Thermal Ionization

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Dedicated, in admiration and friendship, to
Elliott Lieb and Edward Nelson,
on the occasion of their 70^{th} *birthdays.*

Abstract

In the context of an idealized model describing an atom coupled to black-body radiation at a sufficiently high positive temperature, we show that the atom will end up being ionized in the limit of large times. Mathematically, this is translated into the statement that the coupled system does not have any time-translation invariant state of positive (asymptotic) temperature, and that the expectation value of an arbitrary finite-dimensional projection in an arbitrary initial state of positive (asymptotic) temperature tends to zero, as time tends to infinity.

These results are formulated within the general framework of W^*-dynamical systems, and the proofs are based on Mourre's theory of positive commutators and a new virial theorem. Results on the so-called standard form of a von Neumann algebra play an important role in our analysis.

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1 Introduction

In this paper, we study an idealized model describing an atom or molecule consisting of static nuclei and electrons coupled to black-body radiation. Our aim is to show that when the quantized radiation field is in a thermal state corresponding to a sufficiently high positive temperature, and under suitable conditions on the interaction Hamiltonian, including infrared and ultraviolet cutoffs and a small value of the coupling constant, the atom or molecule will always be ionized in the limit of very large times. This process is called *thermal ionization.*

Thus, a very dilute gas of atoms or molecules in intergalactic space and subject to the $3K$ thermal background radiation of the universe will eventually be transformed into a very dilute plasma of nuclei and electrons.

If the temperature of the black-body radiation is small, as compared to a typical atomic ionization energy, then an atom initially prepared in an excited bound state will start to emit light and relax towards its groundstate. After a time much longer than its relaxation time, it will be stripped of its electrons in very unlikely events where an atomic electron is hit by a high-energy photon from the thermal background radiation. The life time of the groundstate of an isolated atom interacting with black body radiation at inverse temperature β, before it is ionized, is expected to be exponentially large in β. A precise description of the temporal evolution of such an atom is difficult to come by; but the claim that, it will eventually be ionized, is highly plausile. To most physicists, this result must look obvious. Unfortunately a complete proof of it is likely to be very involved. The main purpose of this paper is to present some partial results, thermal ionization at sufficiently high temperatures for simplified models, supporting this picture.

If the temperature of electromagnetic radiation is strictly zero then an atom initially prepared in a bound state of maximal energy well below its ionization threshold can be shown to always relax to a groundstate by emitting photons; (for a proof of this statement in some slightly idealized models see [FGS]). This result and our complementary result on thermal ionization provide some qualitative understanding of two fundamental irreversible processes in atomic physics: relaxation to a ground state, and ionization by thermal radiation.

Next, we describe the physical system analyzed in this paper somewhat more precisely; (for further details see Section 2.1). It is composed of a subsystem with finitely many degrees of freedom, the "atom" (or "molecule"), and a subsystem with infinitely many degrees of freedom, the "radiation field". The space of pure state vectors of the atom is a separable Hilbert space, $\mathcal{H}_p$; (where the subscript $_p$ stands for "particle"). Mixed states of the atom are described by density matrices, ρ, where ρ is a non-negative, trace-class operator on $\mathcal{H}_p$ of unit trace. The expectation value of a bounded operator A on $\mathcal{H}_p$ in the state ρ is given by

$$\omega_\rho^p(A) := \mathrm{tr}\,\rho A. \tag{1}$$

Before the "atom" or particle system is coupled to the radiation field the time evolution of a bounded operator A on $\mathcal{H}_p$ in the Heisenberg picture is given by

$$\alpha_t^p(A) := e^{itH_p} A e^{-itH_p}, \tag{2}$$

where H_p is the particle Hamiltonian, which is a selfadjoint operator on $\mathcal{H}_p$ whose spectrum is bounded from below by a constant $E > -\infty$.

To be specific, we may think of $\mathcal{H}_p$ as being the Hilbert space

$$\mathcal{H}_p = \mathbb{C}^n \oplus L^2(\mathbb{R}^3, d^3x), \tag{3}$$

and the Hamiltonian H_p as the operator

$$H_p = \mathrm{diag}\,(E_0 = E, E_1, \ldots, E_{n-1}) \upharpoonright_{\mathbb{C}^n} \oplus (-\Delta) \upharpoonright_{L^2(\mathbb{R}^3, d^3x)}, \tag{4}$$

describing a one-electron atom (with a static nucleus) with n boundstates of energies $E_0, E_1, \ldots, E_{n-1} < 0$ and scattering states of arbitrary energies $k^2 \in [0, \infty)$ spanning the subspace $L^2(\mathbb{R}^3, d^3x)$ of $\mathcal{H}_p$. Thus, the point spectrum of H_p is given by the eigenvalues $\{E_0, E_1, \ldots, E_{n-1}\}$ and the continuous spectrum of H_p covers $[0, \infty)$, has constant (infinite) multiplicity and is absolutely continuous. Just in order to keep things simple, we shall usually assume that $n = 1$.

