrm{ess} \otimes p_E \otimes \mathrm{Id}_\mathrm{f}}{(H_\mathrm{p} \otimes \mathrm{Id}_\mathrm{p} - E + \mathsf{d}\Gamma(\hat{\mathrm{u}}))^2 + \varepsilon^2} \\
&\qquad \times a^*(\tau_\beta(G \otimes \mathrm{Id}_\mathrm{p}))\Pi,
\end{aligned}$$

where we used $\Pi(P_{\text{ess}} \otimes \mathrm{Id}_{\text{p}}) = 0$ in the second to last step and the pull through formula in the last step. Evaluating Π and using the definition of τ_β, we arrive at

$$\begin{aligned}\Pi W R_\varepsilon^2 W \Pi \geq \Big(\mathbb{1}_{L_{\text{p}}=0} \sum_{E \in \sigma_{\text{d}}(H_{\text{p}})} \int_{\mathbb{R}} \int_{\mathbb{S}^2} \tau_\beta(G^* \otimes \mathrm{Id}_{\text{p}})(u,\Sigma) \frac{P_{\text{ess}}}{(H_{\text{p}} - E + u)^2 + \varepsilon^2} \otimes p_E \\ \tau_\beta(G \otimes \mathrm{Id}_{\text{p}})(u,\Sigma) \mathrm{d}\Sigma \mathrm{d}u \mathbb{1}_{L_{\text{p}}=0} \Big) \otimes P_\Omega \\ = \sum_{E \in \sigma_{\text{d}}(H_{\text{p}})} p_E (F^{(1)}_{G,\beta}(E,\varepsilon) + F^{(2)}_{G,\beta}(E,\varepsilon)) p_E \otimes p_E \otimes P_\Omega,\end{aligned}$$

with $F^{(1)}_{G,\beta}(E,\varepsilon)$, $F^{(2)}_{G,\beta}(E,\varepsilon)$ defined as in Section 3.1.3. Applying the projection $\widehat{P}_J$ on both sides yields the desired result. □

The two other terms (7.5) and (7.6) are possibly negative and estimated in the following lemma. It contains sharper bounds than [FMS04], which we later use for a Birman-Schwinger argument.

Lemma 7.2
For all $\varepsilon > 0$ and all $\lambda \in \mathbb{R}$, the following holds.

(a) We have

$$\Pi^\perp \mathrm{i}[L_\lambda, A_0] \Pi^\perp = \mathbb{1}_{\widehat{N}_{\text{f}}=1} \Pi^\perp \mathrm{i}[L_\lambda, A_0] \Pi^\perp \mathbb{1}_{\widehat{N}_{\text{f}}=1}.$$

Moreover,

$$\left\| \Pi^\perp \mathrm{i}[L_\lambda, A_0] \Pi^\perp \right\| \leq 2 \frac{\lambda^2}{\varepsilon^2} \|I\|^2 .$$

(b) For arbitrary $\delta_1, \delta_2 > 0$,

$$\begin{aligned}&\Pi^\perp \mathrm{i}[L_\lambda, A_0]\Pi + \Pi \mathrm{i}[L_\lambda, A_0]\Pi^\perp \\ &\quad \leq (\delta_1 |\lambda| + \delta_2 \lambda^2) \Pi W R_\varepsilon^2 W \Pi + \frac{|\lambda|}{\delta_1} \widehat{P_\Omega}^\perp \\ &\quad + 2 \frac{\lambda^2}{\delta_2} \left(a^*(I) R_\varepsilon^2 a(I) \mathbb{1}_{\widehat{N}_{\text{f}}=2} + \Pi^\perp \int \frac{I(u,\Sigma)^* I(u,\Sigma)}{u^2 + \varepsilon^2} \mathrm{d}(u,\Sigma) \otimes P_\Omega \Pi^\perp \right).\end{aligned}$$

Proof. (a) Consider the first term in (7.5),

$$\Pi^\perp W \Pi W R_\varepsilon^2 \Pi^\perp = a^*(I) \Pi a(I) R_\varepsilon^2 \Pi^\perp .$$

Clearly, this operator vanishes everywhere except on ran $\mathbb{1}_{\widehat{N}_{\text{f}}=1}$. By standard estimates of creation and annihilation operators we obtain

$$\|a^*(I) \Pi a(I)\| \leq \|I\|^2 ,$$

thus,

$$\left\|\Pi^\perp W\Pi W R_\varepsilon^2 \Pi^\perp\right\| \le \frac{\|I\|^2}{\varepsilon^2},$$

which proves the claim, as the second term in (7.5) is just the adjoint of the first one.

(b) Using (7.6), and the operator inequality (5.4) we get

$$\begin{aligned}
&\Pi^\perp \mathrm{i}[L_\lambda, A_0]\Pi + \Pi\mathrm{i}[L_\lambda, A_0]\Pi^\perp \\
&\quad = \lambda(\Pi W R_\varepsilon^2 L_0 \mathbb{1}_{\widehat{N}_\mathrm{f}=1} + \mathbb{1}_{\widehat{N}_\mathrm{f}=1} L_0 R_\varepsilon^2 W\Pi) \\
&\qquad + \lambda^2(\Pi W R_\varepsilon^2 \mathbb{1}_{\widehat{N}_\mathrm{f}=1} W\Pi^\perp + \Pi^\perp W \mathbb{1}_{\widehat{N}_\mathrm{f}=1} R_\varepsilon^2 W\Pi) \\
&\quad \le |\lambda|\,(\delta_1 \Pi W R_\varepsilon^2 W\Pi + \delta_1^{-1} \mathbb{1}_{\widehat{N}_\mathrm{f}=1} L_0 R_\varepsilon^2 L_0 \mathbb{1}_{\widehat{N}_\mathrm{f}=1}) && (7.7)\\
&\qquad + \lambda^2(\delta_2 \Pi W R_\varepsilon^2 W\Pi + \delta_2^{-1}\Pi^\perp W \mathbb{1}_{\widehat{N}_\mathrm{f}=1} R_\varepsilon^2 \mathbb{1}_{\widehat{N}_\mathrm{f}=1} W\Pi^\perp). && (7.8)
\end{aligned}$$

We have

$$\left\|\mathbb{1}_{\widehat{N}_\mathrm{f}=1} L_0 R_\varepsilon^2 L_0 \mathbb{1}_{\widehat{N}_\mathrm{f}=1}\right\| \le 1,$$

which yields a bound for the second operator in (7.7). The second one in (7.8) only operates on the space $\mathrm{ran}(\widehat{P_\Omega} + \mathbb{1}_{\widehat{N}_\mathrm{f}=2})$. So we can write

$$\begin{aligned}
&\Pi^\perp W \mathbb{1}_{\widehat{N}_\mathrm{f}=1} R_\varepsilon^2 \mathbb{1}_{\widehat{N}_\mathrm{f}=1} W\Pi^\perp \\
&\quad = (\widehat{P_\Omega} + \mathbb{1}_{\widehat{N}_\mathrm{f}=2})\Pi^\perp W \mathbb{1}_{\widehat{N}_\mathrm{f}=1} R_\varepsilon^2 \mathbb{1}_{\widehat{N}_\mathrm{f}=1} W\Pi^\perp (\widehat{P_\Omega} + \mathbb{1}_{\widehat{N}_\mathrm{f}=2}). && (7.9)
\end{aligned}$$

Now, we can again use the operator inequality (5.4) and then the pull-through formula to estimate (7.9) by

$$\begin{aligned}
&2a^*(I) R_\varepsilon^2 a(I) \mathbb{1}_{\widehat{N}_\mathrm{f}=2} + 2\Pi^\perp a(I) R_\varepsilon^2\, a^*(I)\Pi^\perp \widehat{P_\Omega} \\
&\le 2\left(a^*(I) R_\varepsilon^2 a(I) \mathbb{1}_{\widehat{N}_\mathrm{f}=2} + \Pi^\perp \int \frac{I^*(u,\Sigma) I(u,\Sigma)}{u^2+\varepsilon^2} \mathrm{d}(u,\Sigma) \otimes P_\Omega \Pi^\perp\right). \qquad \square
\end{aligned}$$

Proposition 7.3
For all $\varepsilon > 0$ there exist constants $c_1, c_2, c_3 > 0$ depending on ε such that for $|\lambda| < 1$,

$$\begin{aligned}
\mathrm{i}[L_\lambda, A_0] \ge (1 - c_1|\lambda|)2\lambda^2 \Pi W R_\varepsilon^2 W\Pi - c_2|\lambda|\,(\|I\|^2 + 1)\widehat{P_\Omega}^\perp \\
- c_3\lambda^2(\mathbb{1}_{L_\mathrm{p}\neq 0} w \mathbb{1}_{L_\mathrm{p}\neq 0}) \otimes P_\Omega.
\end{aligned}$$

Proof. Lemma 7.2 yields for all $\delta_1, \delta_2 > 0$,

$$\begin{aligned}\mathrm{i}[L_\lambda, A_0] &= \Pi\mathrm{i}[L_\lambda, A_0]\Pi + \Pi^\perp\mathrm{i}[L_\lambda, A_0]\Pi^\perp + \Pi^\perp\mathrm{i}[L_\lambda, A_0]\Pi + \Pi\mathrm{i}[L_\lambda, A_0]\Pi^\perp \\ &\geq (1 - (|\lambda|\,\delta_1 + \delta_2\lambda^2))\Pi\mathrm{i}[L_\lambda, A_0]\Pi - 2\frac{\lambda^2}{\varepsilon^2}\,\|I\|^2\,\widehat{P_\Omega}^\perp \\ &\quad - \frac{|\lambda|}{\delta_1}\widehat{P_\Omega}^\perp - 2\frac{\lambda^2}{\delta_2}\left(a^*(I)R_\varepsilon^2 a(I)\mathbb{1}_{\widehat{N}_\mathrm{f}=2} + \frac{1}{\varepsilon^2}\Pi^\perp w \otimes P_\Omega\Pi^\perp\right).\end{aligned}$$

For arriving at the desired estimate note that $\|a^*(I)R_\varepsilon^2 a(I)\mathbb{1}_{N_\mathrm{f}=2}\| \leq C\,\|I\|^2$ for some constant C and $\Pi^\perp w \otimes P_\Omega\Pi^\perp = (\mathbb{1}_{L_\mathrm{p}\neq 0} w \mathbb{1}_{L_\mathrm{p}\neq 0}) \otimes P_\Omega$. □

7.2. Additional Auxiliary Term

To obtain a strictly positive operator on the remaining space $(\ker L_\mathrm{p})^\perp \otimes \operatorname{ran} P_\Omega$ we introduce the following auxiliary term on $\mathcal{H}$. Let $Q \in \mathcal{L}(\mathcal{H}_\mathrm{p} \otimes \mathcal{H}_\mathrm{p})$ such that $\operatorname{ran} Q \subseteq \mathcal{D}(L_\mathrm{p}^{-1})$, and $L_\mathrm{p}^{-1}Q$ is bounded and self-adjoint. Note that L_p^{-1} is to be understood in the sense of functional calculus as an unbounded operator. Then define a bounded operator C_Q on $\mathcal{H}$ by

$$C_Q := Q \otimes P_\Omega + \frac{\lambda}{2}\left(W(L_\mathrm{p}^{-1}Q \otimes P_\Omega) + W(L_\mathrm{p}^{-1}Q \otimes P_\Omega)^*\right).$$

Lemma 7.4
Let $\psi \in \mathcal{D}(L_\lambda)$ with $L_\lambda\psi = 0$. Then

$$\langle \psi, C_Q\psi\rangle = 0.$$

Proof. By assumption $L_\lambda\psi = 0$, and thus

$$\begin{aligned}0 &= \left\langle (L_\mathrm{p}^{-1}Q \otimes P_\Omega)L_\lambda\psi, \psi\right\rangle \\ &= \left\langle \psi, L_\lambda(L_\mathrm{p}^{-1}Q \otimes P_\Omega)\psi\right\rangle \\ &= \left\langle \psi, (L_\mathrm{p} \otimes \mathrm{Id}_\mathrm{f} + \lambda W)(L_\mathrm{p}^{-1}Q \otimes P_\Omega)\psi\right\rangle \\ &= \left\langle \psi, (Q \otimes P_\Omega)\psi + \lambda W(L_\mathrm{p}^{-1}Q \otimes P_\Omega)\psi\right\rangle. \end{aligned} \tag{7.10}$$

Finally, the claim follows by considering the real part of (7.10). □

Now, we make the following concrete choice

$$Q := L_{\mathrm{p}}^2 \mathbb{1}_{[-1,1]}(L_{\mathrm{p}}) + \mathbb{1}_{(-\infty,-1)\cup(1,\infty)}(L_{\mathrm{p}}). \tag{7.11}$$

Indeed, $\operatorname{ran} Q \subseteq \mathcal{D}(L_{\mathrm{p}}^{-1})$, and $L_{\mathrm{p}}^{-1}Q$ is bounded and self-adjoint. Furthermore, the leading term $Q \otimes P_\Omega$ is positive on $(\ker L_{\mathrm{p}})^\perp \otimes \operatorname{ran} P_\Omega$. Together with the possibly negative correction terms we get the following lower bound.

Proposition 7.5
There exists a constant $C > 0$ such that for all $\lambda \in \mathbb{R}$,

$$C_Q \geq (1 - C\,|\lambda|\,\|w\|)Q \otimes P_\Omega - |\lambda|\,\widehat{P_\Omega}^{\perp}.$$

Proof. We have

$$W(L_{\mathrm{p}}^{-1}Q \otimes P_\Omega) = a^*(I)(L_{\mathrm{p}}^{-1}Q \otimes P_\Omega) = a^*(IL_{\mathrm{p}}^{-1}Q)\widehat{P_\Omega}.$$

Thus, Lemma A.4 yields for all $\delta > 0$ on $\mathcal{D}(\widehat{N_{\mathrm{f}}})$,

$$\begin{aligned} &W(L_{\mathrm{p}}^{-1}Q \otimes P_\Omega) + (W(L_{\mathrm{p}}^{-1}Q \otimes P_\Omega))^* \\ &\quad \leq \delta\widehat{N_{\mathrm{f}}} + \delta^{-1}\int L_{\mathrm{p}}^{-1}QI(u,\Sigma)^*I(u,\Sigma)L_{\mathrm{p}}^{-1}Q\mathrm{d}(u,\Sigma) \otimes P_\Omega. \end{aligned}$$

Using this we conclude

$$\begin{aligned} C_Q &\geq Q \otimes P_\Omega - \frac{|\lambda|}{2}\delta\widehat{N_{\mathrm{f}}} - \frac{|\lambda|}{2}\,\|w\|\,\delta^{-1}(L_{\mathrm{p}}^{-1}Q)^2 \otimes P_\Omega \\ &\geq (1 - |\lambda|\,\delta^{-1}\,\|w\|)Q \otimes P_\Omega - \frac{|\lambda|}{2}\delta\widehat{N_{\mathrm{f}}}, \end{aligned} \tag{7.12}$$

where we used that the concrete choice of Q implies

$$(L_{\mathrm{p}}^{-1}Q)^2 = (L_{\mathrm{p}}^2\mathbb{1}_{[-1,1]}(L_{\mathrm{p}}) + L_{\mathrm{p}}^{-2}\mathbb{1}_{(-\infty,-1)\cup(1,\infty)}(L_{\mathrm{p}})) \leq 2Q. \qquad \square$$

7.3. Long-Range

In this part we put everything together in the LR case and prove the positivity of the form $q_{\mathrm{tot}}^{\mathrm{lr}}$. We proceed similarly as in the proof of the virial theorem: we summarize the necessary conditions for the proof in (H1)–(H3), and subsequently show that they are in fact satisfied if J_{d} is finite. We cannot provide a proof for the case of infinitely many coupled eigenvalues, yet, but some ideas and problems are sketched in Remark 7.9.

7.3.1. Positivity for a General Cutoff Function

Recall that we assume that Hypotheses A-LR and B-LR are true and χ is a cutoff function satisfying Hypothesis C.

First, we prove that the interaction terms are bounded and sufficiently localized. This will play an important role for the Birman-Schwinger bounds. The following lemma shows that they decay as $|x|^{-2}$ in spatial infinity.

Lemma 7.6
For all $n, m \in \{0,1\}$ there exists a constant C such that

$$\left\| \partial_u^m \tau_\beta \left(\mathrm{ad}^{(n)}_{A_{\mathrm{p}}^{\mathrm{lr}}}(\tau_\beta(G)) \right) \langle \hat{\mathsf{x}} \rangle^2 \right\|_{L^2(\mathbb{R}\times\mathbb{S}^2, \mathcal{L}(\mathcal{H}_{\mathrm{p}}))} \leq C(1+\beta^{-1/2})$$

for all $\beta > 0$.

Proof. The proof is analogous to Lemma 5.3. Notice that at most one commutator with $A_{\mathrm{p}}^{\mathrm{lr}}$ has to be considered, so the regularity assumptions for

$$\langle \hat{\mathsf{x}} \rangle^{n_1} G \langle \hat{\mathsf{x}} \rangle^{n_2}, \qquad n_1, n_2 \leq 2+1 = 3,$$

given in Hypothesis B-LR are sufficient. The β-dependence follows from (4.8). $\square$

This can be rephrased for the integrated interaction terms, which were introduced at the beginning of this chapter, as follows.

Lemma 7.7
For $\alpha = \mathsf{l}, \mathsf{r}$, the operators w_α and $w_{1,\alpha}^{\mathrm{lr}}$ are well-defined and bounded, and there exist constants C such that for all $\beta > 0$,

(a) $\|I_\alpha\|^2_{L^2(\mathbb{R}\times\mathbb{S}^2,\mathcal{L}(\mathcal{H}_{\mathrm{p}}))} \leq C(1+\beta^{-1})$,

(b) $\left\|I_{1,\alpha}^{\mathrm{lr}}\right\|^2_{L^2(\mathbb{R}\times\mathbb{S}^2,\mathcal{L}(\mathcal{H}_{\mathrm{p}}))} \leq C(1+\beta^{-1})$,

(c) $w_\alpha \leq C(1+\beta^{-1}) V_{\mathsf{c}}^* \langle \hat{\mathsf{x}} \rangle^{-4} V_{\mathsf{c}}$,

(d) $w_{1,\alpha}^{\mathrm{lr}} \leq C(1+\beta^{-1}) V_{\mathsf{c}}^* \langle \hat{\mathsf{x}} \rangle^{-4} V_{\mathsf{c}}$.