The bounded operators on a Hilbert space $\mathcal{H}$ form a von Neumann algebra denoted by $\mathcal{B}(\mathcal{H})$. A convenient algebra of operators encoding the kinematics of the "atom" or particle sytem is the algebra $\mathfrak{A}_p := \mathcal{B}(\mathcal{H}_p)$.

The "radiation field" is described by a free, massless, scalar Bose field φ on physical space $\mathbb{R}^3$, a "phonon field". For purposes of physics, it would be preferable to replace φ by the free electromagnetic field. In our entire analysis, this replacement can be made without any difficulties - at the price of slightly more complicated notation. A convenient algebra of operators to encode the kinematics of the radiation field is a C^*-algebra $\mathfrak{A}_f$ which can be viewed as a time-averaged version of the algebra of Weyl operators generated by φ and its conjugate momentum field π. The time evolution of operators in $\mathfrak{A}_f$, in the Heisenberg picture, *before* the field is coupled to the particle system, is given by the *free-field time evolution* α_t^f, which is a one-parameter group of $*$automorphisms on $\mathfrak{A}_f$.

A one-parameter group $\{\alpha_t | t \in \mathbb{R}\}$ defined on a C^*-algebra $\mathfrak{A}$ is a $*$automorphism group of $\mathfrak{A}$ iff

$$\begin{aligned} \alpha_t(A) &\in \mathfrak{A}, \quad (\alpha_t(A))^* = \alpha_t(A^*), \quad \text{for all } A \in \mathfrak{A}, \\ \alpha_t(A)\alpha_t(B) &= \alpha_t(AB), \quad \text{for all } A, B \in \mathfrak{A}, \\ \alpha_{t=0}(A) &= A, \quad \alpha_t(\alpha_s(A)) = \alpha_{t+s}(A), \quad \text{for all } A \in \mathfrak{A},\ t, s \in \mathbb{R}. \end{aligned} \tag{5}$$

Since we work on a time-averaged Weyl algebra, the free field time evolution is *norm continuous*, i.e., $t \mapsto \alpha_t^f(A)$ is a continuous map from $\mathbb{R}$ to $\mathfrak{A}_f$. General states of the radiation field can be described as states on the algebra $\mathfrak{A}_f$, i.e., as positive, linear functionals, ω, on $\mathfrak{A}_f$ normalized such that $\omega(\mathbb{1}) = 1$.

A convenient algebra of operators to encode the kinematics of the system composed of the "atom" and the "radiation field" is the C^*-algebra, $\mathfrak{A}$, given by

$$\mathfrak{A} = \mathfrak{A}_p \otimes \mathfrak{A}_f. \tag{6}$$

The time evolution of operators in $\mathfrak{A}$, *before* the two subsystems are coupled to each other, is given by

$$\alpha_{t,0} := \alpha_t^p \otimes \alpha_t^f. \tag{7}$$

A regularized interaction coupling the two subsystems can be introduced by choosing a bounded, selfadjoint operator $V^{(\epsilon)} \in \mathfrak{A}$, where the superscript $^{(\epsilon)}$ indicates that a regularization has been imposed on an interaction term, V, in such a way that $\|V^{(\epsilon)}\| = O(1/\epsilon)$. We define the *regularized, interacting time evolution of the coupled system* as a $*$automorphism group $\{\alpha_{t,\lambda}^{(\epsilon)} | t \in \mathbb{R}\}$ on the algebra $\mathfrak{A}$ given by the norm-convergent *Schwinger-Dyson series*

$$\begin{aligned} \alpha_{t,\lambda}^{(\epsilon)}(A) = \alpha_{t,0}(A) + \sum_{n=1}^{\infty} (i\lambda)^n \int_0^t dt_1 \cdots \\ \cdots \int_0^{t_{n-1}} dt_n \ [\alpha_{t_n,0}(V^{(\epsilon)}), [\alpha_{t_{n-1},0}(V^{(\epsilon)}), \ldots, [\alpha_{t_1,0}(V^{(\epsilon)}), \alpha_{t,0}(A)] \cdots]], \end{aligned} \tag{8}$$

for an arbitrary operator $A \in \mathfrak{A}$. In equation (8), λ is a coupling constant, and the interaction term V is chosen in accordance with conventional models describing electrons coupled to the quantized radiation field.

We are interested in analyzing the time evolution of the coupled system in some states ω of physical interest, i.e., in understanding the time-dependence of expectation values

$$\omega(\alpha_{t,\lambda}^{(\epsilon)}(A)), \quad A \in \mathfrak{A}, \tag{9}$$

in the limit where the regularization is removed, i.e., $\epsilon \to 0$, and for large times t. The *states ω of interest* are states "close to" (technically speaking, *normal* with respect to) a *reference state* of the form

$$\omega_{\rho,\beta} := \omega_\rho^p \otimes \omega_\beta^f, \tag{10}$$

where ω_ρ^p is given by a density matrix ρ on $\mathcal{H}_p$, see equation (1), and ω_β^f is the *thermal equilibrium state* of the radiation field at temperature $T = (k_B\beta)^{-1}$, where k_B is Boltzmann's constant. Technically, ω_β^f is defined as the *unique* (α_t^f, β)-KMS *state* on the algebra $\mathfrak{A}_f$; it is invariant under (or "stationary" for) the free-field time evolution α_t^f. If the density matrix ρ describes an arbitrary statistical mixture of bound states of H_p, but ρ vanishes on the subspace $L^2(\mathbb{R}^3, d^3x)$ of $\mathcal{H}_p$, then $\omega_{\rho,\beta}$ is *stationary* for the free time evolution $\alpha_{t,0}$ defined in equation (7). However, it is *not* an equilibrium (KMS) state for $\alpha_{t,0}$. In fact, because H_p has continuous spectrum, there are *no* equilibrium (KMS) states on $\mathfrak{A}$ for the time evolution $\alpha_{t,0}$.

Given the algebra $\mathfrak{A}$ and a reference state $\omega_{\rho,\beta}$ on $\mathfrak{A}$, as in equation (10), the *GNS construction* associates with the pair $(\mathfrak{A}, \omega_{\rho,\beta})$ a Hilbert space $\mathcal{H}$, a $*$representation π_β of $\mathfrak{A}$ on $\mathcal{H}$, and a vector $\Omega_\rho \in \mathcal{H}$, cyclic for the algebra $\pi_\beta(\mathfrak{A})$, such that

$$\omega_{\rho,\beta}(A) = \langle \Omega_\rho, \pi_\beta(A)\Omega_\rho \rangle \,, \tag{11}$$

for all $A \in \mathfrak{A}$. The closure of the algebra $\pi_\beta(\mathfrak{A})$ in the weak operator topology is a von Neumann algebra of bounded operators on $\mathcal{H}$ which we denote by $\mathfrak{M}_\beta$. This algebra depends on β, but is independent of the choice of the density matrix ρ. The states ω on $\mathfrak{A}$ of interest to us are given by vectors $\psi \in \mathcal{H}$ in such a way that

$$\omega(A) = \langle \psi, \pi_\beta(A)\psi \rangle \,, \quad A \in \mathfrak{A}. \tag{12}$$

We shall see that there exists a selfadjoint operator $L_\lambda^{(\epsilon)}$ on $\mathcal{H}$ generating the time evolution of the coupled system, in the sense that

$$\pi_\beta(\alpha_{t,\lambda}^{(\epsilon)}(A)) = e^{itL_\lambda^{(\epsilon)}}\pi_\beta(A)e^{-itL_\lambda^{(\epsilon)}}, \tag{13}$$

for $A \in \mathfrak{A}$; $L_\lambda^{(\epsilon)}$ is called the (regularized) *Liouvillian*. Clearly,

$$\sigma_{t,\lambda}^{(\epsilon)}(K) := e^{itL_\lambda^{(\epsilon)}}Ke^{-itL_\lambda^{(\epsilon)}}, \quad K \in \mathfrak{M}_\beta, \tag{14}$$

defines a $*$automorphism group of time translations on $\mathfrak{M}_\beta$. For an interesting class of models, we shall show that

$$\text{s-}\lim_{\epsilon\to 0} e^{itL_\lambda^{(\epsilon)}} =: e^{itL_\lambda} \tag{15}$$

exists, for all t, and defines a unitary one-parameter group on $\mathcal{H}$. It then follows from (14), (15) that

$$\sigma_{t,\lambda}(K) := e^{itL_\lambda}Ke^{-itL_\lambda} \tag{16}$$

defines a one-parameter group of $*$automorphisms on the von Neumann algebra $\mathfrak{M}_\beta$. The pair $(\mathfrak{M}_\beta, \sigma_{t,\lambda})$ defines a so-called W^**-dynamical system.* If the coupling constant λ vanishes then a state $\omega_{\rho,\beta} = \omega_\rho^p \otimes \omega_\beta^f$, where the density matrix ρ vanishes on the subspace $L^2(\mathbb{R}^3, d^3x) \subset \mathcal{H}_p$ corresponding to the continuous spectrum of $\mathcal{H}_p$ and commutes with H_p, is an invariant state for $\sigma_{t,0}$, in the sense that

$$\omega_{\rho,\beta}(\sigma_{t,0}(K)) := \langle\Omega_\rho, \sigma_{t,0}(K)\Omega_\rho\rangle = \omega_{\rho,\beta}(K), \tag{17}$$

for all $K \in \mathfrak{M}_\beta$.