Proof. By Lemma 7.6 we have

$$I_\alpha,\ I_{1,\alpha}^{\mathrm{lr}},\ I_\alpha V_{\mathsf{c}}^* \hat{\mathsf{x}}_j^2 V_{\mathsf{c}},\ I_{1,\alpha}^{\mathrm{lr}} V_{\mathsf{c}}^* \hat{\mathsf{x}}_j^2 V_{\mathsf{c}} \in L^2(\mathbb{R}\times\mathbb{S}^2, \mathcal{L}(\mathcal{H}_{\mathrm{p}}))$$

for all $j \in \{1,2,3\}$, $\alpha = \mathsf{l}, \mathsf{r}$, and there is a constant C independent of β such that we can estimate the norm of these expressions by

$$C(1+\beta^{-1}).$$

Thus, the same applies to $I_\alpha V_{\mathsf{c}}^* \langle \hat{\mathsf{x}} \rangle^2 V_{\mathsf{c}}$, $I_{1,\alpha}^{\mathrm{lr}} V_{\mathsf{c}}^* \langle \hat{\mathsf{x}} \rangle^2 V_{\mathsf{c}} \in L^2(\mathbb{R}\times\mathbb{S}^2, \mathcal{L}(\mathcal{H}_{\mathrm{p}}))$. Consequently, we obtain

$$\begin{aligned} w_\alpha &= V_{\mathsf{c}}^* \langle \hat{\mathsf{x}} \rangle^{-2} V_{\mathsf{c}} \int (I_\alpha(u,\Sigma) V_{\mathsf{c}}^* \langle \hat{\mathsf{x}} \rangle^2 V_{\mathsf{c}})^* I_\alpha(u,\Sigma) V_{\mathsf{c}}^* \langle \hat{\mathsf{x}} \rangle^2 V_{\mathsf{c}} \mathrm{d}(u,\Sigma) V_{\mathsf{c}}^* \langle \hat{\mathsf{x}} \rangle^{-2} V_{\mathsf{c}} \\ &\le C(1+\beta^{-1}) V_{\mathsf{c}}^* \langle \hat{\mathsf{x}} \rangle^{-4} V_{\mathsf{c}} \end{aligned}$$

for $\alpha = \mathsf{l}, \mathsf{r}$ and some constant $C > 0$ not depending on β. The proof for $w_{1,\alpha}^{\mathrm{lr}}$ is analogous. □

Next, we can estimate C_1^{lr}, the first commutator with A^{lr}, from below. Recall that it was given on $\mathcal{D}^{\mathrm{lr}}$ by

$$C_1^{\mathrm{lr}} = \chi(H_{\mathrm{p}} + \widetilde{V})\chi \otimes \mathrm{Id}_{\mathrm{p}} \otimes \mathrm{Id}_{\mathrm{f}} + \mathrm{Id}_{\mathrm{p}} \otimes \chi(H_{\mathrm{p}} + \widetilde{V})\chi \otimes \mathrm{Id}_{\mathrm{f}} + \widehat{N_{\mathrm{f}}} + \lambda W_1^{\mathrm{lr}}. \tag{7.13}$$

To ensure a positive expression we assume from now on that χ cuts off the negative energy of the coupled eigenmodes, that is,

$$\chi p_{J_{\mathrm{d}}} = 0. \tag{7.14}$$

Proposition 7.8
There exist constants $c_1, c_2, \delta > 0$ such that for all $\beta > 0$ and all $\lambda \in \mathbb{R}$,

$$C_1^{\mathrm{lr}} \ge \Big(P_{\mathrm{ess}}\chi\delta(-\Delta)\chi P_{\mathrm{ess}} \otimes \mathrm{Id}_{\mathrm{p}} + \mathrm{Id}_{\mathrm{p}} \otimes P_{\mathrm{ess}}\chi\delta(-\Delta)\chi P_{\mathrm{ess}} - c_1\lambda^2 w_1^{\mathrm{lr}}\Big) \otimes \mathrm{Id}_{\mathrm{f}} + c_2 \widehat{P_\Omega}^\perp \tag{7.15}$$

holds on $\mathcal{D}(\widehat{N_{\mathrm{f}}}) \cap \operatorname{ran} \widehat{P}_J$. In particular, C_1^{lr} is bounded from below and the lower bound (7.15) extends to the corresponding form $q_1^{\mathrm{lr}}|_{\operatorname{ran}\widehat{P}_J}$.

Proof. As $I_1^{\mathrm{lr}} \in L^2(\mathbb{R}\times\mathbb{S}^2, \mathcal{L}(\mathcal{H}_{\mathrm{p}}))$ by Lemma 7.7, Lemma A.4 yields for any $\delta_1 > 0$,

$$\pm\lambda W_1^{\mathrm{lr}} \le \delta_1 \widehat{N_{\mathrm{f}}} + \frac{1}{\delta_1}\lambda^2 w_1^{\mathrm{lr}} \otimes \mathrm{Id}_{\mathrm{f}}.$$

Therefore, (7.13) also holds on $\mathcal{D}(\widehat{N_{\mathrm{f}}})$. By (7.14), we have $\chi P_J = \chi P_{\mathrm{ess}}$. Then we find on $\mathcal{D}(\widehat{N_{\mathrm{f}}}) \cap \operatorname{ran} \widehat{P}_J$ for any $\delta_1 > 0$,

$$\begin{aligned} C_1^{\mathrm{lr}} &= \chi P_{\mathrm{ess}}(H_{\mathrm{p}} + \widetilde{V})P_{\mathrm{ess}}\chi \otimes \mathrm{Id}_{\mathrm{p}} + \mathrm{Id}_{\mathrm{p}} \otimes \chi P_{\mathrm{ess}}(H_{\mathrm{p}} + \widetilde{V})P_{\mathrm{ess}}\chi \otimes \mathrm{Id}_{\mathrm{f}} + \widehat{N_{\mathrm{f}}} + \lambda W_1^{\mathrm{lr}} \\ &\ge \chi P_{\mathrm{ess}}(H_{\mathrm{p}} + \widetilde{V})P_{\mathrm{ess}}\chi \otimes \mathrm{Id}_{\mathrm{p}} + \mathrm{Id}_{\mathrm{p}} \otimes \chi P_{\mathrm{ess}}(H_{\mathrm{p}} + \widetilde{V})P_{\mathrm{ess}}\chi \otimes \mathrm{Id}_{\mathrm{f}} + (1-\delta_1)\widehat{N_{\mathrm{f}}} \\ &\quad - \frac{\lambda^2}{\delta_1} w_1^{\mathrm{lr}} \otimes \mathrm{Id}_{\mathrm{f}}. \end{aligned}$$

Next, we estimate the first two terms. Choose $\delta > 0$ as in Hypothesis A-LR (2). Then

$$P_{\mathrm{ess}}(H_{\mathrm{p}} + \widetilde{V})P_{\mathrm{ess}} \geq \frac{\delta}{2} P_{\mathrm{ess}}(-\Delta)P_{\mathrm{ess}}.$$

Combining this with the previous estimate and setting for example $\delta_1 = \frac{1}{2}$ yields (7.15) on $\mathcal{D}(\widehat{N}_{\mathrm{f}}) \cap \operatorname{ran} \widehat{P}_J$. As $\mathcal{D}(\widehat{N}_{\mathrm{f}})$ is a core for C_1^{lr}, it is also a form core for q_1^{lr}. Notice that the right-hand side of (7.15) consists only of bounded operators, so the inequality carries over to $q_1^{\mathrm{lr}}|_{\operatorname{ran} \widehat{P}_J}$ by approximation. $\square$

Before presenting the final proof, we want to identify the necessary positivity conditions. For $\beta > 0, \varepsilon > 0$ and $\delta \geq 0$ they are as follows.

(H1) $P_{\mathrm{ess}}(\chi(-\Delta)\chi - \delta(w_{\mathsf{l}} + w_{1,\mathsf{l}}^{\mathrm{lr}}))P_{\mathrm{ess}} \geq 0,$

(H2) on $\operatorname{ran} \mathbb{1}_{L_{\mathrm{p}} \neq 0}(P_J \otimes P_J)$:

$$Q - \delta\Big(P_{\mathrm{disc}}(w_{\mathsf{l}} + w_{1,\mathsf{l}}^{\mathrm{lr}})P_{\mathrm{disc}} \otimes P_{\mathrm{ess}} + P_{\mathrm{ess}} \otimes P_{\mathrm{disc}}(w_{\mathsf{r}} + w_{1,\mathsf{r}}^{\mathrm{lr}})P_{\mathrm{disc}}$$
$$+ \mathbb{1}_{L_{\mathrm{p}} \neq 0}(P_{\mathrm{disc}} w_{1,\mathsf{l}}^{\mathrm{lr}} P_{\mathrm{disc}} \otimes P_{\mathrm{disc}} + P_{\mathrm{disc}} \otimes P_{\mathrm{disc}} w_{1,\mathsf{r}}^{\mathrm{lr}} P_{\mathrm{disc}})\mathbb{1}_{L_{\mathrm{p}} \neq 0}\Big) > 0,$$

(H3) on $\operatorname{ran} \Pi \widehat{P}_J$:

$$\Pi W R_\varepsilon^2 W \Pi - \delta \mathbb{1}_{L_{\mathrm{p}} = 0}\Big(P_{\mathrm{disc}} w_{1,\mathsf{l}}^{\mathrm{lr}} P_{\mathrm{disc}} \otimes P_{\mathrm{disc}}$$
$$+ P_{\mathrm{disc}} \otimes P_{\mathrm{disc}} w_{1,\mathsf{r}}^{\mathrm{lr}} P_{\mathrm{disc}}\Big)\mathbb{1}_{L_{\mathrm{p}} = 0} \otimes P_\Omega > 0.$$

Let $\delta_1^{(\beta)}, \delta_2^{(\beta)}, \delta_3^{(\beta,\varepsilon)} \in [0, \infty]$ be the supremum of all δ such that (H1), (H2) and (H3) holds true, respectively. Obviously, all three conditions are trivially satisfied for $\delta = 0$, since the leading terms are strictly positive. However, in order to show that the total form $q_{\mathrm{tot}}^{\mathrm{lr}}$ is strictly positive for non-zero coupling constants, one needs actually a positive value.

Remark 7.9

(H1)–(H3) can be regarded both as collection of the essential ingredients for the proof of positivity as well as a possible guide for future work about this problem, in particular for treating potentials with infinitely many eigenvalues.

Condition (H1) is basically a generalization of a Birman-Schwinger bound, which in its classical form corresponds to $\chi = \mathrm{Id}_{\mathrm{p}}$. The interaction terms $w_\alpha + w_{1,\alpha}^{\mathrm{lr}}$ will be estimated by some function decaying at spatial infinity fast enough. In fact, in case of finitely many eigenvalues χ can be chosen in such a way that it equals the identity near zero energy and decays appropriately at infinity (cf.

Proposition 7.11). In this case a Birman-Schwinger bound can be proven, see Proposition B.13.

For infinitely many eigenvalues χ has to vanish at zero energy. This implies that one is confronted with an additional decay near zero and the Birman-Schwinger bound has to be improved in this way. Another idea would be to consider a sharp cutoff at zero energy. In this case, condition (H1) can be dropped for the price that certain commutators of the projection p_{J_d} with A_D and other expressions have to be bounded, see Remark 5.8.

The crucial point in (H2) is that Q decays to zero if one approaches $\ker L_\mathrm{p}$. As the interaction terms are bounded, the negative terms in (H2) become only problematic if we consider two discrete eigenvalues close to zero or a discrete eigenvalue and a point in the essential spectrum close to zero. In case of finitely many eigenvalues this does not occur as the distances of two different eigenvalues and the distance between the essential and the discrete spectrum are bounded from below by a positive constant. However, this is no longer true for infinitely many. For a proof of (H2) one could then use that the eigenfunctions of a Schrödinger operator are expected to smear out if their energy approaches zero. Based on the localization of the interaction terms $w_\alpha + w_{1,\alpha}^{\mathrm{lr}}$, one might be able to prove that their application to a spatially extended eigenfunction is sufficiently small such that the inequality in (H2) holds true.

Condition (H3) is the counterpart to the Fermi Golden Rule condition and might pose the biggest challenge for a generalization to infinitely many eigenvalues. The philosophy is similar as in (H2): The operator $\widehat{P}_J \Pi W R_\varepsilon^2 W \Pi \widehat{P}_J$ is bounded from below by a positive constant for a finite set J_d, but it might decay to zero on the eigenspaces if we consider infinitely many eigenmodes. However, with the same arguments as in the prior discussion, the hope would be that the negative terms decay as well if one approaches zero in the discrete spectrum. Here a careful analysis of the Fermi Golden Rule term and of the interaction terms depending on the energy would be necessary.

Now, the final result of this section, the positivity of the total form (7.1) will be the content of the following theorem.

Theorem 7.10
Let $\beta_0 > 0$ and $\varepsilon > 0$. Then there exists a constant C such that for all $\beta > 0$ and

$$|\lambda| < C \min\{1 + \beta^{-2}, (\delta_1^{(\beta)})^{2/3}, (\delta_2^{(\beta)})^{2/3}, (\delta_3^{(\beta,\varepsilon)})^2\},$$

we have $q_{\mathrm{tot}}^{\mathrm{lr}}|_{\mathrm{ran}\,\widehat{P}_J} > 0$ for $\theta = |\lambda|^{-1/2}$. That is, $q_{\mathrm{tot}}^{\mathrm{lr}} \geq 0$ and $q_{\mathrm{tot}}^{\mathrm{lr}}(\psi) = 0$ for some $\psi \in \mathcal{D}(q_1^{\mathrm{lr}}) \cap \mathrm{ran}\,\widehat{P}_J$ implies $\psi = 0$.

Proof. By Propositions 7.3, 7.5 and 7.8, and Lemma 7.7 (from which we infer $\|w\|^2 \leq \|I\|^2 \leq C(1+\beta^{-1})$ for some constant C), we obtain on $\mathcal{D}(q_1^{\mathrm{lr}}) \cap \operatorname{ran} \widehat{P}_J$,

$$\begin{aligned} q_{\mathrm{tot}}^{\mathrm{lr}} \geq{}& (P_{\mathrm{ess}}\chi\delta(-\Delta)\chi P_{\mathrm{ess}} \otimes \mathrm{Id}_{\mathrm{p}} + \mathrm{Id}_{\mathrm{p}} \otimes P_{\mathrm{ess}}\chi\delta(-\Delta)\chi P_{\mathrm{ess}} - c_1\lambda^2 w_1^{\mathrm{lr}}) \otimes \mathrm{Id}_{\mathrm{f}} + c_2\widehat{P_\Omega}^{\perp} \\ &+ 2\theta(1-c_3|\lambda|)\lambda^2\Pi W R_\varepsilon^2 W\Pi - c_4\theta|\lambda|(1+\beta^{-1})\widehat{P_\Omega}^{\perp} \\ &- c_5\theta\lambda^2(\mathbb{1}_{L_{\mathrm{p}}\neq 0} w \mathbb{1}_{L_{\mathrm{p}}\neq 0}) \otimes P_\Omega + (1 - c_6|\lambda|(1+\beta^{-1}))Q \otimes P_\Omega - |\lambda|\widehat{P_\Omega}^{\perp} \end{aligned}$$

for some constants $c_i > 0$, $i \in \mathbb{N}$. The operator inequality (5.4) yields

$$\begin{aligned} w &\leq 2w_{\mathsf{l}} \otimes \mathrm{Id}_{\mathrm{p}} + 2\,\mathrm{Id}_{\mathrm{p}} \otimes w_{\mathsf{r}} \\ &\leq 4(P_{\mathrm{disc}} w_{\mathsf{l}} P_{\mathrm{disc}} + P_{\mathrm{ess}} w_{\mathsf{l}} P_{\mathrm{ess}}) \otimes \mathrm{Id}_{\mathrm{p}} \\ &\qquad + 4\,\mathrm{Id}_{\mathrm{p}} \otimes (P_{\mathrm{disc}} w_{\mathsf{r}} P_{\mathrm{disc}} + P_{\mathrm{ess}} w_{\mathsf{r}} P_{\mathrm{ess}}), \end{aligned}$$

and analogously for w_1^{lr}. Using these in the above estimate for $q_{\mathrm{tot}}^{\mathrm{lr}}$, we find on $\mathcal{D}(q_1^{\mathrm{lr}}) \cap \operatorname{ran} \widehat{P}_J$,

$$\begin{aligned} q_{\mathrm{tot}}^{\mathrm{lr}} \geq{}& P_{\mathrm{ess}}\left(\delta\chi(-\Delta)\chi - c_1\lambda^2(\theta w_{\mathsf{l}} + w_{1,\mathsf{l}}^{\mathrm{lr}})\right)P_{\mathrm{ess}} \otimes \mathrm{Id}_{\mathrm{p}} \otimes \mathrm{Id}_{\mathrm{f}} && (7.16) \\ &+ \mathrm{Id}_{\mathrm{p}} \otimes P_{\mathrm{ess}}\left(\delta\chi(-\Delta)\chi - c_1\lambda^2(\theta w_{\mathsf{r}} + w_{1,\mathsf{r}}^{\mathrm{lr}})\right)P_{\mathrm{ess}} \otimes \mathrm{Id}_{\mathrm{f}} && (7.17) \\ &+ (c_2 - c_3(1+\theta(1+\beta^{-1}))|\lambda|)\widehat{P_\Omega}^{\perp} && (7.18) \\ &+ \Big((1 - c_4(1+\beta^{-1})|\lambda|)Q - c_5\lambda^2[P_{\mathrm{disc}}(\theta w_{\mathsf{l}} + w_{1,\mathsf{l}}^{\mathrm{lr}})P_{\mathrm{disc}} \otimes P_{\mathrm{ess}} \\ &\qquad + P_{\mathrm{ess}} \otimes P_{\mathrm{disc}}(\theta w_{\mathsf{r}} + w_{1,\mathsf{r}}^{\mathrm{lr}})P_{\mathrm{disc}} \\ &\qquad - \mathbb{1}_{L_{\mathrm{p}}\neq 0}((P_{\mathrm{disc}}(\theta w_{\mathsf{l}} + w_{1,\mathsf{l}}^{\mathrm{lr}})P_{\mathrm{disc}} \otimes P_{\mathrm{disc}} \\ &\qquad + P_{\mathrm{disc}} \otimes P_{\mathrm{disc}}(\theta w_{\mathsf{r}} + w_{1,\mathsf{r}}^{\mathrm{lr}})P_{\mathrm{disc}})\mathbb{1}_{L_{\mathrm{p}}\neq 0}]\Big) \otimes P_\Omega && (7.19) \\ &+ 2\theta\lambda^2(1 - c_6|\lambda|)\Pi W R_\varepsilon^2 W\Pi \\ &\qquad - c_7\lambda^2\Pi(P_{\mathrm{disc}} w_{1,\mathsf{l}}^{\mathrm{lr}} P_{\mathrm{disc}} \otimes P_{\mathrm{disc}} + P_{\mathrm{disc}} \otimes P_{\mathrm{disc}} w_{1,\mathsf{r}}^{\mathrm{lr}} P_{\mathrm{disc}})\Pi && (7.20) \end{aligned}$$

for some other constants $c_i > 0$, $i \in \mathbb{N}$. Then we can restrict the right-hand side of the operator inequality above to $\operatorname{ran} \widehat{P}_J$ and set $\theta = |\lambda|^{-1/2}$. Now we make $|\lambda| \geq 0$ small enough so that (H1)–(H3) are applicable.

First, it has to be small enough such that (7.16) and (7.17) are non-negative operators, which requires $\lambda^{3/2} < C\delta_1^{(\beta)}$ for a suitable constant C. Next, it has to be small enough ($|\lambda|^{1/2} < C(1+\beta^{-1})$) such that (7.18) is a strictly positive operator on $\operatorname{ran} \widehat{P_\Omega}^{\perp}\widehat{P}_J$, (7.19) is a strictly positive operator on $\operatorname{ran}\left((\mathbb{1}_{L_{\mathrm{p}}\neq 0} \otimes P_\Omega)\widehat{P}_J\right)$ ($|\lambda|^{3/2} < C\delta_2^{(\beta)}$) and (7.20) is a strictly positive operator on $\operatorname{ran} \Pi\widehat{P}_J$ ($|\lambda|^{1/2} < C\delta_3^{(\beta,\varepsilon)}$).

The claim now follows in view of the decomposition (4.15). $\square$

7.3.2. Finitely Many Coupled Bound States

In this part we verify in case of finitely many coupled eigenmodes that the constants $\delta_1^{(\beta)}, \delta_2^{(\beta)}, \delta_3^{(\beta,\varepsilon)}$ appearing in (H1)–(H3) are actually positive. This shows the applicability of Theorem 7.10 for the proof of the main theorem. In this situation we have a gap between the discrete and essential spectrum, that is,

$$\max_{m \in J_{\mathrm{d}}} E_m < 0,$$

which turns out to be essential.

Proposition 7.11
Assume that J_{d} is finite and let $\chi = \chi_0 \chi_1(H_{\mathrm{p}})$, where χ_0 is defined as in (5.10) and χ_1 is a smooth function on $\mathbb{R}$ which satisfies

$$\chi_1(e) = \begin{cases} 0 & : e \leq \max_{m \in J_{\mathrm{d}}} E_m, \\ 1 & : e \geq 0. \end{cases}$$

Assume that Hypotheses A-LR and B-LR hold. Let $\beta_0 > 0$ and $\varepsilon > 0$. Then there exist constants $\delta_1, \delta_2, C > 0$ such that for all $\beta \geq \beta_0$, we have $\delta_1^{(\beta)} \geq \delta_1$, $\delta_2^{(\beta)} \geq \delta_2$ and $\delta_3^{(\beta,\varepsilon)} \geq C\gamma_\beta(\varepsilon, J_{\mathrm{d}})$, where the latter is defined as in (3.8). If the Fermi Golden Rule condition (3.9) is satisfied, $\gamma_\beta(\varepsilon, J_{\mathrm{d}}) > 0$.

Proof. First notice that χ satisfies Hypothesis C due to Proposition 5.7.

(H1) By definition of χ, we have $P_{\mathrm{ess}}\chi = P_{\mathrm{ess}}\chi_0$. Therefore, for all $\delta > 0$,

$$\begin{aligned} &P_{\mathrm{ess}}(\chi(-\Delta)\chi - \delta(w_{\mathsf{l}} + w_{1,\mathsf{l}}^{\mathrm{lr}}))P_{\mathrm{ess}} \\ &\qquad = P_{\mathrm{ess}}(\chi_0(-\Delta)\chi_0 - \delta(w_{\mathsf{l}} + w_{1,\mathsf{l}}^{\mathrm{lr}}))P_{\mathrm{ess}} \\ &\qquad \geq P_{\mathrm{ess}}(\chi_0(-\Delta)\chi_0 - C\delta(1+\beta^{-1})\langle \hat{\mathsf{x}} \rangle^{-4})P_{\mathrm{ess}} \end{aligned}$$

for some constant $C > 0$ where we used Lemma 7.7. By Proposition B.13 this expression is non-negative if we choose $\delta > 0$ small enough.

(H2) By assumption, $P_J G(k) P_J = G(k)$ for a.e. $k \in \mathbb{R}^3$. We conclude that for a.e. $(u, \Sigma) \in \mathbb{R} \times \mathbb{S}^2$ we have $P_J \tau_\beta(G)(u,\Sigma) P_J = \tau_\beta(G)(u,\Sigma)$, which implies

$$P_{\mathrm{disc}} T P_{\mathrm{disc}} = p_{J_{\mathrm{d}}} T p_{J_{\mathrm{d}}}, \qquad \text{for } T = w_{\mathsf{l}}, w_{\mathsf{r}}, w_{1,\mathsf{l}}^{\mathrm{lr}}, w_{1,\mathsf{r}}^{\mathrm{lr}}.$$

By Lemma 7.7, we find a constant C such that for all $\beta > 0$,

$$\begin{aligned} &P_{\mathrm{disc}}(w_{\mathsf{l}} + w_{1,\mathsf{l}}^{\mathrm{lr}})P_{\mathrm{disc}} \otimes P_{\mathrm{ess}} + P_{\mathrm{ess}} \otimes P_{\mathrm{disc}}(w_{\mathsf{r}} + w_{1,\mathsf{r}}^{\mathrm{lr}})P_{\mathrm{disc}} &\quad (7.21)\\ &\quad + \mathbb{1}_{L_{\mathrm{p}} \neq 0}(P_{\mathrm{disc}} w_{1,\mathsf{l}}^{\mathrm{lr}} P_{\mathrm{disc}} \otimes P_{\mathrm{disc}} + P_{\mathrm{disc}} \otimes P_{\mathrm{disc}} w_{1,\mathsf{r}}^{\mathrm{lr}} P_{\mathrm{disc}})\mathbb{1}_{L_{\mathrm{p}} \neq 0} \\ &\leq C(1+\beta^{-1})(p_{J_{\mathrm{d}}} \otimes P_{\mathrm{ess}} + P_{\mathrm{ess}} \otimes p_{J_{\mathrm{d}}} + P_{\mathrm{disc}} \otimes P_{\mathrm{disc}} \mathbb{1}_{L_{\mathrm{p}} \neq 0}). &\quad (7.22) \end{aligned}$$

The essential feature of finitely many eigenvalues is that there is no accumulation at zero. The distance between two different eigenvalues as well as the distance of eigenvalues to the essential spectrum starting at zero is bounded from below by a positive constant. Hence,

$$\Xi := \inf_{\substack{\lambda\in E(J_\mathrm{d}),\mu\in E(J_\mathrm{d})\cup\sigma_\mathrm{ess}(H_\mathrm{p}),\\ \lambda\neq\mu}} (\lambda-\mu)^2 > 0,$$

where $E(J_\mathrm{d}) := \{E_m : m \in J_\mathrm{d}\}$. We can estimate the projections in (7.22) by

$$(P_J\otimes P_J)(p_{J_\mathrm{d}}\otimes P_\mathrm{ess} + P_\mathrm{ess}\otimes p_{J_\mathrm{d}} + P_\mathrm{disc}\otimes P_\mathrm{disc}\mathbb{1}_{L_\mathrm{p}\neq 0})(P_J\otimes P_J) \le \mathbb{1}_{[\Xi,\infty)}(L_\mathrm{p}^2).$$

Recall that $Q = L_\mathrm{p}^2\mathbb{1}_{[0,1]}(L_\mathrm{p}^2) + \mathbb{1}_{(1,\infty)}(L_\mathrm{p}^2)$. Then, writing $C_\beta := C(1+\beta^{-1})$, we get for $\delta < \frac{\min\{\Xi,1\}}{C_{\beta_0}}$,

$$\begin{aligned} Q-&\delta C_\beta\mathbb{1}_{[\Xi,\infty)}(L_\mathrm{p}^2)\\ &= L_\mathrm{p}^2\mathbb{1}_{[0,\Xi)}(L_\mathrm{p}^2) + (L_\mathrm{p}^2-\delta C_\beta)\mathbb{1}_{[\Xi,1]}(L_\mathrm{p}^2) + (1-\delta C_\beta)\mathbb{1}_{(1,\infty)}(L_\mathrm{p}^2)\\ &> 0 \end{aligned}$$

on $\operatorname{ran}\mathbb{1}_{L_\mathrm{p}\neq 0}$.

(H3) Proposition 7.1 yields

$$\widehat{P}_J\Pi W R_\varepsilon^2 W\Pi\widehat{P}_J \ge \gamma_\beta(\varepsilon, J_\mathrm{d})\Pi\widehat{P}_J.$$

Again, we can use that the interaction terms are bounded, i.e., there is a constant C such that for all $\beta > 0$,

$$\widehat{P}_J\mathbb{1}_{L_\mathrm{p}=0}(P_\mathrm{disc}w_{1,\mathrm{l}}^\mathrm{lr}P_\mathrm{disc}\otimes P_\mathrm{disc}+P_\mathrm{disc}\otimes P_\mathrm{disc}w_{1,\mathrm{r}}^\mathrm{lr}P_\mathrm{disc})\mathbb{1}_{L_\mathrm{p}=0}\widehat{P}_J \le C(1+\beta^{-1})\Pi\widehat{P}_J.$$

This shows $\delta_3^{(\beta,\varepsilon)} \ge \frac{\gamma_\beta(\varepsilon,J_\mathrm{d})}{C(1+\beta_0^{-1})} > 0.$ $\square$

7.4. Short-Range

In the SR setting we proceed analogously as in the previous section. First we give some decay estimates for the interaction terms. Then we prove a lower bound for the first commutator with A^sr. Finally, Theorem 7.14 states that the total form $q_\mathrm{tot}^\mathrm{sr}$ is positive, where the conditions (H1)–(H3) and their verification are effectively included in the proof.

Lemma 7.12
There exist constants C independent of β such that, for $\alpha = \mathsf{l}, \mathsf{r}$,

(a) $\|I_\alpha\|^2_{L^2(\mathbb{R}\times\mathbb{S}^2,\mathcal{L}(\mathcal{H}_\mathrm{p}))} \leq C(1+\beta^{-1})$,

(b) $\left\|I^{\mathrm{sr}}_{1,\alpha}\right\|^2_{L^2(\mathbb{R}\times\mathbb{S}^2,\mathcal{L}(\mathcal{H}_\mathrm{p}))} \leq C(1+\beta^{-1})$,

(c) $P_{\mathrm{ess}} w_\alpha P_{\mathrm{ess}} \leq C(1+\beta^{-1}) V_\mathsf{c}^* \langle \hat{\mathsf{q}} \rangle^{-2} V_\mathsf{c}$,

(d) $P_{\mathrm{ess}} w^{\mathrm{sr}}_{1,\alpha} P_{\mathrm{ess}} \leq C(1+\beta^{-1}) V_\mathsf{c}^* \langle \hat{\mathsf{q}} \rangle^{-2} V_\mathsf{c}$.

Proof. By Proposition 6.2 we have

$$I_\alpha,\ I^{\mathrm{sr}}_{1,\alpha},\ I_\alpha V_\mathsf{c}^* \hat{\mathsf{q}}_j V_\mathsf{c},\ I^{\mathrm{sr}}_{1,\alpha} V_\mathsf{c}^* \hat{\mathsf{q}}_j V_\mathsf{c} \in L^2(\mathbb{R}\times\mathbb{S}^2,\mathcal{L}(\mathcal{H}_\mathrm{p})),$$

for all $j \in \{1,2,3\}$, $\alpha = \mathsf{l},\mathsf{r}$, and there is a constant C independent of β such that we can estimate the norm of these expressions by

$$C(1+\beta^{-1}).$$

Thus, the same applies to $I_\alpha V_\mathsf{c}^* \langle \hat{\mathsf{q}} \rangle V_\mathsf{c},\ I^{\mathrm{sr}}_{1,\alpha} V_\mathsf{c}^* \langle \hat{\mathsf{q}} \rangle V_\mathsf{c} \in L^2(\mathbb{R}\times\mathbb{S}^2,\mathcal{L}(\mathcal{H}_\mathrm{p}))$. Consequently, we obtain for $\alpha = \mathsf{l},\mathsf{r}$ and a constant $C > 0$ not depending on β,

$$\begin{aligned}
&P_{\mathrm{ess}} w_\alpha P_{\mathrm{ess}} \\
&\quad = V_\mathsf{c}^* \langle \hat{\mathsf{q}} \rangle^{-1} V_\mathsf{c} \int (I_\alpha(u,\Sigma) V_\mathsf{c}^* \langle \hat{\mathsf{q}} \rangle V_\mathsf{c})^* I_\alpha(u,\Sigma) V_\mathsf{c}^* \langle \hat{\mathsf{q}} \rangle V_\mathsf{c} \mathrm{d}(u,\Sigma) V_\mathsf{c}^* \langle \hat{\mathsf{q}} \rangle^{-1} V_\mathsf{c} \\
&\quad \leq C(1+\beta^{-1}) V_\mathsf{c}^* \langle \hat{\mathsf{q}} \rangle^{-2} V_\mathsf{c}.
\end{aligned}$$

The proof for $w^{\mathrm{sr}}_{1,\alpha}$ is analogous. □

Proposition 7.13
There exist constants $c_1, c_2 > 0$ such that for all $\beta > 0$ and all $\lambda \in \mathbb{R}$,

$$\begin{aligned}
C^{\mathrm{sr}}_1 \geq \Big[&V_\mathsf{c}^* \hat{\mathsf{k}}^2 V_\mathsf{c} \otimes \mathrm{Id}_\mathrm{p} + \mathrm{Id}_\mathrm{p} \otimes V_\mathsf{c}^* \hat{\mathsf{k}}^2 V_\mathsf{c} \\
&- c_1(1+\beta^{-1})\lambda^2 \Big(V_\mathsf{c}^* \langle \hat{\mathsf{q}} \rangle^{-2} V_\mathsf{c} \otimes \mathrm{Id}_\mathrm{p} + \mathrm{Id}_\mathrm{p} \otimes V_\mathsf{c}^* \langle \hat{\mathsf{q}} \rangle^{-2} V_\mathsf{c} + (P_{\mathrm{ess}} \otimes P_{\mathrm{ess}})^\perp\Big)\Big] \\
&\quad \otimes \mathrm{Id}_\mathrm{f} + c_2 \widehat{P_\Omega}^\perp
\end{aligned} \tag{7.23}$$

holds on $\mathcal{D}^{\mathrm{sr}}$. In particular, C^{sr}_1 is bounded from below and the lower bound (7.23) extends to the corresponding form q^{sr}_1.

Proof. As $I_1^{\mathrm{sr}} \in L^2(\mathbb{R} \times \mathbb{S}^2, \mathcal{L}(\mathcal{H}_\mathrm{p}))$ by Lemma 7.12, Lemma A.4 yields for any $\delta > 0$,

$$\pm\lambda W_1^{\mathrm{sr}} \le \delta \widehat{N}_\mathrm{f} + \frac{1}{\delta}\lambda^2 w_1^{\mathrm{sr}} \otimes \mathrm{Id}_\mathrm{f} \,.$$

Using this and the explicit form of C_1^{sr} on $\mathcal{D}^{\mathrm{sr}}$, we find

$$\begin{aligned} C_1^{\mathrm{sr}} &= V_\mathsf{c}^* \hat{\mathsf{k}}^2 V_\mathsf{c} \otimes \mathrm{Id}_\mathrm{p} + \mathrm{Id}_\mathrm{p} \otimes V_\mathsf{c}^* \hat{\mathsf{k}}^2 V_\mathsf{c} \otimes \mathrm{Id}_\mathrm{f} + \widehat{N}_\mathrm{f} + \lambda W_1^{\mathrm{sr}} \\ &\ge V_\mathsf{c}^* \hat{\mathsf{k}}^2 V_\mathsf{c} \otimes \mathrm{Id}_\mathrm{p} + \mathrm{Id}_\mathrm{p} \otimes V_\mathsf{c}^* \hat{\mathsf{k}}^2 V_\mathsf{c} \otimes \mathrm{Id}_\mathrm{f} + (1-\delta_1)\widehat{N}_\mathrm{f} - \frac{\lambda^2}{\delta_1} w_1^{\mathrm{sr}} \end{aligned}$$

for any $\delta_1 > 0$. By the operator inequality (5.4),

$$w_1^{\mathrm{sr}} \le 2(w_{1,\mathsf{l}}^{\mathrm{sr}} \otimes \mathrm{Id}_\mathrm{p} + \mathrm{Id}_\mathrm{p} \otimes w_{1,\mathsf{r}}^{\mathrm{sr}}).$$

Then, a decomposition into $\operatorname{ran} P_{\mathrm{ess}}$ and $\operatorname{ran} P_{\mathrm{disc}}$, the operator inequality (5.4) and subsequently Lemma 7.12 yield, for $\alpha = \mathsf{l}, \mathsf{r}$ and some constant C,

$$\begin{aligned} w_{1,\alpha}^{\mathrm{sr}} &\le 2(P_{\mathrm{ess}} w_{1,\alpha}^{\mathrm{sr}} P_{\mathrm{ess}} + P_{\mathrm{disc}} w_{1,\alpha}^{\mathrm{sr}} P_{\mathrm{disc}}) \\ &\le C(1+\beta^{-1})(V_\mathsf{c}^* \langle \hat{\mathsf{q}} \rangle^{-2} V_\mathsf{c} + P_{\mathrm{disc}}). \end{aligned}$$

Choosing any $0 < \delta_1 < 1$ shows (7.23) on $\mathcal{D}^{\mathrm{sr}}$. As $\mathcal{D}^{\mathrm{sr}}$ is a core for C_1^{sr}, it is also a form core for q_1^{sr}, so the operator inequality can be extended on $\mathcal{D}(q_1^{\mathrm{sr}})$ to the corresponding forms. □

After the preparations we are now able to put all the estimates of this chapter together in order to prove positivity.

Theorem 7.14
Let $\varepsilon > 0$ and $\beta_0 > 0$. Then there exists a constant C such that for all $\beta \ge \beta_0$ and $0 < |\lambda| < C \min\{1, \gamma_\beta(\varepsilon, \mathcal{M})^2\}$, we have $q_{\mathrm{tot}}^{\mathrm{sr}} > 0$ for $\theta = |\lambda|^{-1/2}$. That is, $q_{\mathrm{tot}}^{\mathrm{sr}} \ge 0$, and $q_{\mathrm{tot}}^{\mathrm{sr}}(\psi) = 0$ for some $\psi \in \mathcal{D}(q_1^{\mathrm{sr}}) \cap \mathcal{D}(L_\lambda)$ implies $\psi = 0$.