The *main result* proven in this paper can be described as follows: For an interesting class of interactions, V, for an arbitrary inverse temperature $0 < \beta < \infty$, and for all real coupling constants λ with $0 < |\lambda| < \lambda_0(\beta)$, where $\lambda_0(\beta)$ depends on the choice of V, and on β as $\lambda_0(\beta) \sim e^{\beta E_0}$, where $E_0 < 0$ is the ground state energy of the particle system, there *do not exist any* states ω on $\mathfrak{M}_\beta$ close, in the sense of equation (12), to a reference state $\omega_{\rho,\beta}$, as in equation (10), which are *invariant* under the time evolution $\sigma_{t,\lambda}$ on $\mathfrak{M}_\beta$, (in the sense that $\omega(\sigma_{t,\lambda}(K)) = \omega(K)$, for $K \in \mathfrak{M}_\beta$).

In other words, we show that, under the hypotheses described above, there are no time-translation invariant states of the coupled system of asymptotic temperature $T = (k_B\beta)^{-1} > 0$. It will turn out that this result is a consequence of the following one: For a certain canonical definition of the Liouvillian L_λ of the coupled system, and under the hypotheses sketched above, L_λ does not have any eigenvectors $\psi \in \mathcal{H}$, in particular, $\ker L_\lambda = \{0\}$. This result will be proven with the help of *Mourre's theory of positive commutators* applied to L_λ and a new virial theorem.

As a corollary of our results it follows that, for an arbitrary vector $\psi \in \mathcal{H}$ and an arbitrary compact operator K on $\mathcal{H}$,

$$\left\langle \psi, e^{itL_\lambda} K e^{-itL_\lambda} \psi \right\rangle \to 0, \tag{18}$$

as time $t \to \infty$, (at least in the sense of ergodic means). This means that the survival probability of an arbitrary bound state of the atom coupled to the quantized radiation field in a thermal equilibrium state at positive temperature tends to zero, as time $t \to \infty$. Heuristically, this can be understood by using Fermi's Golden Rule.

One may wonder how the quantum-mechanical motion of an electron looks like, after it has been knocked off the atom by a high-energy boson, i.e., after thermal ionization. We cannot give an answer to this question, in this paper, because we are not able to analyze appropriately realistic models, yet. But it is natural to expect that this motion will be *diffusive*, furnishing an example of "quantum Brownian motion". Progress on this question would be highly desirable.

Organization of the paper. In Section 2, we define the model, and state our main result on thermal ionization, Theorem 2.4, which follows from spectral properties of the Liouvillian proven in our key technical theorem, Theorem 2.3. In Section 3, we state two general virial theorems, Theorems 3.2 and 3.3, we present a result on regularity of eigenfunctions of Liouvillians, Theorem 3.4, and explain some basic ideas of the positive commutator method. The proof of Theorem 2.3 (spectrum of Liouvillian) is given in Section 4. It consists of two main parts: verification that the virial theorems are applicable in the particular situation encountered in the analysis of our models (Subsection 4.2), and proof of a lower bound on a commutator of the Liouvillian with a suitable conjugate operator (Subsections 4.3, 4.4). In Section 5, we establish some technical results on the invariance of operator domains and on certain commutator expansions that are needed in the proofs of the virial theorems and of the theorem on regularity of eigenfunctions. Proofs of the latter results are presented in Section 6. In Section 7, we describe some results on unitary groups generated by vector fields which are needed in the definition of our "conjugate operator" A_p^a in the positive commutator method. The last section, Section 8, contains proofs of several propositions used in earlier sections of the paper.

2 Definition of models and main results on thermal ionization

In Section 2.1, we introduce our model and use it to define a W^*-dynamical system $(\mathfrak{M}_\beta, \sigma_{t,\lambda})$. Our main results on thermal ionization are described in Section 2.2.

2.1 Definition of the model

Starting with the algebra $\mathfrak{A}$ and a (regularized) dynamics $\alpha_{t,\lambda}^{(\epsilon)}$ on it, we introduce a reference state $\omega_{\rho_0,\beta}$, and consider the induced (regularized) dynamics $\sigma_{t,\lambda}^{(\epsilon)}$ on $\pi_\beta(\mathfrak{A})$, where $(\mathcal{H}, \pi_\beta, \Omega_{\rho_0})$ denotes the GNS representation corresponding to $(\mathfrak{A}, \omega_{\rho_0,\beta})$. We show that, as $\epsilon \to 0$, $\sigma_{t,\lambda}^{(\epsilon)}$ tends to a $*$automorphism group, $\sigma_{t,\lambda}$, of the von Neumann algebra $\mathfrak{M}_\beta$, defined as the weak closure of $\pi_\beta(\mathfrak{A})$ in $\mathcal{B}(\mathcal{H})$. We determine the generator, L_λ, of the unitary group, e^{itL_λ}, on $\mathcal{H}$ implementing $\sigma_{t,\lambda}$; L_λ is called a *Liouvillian*. The relation between eigenvalues of L_λ and invariant normal states on $\mathfrak{M}_\beta$ will be explained later in this section, (see Theorem 2.2). We will sometimes write simply L instead of L_λ, for $\lambda \neq 0$.

2.1.1 The algebra $\mathfrak{A}_f$

We introduce a C^*-algebra suitable for the description of the dynamics of the free field, and, as we explain below, for the description of the interacting dynamics.

Let $\mathfrak{W} = \mathfrak{W}(L_0^2)$ be the Weyl CCR algebra over

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

i.e., the C^*-algebra generated by the Weyl operators, $W(f)$, for $f \in L^2_0$, satisfying

$$W(-f) = W(f)^*, \quad W(f)W(g) = e^{-i\mathrm{Im}\langle f,g\rangle/2} W(f+g).$$

Here, $\langle\cdot,\cdot\rangle$ denotes the inner product of L^2_0. The latter relation implies the CCR

$$W(f)W(g) = e^{-i\mathrm{Im}\langle f,g\rangle} W(g)W(f). \tag{19}$$

The expectation functional for the KMS state of an infinitely extended free Bose field in thermal equilibrium at inverse temperature β is given by

$$g \mapsto \omega^f_\beta(W(g)) = \exp\left\{ -\frac{1}{4}\int_{\mathbb{R}^3} \left(1 + \frac{2}{e^{\beta|k|}-1}\right) |g(k)|^2 d^3k \right\},$$

which motivates the choice of the space L^2_0 (as opposed to $g \in L^2(\mathbb{R}^3)$).

The free field dynamics on $\mathfrak{W}$ is given by the $*$automorphism group

$$\alpha^{\mathfrak{W}}_t(W(f)) = W(e^{i|k|t}f). \tag{20}$$

It is well known that for $f \neq 0$, $t \mapsto \alpha^{\mathfrak{W}}_t(W(f))$ is not a continuous map from $\mathbb{R}$ to $\mathfrak{W}$, but $t \mapsto \omega(\alpha^{\mathfrak{W}}_t(W(f)))$ is continuous for a large (weak* dense) class of states ω on $\mathfrak{W}$. An interacting dynamics is commonly defined using a Dyson series expansion, hence we should be able to give a sense to time integrals over $\alpha^{\mathfrak{W}}_t(a)$, for $a \in \mathfrak{W}$. Because of the lack of norm-continuity of the free dynamics, such an integral cannot be interpreted in norm sense, but only in a weak hence representation dependent way. In order to give a representation independent definition of the (coupled) dynamics, we modify the algebra in such a way that the free dynamics becomes norm continuous. The idea is to introduce a time-averaged Weyl algebra, generated by elements given by

$$a(h) = \int_{\mathbb{R}} ds\ h(s)\alpha^{\mathfrak{W}}_s(a), \tag{21}$$

for functions h in a certain class, and $a \in \mathfrak{W}$ (if h is sharply localized at zero, the integral approximates $a \in \mathfrak{W}$). The free dynamics is then given by

$$\alpha^f_t(a(h)) = \int_{\mathbb{R}} ds\ h(s)\alpha^{\mathfrak{W}}_s(\alpha^{\mathfrak{W}}_t(a)) = \int_{\mathbb{R}} ds\ h(s-t)\alpha^{\mathfrak{W}}_s(a).$$

We now construct a C^*-algebra whose elements, when represented on a Hilbert space, are given by (21), where the integral is understood in a weak sense.

Let $\mathfrak{P}$ be the free algebra generated by elements

$$\left\{ a(h) \mid a \in \mathfrak{W}, \widehat{h} \in C_0^\infty(\mathbb{R}) \right\},$$

where $\widehat{}$ denotes the Fourier transform. Taking the functions h to be analytic (i.e., having a Fourier transform in C_0^∞) allows us to construct KMS states w.r.t. the free dynamics, as we explain below. We equip the algebra $\mathfrak{P}$ with the star operation defined by $(a(h))^* = (a^*)(\overline{h})$, and introduce the seminorm

$$p(a(h)) = \sup_{\pi \in \mathrm{Rep}\, \mathfrak{W}} \left\| \int_{\mathbb{R}} dt\ h(t) \pi \left(\alpha_t^{\mathfrak{W}}(a) \right) \right\|, \tag{22}$$