Proof. By Propositions 7.3, 7.5 and 7.13, and Lemma 7.12, we obtain in the sense of forms on $\mathcal{D}(q_1^{\mathrm{sr}})$,

$$\begin{aligned} q_{\mathrm{tot}}^{\mathrm{sr}} \ge \Big[& V_\mathsf{c}^* \hat{\mathsf{k}}^2 V_\mathsf{c} \otimes \mathrm{Id}_\mathrm{p} + \mathrm{Id}_\mathrm{p} \otimes V_\mathsf{c}^* \hat{\mathsf{k}}^2 V_\mathsf{c} - c_1(1+\beta^{-1})\lambda^2 \\ & \times \Big(V_\mathsf{c}^* \langle \hat{\mathsf{q}} \rangle^{-2} V_\mathsf{c} \otimes \mathrm{Id}_\mathrm{p} + \mathrm{Id}_\mathrm{p} \otimes V_\mathsf{c}^* \langle \hat{\mathsf{q}} \rangle^{-2} V_\mathsf{c} + (P_{\mathrm{ess}} \otimes P_{\mathrm{ess}})^\perp \Big) \Big] \otimes \mathrm{Id}_\mathrm{f} + c_2 \widehat{P_\Omega}^\perp \\ & + (1 - c_3 |\lambda|) 2\lambda^2 \Pi W R_\varepsilon^2 W \Pi - c_4(1+\beta^{-1}) |\lambda| \widehat{P_\Omega}^\perp \\ & \quad - c_5(1+\beta^{-1})\lambda^2 \mathbb{1}_{L_\mathrm{p} \neq 0} \Big(V_\mathsf{c}^* \langle \hat{\mathsf{q}} \rangle^{-2} V_\mathsf{c} \otimes \mathrm{Id}_\mathrm{p} + \mathrm{Id}_\mathrm{p} \otimes V_\mathsf{c}^* \langle \hat{\mathsf{q}} \rangle^{-2} V_\mathsf{c} \\ & \quad + (P_{\mathrm{ess}} \otimes P_{\mathrm{ess}})^\perp \Big) \mathbb{1}_{L_\mathrm{p} \neq 0} \otimes P_\Omega \\ & + (1 - c_6 |\lambda| (1+\beta^{-1})) Q \otimes P_\Omega - |\lambda| \widehat{P_\Omega}^\perp , \end{aligned}$$

for constants $c_i > 0$, $i \in \mathbb{N}$, independent of λ and β. Rearranging the terms, we find

$$
\begin{aligned}
q^{\mathrm{sr}}_{\mathrm{tot}} \geq V_{\mathsf{c}}^* &\left(\hat{\mathsf{k}}^2 - c_1\lambda^2(1+\theta)(1+\beta^{-1})\,\langle\hat{\mathsf{q}}\rangle^{-2}\right) V_{\mathsf{c}} \otimes \mathrm{Id}_{\mathrm{p}} \otimes \mathrm{Id}_{\mathrm{f}} \\
&+ \mathrm{Id}_{\mathrm{p}} \otimes V_{\mathsf{c}}^* \left(\hat{\mathsf{k}}^2 - c_1\lambda^2(1+\theta)(1+\beta^{-1})\,\langle\hat{\mathsf{q}}\rangle^{-2}\right) V_{\mathsf{c}} \otimes \mathrm{Id}_{\mathrm{f}} \\
&+ \Big(c_2 - c_3(1+\theta)\,|\lambda|\,(1+\beta^{-1})\Big)\,\widehat{P_\Omega}^{\perp} && (7.24)\\
&+ 2\theta\lambda^2(1-c_4\,|\lambda|)\gamma_\beta(\varepsilon)\Pi - c_5\lambda^2(1+\beta^{-1})\Pi && (7.25)\\
&+ \Big[\Big(1 - c_6\,|\lambda|\,(1+\beta^{-1})\Big)\,Q \\
&\qquad - c_7\lambda^2(1+\theta)(1+\beta^{-1})(P_{\mathrm{ess}}\otimes P_{\mathrm{ess}})^{\perp}\mathbb{1}_{L_{\mathrm{p}}\neq 0}\Big] \otimes P_\Omega, && (7.26)
\end{aligned}
$$

with other constants $c_i > 0$, $i \in \mathbb{N}$, independent of λ and β. Then we set $\theta = |\lambda|^{-1/2}$ in order to have a positive term in (7.25) of smaller order in $|\lambda|$. Next, we make $|\lambda| > 0$ sufficiently small in the following sense: First we make it so small such that, by the uncertainty principle lemma (cf. [RS2, section X.2])

$$
\hat{\mathsf{k}}^2 - \max\{c_1, c_2\}\lambda^2(1+|\lambda|^{-\frac{1}{2}})(1+\beta_0^{-1})\,\langle\hat{\mathsf{q}}\rangle^{-2} > 0.
$$

Furthermore, we can make it small enough such that we get strictly positive operators in (7.24) and (7.25) on $\operatorname{ran}\widehat{P_\Omega}^{\perp}$ and $\operatorname{ran}\Pi$, respectively. Note that we have to choose $|\lambda|$ small enough proportional to $\gamma_\beta(\varepsilon,\mathcal{M})^2$ due to (7.25). For the last term, we have

$$
(P_{\mathrm{ess}}\otimes P_{\mathrm{ess}})^{\perp}\mathbb{1}_{L_{\mathrm{p}}\neq 0} \leq \mathbb{1}_{[\Xi,\infty)}(L_{\mathrm{p}}^2),
$$

where

$$
\Xi := \inf_{\substack{\lambda\in\sigma_{\mathrm{disc}}(H_{\mathrm{p}}),\mu\in\sigma(H_p)\\ \lambda\neq\mu}} (\lambda-\mu)^2 > 0.
$$

Now we can plug in $Q = L_{\mathrm{p}}^2\mathbb{1}_{[0,1]}(L_{\mathrm{p}}^2) + \mathbb{1}_{(1,\infty)}(L_{\mathrm{p}}^2)$, and use that

$$
\begin{aligned}
Q - \delta\mathbb{1}_{[\Xi,\infty)}(L_{\mathrm{p}}^2) &= L_{\mathrm{p}}^2\mathbb{1}_{[0,\Xi)}(L_{\mathrm{p}}^2) + (L_{\mathrm{p}}^2-\delta)\mathbb{1}_{[\Xi,1]}(L_{\mathrm{p}}^2) + (1-\delta)\mathbb{1}_{(1,\infty)}(L_{\mathrm{p}}^2)\\
&> 0
\end{aligned}
$$

on $\operatorname{ran}\mathbb{1}_{L_{\mathrm{p}}\neq 0}$ for $\delta < \min\{\Xi, 1\}$. Thus, we can achieve that (7.26) is strictly positive on

$$
\operatorname{ran}(\mathbb{1}_{L_{\mathrm{p}}\neq 0}\otimes P_\Omega)
$$

for $|\lambda|$ small enough. The claim now follows in view of the decomposition (4.15). $\square$

A. Basic Theory

A.1. Second Quantization

Bosonic Fock spaces

The quantized field will be described by operators on Fock spaces. It is known from physics that the particles we consider, photons and phonons, are so-called bosonic particles. This means, they are indistinguishable and able to occupy the same quantum state. Mathematically this is reflected in the fact that the corresponding many-body wave functions commute in their arguments. Hence, in the construction we need a symmetrization of tensor products.

Definition A.1 (Bosonic Fock space)
For a Hilbert space $\mathfrak{h}$, also called the one-particle space, we set

$$\mathfrak{F}(\mathfrak{h}) := \mathbb{C} \oplus \bigoplus_{n=1}^{\infty} \mathfrak{h}^{\otimes_{\mathsf{s}} n},$$

where $\otimes_{\mathsf{s}} n$ is the n-times symmetric tensor product of Hilbert spaces (cf. [Asa17, section 2.9] for a detailed explanation), and the direct sum is to be understood as an infinite direct sum of Hilbert spaces (cf. [Asa17, section 4.1]).

For $\psi \in \mathfrak{F}(\mathfrak{h})$, we write ψ_n for the n-th element in the direct sum and we use the notation $\psi = (\psi_0, \psi_1, \psi_2, \ldots)$. The vacuum vector is defined as

$$\Omega := (1, 0, 0, \ldots).$$

For a subspace $\mathfrak{d} \subseteq \mathfrak{h}$ we define the space of finitely many particles in $\mathfrak{F}(\mathfrak{h})$ by

$$\begin{aligned} \mathfrak{F}_{\text{fin}}(\mathfrak{d}) :=&\{(\psi_0, \psi_1, \psi_2, \dots) \in \mathfrak{F}(\mathfrak{h}) : \psi_n \in \mathfrak{d}^{\hat{\otimes}_{\mathsf{s}} n} \text{ for all } n \in \mathbb{N}_0 \\ &\text{and there exists } N \in \mathbb{N}_0 : \psi_n = 0 \text{ for } n \geq N\}, \end{aligned}$$

where $\hat{\otimes}_{\mathsf{s}} n$ now represents n-times symmetric algebraic tensor product of vector spaces. If $\mathfrak{d}$ is dense in $\mathfrak{h}$, one can show that $\mathfrak{F}_{\text{fin}}(\mathfrak{d})$ is dense in $\mathfrak{F}(\mathfrak{h})$ as well.

Second quantization of operators

We can naturally lift unitary and self-adjoint operators from $\mathfrak{h}$ to $\mathfrak{F}(\mathfrak{h})$ (cf. [RS2, section X.7]). Let U be a unitary operator on $\mathfrak{h}$. We define a unitary operator $\Gamma(U)$ on $\mathfrak{F}(\mathfrak{h})$ by

$$(\Gamma(U)\psi)_n := \begin{cases} \psi_0 & : n = 0, \\ (\underbrace{U \otimes \cdots \otimes U}_{n \text{ times}})\psi_n & : n \geq 1. \end{cases}$$

Let A be a self-adjoint operator on $\mathfrak{h}$ and $\mathcal{D}(A)$ a core for A. For $\psi \in \mathfrak{F}_{\text{fin}}(\mathcal{D}(A))$ we define $(\mathsf{d}\Gamma(A)\psi)_0 := 0$ and for $n \geq 1$,

$$\begin{aligned}&(\mathsf{d}\Gamma(A)\psi)_n \\ &\quad := (A \otimes \mathrm{Id}_{\mathfrak{h}} \otimes \cdots \otimes \mathrm{Id}_{\mathfrak{h}} + \mathrm{Id}_{\mathfrak{h}} \otimes A \otimes \cdots \otimes \mathrm{Id}_{\mathfrak{h}} + \ldots + \mathrm{Id}_{\mathfrak{h}} \otimes \cdots \otimes \mathrm{Id}_{\mathfrak{h}} \otimes A)\psi_n.\end{aligned}$$

It is well-known that $\mathsf{d}\Gamma(A)$, the so-called *second quantization* of A, is essentially self-adjoint on $\mathfrak{F}_{\text{fin}}(\mathcal{D}(A))$. In the following its self-adjoint extension shall be denoted by the same symbol $\mathsf{d}\Gamma(A)$. The second quantization of A can also be obtained as self-adjoint generator of the strongly-continuous unitary group $t \mapsto \Gamma(e^{\mathrm{i}tA})$ (cf. [Asa17, section 4.11]):

$$\Gamma(e^{\mathrm{i}tA}) = e^{\mathrm{i}t\mathsf{d}\Gamma(A)}, \qquad t \in \mathbb{R}.$$

A very important example of a second-quantized operator is the *number operator*

$$N_{\mathrm{f}} := \mathsf{d}\Gamma(\mathrm{Id}_{\mathfrak{h}}).$$

Its domain is explicitly given by

$$\mathcal{D}(N_{\mathrm{f}}) = \{\psi \in \mathfrak{F}(\mathfrak{h}) : \sum_{n=1}^{\infty} n^2 \left\|\psi_n\right\|^2 < \infty\}.$$

Generalized creation and annihilation operators on L^2 spaces

Let $(\mathbb{X}, \mu)$ be a measure space. We use the abbreviations $L^2(\mathbb{X}) := L^2(\mathbb{X}, \mu)$, and write

$$\int_{\mathbb{X}} \overline{f(X)} g(X) \mathrm{d}X := \int_{\mathbb{X}} \overline{f} g \mathrm{d}\mu.$$

for its inner product. In the following we write $\mathfrak{F} := \mathfrak{F}(L^2(\mathbb{X}, \mu))$ and $\mathfrak{F}_{\text{fin}} := \mathfrak{F}_{\text{fin}}(L^2(\mathbb{X}, \mu))$. For $\psi \in \mathfrak{F}$ notice that ψ_n, $n \geq 1$, can be understood as an L^2 function in n symmetric variables $X_i \in \mathbb{X}$, $i = 1, \ldots, n$. The space of all such functions will be denoted by $L^2_{\mathsf{s}}(\mathbb{X}^n, \mu)$. Furthermore, we can tensorize the Fock space with another Hilbert space $\mathcal{H}$ usually describing another system interacting with the field and use the natural identification

$$\mathcal{H} \otimes \mathfrak{F} \cong \bigoplus_{n=0}^{\infty} \mathcal{H} \otimes L^2_{\mathsf{s}}(\mathbb{X}^n) \cong \bigoplus_{n=0}^{\infty} L^2_{\mathsf{s}}(\mathbb{X}^n, \mathcal{H}),$$

where $L^2_{\mathsf{s}}(\mathbb{X}^n, \mathcal{H})$ is the Bochner space of symmetric square-integrable $\mathcal{H}$-valued functions. That is, we can write any element $\psi \in \mathcal{H} \otimes \mathfrak{F}$ as sequence $(\psi_0, \psi_1, \psi_2, \dots)$ where $\psi_n \in L^2_{\mathsf{s}}(\mathbb{X}^n, \mathcal{H})$ and we define again $(\mathcal{H} \otimes \mathfrak{F})_{\text{fin}}$ as the space of all such sequences where all but finitely many entries vanish. Now, on $(\mathcal{H} \otimes \mathfrak{F})_{\text{fin}}$ we introduce the (generalized) creation and annihilation operator for a function $F \in L^2(\mathbb{X}, \mathcal{L}(\mathcal{H}))$ and $\psi \in \mathcal{H} \mathbin{\widehat{\otimes}} \mathfrak{F}_{\text{fin}}$,

$$\begin{aligned}
(a(F)\psi)_n(X_1, \dots, X_n) &:= \sqrt{n+1} \int F(X)^* \psi_{n+1}(X, X_1, \dots, X_n) \mathrm{d}X, \quad n \in \mathbb{N}_0, \\
(a^*(F)\psi)_n(X_1, \dots, X_n) &:= n^{-\frac{1}{2}} \sum_{i=1}^{n} F(X_i) \psi_{n-1}(X_1, \dots, \hat{X}_i, \dots, X_n), \quad n \in \mathbb{N},
\end{aligned}$$

and set $(a^*(F)\psi)_0 := 0$. The symbol $\hat{X}_i$ represents the omission of the i-th argument. Note that $a(F)\Omega = 0$, and that both operators leave the space $(\mathcal{H} \otimes \mathfrak{F})_{\text{fin}}$ invariant. Moreover, as the notation suggests, both operators are formally adjoint to each other on that space. By definition, $F \mapsto a^*(F)$ is linear whereas $F \mapsto a(F)$ is anti-linear in F.

Next, we define the field operators on $(\mathcal{H} \otimes \mathfrak{F})_{\text{fin}}$ as

$$\Phi(F) := a(F) + a^*(F), \qquad F \in L^2(\mathbb{X}, \mathcal{L}(\mathcal{H})). \tag{A.1}$$

It is easy to see that $\Phi(F)$ is symmetric and in fact also essentially self-adjoint (cf. [RS2, Theorem X.41] for the classical case $\mathcal{H}_{\mathrm{p}} = \mathbb{C}$, which can be transferred to our cases using the estimates of Lemma A.3). Their self-adjoint extension will be denoted by the same symbol. Furthermore, we have by definition on $(\mathcal{H} \otimes \mathfrak{F})_{\text{fin}}$,

$$\begin{aligned}
a^*(F) &= \frac{1}{2}(\Phi(F) - \mathrm{i}\Phi(\mathrm{i}F)), \\
a(F) &= \frac{1}{2}(\Phi(F) + \mathrm{i}\Phi(\mathrm{i}F)).
\end{aligned}$$

In the classical case $\mathcal{H}_{\mathrm{p}} = \mathbb{C}$, $\mathcal{H}_{\mathrm{p}} \otimes \mathfrak{F} \cong \mathfrak{F}$, the creation and annihilation operators satisfy the canonical commutation relations (cf. [Asa17, section 5.7.2])

$$[a(f), a^*(g)] = \langle f, g \rangle, \qquad [a(f), a(g)] = 0, \qquad [a^*(f), a^*(g)] = 0,$$

for all $f, g \in L^2(\mathbb{X})$. Furthermore, it is important to note that finite products of creation operators applied to the vacuum span the dense subspace $\mathfrak{F}_{\text{fin}}$. The same is true for the field operators.

Lemma A.2
For a dense subspace $\mathfrak{d} \subseteq L^2(\mathbb{X})$ *the sets*

$$\begin{aligned}\operatorname{lin}\{a^*(f_1)\dots a^*(f_n)\Omega : n \in \mathbb{N},\ f_1,\dots,f_n \in \mathfrak{d}\},\\ \operatorname{lin}\{\Phi(f_1)\dots \Phi(f_n)\Omega : n \in \mathbb{N},\ f_1,\dots,f_n \in \mathfrak{d}\},\end{aligned}$$

equal $\mathfrak{F}_{\mathrm{fin}}(\mathfrak{d})$ *and therefore are dense in* $\mathfrak{F}$.

Proof. It is clear for the first set and for the second one it follows by applying the canonical commutation relations (cf. [Asa17, Proposition 5.14]). □

For a function $\omega\colon \mathbb{X} \to \mathbb{R}$ we just write ω for the corresponding multiplication operator on $L^2(\mathbb{X})$. The following classical estimates for creation and annihilation operators will be often used in the thesis.