where the supremum extends over all representations of $\mathfrak{W}$. The integral on the r.h.s. of (22) is understood in the weak sense ($t \mapsto \pi(\alpha_t^{\mathfrak{W}}(a))$ is weakly measurable for any $\pi \in \mathrm{Rep}\, \mathfrak{W}$), and the norm is the one of operators acting on the representation Hilbert space. It is not difficult to verify that

$$\mathfrak{N} = \{ a \in \mathfrak{P} \mid p(a) = 0 \}$$

is a two-sided $*$ideal in $\mathfrak{P}$. We can therefore build the quotient $*$algebra $\mathfrak{P}/\mathfrak{N}$ consisting of equivalence classes $[a] = \{ a + n \mid a \in \mathfrak{P}, n \in \mathfrak{N} \}$, on which p defines a norm

$$\| [a] \| = p(a), \quad [a] \in \mathfrak{P}/\mathfrak{N},$$

having the C^* property

$$\| [a]^*[a] \| = \| [a] \|^2.$$

The C^*-algebra $\mathfrak{A}_f$ of the field is defined to be the closure of the quotient in this norm,

$$\mathfrak{A}_f = \overline{\mathfrak{P}/\mathfrak{N}}^{\|\cdot\|}.$$

Notice that every $\pi_{\mathfrak{W}} \in \mathrm{Rep}\, \mathfrak{W}$ induces a representation $\pi_f \in \mathrm{Rep}\, \mathfrak{A}_f$ according to $\pi_f(a(h)) = \int dt\, h(t) \pi_{\mathfrak{W}}(\alpha_t^{\mathfrak{W}}(a))$. The algebra $\mathfrak{A}_f$ can be viewed as a time-averaged version of the Weyl algebra. The advantage of $\mathfrak{A}_f$ over $\mathfrak{W}$ is that the free field dynamics on $\mathfrak{A}$, defined by

$$\alpha_t^f(a(h)) = a(h_t), \quad h_t(x) = h(x-t), \tag{23}$$

is a norm-continous $*$automorphism group, i.e., $\|\alpha_t^f(a) - a\| \to 0$, as $t \to 0$, for any $a \in \mathfrak{A}_f$.

There is a one-to-one correspondence between $(\beta, \alpha_t^{\mathfrak{W}})$-KMS states $\omega_\beta^{\mathfrak{W}}$ on $\mathfrak{W}$ and (β, α_t^f)-KMS states ω_β^f on $\mathfrak{A}_f$, given by the relation

$$\omega_\beta^f(a_1(f_1)\cdots a_n(f_n)) = \int dt_1 \cdots dt_n\, f_1(t_1)\cdots f_n(t_n)\, \omega_\beta^{\mathfrak{W}}\left(\alpha_{t_1}^{\mathfrak{W}}(a_1)\cdots \alpha_{t_n}^{\mathfrak{W}}(a_n)\right).$$

If $(\mathcal{H}, \pi_{\mathfrak{W}}^\beta, \Omega)$ is the GNS representation of $(\mathfrak{W}, \omega_\beta^{\mathfrak{W}})$ then the one of $(\mathfrak{A}_f, \omega_\beta^f)$ is given by $(\mathcal{H}, \pi_f^\beta, \Omega)$, where

$$\begin{aligned} &\pi_f^\beta\left(a_1(f_1)\cdots a_n(f_n)\right) \\ &\quad = \int dt_1 \cdots dt_n\ f_1(t_1)\cdots f_n(t_n)\pi_{\mathfrak{W}}^\beta\left(\alpha_{t_1}^{\mathfrak{W}}(a_0)\cdots \alpha_{t_n}^{\mathfrak{W}}(a_n)\right). \end{aligned} \tag{24}$$

It follows that any unitary group implementing the free dynamics relative to $\pi_{\mathfrak{W}}^\beta$ implements it in the representation π_f^β, and conversely.

2.1.2 The algebra $\mathfrak{A}$ and the regularized dynamics $\alpha_{t,\lambda}^{(\epsilon)}$

The C^*-algebra $\mathfrak{A}$ describing the "observables" of the combined system is the tensor product algebra

$$\mathfrak{A} = \mathfrak{A}_p \otimes \mathfrak{A}_f. \tag{25}$$

Here, $\mathfrak{A}_p = \mathcal{B}(\mathcal{H}_p)$ is the C^*-algebra of all bounded operators on the particle Hilbert space

$$\mathcal{H}_p = \mathbb{C} \oplus L^2(\mathbb{R}_+, de; \mathfrak{H}) \equiv \mathbb{C} \oplus \int_{\mathbb{R}_+}^{\oplus} \mathfrak{H}_e\ de, \tag{26}$$