Lemma A.3
Let $\omega\colon \mathbb{X} \to \mathbb{R}$ *be measurable and* $\omega > 0$ *almost everywhere. Furthermore assume that* $F, \frac{F}{\sqrt{\omega}} \in L^2(\mathbb{X}, \mathcal{L}(\mathcal{H}))$*, Then for all* $\psi \in \mathcal{H} \mathbin{\widehat{\otimes}} \mathfrak{F}_{\mathrm{fin}}$*,*

$$\begin{aligned}\|a(F)\psi\| &\le \left\|\frac{F}{\sqrt{\omega}}\right\| \left\|\mathrm{Id}_{\mathcal{H}} \otimes \mathsf{d}\Gamma(\omega)^{1/2}\psi\right\|,\\ \|a^*(F)\psi\| &\le \left\|\frac{F}{\sqrt{\omega}}\right\| \left\|(\mathrm{Id}_{\mathcal{H}} \otimes \mathsf{d}\Gamma(\omega)+1)^{1/2}\psi\right\|,\end{aligned}$$

so the operators can be uniquely extended to $\mathcal{D}(\mathrm{Id}_{\mathfrak{h}} \otimes \mathsf{d}\Gamma(\omega)^{1/2})$ *and will be denoted by the same symbols. In particular, we get for* $\psi \in \mathcal{D}(\mathrm{Id}_{\mathfrak{h}} \otimes N_{\mathrm{f}}^{1/2})$*,*

$$\begin{aligned}\|a(F)\psi\| &\le \|F\| \left\|(\mathrm{Id}_{\mathcal{H}} \otimes N_{\mathrm{f}})^{1/2}\psi\right\|,\\ \|a^*(F)\psi\| &\le \|F\| \left\|(\mathrm{Id}_{\mathcal{H}} \otimes N_{\mathrm{f}}+1)^{1/2}\psi\right\|.\end{aligned}$$

Proof. The estimates for the case $\mathcal{H}_{\mathrm{p}} = \mathbb{C}$ can be found in [Asa17, section 5.8.1] and one can mimic the proof to cover also the more general case, see for example [Lan18, Lemma 3.3.12] or [BFS98a]. □

Lemma A.4
Let $F \in L^2(\mathbb{X}, \mathcal{L}(\mathcal{H}))$*, and assume we have a* $T \in \mathcal{L}(\mathcal{H} \otimes \mathfrak{F})$ *which leaves* $\mathcal{D}(\mathrm{Id}_{\mathcal{H}} \otimes N_{\mathrm{f}})$ *invariant. Then it holds on* $\mathcal{D}(\mathrm{Id}_{\mathcal{H}} \otimes N_{\mathrm{f}})$ *for all* $\delta > 0$*,*

$$T^*a(F) + a^*(F)T \le \delta\, \mathrm{Id}_{\mathcal{H}} \otimes N_{\mathrm{f}} + \delta^{-1} T^* \left(\int F(X)^* F(X) \mathrm{d}X \otimes \mathrm{Id}_{\mathfrak{F}}\right) T.$$

Proof. By the definition of $a(F)$ we have

$$\langle T\psi, a(F)\psi\rangle = \sum_{n=0}^{\infty} \sqrt{n+1} \int \langle (T\psi)_n(X_1,\dots,X_n), F^*(X)\psi_{n+1}(X,X_1,\dots,X_n)\rangle \\ \mathrm{d}(X,X_1,\dots,X_n).$$

Thus,

$$\begin{aligned} |\langle T\psi, a(F)\psi\rangle| &\leq \frac{1}{2}\sum_{n=0}^{\infty}\int \Big(\delta \left\|F(X)(T\psi)_n(X_1,\dots,X_n)\right\|^2 \\ &\qquad + \delta^{-1}(n+1)\left\|\psi_{n+1}(X,X_1,\dots,X_n)\right\|^2\Big)\mathrm{d}(X,X_1,\dots,X_n) \\ &\leq \frac{\delta}{2}\int \langle \psi, T^*(F(X)^*F(X)\otimes \mathrm{Id}_{\mathfrak{F}})T\psi\rangle \,\mathrm{d}X + \frac{\delta^{-1}}{2}\langle \psi, \mathrm{Id}_{\mathcal{H}}\otimes N_{\mathrm{f}}\psi\rangle . \end{aligned}$$ □

Lemma A.5
Let $\omega\colon \mathbb{X}\to\mathbb{R}$ be a measurable function and let $F \in L^2(\mathbb{X},\mathcal{L}(\mathcal{H}))$ such that $\omega F \in L^2(\mathbb{X},\mathcal{L}(\mathcal{H}))$. Then we have on $(\mathcal{H}\otimes\mathfrak{F})_{\mathrm{fin}} \cap \mathcal{D}(\mathrm{Id}_{\mathcal{H}}\otimes \mathsf{d}\Gamma(\omega))$,

$$\begin{aligned} [\mathrm{Id}_{\mathcal{H}}\otimes \mathsf{d}\Gamma(\omega), a^*(F)] &= a^*(\omega F), \\ [a(F), \mathrm{Id}_{\mathcal{H}}\otimes \mathsf{d}\Gamma(\omega)] &= a(\omega F). \end{aligned}$$

Proof. Notice that for $\psi \in (\mathcal{H}\otimes\mathfrak{F})_{\mathrm{fin}} \cap \mathcal{D}(\mathrm{Id}_{\mathcal{H}}\otimes \mathsf{d}\Gamma(\omega))$,

$$(\mathrm{Id}_{\mathfrak{h}}\otimes \mathsf{d}\Gamma(\omega)\psi)_n(X_1,\dots,X_n) = \sum_{j=1}^{n}\omega(X_j)\psi_n(X_1,\dots,X_n).$$

Combining this with the definition of the creation and annihilation operators yields the given formulas. □

Tensor product of Fock spaces

The Fock space over a direct sum of Hilbert spaces can be identified in a natural way with the tensor product of the two Fock spaces of the respective spaces.

Theorem A.6 (cf. [JP96a] and [Asa17, Theorem 5.38])
Let $\mathfrak{h}_1$ and $\mathfrak{h}_2$ be separable Hilbert spaces. There exists a unitary map

$$U\colon \mathfrak{F}(\mathfrak{h}_1)\otimes\mathfrak{F}(\mathfrak{h}_2) \longrightarrow \mathfrak{F}(\mathfrak{h}_1\oplus\mathfrak{h}_2)$$

with the following properties:

(1) $U(\Omega_{\mathfrak{h}_1} \otimes \Omega_{\mathfrak{h}_2}) = \Omega_{\mathfrak{h}_1 \oplus \mathfrak{h}_2}$.

(2) $U(\mathfrak{F}_{\text{fin}}(\mathfrak{h}_1) \widehat{\otimes} \mathfrak{F}_{\text{fin}}(\mathfrak{h}_1)) = \mathfrak{F}_{\text{fin}}(\mathfrak{h}_1 \oplus \mathfrak{h}_2)$.

(3) For unitary operators u_1, u_2 on $\mathfrak{h}_1$, $\mathfrak{h}_2$, we have

$$U(\Gamma(u_1) \otimes \Gamma(u_2))U^{-1} = \Gamma(u_1 \oplus u_2).$$

(4) For self-adjoint operators T_1, T_2 on $\mathfrak{h}_1$, $\mathfrak{h}_2$, we have

$$U\overline{\mathsf{d}\Gamma(T_1) \otimes \mathrm{Id} + \mathrm{Id} \otimes \mathsf{d}\Gamma(T_2)}U^{-1} = \mathsf{d}\Gamma(T_1 \oplus T_2).$$

(5) If $\mathfrak{h}_1$ and $\mathfrak{h}_2$ are two L^2 spaces and $f \in \mathfrak{h}_1$, $g \in \mathfrak{h}_2$, we have

$$U\overline{a^*(f) \otimes \mathrm{Id} + \mathrm{Id} \otimes a^*(g)}U^{-1} = a^*(f \oplus g),$$
$$U\overline{a(f) \otimes \mathrm{Id} + \mathrm{Id} \otimes a(g)}U^{-1} = a(f \oplus g).$$

A.2. Special Topics of Operator Algebras

A.2.1. Tensor Products

In the thesis we use multiple times tensor products of C^*-algebras as well as states and morphisms operating on them. As there are different C^*-norms on the *algebraic* tensor product of two C^*-algebras with the multiplicative property

$$\|A \otimes B\| = \|A\| \, \|B\| \, ,$$

we want to clarify here that we only consider the *minimal* (also called *spatial*) norm. We recall the definition and some properties we need, especially in Chapter 2. A detailed reference for tensor products can be found in [Ols94], a brief description also in [Brü99] and [BR2].

Definition A.7 (Spatial tensor product)
Let $\mathfrak{A}_1$, $\mathfrak{A}_2$ be C^*-algebras. The spatial tensor product $\mathfrak{A}_1 \otimes \mathfrak{A}_2$ is the completion of the algebraic tensor product $\mathfrak{A}_1 \mathbin{\widehat{\otimes}} \mathfrak{A}_2$ with respect to the spatial C^*-norm, that is, for $A \in \mathfrak{A}_1 \mathbin{\widehat{\otimes}} \mathfrak{A}_2$,

$$\|A\| := \|(\pi_1 \otimes \pi_2)(A)\|_{\mathcal{L}(\mathcal{H}_1 \otimes \mathcal{H}_2)} \, ,$$

where for $i = 1, 2$, π_i is some faithful representation of $\mathfrak{A}_i$ on a Hilbert space $\mathcal{H}_i$, and

$$(\pi_1 \otimes \pi_2)\left(\sum_i A_i^{(1)} \otimes A_i^{(2)}\right) := \sum_i \pi_1(A_i^{(1)}) \otimes \pi_2(A_i^{(2)}).$$

One can show that the definition is independent of the choice of π_1 and π_2. A key property for our application is a natural embedding for the tensor product, that is,

$$\mathfrak{A}_1 \otimes \mathfrak{A}_2 \subseteq \mathcal{L}(\mathcal{H}_1 \otimes \mathcal{H}_2).$$

for C^*-algebras $\mathfrak{A}_i \subseteq \mathcal{L}(\mathcal{H}_i)$, and Hilbert spaces $\mathcal{H}_i$, $i = 1, 2$.

Furthermore, we can extend $*$-morphisms to the tensor product.

Proposition A.8
For $i = 1, 2$, let $\mathfrak{A}_i$, $\mathfrak{B}_i$ be C^*-algebras and let $\phi_i \colon \mathfrak{A}_i \to \mathfrak{B}_i$ be $*$-morphisms. Then there exists a unique $*$-morphism

$$\phi_1 \otimes \phi_2 \colon \mathfrak{A}_1 \otimes \mathfrak{A}_2 \longrightarrow \mathfrak{B}_1 \otimes \mathfrak{B}_2,$$

such that

$$(\phi_1 \otimes \phi_2)(A_1 \otimes A_2) = \phi_1(A_1) \otimes \phi_2(A_2), \;\; A_1 \in \mathfrak{A}_1, \;\; A_2 \in \mathfrak{A}_2.$$

Furthermore, if ϕ_1 and ϕ_2 are injective, so is $\phi_1 \otimes \phi_2$.

Corollary A.9
Let $\mathfrak{A}_1$, $\mathfrak{A}_2$ be C^*-algebras.

(a) If π_i is a representation of $\mathfrak{A}_i$ on $\mathcal{L}(\mathcal{H}_i)$, $i = 1, 2$, then $\pi_1 \otimes \pi_2$ is a representation of $\mathfrak{A}_1 \otimes \mathfrak{A}_2$ on $\mathcal{H}_1 \otimes \mathcal{H}_2$.

(b) If ω_i is a state on $\mathfrak{A}_i$, $i = 1, 2$, then $\omega_1 \otimes \omega_2$ (in the sense of Proposition A.8 as a $*$-morphism to $\mathbb{C}$) is a state on $\mathfrak{A}_1 \otimes \mathfrak{A}_2$.

(c) If ω_i is a state on $\mathfrak{A}_i$, and $(\pi_i, \mathcal{H}_i, \Omega_i)$ the GNS representation with respect to ω_i, $i = 1, 2$, then $(\pi_1 \otimes \pi_2, \mathcal{H}_1 \otimes \mathcal{H}_2, \Omega_1 \otimes \Omega_2)$ is the GNS representation of $\mathfrak{A}_1 \otimes \mathfrak{A}_2$ with respect to $\omega_1 \otimes \omega_2$.

A.2.2. Some Aspects of Modular Theory

In this subsection we collect some results of modular theory for von Neumann algebras. For more details we refer the reader to [KR97] or [BR2]. Let $\mathfrak{M}$ be a von Neumann algebra operating on a Hilbert space $\mathcal{H}$. Let $\Omega \in \mathcal{H}$ be *cyclic*, i.e.,

$$\overline{\{A\Omega : A \in \mathfrak{M}\}} = \mathcal{H},$$

and *separating*, i.e., that is, $A\Omega = 0$ for some $A \in \mathfrak{M}$ implies $A = 0$. We define an antilinear operator

$$S_0 \colon \mathcal{D}(S_0) \subseteq \mathcal{H} \longrightarrow \mathcal{H}, \;\; A\Omega \mapsto A^*\Omega,$$

on the dense domain $\mathcal{D}(S_0) := \{A\Omega : A \in \mathfrak{M}\}$. One can show that S_0 is closable (cf. [BR1, Proposition 2.5.9]) and its closure shall be denoted by S. By the polar decomposition of S one obtains a unique positive self-adjoint operator $\Delta_{\mathfrak{M}}$ and a unique antiunitary operator J such that

$$S = J\sqrt{\Delta_{\mathfrak{M}}}.$$

Definition A.10
One calls $\Delta_{\mathfrak{M}}$ the modular operator and J the modular conjugation associated to $(\mathfrak{M}, \Omega)$.

One of the main results of Tomita-Takesaki theory we will use is that the conjugation with J yields all elements which commute with all other elements of the algebra.

Theorem A.11 (Tomita's theorem)
We have $J\Omega = \Delta_{\mathfrak{M}}\Omega = \Omega$, and

$$J\mathfrak{M}J = \mathfrak{M}', \qquad \Delta_{\mathfrak{M}}^{\mathrm{i}t}\mathfrak{M}\Delta_{\mathfrak{M}}^{-\mathrm{i}t} = \mathfrak{M},\ t \in \mathbb{R}.$$

Another object we want to introduce is the so-called natural cone. It is of great importance in our setting, because each normal state can be represented uniquely by a vector in this cone.

Definition A.12 (Positive cone)
The natural positive cone $\mathcal{P}$ associated to $(\mathfrak{M}, \Omega)$ is defined as the closure of the set

$$\{AJA\Omega : A \in \mathfrak{M}\}.$$

Theorem A.13 (cf. [BR2, Theorem 2.5.31])
For each normal state ω there exists a unique $\xi \in \mathcal{P}$ such that for all $A \in \mathfrak{M}$,

$$\omega(A) = \omega_\xi(A) := \langle \xi, A\xi \rangle\,.$$

B. Technical Requirements

This part contains some variations of different well-known concepts, which could not be found explicitly in the literature, but whose proofs are rather straightforward.

In the following we assume that $H_\mathrm{p} = -\Delta + V$ is a Schrödinger operator on $L^2(\mathbb{R}^d)$ in some dimension $d \in \mathbb{N}$. $V \leq 0$ is a bounded continuous function with $V(x) \to 0$ as $|x| \to \infty$. Furthermore, we choose a constant $C_\mathrm{p} > 0$ big enough such that $\inf H_\mathrm{p} + C_\mathrm{p} > 0$ and $\|(-\Delta + C_\mathrm{p})^{-1} V\| < 1$. For $t \geq 0$, we set $R_\mathrm{p}(t) := (H_\mathrm{p} + C_\mathrm{p} + t)^{-1}$, $R_\mathrm{p} := R_\mathrm{p}(0)$ and $\chi_0 := R_\mathrm{p}^{1/2}$.

B.1. Combes Thomas Estimates

Combes Thomas estimates, tracing back originally to ideas of [CT73], describe an exponential decay of Green's functions of Schrödinger operators. A classical result for Schrödinger operators in $\mathbb{R}^d$ can be found in [Sim82] and a result for generalized Schrödinger operators in $\mathbb{R}^d$ with the explicit statement of the constants in [GK03]. In our setting we need a Combes Thomas estimate for the operators

$$\hat{\mathsf{p}}_j^s (H_\mathrm{p} + C_\mathrm{p})^{-1/2} \hat{\mathsf{p}}_j^t, \quad j \in \{1, \dots, d\},\ s, t \in \{0, 1\}, s + t \leq 1, \tag{B.1}$$

which does not seem to available explicitly in the literature. In this section we assume that V is differentiable and its derivative is bounded.

B.1.1. Standard Version

First, we recall a standard version of a Combes Thomas estimate for Schrödinger operators. This could also be deduced from [GK03]. However, we rather give a short direct proof, as the techniques here are reused in the second part to discuss the operators (B.1).

In the following let $\langle x \rangle_\beta := (\beta + x^2)^{\frac{1}{2}}$ for $\beta \geq 0$ and recall that $\langle x \rangle = \langle x \rangle_1$.

Lemma B.1
There exists a $\delta > 0$ such that for all $W \in C^2(\mathbb{R}^d)$, which are bounded from below,

satisfying $\sup_x |\nabla W(x)| < \delta$ *and* $\sup_x |\Delta W(x)| < \delta$, *and all* $t \geq 0$, *we have*

$$\left\| e^{-W} R_{\mathrm{p}}(t) e^{W} \Big|_{C_{\mathsf{c}}^{\infty}(\mathbb{R}^d)} \right\| \leq \frac{C}{1+t}$$

for some constant C *independent of* t.

Proof. We set on $\mathcal{D}(\hat{\mathsf{p}}^2)$,

$$H_W := H_{\mathrm{p}} + D_W, \tag{B.2}$$

where we define on $C_{\mathsf{c}}^{\infty}(\mathbb{R}^d)$,

$$D_W := e^{-W}[\hat{\mathsf{p}}^2, e^W] = -\Delta W - (\nabla W)^2 - 2\mathrm{i}\nabla W \hat{\mathsf{p}}, \tag{B.3}$$

which clearly extends to $\mathcal{D}(\hat{\mathsf{p}}^2)$. By assumption, there is for all $\epsilon > 0$ a $\delta > 0$ such that for all $W \in C^2(\mathbb{R}^d)$ with $\sup_x |\nabla W(x)| < \delta$ and $\sup_x |\Delta W(x)| < \delta$,

$$\|D_W \psi\| \leq \epsilon(\|H_{\mathrm{p}}\psi\| + \|\psi\|), \qquad \psi \in \mathcal{D}(H_{\mathrm{p}}).$$

We can now choose $\epsilon > 0$ (and therefore accordingly $\delta > 0$) small enough such that $\|D_W R_{\mathrm{p}}(t)\| \leq \frac{1}{2}$ for all $t \geq 0$. Then,

$$H_W + C_{\mathrm{p}} + t = (H_{\mathrm{p}} + C_{\mathrm{p}} + t)(1 + R_{\mathrm{p}}(t) D_W)$$

is invertible. Now, we have on $\mathcal{D}(\Delta)$, on the level of measurable functions (the single operators do not map L^2 functions necessarily into L^2 functions),

$$H_W = e^{-W}(-\Delta + V)e^W.$$

Notice by the explicit form of D_W we do not have $e^W\psi \in \mathcal{D}(\Delta)$ for $\psi \in \mathcal{D}(\Delta)$, but $e^W\psi$ is still two times weakly differentiable. Thus, for $\psi \in C_{\mathsf{c}}^{\infty}(\mathbb{R}^d)$,

$$\begin{aligned} \left\| e^{-W} R_{\mathrm{p}}(t) e^W \psi \right\| &= \left\| (H_W + C_{\mathrm{p}} + t)^{-1} (H_W + C_{\mathrm{p}} + t) e^{-W} R_{\mathrm{p}}(t) p^s e^W \psi \right\| \\ &= \left\| (H_W + C_{\mathrm{p}} + t)^{-1} \psi \right\| \\ &= \left\| (1 + R_{\mathrm{p}}(t) D_W)^{-1} R_{\mathrm{p}}(t) \psi \right\|. \end{aligned}$$

Since $D_W R_{\mathrm{p}}(t)$ is bounded independently of $t \geq 0$ and $\|R_{\mathrm{p}}(t)\| \leq \frac{C}{1+t}$ for some constant C, this yields the desired statement. □

In particular, the exponential decay allows us to conclude that the kernel of the resolvent decays faster than any polynomial. This is the content of the following proposition.

Proposition B.2
For all $\alpha \in \mathbb{R}$, we have for all $t \geq 0$,

$$\left\| \langle \hat{\mathsf{x}} \rangle^{-\alpha} R_{\mathrm{p}}(t) \langle \hat{\mathsf{x}} \rangle^{\alpha} \big|_{C_{\mathsf{c}}^{\infty}(\mathbb{R}^d)} \right\| \leq \frac{C}{1+t} \tag{B.4}$$

for some constant C independent of t. In particular, (B.4) is well-defined for $\alpha < 0$, i.e., $(H_{\mathrm{p}} + C_{\mathrm{p}})^{-1}$ maps $\mathcal{D}(|\hat{\mathsf{x}}|^{\alpha})$ to $\mathcal{D}(|\hat{\mathsf{x}}|^{\alpha})$ for all $\alpha > 0$.

Proof. We first consider the case $\alpha \geq 0$. For $\beta > 0$ we set $W(x) = \alpha \ln(\beta + x^2)$. A direct calculation yields $\sup_x |\nabla W(x)| \leq C\beta^{-1/2}$ and $\sup_x |\Delta W(x)| \leq C\beta^{-1}$ for some constants C not depending on β. We make $\beta > 0$ big enough and therefore also the derivatives of W small enough such that Lemma B.1 is applicable. Then it follows that

$$\langle \hat{\mathsf{x}} \rangle^{-\alpha} (H_{\mathrm{p}} + C_{\mathrm{p}})^{-1} \langle \hat{\mathsf{x}} \rangle^{\alpha} = \langle \hat{\mathsf{x}} \rangle^{-\alpha} \langle \hat{\mathsf{x}} \rangle_{\beta}^{\alpha} \langle \hat{\mathsf{x}} \rangle_{\beta}^{-\alpha} (H_{\mathrm{p}} + C_{\mathrm{p}})^{-1} \langle \hat{\mathsf{x}} \rangle_{\beta}^{\alpha} \langle \hat{\mathsf{x}} \rangle_{\beta}^{-\alpha} \langle \hat{\mathsf{x}} \rangle^{\alpha}$$

is bounded on $C_{\mathsf{c}}^{\infty}(\mathbb{R}^d)$ and extends to $\mathcal{D}(|\hat{\mathsf{x}}|^{\alpha})$. This also shows that $(H_{\mathrm{p}} + C_{\mathrm{p}})^{-1}$ leaves $\mathcal{D}(|\hat{\mathsf{x}}|^{\alpha})$ invariant, and the boundedness of

$$\langle \hat{\mathsf{x}} \rangle^{\alpha} \hat{\mathsf{p}}_j^{s} (H_{\mathrm{p}} + C_{\mathrm{p}})^{-1/2} \hat{\mathsf{p}}_j^{t} \langle \hat{\mathsf{x}} \rangle^{-\alpha}$$

follows since it is the adjoint operator. □

B.1.2. Square Root of the Resolvent

Now, the operators (B.1) can be discussed. The main idea is to use the relation

$$(H_{\mathrm{p}} + C_{\mathrm{p}})^{-1/2} = \frac{1}{\pi} \int_0^{\infty} \frac{1}{\sqrt{t}} R_{\mathrm{p}}(t) \mathrm{d}t, \tag{B.5}$$

and apply the standard Combes Thomas estimate. We start with two technical preparatory lemmas.

Lemma B.3
Let

$$\xi \colon \mathbb{R}^d \times \mathbb{R}_+ \longrightarrow \mathbb{R}, \ \xi(p,t) := \sqrt{\frac{p^2 + C_{\mathrm{p}} + t}{|p| + 1}}.$$

For all $t \geq 0$, $j = 1, \ldots, d$, the following operator, defined on $C_{\mathsf{c}}^{\infty}(\mathbb{R}^d)$,

$$\xi(\hat{\mathsf{p}}, t)(H_{\mathrm{p}} + C_{\mathrm{p}} + t)^{-1} \hat{\mathsf{p}}_j \xi(\hat{\mathsf{p}}, t),$$

is bounded with norm bound independent of t.

Proof. As $\|(-\Delta + C_\mathrm{p})V\| < 1$, a von Neumann series expansions yields for all $t \geq 0$,

$$\begin{aligned}(H_\mathrm{p} + C_\mathrm{p} + t)^{-1} &= ((\hat{\mathsf{p}}^2 + C_\mathrm{p} + t)(1 + (\hat{\mathsf{p}}^2 + C_\mathrm{p} + t)^{-1}V))^{-1} \\ &= (1 + (\hat{\mathsf{p}}^2 + C_\mathrm{p} + t)^{-1}V)^{-1}(\hat{\mathsf{p}}^2 + C_\mathrm{p} + t)^{-1} \\ &= \sum_{n=0}^{\infty}(-(\hat{\mathsf{p}}^2 + C_\mathrm{p} + t)^{-1}V)^n(\hat{\mathsf{p}}^2 + C_\mathrm{p} + t)^{-1}.\end{aligned}$$

Thus,

$$\begin{aligned}&\xi(\hat{\mathsf{p}}, t)(H_\mathrm{p} + C_\mathrm{p} + t)^{-1}\hat{\mathsf{p}}_j\xi(\hat{\mathsf{p}}, t) \\ &= -\frac{\xi(\hat{\mathsf{p}}, t)}{\hat{\mathsf{p}}^2 + C_\mathrm{p} + t}\left(\sum_{n=1}^{\infty}(-(\hat{\mathsf{p}}^2 + C_\mathrm{p} + t)^{-1}V)^{n-1}\right)\frac{\hat{\mathsf{p}}_j\xi(\hat{\mathsf{p}}, t)}{\hat{\mathsf{p}}^2 + C_\mathrm{p} + t} \\ &\qquad + \xi(\hat{\mathsf{p}}, t)(\hat{\mathsf{p}}^2 + C_\mathrm{p} + t)^{-1}\hat{\mathsf{p}}_j\xi(\hat{\mathsf{p}}, t)\end{aligned}$$

is bounded independent of t. $\square$

Lemma B.4
Assume that W satisfy the same assumptions as in Lemma B.1, and let H_W and D_W defined as in (B.2) and (B.3), respectively. Then for all j, the operator

$$\int_0^\infty \frac{1}{\sqrt{t}}(H_W + C_\mathrm{p} + t)^{-1}\hat{\mathsf{p}}_j \mathrm{d}t,$$

where the integral is to be understood in the strong sense on $C_\mathsf{c}^\infty(\mathbb{R}^d)$, is bounded.

Proof. Let ξ be given as in Lemma B.3. Notice that

$$\begin{aligned}&\xi(\hat{\mathsf{p}}, t)(\mathrm{Id} + (H_\mathrm{p} + C_\mathrm{p} + t)^{-1}D_W)^{-1}\xi(\hat{\mathsf{p}}, t)^{-1} \\ &\qquad = \mathrm{Id} - \xi(\hat{\mathsf{p}}, t)(H_\mathrm{p} + C_\mathrm{p} + t)^{-1}D_W\sum_{n=1}^{\infty}(-(H_\mathrm{p} + C_\mathrm{p} + t)^{-1}D_W)^n\xi(\hat{\mathsf{p}}, t)^{-1}\end{aligned}$$

is bounded (independent of t) since $\xi(\hat{\mathsf{p}}, t)(H_\mathrm{p} + C_\mathrm{p} + t)^{-1}D_W$ is bounded by definition of ξ. This together with Lemma B.3 yields that the following operator is also bounded by a constant C independent of t:

$$\begin{aligned}&\xi(\hat{\mathsf{p}}, t)(H_W + C_\mathrm{p} + t)^{-1}\hat{\mathsf{p}}_j\xi(\hat{\mathsf{p}}, t) \\ &\qquad = \xi(\hat{\mathsf{p}}, t)(1 + (H_\mathrm{p} + C_\mathrm{p} + t)^{-1}D_W)^{-1}\xi(\hat{\mathsf{p}}, t)^{-1}\xi(\hat{\mathsf{p}}, t)(H_\mathrm{p} + C_\mathrm{p} + t)^{-1}\hat{\mathsf{p}}_j\xi(\hat{\mathsf{p}}, t).\end{aligned}$$

Therefore, for $\psi \in C_c^\infty(\mathbb{R}^d)$,

$$\left\| \int_0^\infty \frac{1}{\sqrt{t}} (H_W + C_\mathrm{p} + t)^{-1} \hat{\mathsf{p}}_j \mathrm{d}t \psi \right\| \le C \int_0^\infty \frac{1}{\sqrt{t}} \left\| \xi(\hat{\mathsf{p}}, t)^{-2} \psi \right\| \mathrm{d}t.$$

As the following expression

$$\frac{1}{\pi} \int_0^\infty \frac{1}{\sqrt{t}} \xi(p,t)^{-2} \mathrm{d}t = \frac{1}{\pi} \int_0^\infty \frac{1}{\sqrt{t}} \frac{|p|+1}{p^2 + C_\mathrm{p} + t} \mathrm{d}t = (|p|+1)(p^2 + C_\mathrm{p})^{-1/2}$$

is bounded in p, this completes the proof. □

Now we can state a similar result as in Lemma B.1 for the square root of the resolvent.

Lemma B.5
There exists a $\delta > 0$ such that for all $W \in C^2(\mathbb{R}^d)$, which are bounded from below, satisfying $\sup_x |\nabla W(x)| < \delta$ and $\sup_x |\Delta W(x)| < \delta$, and for all $j \in \{1, \dots, d\}$, $s, t \in \{0, 1\}$, $s + t \le 1$, the operator

$$e^{-W} \hat{\mathsf{p}}_j^s (H_\mathrm{p} + C_\mathrm{p})^{-1/2} \hat{\mathsf{p}}_j^t e^W \tag{B.6}$$

defined on $C_c^\infty(\mathbb{R}^d)$, is bounded.

Proof. For $s = 0$ and $t \in \{0, 1\}$ we proceed as in the proof of Lemma B.1 and compute on $C_c^\infty(\mathbb{R}^d)$, using (B.5),

$$\begin{aligned}
&e^{-W} (H_\mathrm{p} + C_\mathrm{p})^{-1/2} \hat{\mathsf{p}}_j^t e^W \\
&\quad = \frac{1}{\pi} \int_0^\infty \frac{1}{\sqrt{t'}} e^{-W} R_\mathrm{p}(t') \hat{\mathsf{p}}_j^t e^W \mathrm{d}t' \\
&\quad = \frac{1}{\pi} \int_0^\infty \frac{1}{\sqrt{t'}} (H_W + C_\mathrm{p} + t')^{-1} (H_W + C_\mathrm{p} + t') e^{-W} R_\mathrm{p}(t') \hat{\mathsf{p}}_j^t e^W \mathrm{d}t' \\
&\quad = \frac{1}{\pi} \int_0^\infty \frac{1}{\sqrt{t'}} (H_W + C_\mathrm{p} + t')^{-1} e^{-W} \hat{\mathsf{p}}_j^t e^W \mathrm{d}t' \\
&\quad = \int_0^\infty \frac{1}{\sqrt{t'}} (H_W + C_\mathrm{p} + t')^{-1} [e^{-W}, \hat{\mathsf{p}}_j^t] e^W \mathrm{d}t' + \int_0^\infty \frac{1}{\sqrt{t'}} (H_W + C_\mathrm{p} + t')^{-1} \hat{\mathsf{p}}_j^t \mathrm{d}t'.
\end{aligned}$$

The first integral is bounded since $\|(H_W + C_\mathrm{p} + t')^{-1}\| \le \frac{C}{1+t'}$, $t' \ge 0$, for some constant C and $[e^{-W}, \hat{\mathsf{p}}_j] e^W$ is a bounded operator. The second one is bounded due to Lemma B.4. This shows the claim for $s = 0$.

Finally, with regard to $s = 1$, $t = 0$ in (B.6), we compute on $C_{\mathsf{c}}^{\infty}(\mathbb{R}^d)$,

$$\begin{aligned}
&e^{-W}[\hat{\mathsf{p}}_j, (H_{\mathrm{p}} + C_{\mathrm{p}})^{-1/2}]e^{W} \\
&\quad = \frac{1}{\pi}\int_0^\infty \frac{1}{\sqrt{t}} e^{-W}\left[\hat{\mathsf{p}}_j, \frac{1}{H_{\mathrm{p}} + C_{\mathrm{p}} + t}\right] e^{W} \mathrm{d}t \\
&\quad = \frac{1}{\pi}\int_0^\infty \frac{1}{\sqrt{t}} e^{-W} \frac{1}{H_{\mathrm{p}} + C_{\mathrm{p}} + t} (\mathrm{i}\partial_j V) \frac{1}{H_{\mathrm{p}} + C_{\mathrm{p}} + t} e^{W} \mathrm{d}t.
\end{aligned}$$

Then, we can estimate the integrand in norm using Lemma B.1 by

$$\left\| e^{-W} \frac{1}{H_{\mathrm{p}} + C_{\mathrm{p}} + t} (\mathrm{i}\partial_j V) \frac{1}{H_{\mathrm{p}} + C_{\mathrm{p}} + t} e^{W} \right\| \leq \frac{C}{(1+t)^2},$$

with a constant C indepedent of t, which shows that the integral is bounded. $\square$

Proposition B.6

For all $\alpha \in \mathbb{R}$, $j \in \{1, \ldots, d\}$ and $s, t \in \{0, 1\}$, $s + t \leq 1$, the operators,

$$\langle \hat{\mathsf{x}} \rangle^{-\alpha} \hat{\mathsf{p}}_j^s (H_{\mathrm{p}} + C_{\mathrm{p}})^{-1/2} \hat{\mathsf{p}}_j^t \langle \hat{\mathsf{x}} \rangle^{\alpha},$$

defined on $C_{\mathsf{c}}^{\infty}(\mathbb{R}^d)$, are bounded. In particular, the operators are well-defined for $\alpha < 0$, i.e., the operators $\hat{\mathsf{p}}_j^s (H_{\mathrm{p}} + C_{\mathrm{p}})^{-1/2} \hat{\mathsf{p}}_j^t$ map $\mathcal{D}(|\hat{\mathsf{x}}|^{-\alpha})$ to $\mathcal{D}(|\hat{\mathsf{x}}|^{-\alpha})$.

Proof. The statement follows from Lemma B.5 in the same way as in the proof of Proposition B.2. $\square$

Proposition B.7

For all $n \in \mathbb{N}$, $j \in \{1, \ldots, d\}$ and $s, t \in \{0, 1\}$, $s + t \leq 1$, the operators

$$\langle \hat{\mathsf{x}} \rangle^{-(n+1)} \hat{\mathsf{p}}_j^s \chi_0 A_{\mathsf{D}} \chi_0 \hat{\mathsf{p}}_j^t \langle \hat{\mathsf{x}} \rangle^{n}, \quad \langle \hat{\mathsf{x}} \rangle^{n} \hat{\mathsf{p}}_j^s \chi_0 A_{\mathsf{D}} \chi_0 \hat{\mathsf{p}}_j^t \langle \hat{\mathsf{x}} \rangle^{-(n+1)}, \tag{B.7}$$

defined on $C_{\mathsf{c}}^{\infty}(\mathbb{R}^d)$, are bounded. In particular, the operators are well-defined, i.e., the operators $\hat{\mathsf{p}}_j^s \chi_0 A_{\mathsf{D}} \chi_0 \hat{\mathsf{p}}_j^t$ map $\mathcal{D}(|\hat{\mathsf{x}}|^{n+1})$ to $\mathcal{D}(|\hat{\mathsf{x}}|^{n})$.

Proof. It suffices to show that the first operators in (B.7) are bounded. Then it follows by the standard arguments that the second ones are well-defined and bounded.

Now, for $s = 0$ we can write $A_{\mathsf{D}} = \frac{1}{4}\sum_k (2\hat{\mathsf{p}}_k \hat{\mathsf{x}}_k + \mathrm{i})$ and we obtain that for all k,

$$\langle \hat{\mathsf{x}} \rangle^{-(n+1)} \chi_0 \hat{\mathsf{p}}_k \hat{\mathsf{x}}_k \chi_0 \hat{\mathsf{p}}_j^t \langle \hat{\mathsf{x}} \rangle^{n} = \langle \hat{\mathsf{x}} \rangle^{-(n+1)} \chi_0 \hat{\mathsf{p}}_k \langle \hat{\mathsf{x}} \rangle^{-(n+1)} \langle \hat{\mathsf{x}} \rangle^{n+1} \hat{\mathsf{x}}_k \langle \hat{\mathsf{x}} \rangle^{-n} \langle \hat{\mathsf{x}} \rangle^{n} \chi_0 \hat{\mathsf{p}}_j^t \langle \hat{\mathsf{x}} \rangle^{n}$$

is bounded by Proposition B.6. Clearly, with the same argument $\langle \hat{\mathsf{x}} \rangle^{-(n+1)} \chi_0^2 \hat{\mathsf{p}}_j^t \langle \hat{\mathsf{x}} \rangle^{n}$ and therefore $\langle \hat{\mathsf{x}} \rangle^{-(n+1)} \chi_0 A_{\mathsf{D}} \chi_0 \hat{\mathsf{p}}_j^t \langle \hat{\mathsf{x}} \rangle^{n}$ are bounded as well.

In the case $s = 1$, $t = 0$ we can write $A_{\mathsf{D}} = \frac{1}{4}\sum_k (2\hat{\mathsf{x}}_k \hat{\mathsf{p}}_k - \mathrm{i})$ and use the same argument. $\square$

B.1.3. Combination with the Helffer-Sjöstrand Formula

In this part we want to state a similar result as Proposition B.7 for compactly supported functions which are sufficiently smooth. We use a result of [GK03], where the authors combined Combes Thomas estimates with the so-called Helffer-Sjöstrand formula (cf. [HS89; Dav95]),

$$\chi(H) = -\frac{1}{\pi}\int_{\mathbb{C}} \frac{\partial\widehat{\chi}}{\partial\overline{z}}(H-z)^{-1}\mathrm{d}z, \tag{B.8}$$

which provides an approach for the functional calculus for self-adjoint operators H with suitable real functions χ. Here, $\widehat{\chi}$ is a so-called almost analytic extension of χ to $\mathbb{C}$. The occurrence of the resolvent in (B.8) indeed motivates the combination with Combes Thomas estimates.

For any function $\chi \in C_{\mathrm{c}}^{n}(\mathbb{R})$, $n \in \mathbb{N}$, we define the norm (cf. [Dav95, eq. (1)])

$$\|\chi\|_{\mathrm{D}}^{(n)} := \sum_{r=0}^{n}\int_{\mathbb{R}} \left|\chi^{(r)}(x)\right| \langle x\rangle^{r-1}\,\mathrm{d}x.$$

In [GK03, Theorem 2] it is proven that the operator kernel of $\chi(H_{\mathrm{p}})$ for a function $\chi \in C_{\mathsf{c}}^{\infty}(\mathbb{R}^d)$ decays for any $n \in \mathbb{N}$ polynomially with order n at spatial infinity, with a multiplicative constant $C_n\,\|\chi\|_{\mathrm{D}}^{(2+n)}$ where C_n does not depend on χ. To obtain a bounded operator, one needs, by Young's inequality for convolutions, additional decay of $d+1$. Therefore, it is straightforward to deduce the following proposition.

Proposition B.8 (cf. [GK03, Theorem 2])
For all $n \in \mathbb{N}$ there is a constant C_n such that for all $\chi \in C_{\mathsf{c}}^{\infty}(\mathbb{R}^d)$,

$$\left\|\langle\hat{\mathsf{x}}\rangle^{-n}\,\chi(H_{\mathrm{p}})\,\langle\hat{\mathsf{x}}\rangle^{n}\right\| \leq C_n\,\|\chi\|_{D}^{(2+n+d+1)}\,,$$

where the constants C_n do not depend on χ.