where de is the Lebesgue measure on $\mathbb{R}_+$, $\mathfrak{H}$ is a (separable) Hilbert space, and the r.h.s. is the constant fibre direct integral with $\mathfrak{H}_e \cong \mathfrak{H}$, $e \in \mathbb{R}_+$. An element in $\mathcal{H}_p$ is given by $\psi = \{\psi(e)\}_{e\in\{E\}\cup\mathbb{R}_+}$, where $\psi(E) \in \mathbb{C}$, and $\psi(e) \in \mathfrak{H}$, $e \in \mathbb{R}_+$. $\mathcal{H}_p$ is a Hilbert space with inner product

$$\langle \psi, \phi\rangle = \overline{\psi(E)}\phi(E) + \int_{\mathbb{R}_+} \langle \psi(e), \phi(e)\rangle_{\mathfrak{H}}\ de.$$

Let α_t^p denote the $*$automorphism group on $\mathfrak{A}_p$ given by

$$\alpha_t^p(A) = e^{itH_p} A e^{-itH_p},$$

where H_p is a selfadjoint operator on $\mathcal{H}_p$, which is diagonalized by the direct integral decomposition of $\mathcal{H}_p$:

$$H_p = E \oplus \int_{\mathbb{R}_+}^{\oplus} e\ de, \qquad \text{for some } E < 0. \tag{27}$$

The domain of definition of H_p is given by

$$\mathcal{D}(H_p) = \mathbb{C} \oplus \left\{ \psi \in \int_{\mathbb{R}_+}^{\oplus} \mathfrak{H}_e de \;\middle|\; \int_{\mathbb{R}_+} e^2 \|\psi(e)\|_{\mathfrak{H}}^2 de < \infty \right\}. \tag{28}$$

The dense set $C_0^\infty(\mathbb{R}_+;\mathfrak{H}) \equiv C_0^\infty$ consists of all elements $\psi \in \mathcal{H}_p$ s.t. the support, $\mathrm{supp}(\psi \restriction \mathbb{R}_+)$, is a compact set in the open half-axis $(0,\infty)$, and s.t. ψ is infinitely many times continuously differentiable as an $\mathfrak{H}$-valued function. Clearly, $C_0^\infty \subset \mathcal{D}(H_p)$, and since e^{itH_p} leaves C_0^∞ invariant, it follows that C_0^∞ is a core for H_p. It is sometimes practical to identify $\mathbb{C} \cong \mathbb{C}\varphi_0$, and we say that φ_0 is the eigenfunction of H_p corresponding to the eigenvalue E.

Example. This model is inspired by considering a block-diagonal Hamiltonian H_p on the Hilbert space $\mathbb{C} \oplus L^2(\mathbb{R}^3, d^3x)$, with $H_p \restriction \mathbb{C} = E < 0$, $H_p \restriction L^2(\mathbb{R}^3, d^3x) = -\Delta$. Passing to a diagonal representation of the Laplacian (Fourier transform), we have the following identifications, using polar coordinates:

$$\begin{aligned}
\mathcal{H}_p &= \mathbb{C} \oplus L^2(\mathbb{R}^3, d^3k) \\
&= \mathbb{C} \oplus L^2(\mathbb{R}_+ \times S^2, |k|^2 d|k| \times d\Sigma) \\
&= \mathbb{C} \oplus L^2(\mathbb{R}_+, |k|^2 d|k|; L^2(S^2, d\Sigma)) \\
&= \mathbb{C} \oplus L^2(\mathbb{R}_+, d\mu; \mathfrak{H}),
\end{aligned}$$

where we set $\mathfrak{H} = L^2(S^2, d\Sigma)$, and make the change of variables $|k|^2 = e$, so that $d\mu(e) = \mu(e)de$, with $\mu(e) = \frac{1}{2}\sqrt{e}$. To arrive at the form (26), (27) of $\mathcal{H}_p$, H_p, we use the unitary map $U : L^2(\mathbb{R}_+, d\mu; \mathfrak{H}) \to L^2(\mathbb{R}_+, de; \mathfrak{H})$, given by

$$\psi \mapsto U\psi = \sqrt{\mu}\psi.$$

If H_p is the operator of multiplication by e on $L^2(\mathbb{R}_+, d\mu; \mathfrak{H})$, then its transform, UH_pU^{-1}, is the operator of multiplication by e on $L^2(\mathbb{R}_+, de; \mathfrak{H})$.