Corollary B.9
Let $n_0 \in \mathbb{N}$ and $\chi \in C_{\mathrm{c}}^{n_0+d+3}(\mathbb{R})$. Then for all $0 \leq n \leq n_0$, the operators

$$\langle\hat{\mathsf{x}}\rangle^{\pm n}\,\hat{\mathsf{p}}_j^{s}\chi(H_{\mathrm{p}})\hat{\mathsf{p}}_j^{t}\,\langle\hat{\mathsf{x}}\rangle^{\mp n}\,,\qquad j\in\{1,\dots,d\},\;\; s,t\in\{0,1\}, s+t\leq 1,$$

are well-defined and bounded.

Proof. Let us first consider the case $s=t=0$. Let $0 \leq n \leq n_0$. By convolution with a suitable smooth Dirac sequence supported in a common compact set, one finds a sequence $(\chi_k)_{k\in\mathbb{N}}$ of functions in $C^\infty_\mathsf{c}(\mathbb{R})$ such that $\chi_k \overset{k\to\infty}{\to} \chi$ in the norm $\|\chi\|_{\mathrm{D}}^{(n+d+3)}$. This yields $\chi_k(H_\mathrm{p}) \overset{k\to\infty}{\to} \chi(H_\mathrm{p})$ in norm, so for all $\psi \in C^\infty_\mathsf{c}(\mathbb{R}^d)$,

$$\left\| \langle \hat{\mathsf{x}} \rangle^{-n} \chi(H_\mathrm{p}) \langle \hat{\mathsf{x}} \rangle^{n} \psi \right\| = \lim_{k\to\infty} \left\| \langle \hat{\mathsf{x}} \rangle^{-n} \chi_k(H_\mathrm{p}) \langle \hat{\mathsf{x}} \rangle^{n} \psi \right\| \leq C_n \|\chi\|_{\mathrm{D}}^{(n+d+3)} \|\psi\| .$$

Now, for $s = 1$, we can write $\widetilde{\chi}(e) := (e + C_\mathrm{p})\chi(e)$. Then $\widetilde{\chi} \in C_\mathrm{c}^{n_0+d+3}(\mathbb{R})$ as well, and we obtain that

$$\langle \hat{\mathsf{x}} \rangle^{-n} \hat{\mathsf{p}}_j \chi(H_\mathrm{p}) \langle \hat{\mathsf{x}} \rangle^{n} = \langle \hat{\mathsf{x}} \rangle^{-n} \hat{\mathsf{p}}_j (H_\mathrm{p} + C_\mathrm{p})^{-1} \langle \hat{\mathsf{x}} \rangle^{n} \langle \hat{\mathsf{x}} \rangle^{-n} \widetilde{\chi}(H_\mathrm{p}) \langle \hat{\mathsf{x}} \rangle^{n}$$

is bounded, where we used Proposition B.6 and the case $s = t = 0$.

The proof for $t = 1$ is analogous and by the standard arguments it also follows that the adjoint operators

$$\langle \hat{\mathsf{x}} \rangle^{-n} \hat{\mathsf{p}}_j^s \chi(H_\mathrm{p}) \hat{\mathsf{p}}_j^t \langle \hat{\mathsf{x}} \rangle^{n}$$

are bounded and well-defined, and for all $\psi \in C^\infty_\mathsf{c}(\mathbb{R}^d)$,

$$\langle \hat{\mathsf{x}} \rangle^{-n} \hat{\mathsf{p}}_j^s \chi_k(H_\mathrm{p}) \hat{\mathsf{p}}_j^t \langle \hat{\mathsf{x}} \rangle^{n} \psi \overset{k\to\infty}{\longrightarrow} \langle \hat{\mathsf{x}} \rangle^{-n} \hat{\mathsf{p}}_j^s \chi(H_\mathrm{p}) \hat{\mathsf{p}}_j^t \langle \hat{\mathsf{x}} \rangle^{n} \psi.$$

Then, by the Helffer-Sjöstrand formula, we obtain

$$\langle \hat{\mathsf{x}} \rangle^{-n} \hat{\mathsf{p}}_j^s \chi_k(H_\mathrm{p}) \hat{\mathsf{p}}_j^t \langle \hat{\mathsf{x}} \rangle^{n} \psi = -\frac{1}{\pi} \int_\mathbb{C} \frac{\partial \widetilde{\chi}_k}{\partial \bar{z}} \langle \hat{\mathsf{x}} \rangle^{-n} \hat{\mathsf{p}}_j^s (H_\mathrm{p} - z)^{-1} \hat{\mathsf{p}}_j^t \langle \hat{\mathsf{x}} \rangle^{n} \psi.$$

Using that $\left\| \langle \hat{\mathsf{x}} \rangle^{-n} \hat{\mathsf{p}}_j^s (H_\mathrm{p} - z)^{-1} \hat{\mathsf{p}}_j^t \langle \hat{\mathsf{x}} \rangle^{n} \right\| \leq \frac{C}{|\mathrm{Im}\, z|}$ for some constant C (Proposition B.6), the last term can estimated by $C \|\chi_k\|_{\mathrm{D}2}$ for another constant C independent of k (see [Dav95, Lemma 1]).

This proves that the operators $\langle \hat{\mathsf{x}} \rangle^{-n} \hat{\mathsf{p}}_j^s \chi_k(H_\mathrm{p}) \hat{\mathsf{p}}_j^t \langle \hat{\mathsf{x}} \rangle^{n}$, $j \in \{1, \dots, d\}$, $s, t \in \{0, 1\}, s + t \leq 1$, are bounded. With the usual argumentation it follows that the formal adjoint operator is well-defined (i.e., $\hat{\mathsf{p}}_j^s \chi_k(H_\mathrm{p}) \hat{\mathsf{p}}_j^t \langle \hat{\mathsf{x}} \rangle^{-n}$ maps to $\mathcal{D}(|\hat{\mathsf{x}}|^n)$) and bounded. □

B.2. Commutator with a Cutoff Function

In this section a modification of an auxiliary result of [FMS04, section A.1] about the boundedness of commutators with a cutoff function is proven. In contrast to the original version we would like to treat non-smooth cutoff functions.

For the proof we repeat a theorem about the commutator expansion of unbounded operators, sometimes also referred to as *Hadamard's Lemma*. It is stated in this form in [FMS04, section A.1], but originally appeared in [Frö77].

Theorem B.10 (Commutator expansion, [FMS04, Theorem A.2])
Let $Y \geq \mathrm{Id}$ be self-adjoint and let $\mathcal{D}$ be a core for Y. Let $M \in \mathbb{N}$ and X, Z, $\mathrm{ad}_X^{(n)}(Z)$, $n = 1, \ldots, M$, be symmetric operators on $\mathcal{D}$ satisfying

$$\mathrm{ad}_X^{(0)}(Z) = Z, \tag{B.9}$$

$$\left\langle \psi, \mathrm{ad}_X^{(n)}(Z)\psi \right\rangle = \mathrm{i}\left(\left\langle \mathrm{ad}_X^{(n-1)}(Z)\psi, X\psi \right\rangle - \left\langle X\psi, \mathrm{ad}_X^{(n-1)}(Z)\psi \right\rangle \right), \tag{B.10}$$

for all $\psi \in \mathcal{D}$. Furthermore, assume that $(\mathrm{ad}_X^{(n)}(Z), Y, \mathcal{D})$, $n = 0, \ldots, M$, satisfy the GJN condition, that X is self-adjoint, $\mathcal{D} \subseteq \mathcal{D}(X)$, $e^{\mathrm{i}tX}$ leaves $\mathcal{D}(Y)$ invariant for all $t \in \mathbb{R}$, and (4.19) holds. Then we have on $\mathcal{D}(Y)$ for all $t \in \mathbb{R}$,

$$e^{\mathrm{i}tX} Z e^{-\mathrm{i}tX} = Z - \sum_{n=1}^{M-1} \frac{t^n}{n!} \mathrm{ad}_X^{(n)}(Z) - \int_0^t \cdots \int_0^{t_{M-1}} e^{\mathrm{i}t_M X} \mathrm{ad}_X^{(M)}(Z) e^{-\mathrm{i}t_M X} \mathrm{d}t_M \ldots \mathrm{d}t_1.$$

Now, we can prove our result to treat cutoff functions χ which are only M times differentiable. As tradeoff one has to impose certain assumptions with respect to the resolvent of X. The proof uses the same commutator expansion as in [FMS04, Lemma A.1], and it combines it with the approach in the proof of [FM04b, Lemma A.1].

Proposition B.11 (cf. [FMS04, Lemma A.2])
Let $M \in \mathbb{N}$ and $\chi \in C_c^{M+2}(\mathbb{R})$. Let $(X, Y, \mathcal{D})$ be a GJN triple, Z a symmetric operator on $\mathcal{D}$. Suppose $\chi(X)$ leaves $\mathcal{D}(Y)$ invariant and that $(\mathrm{ad}_X^{(n)}(Z), Y, \mathcal{D})$ satisfies the GJN condition for all $n = 0, \ldots, M$. In particular, Z extends to a self-adjoint operator, which will be denoted by the same symbol. Furthermore, assume there exist constants C such that for all $\psi \in \mathcal{D}(Y)$,

$$\begin{aligned} \left\| \mathrm{ad}_X^{(n)}(Z)\psi \right\| &\leq C \left\| \psi \right\|, \qquad n = 1, \ldots, M-1, \\ \left\| \mathrm{ad}_X^{(M)}(Z)\psi \right\| &\leq C(\|X\psi\| + \|\psi\|). \end{aligned}$$

Moreover, we assume that for some $\mu \in \rho(X)$, $(X-\mu)^{-1}$ leaves $\mathcal{D}(Y)$ invariant and $[(X-\mu)^{-1}, Z]$ (defined on $\mathcal{D}(Y)$) is bounded. Then, the commutator $[\chi(X), Z]$, defined on $\mathcal{D}(Y)$, is bounded.

Proof. Let $\chi_1(x) := (x-\mu)\chi(x)$. For $R \geq 0$ let

$$\chi_{1,R}(X) := (2\pi)^{-1/2} \int_{-R}^{R} (\mathcal{F}\chi_1)(s) e^{\mathrm{i}sX} \mathrm{d}s,$$

which exists as $\mathcal{F}\chi_1$ is continuous. Furthermore, we have by assumption $\chi_1 \in C^{M+2}(\mathbb{R})$ and therefore, using a standard stationary phase argument (see also

Lemma 6.11), there exists a constant C such that $|(\mathcal{F}\chi_1)(s)| \leq C \langle s \rangle^{-2}$ holds for all $s \in \mathbb{R}$. We then get $\chi_{1,R}(X) \to \chi_1(X)$ as $R \to \infty$, since $\mathcal{F}\chi_1 \in L^1(\mathbb{R})$.

By functional calculus, $\chi(X) = \chi_1(X)(X-\mu)^{-1}$ and given that $\chi_1(X)$ leaves $\mathcal{D}(Y)$ invariant, we obtain on $\mathcal{D}(Y)$,

$$[\chi(X), Z] = \chi_1(X)[(X-\mu)^{-1}, Z] + [\chi_1(X), Z](X-\mu)^{-1}. \tag{B.11}$$

The first term on the right-hand side of (B.11) is bounded by assumption. It remains to consider the second term.

Let $\psi \in \mathcal{D}(Y)$. By Theorem 4.7, $e^{\mathrm{i}sX}\psi \in \mathcal{D}(Y)$ for all $s \in \mathbb{R}$ and thus, $\chi_{1,R}(X) \in \mathcal{D}(Y)$, as

$$\int_{-R}^{R} |(\mathcal{F}\chi_1)(s)| \left\| Y e^{\mathrm{i}sX}\psi \right\| \mathrm{d}s \leq \int_{-R}^{R} |(\mathcal{F}\chi_1)(s)| \, e^{\kappa|s|} \mathrm{d}s < \infty,$$

for some $\kappa \geq 0$, where we used (4.19).

Then by Theorem B.10,

$$\begin{aligned} Z\chi_{1,R}(X)\psi &= \chi_{1,R}(X)Z\psi + (2\pi)^{-1/2} \int_{-R}^{R} (\mathcal{F}\chi_1)(s) e^{\mathrm{i}sX} (e^{-\mathrm{i}sX} Z e^{\mathrm{i}sX} - Z)\psi \\ &= \chi_{1,R}(X)Z\psi - (2\pi)^{-1/2} \int_{-R}^{R} (\mathcal{F}\chi_1)(s) e^{\mathrm{i}sX} \Bigg(\sum_{n=1}^{M-1} \frac{(-s)^n}{n!} \operatorname{ad}_X^{(n)}(Z)\psi \\ &\quad + (-1)^M \int_0^s \dots \int_0^{s_{M-1}} e^{-\mathrm{i}s_M X} \operatorname{ad}_X^{(M)}(Z) e^{\mathrm{i}s_M X} \mathrm{d}s_M \dots \mathrm{d}s_1 \Bigg) \psi \mathrm{d}s. \end{aligned} \tag{B.12}$$

Using that $\operatorname{ad}_X^{(n)}(Z)$, $n = 1, \dots, M$, is bounded, and by assumption,

$$\left\| \operatorname{ad}_X^{(M)}(Z) e^{\mathrm{i}s_M X}\psi \right\| \leq C(\|X\psi\| + \|\psi\|)$$

holds for some constant C independent of s and ψ, we can estimate the norm of the integrand in s in (B.12) by

$$C \langle s \rangle^M (\|X\psi\| + \|\psi\|),$$

with another constant C independent of s and ψ. Since all derivatives $\chi^{(n)}$, $n = 0, \dots, M+2$, are compactly supported, the stationary phase argument yields for $n = 0, \dots, M$,

$$\left| \mathcal{F}(\chi^{(n)})(k) \right| \leq C \langle k \rangle^{-2}$$

and thus, $\langle \cdot \rangle^M \mathcal{F}\chi \in L^1(\mathbb{R})$. Hence, $\lim_{R\to\infty} Z\chi_{1,R}(X)\psi$ exists, and since Z is closed, $\chi_1(X)\psi \in \mathcal{D}(Z)$ and $\lim_{R\to\infty} Z\chi_{1,R}(X)\psi = Z\chi_1(X)\psi$. Finally, it follows from (B.12) and the subsequent considerations that there is a constant C such that for all $\psi \in \mathcal{D}(Y)$,

$$\|[Z, \chi_1(X)]\psi\| \leq C(\|X\psi\| + \|\psi\|),$$

which shows that the second term in (B.11) is bounded. □

B.3. Absence of Negative Spectrum with Birman-Schwinger

The Birman-Schwinger principle (originating from [Bir61] and [Sch61], see also [BEG20]) in its classical form states that E is an eigenvalue of a Schrödinger operator $-\Delta + V$ if and only if -1 is an eigenvalue of the so-called Birman-Schwinger operator

$$V^{1/2}(-\Delta - E)\,|V|^{1/2}.$$

A common application are upper (so-called Birman-Schwinger) bounds for the number of (negative) eigenvalues. In particular, one can show that $-\Delta + V \geq 0$ if the Birman-Schwinger operator for all $E < 0$ is sufficiently small.

In this section we want to prove the same if we replace the operator $-\Delta + V$ by

$$(H_{\mathrm{p}} + C_{\mathrm{p}})^{-1/2}(-\Delta)(H_{\mathrm{p}} + C_{\mathrm{p}})^{-1/2} + V. \tag{B.13}$$

First, it will be shown in Lemma B.12 that the corresponding Birman-Schwinger operator for (B.13) is sufficiently small. This will imply the absence of any negative spectrum by means of the Birman-Schwinger principle (Proposition B.13).

In the following we assume to be in dimension $d = 3$.

Lemma B.12
Let $U\colon \mathbb{R}^3 \to \mathbb{R}$ be a measurable and non-negative function, satisfying

$$U(x) \leq C\,\langle x\rangle^{-\alpha}, \qquad x \in \mathbb{R}^3,$$

for some constants C and $\alpha > 2$. Then for any $E < 0$ the operator

$$\sqrt{U}((H_{\mathrm{p}} + C_{\mathrm{p}})^{-1/2}(-\Delta)(H_{\mathrm{p}} + C_{\mathrm{p}})^{-1/2} - E)^{-1}\sqrt{U} \tag{B.14}$$

is bounded by a constant independent of E.

Proof. We can write (B.14) as

$$\sqrt{U}(H_{\rm p}+C_{\rm p})^{1/2}(\hat{\mathsf{p}}^2 - E(H_{\rm p}+C_{\rm p}))^{-1}(H_{\rm p}+C_{\rm p})^{1/2}\sqrt{U}. \tag{B.15}$$

Notice that the operator $\hat{\mathsf{p}}^2 - E(H_{\rm p}+C_{\rm p})$ is self-adjoint on $\mathcal{D}(\Delta)$ and bounded from below by a positive constant. Therefore,

$$\operatorname{ran}(\hat{\mathsf{p}}^2 - E(H_{\rm p}+C_{\rm p}))^{-1} \subseteq \mathcal{D}(\Delta) \subseteq \mathcal{D}((H_{\rm p}+C_{\rm p})^{1/2}),$$

so the expression (B.15) is indeed well-defined. Using the operator inequality (5.4) with

$$\begin{aligned} A &= \sqrt{U}(H_{\rm p}+C_{\rm p})^{1/2}\mathbb{1}_{\hat{\mathsf{p}}^2<1}(\hat{\mathsf{p}}^2 - E(H_{\rm p}+C_{\rm p}))^{-1/2}, \\ B &= \sqrt{U}(H_{\rm p}+C_{\rm p})^{1/2}\mathbb{1}_{\hat{\mathsf{p}}^2\geq 1}(\hat{\mathsf{p}}^2 - E(H_{\rm p}+C_{\rm p}))^{-1/2}, \end{aligned}$$

we can estimate (B.15) from above by

$$2\sqrt{U}(H_{\rm p}+C_{\rm p})^{1/2}\mathbb{1}_{\hat{\mathsf{p}}^2<1}(\hat{\mathsf{p}}^2 - E(H_{\rm p}+C_{\rm p}))^{-1}\mathbb{1}_{\hat{\mathsf{p}}^2<1}(H_{\rm p}+C_{\rm p})^{1/2}\sqrt{U} \tag{B.16}$$

$$+2\sqrt{U}(H_{\rm p}+C_{\rm p})^{1/2}\mathbb{1}_{\hat{\mathsf{p}}^2\geq 1}(\hat{\mathsf{p}}^2 - E(H_{\rm p}+C_{\rm p}))^{-1}\mathbb{1}_{\hat{\mathsf{p}}^2\geq 1}(H_{\rm p}+C_{\rm p})^{1/2}\sqrt{U}. \tag{B.17}$$

To prove that (B.17) is bounded uniformly in E, it suffices to show that the operator

$$(H_{\rm p}+C_{\rm p})^{1/2}\hat{\mathsf{p}}^{-1}\mathbb{1}_{\hat{\mathsf{p}}^2\geq 1}$$

is bounded. This follows by

$$\begin{aligned} \left\|(H_{\rm p}+C_{\rm p})^{1/2}\hat{\mathsf{p}}^{-1}\mathbb{1}_{\hat{\mathsf{p}}^2\geq 1}\right\|^2 &= \sup_{\|\psi\|=1}\left\langle \hat{\mathsf{p}}^{-1}\mathbb{1}_{\hat{\mathsf{p}}^2\geq 1}\psi, (\hat{\mathsf{p}}^2+V+C_{\rm p})\hat{\mathsf{p}}^{-1}\mathbb{1}_{\hat{\mathsf{p}}^2\geq 1}\psi\right\rangle \\ &\leq \sup_{\|\psi\|=1}\left\langle \hat{\mathsf{p}}^{-1}\mathbb{1}_{\hat{\mathsf{p}}^2\geq 1}\psi, (\hat{\mathsf{p}}^2+C_{\rm p})\hat{\mathsf{p}}^{-1}\mathbb{1}_{\hat{\mathsf{p}}^2\geq 1}\psi\right\rangle \\ &\leq 1+C_{\rm p}. \end{aligned}$$

Therefore, the operator $\hat{\mathsf{p}}^{-1}\mathbb{1}_{\hat{\mathsf{p}}^2\geq 1}(H_{\rm p}+C_{\rm p})^{1/2}$, defined on $\mathcal{D}(\Delta)$, is bounded as its formal adjoint.

It remains to show that (B.16) is uniformly bounded in E. The relation

$$(H_{\rm p}+C_{\rm p})^{1/2} = (H_{\rm p}+C_{\rm p})\frac{1}{\pi}\int_0^\infty \frac{1}{\sqrt{t}}R_{\rm p}(t)\mathrm{d}t,$$

which follows from (B.5), allows us to write (B.16) up to positive constants as

$$\int_0^\infty\int_0^\infty \frac{\sqrt{U}}{\sqrt{st}}R_{\rm p}(t)(H_{\rm p}+C_{\rm p})\mathbb{1}_{\hat{\mathsf{p}}^2<1}(\hat{\mathsf{p}}^2 - E(H_{\rm p}+C_{\rm p}))^{-1}\mathbb{1}_{\hat{\mathsf{p}}^2<1}(H_{\rm p}+C_{\rm p})R_{\rm p}(s)\sqrt{U}\mathrm{d}s\mathrm{d}t$$

Now, by Proposition B.2, there exist constants C such that $\left\| \langle \hat{\mathsf{x}} \rangle^{-\alpha/2} R_{\mathrm{p}}(t) \langle \hat{\mathsf{x}} \rangle^{\alpha/2} \right\| \leq \frac{C}{1+t}$ and $\left\| \langle \hat{\mathsf{x}} \rangle^{\alpha/2} R_{\mathrm{p}}(t) \langle \hat{\mathsf{x}} \rangle^{-\alpha/2} \right\| \leq \frac{C}{1+s}$, $s, t \geq 0$. Furthermore, $\langle \hat{\mathsf{x}} \rangle^{\alpha/2} \sqrt{U}$ is bounded by assumption. Thus, it suffices to show that

$$\langle \hat{\mathsf{x}} \rangle^{-\alpha/2} (H_{\mathrm{p}} + C_{\mathrm{p}}) \mathbb{1}_{\hat{\mathsf{p}}^2 < 1} (\hat{\mathsf{p}}^2 - E(H_{\mathrm{p}} + C_{\mathrm{p}}))^{-1} \mathbb{1}_{\hat{\mathsf{p}}^2 < 1} (H_{\mathrm{p}} + C_{\mathrm{p}}) \langle \hat{\mathsf{x}} \rangle^{-\alpha/2} \tag{B.18}$$

is bounded uniformly in E. We have $\hat{\mathsf{p}}^2 - E(H_{\mathrm{p}} + C_{\mathrm{p}}) \geq \hat{\mathsf{p}}^2 - EC$, where $C := C_{\mathrm{p}} + \inf(H_{\mathrm{p}}) > 0$. Thus, we can estimate (B.18) in the operator sense by

$$\langle \hat{\mathsf{x}} \rangle^{-\alpha/2} (H_{\mathrm{p}} + C_{\mathrm{p}}) \mathbb{1}_{\hat{\mathsf{p}}^2 < 1} (\hat{\mathsf{p}}^2 - EC)^{-1} \mathbb{1}_{\hat{\mathsf{p}}^2 < 1} (H_{\mathrm{p}} + C_{\mathrm{p}}) \langle \hat{\mathsf{x}} \rangle^{-\alpha/2} .$$

Now decomposing $H_{\mathrm{p}} + C_{\mathrm{p}} = \hat{\mathsf{p}}^2 + V + C_{\mathrm{p}}$ and using again the operator inequality (5.4) it suffices to consider the diagonal parts. Obviously, $\langle \hat{\mathsf{x}} \rangle^{-\alpha/2} \hat{\mathsf{p}}^2 \mathbb{1}_{\hat{\mathsf{p}}^2 < 1} (\hat{\mathsf{p}}^2 - EC)^{-1} \mathbb{1}_{\hat{\mathsf{p}}^2 < 1} \hat{\mathsf{p}}^2 \langle \hat{\mathsf{x}} \rangle^{-\alpha/2}$ is bounded independent of E. It remains to show that the operator

$$\langle \hat{\mathsf{x}} \rangle^{-\alpha/2} \mathbb{1}_{\hat{\mathsf{p}}^2 < 1} (\hat{\mathsf{p}}^2 - EC)^{-1} \mathbb{1}_{\hat{\mathsf{p}}^2 < 1} \langle \hat{\mathsf{x}} \rangle^{-\alpha/2} \leq \langle \hat{\mathsf{x}} \rangle^{-\alpha/2} (\hat{\mathsf{p}}^2 - EC)^{-1} \langle \hat{\mathsf{x}} \rangle^{-\alpha/2} \tag{B.19}$$

is bounded uniformly in E. Using the Green's function for the Laplace operator, the right-hand side of (B.19) can be written as integral operator with integral kernel

$$K(x, y) = \langle x \rangle^{-\alpha/2} \frac{e^{-\sqrt{-EC}|x-y|}}{4\pi |x - y|} \langle y \rangle^{-\alpha/2} .$$

Recall that $\alpha > 2$. As $x \mapsto \langle x \rangle^{-\alpha} \in L^{3/2}(\mathbb{R}^3)$, it follows by [RS4, section X.9] that $x \mapsto \langle x \rangle^{-\alpha}$ is in the Rollnik class, that is,

$$\int_{\mathbb{R}^3} \int_{\mathbb{R}^3} \frac{\langle x \rangle^{-\alpha} \langle y \rangle^{-\alpha}}{|x - y|^2} \mathrm{d}x \mathrm{d}y < \infty,$$

which shows that $K(\cdot, \cdot) \in L^2(\mathbb{R}^3 \times \mathbb{R}^3)$ and $\|K(\cdot, \cdot)\|_2$ can be estimated independently of E. $\square$

Proposition B.13
Let $U \colon \mathbb{R}^3 \to \mathbb{R}$ be a measurable and non-negative function, satisfying

$$U(x) \leq C \langle x \rangle^{-\alpha} , \qquad x \in \mathbb{R}^3,$$

for some constants C and $\alpha > 2$. Then there exists $\lambda_0 > 0$ such that for all $\lambda < \lambda_0$,

$$(H_{\mathrm{p}} + C_{\mathrm{p}})^{-1/2} (-\Delta) (H_{\mathrm{p}} + C_{\mathrm{p}})^{-1/2} - \lambda U \geq 0. \tag{B.20}$$

Proof. Assume w.l.o.g. $\lambda > 0$ and let

$$T := (H_\mathrm{p} + C_\mathrm{p})^{-1/2}(-\Delta)(H_\mathrm{p} + C_\mathrm{p})^{-1/2}.$$

First notice that T is in fact well-defined on $\mathcal{D}((H_\mathrm{p} + C_\mathrm{p})^{1/2})$ and non-negative. Thus, it has a self-adjoint extension, which we denote by the same symbol.

Assume that $E < 0$ and $E \in \sigma(T - \lambda U)$. Then we find a sequence $(\widetilde{\psi}_n)$ with $\left\|\widetilde{\psi}_n\right\| = 1$ and

$$\lim_{n\to\infty} (T - \lambda U - E)\widetilde{\psi}_n = 0.$$

Using the Birman Schwinger principle we get with $\psi_n = \sqrt{U}\widetilde{\psi}_n$,

$$\lim_{n\to\infty} \left(\lambda\sqrt{U}(T - E)^{-1}\sqrt{U}\psi_n - \psi_n\right) = 0. \tag{B.21}$$

On the other hand, the operator $\sqrt{U}(T-E)^{-1}\sqrt{U}$ is bounded by a constant $C > 0$ independent of E due to Lemma B.12. So for $\lambda < \frac{1}{C}$, we obtain

$$\left\|\lambda\sqrt{U}(T - E)^{-1}\sqrt{U}\psi_n - \psi_n\right\| \geq (1 - C\lambda) \|\psi_n\|. \tag{B.22}$$

Furthermore, from

$$\begin{aligned}
\|\psi_n\|^2 &= \left\langle \widetilde{\psi}_n, U\widetilde{\psi}_n \right\rangle \\
&= \frac{1}{\lambda}\left(\left\langle \widetilde{\psi}_n, (T - E)\widetilde{\psi}_n \right\rangle - \left\langle \widetilde{\psi}_n, (T - \lambda U - E)\widetilde{\psi}_n \right\rangle\right) \\
&\geq \frac{1}{\lambda}(-E) - \left\langle \widetilde{\psi}_n, (T - \lambda U - E)\widetilde{\psi}_n \right\rangle \\
&\overset{n\to\infty}{\to} \frac{-E}{\lambda} > 0
\end{aligned}$$

we conclude $\liminf_{n\to\infty} \|\psi_n\| > 0$. This together with (B.22) is in contradiction to (B.21). □

B.4. Decay Behavior of Planck's Law

Here some elementary decay properties of the derivatives of the functions $\sqrt{\rho_\beta}$ and $\sqrt{1 + \rho_\beta}$, which appear in the Araki Woods representation, are collected. Remember we set for $\beta > 0$,

$$\rho_\beta(u) = \frac{1}{e^{\beta u} - 1}, \qquad u \in \mathbb{R} \setminus \{0\}.$$

We start with some explicit bounds for $\sqrt{\rho_\beta}$ and $\sqrt{1 + \rho_\beta}$, and their first derivatives. In particular, we consider the β-dependence of the constants.

Lemma B.14
There exists constants C such that for all $\omega \geq 0$, $\beta > 0$,

(a) $\sqrt{\rho_\beta(\omega)} \leq \frac{1}{\sqrt{\beta\omega}}$,

(b) $\sqrt{1+\rho_\beta(\omega)} \leq 1 + \frac{1}{\sqrt{\beta\omega}}$,

(c) $\partial_\omega \sqrt{\rho_\beta(\omega)} \leq C(\omega^{-1} + \beta^{-\frac{1}{2}}\omega^{-\frac{3}{2}})$,

(d) $\partial_\omega \sqrt{1+\rho_\beta(\omega)} \leq C(\omega^{-1} + \beta^{-\frac{1}{2}}\omega^{-\frac{3}{2}})$.

Proof. (a) Since $e^{\beta\omega} - 1 \geq \beta\omega$, we have $\rho_\beta(\omega) = (e^{\beta\omega}-1)^{-1} \leq \frac{1}{\beta\omega}$.

(b) Using (a), we obtain

$$\sqrt{1+\rho_\beta(\omega)} \leq 1 + \sqrt{\rho_\beta(\omega)} \leq 1 + \frac{1}{\sqrt{\beta\omega}}.$$

(c) Using (a) again, we find

$$\begin{aligned}
\left|\partial_\omega \sqrt{\rho_\beta(\omega)}\right| &= \frac{1}{2}(e^{\beta\omega}-1)^{-3/2}\beta e^{\beta\omega} \\
&= \frac{1}{2}(e^{\beta\omega}-1)^{-1/2}\beta \frac{e^{\beta\omega}}{e^{\beta\omega}-1} \\
&\leq \frac{1}{2}(e^{\beta\omega}-1)^{-1/2}\beta \left(1 + \frac{1}{\beta\omega}\right) \\
&\leq \frac{1}{2}(e^{\beta\omega}-1)^{-1/2}\beta + \frac{1}{2}(e^{\beta\omega}-1)^{-1/2}\frac{1}{\omega} \\
&\leq \frac{1}{2}\left(\frac{\beta^2\omega^2}{2}\right)^{-1/2}\beta + \frac{1}{2}\frac{1}{\sqrt{\beta\omega}}\frac{1}{\omega} \\
&\leq C\left(\omega^{-1} + \frac{1}{\sqrt{\beta}}\omega^{-3/2}\right)
\end{aligned}$$

for some constant C.

(d) We have

$$\left|\partial_\omega \sqrt{1+\rho_\beta(\omega)}\right| = \frac{1}{2}(1+\rho_\beta(\omega))^{-1/2}\beta e^{\beta\omega}\rho_\beta(\omega)^2 \leq \frac{1}{2}\beta e^{\beta\omega}\rho_\beta(\omega)^{3/2} = \left|\partial_\omega \sqrt{\rho_\beta(\omega)}\right|,$$

and therefore the same bound as in (c). $\square$

Next, we consider higher derivatives. As it is not needed in the applications, we do not keep track of the β-dependence of the constants.

Lemma B.15

(a) We have for all $n \in \mathbb{N}_0$,

$$\limsup_{\omega \downarrow 0} \frac{\partial_\omega^n \sqrt{1+\rho_\beta(\omega)}}{\omega^{-\frac{1}{2}-n}} < \infty, \qquad \limsup_{\omega \downarrow 0} \frac{\partial_\omega^n \sqrt{\rho_\beta(\omega)}}{\omega^{-\frac{1}{2}-n}} < \infty,$$

(b) and for all $n, k \in \mathbb{N}$,

$$\lim_{\omega \to \infty} \omega^k \partial_\omega^n \sqrt{1+\rho_\beta(\omega)} = 0, \qquad \lim_{\omega \to \infty} \omega^k \partial_\omega^n \sqrt{\rho_\beta(\omega)} = 0.$$

Proof. Using $\sqrt{1+\rho_\beta(\omega)} = \frac{1}{\sqrt{1-e^{-\beta\omega}}}$ we get by induction that for all $n \in \mathbb{N}$ and $\beta > 0$, there is a finite set $\mathcal{A}$ and $c_\alpha \in \mathbb{R}, d_\alpha \in \mathbb{N}$, $\alpha \in \mathcal{A}$, with $d_\alpha \leq n$, such that

$$\partial_\omega^n \sqrt{1+\rho_\beta(\omega)} = \sum_{\alpha \in \mathcal{A}} c_\alpha \frac{(e^{-\beta\omega})^{d_\alpha}}{(1-e^{-\beta\omega})^{\frac{1}{2}+d_\alpha}}, \qquad \omega \geq 0.$$

Then the first claims of (a) and (b) follow, since $\limsup_{\omega \downarrow 0} \frac{\omega}{1-e^{-\beta\omega}} < \infty$ and $\lim_{\omega \to \infty} \omega^k \frac{e^{-\beta\omega}}{1-e^{-\beta\omega}} = 0$ for all $k \in \mathbb{N}_0$, respectively.

Next, we can write analogously for all $n \in \mathbb{N}_0$, with constants $c_\alpha \in \mathbb{R}, d_\alpha \in \mathbb{N}$, $\alpha \in \mathcal{A}$, with $d_\alpha \leq n$,

$$\partial_\omega^n \sqrt{\rho_\beta(\omega)} = \sum_{\alpha \in \mathcal{A}} c_\alpha \frac{(e^{\beta\omega})^{d_\alpha}}{(e^{\beta\omega}-1)^{\frac{1}{2}+d_\alpha}}, \qquad \omega \geq 0.$$

Then the second claims of (a) and (b) follow, since $\limsup_{\omega \downarrow 0} \frac{\omega}{e^{\beta\omega}-1} < \infty$ and $\lim_{\omega \to \infty} \omega^k \frac{1}{(e^{\beta\omega}-1)^{1/2}} = 0$ for all $k \in \mathbb{N}_0$, respectively. □

Lemma B.16

The function

$$[0, \infty) \longrightarrow \mathbb{R}, \ \omega \mapsto \omega\rho_\beta(\omega)$$

is infinitely often differentiable and $\lim_{\omega \to \infty} \partial_\omega^n (\omega \rho_\beta(\omega)) = 0$ for all $n \in \mathbb{N}_0$.

Proof. This can be seen explicitly by writing

$$\omega\rho_\beta(\omega) = \frac{1}{\beta} \frac{\beta\omega}{e^{\beta\omega}-1} = \frac{1}{\beta} \left(\sum_{n=1}^{\infty} \frac{(\beta\omega)^{n-1}}{n!} \right)^{-1}.$$ □

Nomenclature

$\hat{\otimes}$	Algebraic tensor product
Δ	Laplace operator with the convention $-\Delta \geq 0$
$\mathbb{1}_{A=a}$	Projection to the eigenspace with eigenvalue a of an operator A
$\mathbb{1}_{A\neq a}$	$\mathbb{1}_{A=a}^{\perp}$
$\mathbb{1}_M$	Indicator function with respect to a set M
$\sigma(H)$	Spectrum of the operator H
$\sigma_{\mathrm{d}}(H)$	Discrete spectrum of the operator H
$\overline{A}$	Closure of A (as set or operator)
A^*	Adjoint operator
$[A, B]$	Commutator of A and B
$A > 0$	Strict positivity of the operator A, i.e., $A \geq 0$ and $\ker A = \{0\}$
$B_R(x)$	Closed ball of radius R around x
C_{c}^{∞}	Compactly supported smooth functions
$C^n(X)$	n times continuously differentiable functions on X
$\mathcal{D}(A)$	Domain of an operator A
$\mathcal{F}$	Fourier transform in $\mathbb{R}^d$
Id	Identity operator (sometimes with subindex referring to the underlying space)
$\hat{\mathsf{k}}$	Multiplication operator in the scattering space
$\mathcal{L}(\mathcal{H})$	Bounded linear operators on $\mathcal{H}$

$\operatorname{lin} M$	Linear span of a set M
$\mathbb{N}$	Natural numbers (without zero)
$\mathbb{N}_0$	Natural numbers (including zero)
$\hat{\mathsf{p}}$	Momentum (derivative) operator $-\mathrm{i}\nabla_x$
$P^\perp$	Orthogonal projection $\mathrm{Id} - P$
$\hat{\mathsf{q}}$	Derivative operator $\mathrm{i}\nabla_k$ in the scattering space
ran	Range (image) of an operator
$\mathbb{R}_+$	Positive real line $(0, \infty)$
$\mathbb{S}^n$	n-dimensional sphere
$\mathcal{S}(\mathbb{R}^d)$	Schwartz functions on $\mathbb{R}^d$
$V^\perp$	Orthogonal complement of a space V
$\langle x \rangle$	$(1 + x^2)^{1/2}$
$\hat{\mathsf{x}}$	Position (multiplication) operator

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- Bei der Auswahl des Materials sowie der Herstellung des Manuskripts haben mich durch ihr Mitwirken an Arbeiten, die Teil dieser Dissertation sind, folgende Personen unterstützt:
  - David Hasler.

Jena, den 15. März 2021

Oliver Siebert