We define the non-interacting time-translation $*$automorphism group of $\mathfrak{A}$ (the free dynamics) by

$$\alpha_{t,0} := \alpha_t^p \otimes \alpha_t^f.$$

Given $\epsilon \neq 0$, set

$$V^{(\epsilon)} := \sum_\alpha G_\alpha \otimes \frac{1}{2i\epsilon}\left\{(W(\epsilon g_\alpha))(h_\epsilon) - (W(\epsilon g_\alpha))(h_\epsilon)^*\right\} \in \mathfrak{A}, \tag{29}$$

where the sum is over finitely many indices α, with $G_\alpha = G_\alpha^* \in \mathcal{B}(\mathcal{H}_p)$, $g_\alpha \in L_0^2$, for all α, and where h_ϵ is an approximation of the Dirac distribution localized at zero. To be specific, we can take $h_\epsilon(t) = \frac{1}{\epsilon}e^{-t^2/\epsilon^2}$. For any value of the real coupling constant λ, the norm-convergent Dyson series

$$\begin{aligned}
&\alpha_{t,0}(A) \\
&+ \sum_{n\geq 1}(i\lambda)^n \int_0^t dt_1 \cdots \int_0^{t_{n-1}} dt_n \left[\alpha_{t_n,0}(V^{(\epsilon)}), \left[\cdots\left[\alpha_{t_1,0}(V^{(\epsilon)}), \alpha_{t,0}(A)\right]\cdots\right]\right] \\
&=: \alpha_{t,\lambda}^{(\epsilon)}(A),
\end{aligned} \tag{30}$$

where $A \in \mathfrak{A}$, defines a $*$automorphism group on $\mathfrak{A}$. The multiple integral in (30) is understood in the product topology coming from the strong topology of $\mathcal{B}(\mathcal{H}_p)$ and the norm topology of $\mathfrak{A}_f$.

One should view $\alpha_{t,\lambda}^{(\epsilon)}$ as a *regularized dynamics*, in the sense that it has a limit, as $\epsilon \to 0$, in suitably chosen representations of $\mathfrak{A}$; (this is shown below).

The functions $g_\alpha \in L_0^2$ are called *form factors*. Using spherical coordinates in $\mathbb{R}^3$, we often write $g_\alpha = g_\alpha(\omega, \Sigma)$, where $(\omega, \Sigma) \in \mathbb{R}_+ \times S^2$.

In accordance with the direct integral decomposition of H_p, the operators G_α are determined by integral kernels. For $\psi = \{\psi(e)\} \in \mathcal{H}_p$, we set

$$(G_\alpha\psi)(e) = \begin{cases} G_\alpha(E,E)\psi(E) + \int_{\mathbb{R}_+} G_\alpha(E,e')\psi(e')de', & \text{if } e = E, \\ G_\alpha(e,E)\psi(E) + \int_{\mathbb{R}_+} G_\alpha(e,e')\psi(e')de', & \text{if } e \in \mathbb{R}_+. \end{cases} \tag{31}$$

The families of bounded operators $G_\alpha(e,e'):\mathfrak{H}_{e'}\to\mathfrak{H}_e$, with $\mathfrak{H}_E=\mathbb{C}$, have the following symmetry properties (guaranteeing that G_α is selfadjoint):

$$\begin{aligned} G_\alpha(E,E) &\in \mathbb{R}, \\ G_\alpha(E,e)^* &= G_\alpha(e,E), \quad \forall e\in\mathbb{R}_+, \\ G_\alpha(e,e')^* &= G_\alpha(e',e), \quad \forall e,e'\in\mathbb{R}_+. \end{aligned}$$

Here, * indicates taking the adjoint of an operator in $\mathcal{B}(\mathfrak{H},\mathbb{C})$ or $\mathcal{B}(\mathfrak{H})$.

Remarks. 1) The map $G_\alpha(E,e):\mathfrak{H}_e\to\mathbb{C}$ is identified (Riesz) with an element $\Gamma_\alpha(e)\in\mathfrak{H}_e$, so that $G_\alpha(E,e)\psi(e)=\langle\Gamma_\alpha(e),\psi(e)\rangle_{\mathfrak{H}_e}$. Then $G_\alpha(E,e)^*:\mathbb{C}\to\mathfrak{H}_e$ is given by $G_\alpha(E,e)^*z=z\Gamma_\alpha(e)$, for all $z\in\mathbb{C}$. Consequently, the above symmetry condition implies that $G_\alpha(e,E)z=z\Gamma_\alpha(e)$.

2) Assuming the strong derivatives w.r.t. the two arguments $(e,e')\in\mathbb{R}_+^2$ of $G_\alpha(\cdot,\cdot)$ exist, we have that $\partial_{1,2}G_\alpha(e,e')$ are operators $\mathfrak{H}\to\mathfrak{H}$. Similarly, one introduces higher derivatives. We assume that all derivatives occuring are bounded operators on $\mathfrak{H}$. For $G_\alpha(\cdot,\cdot)\in C^n(\mathbb{R}_+\times\mathbb{R}_+,\mathcal{B}(\mathfrak{H}))$, it is easily verified that the above symmetry conditions imply that

$$\left(\partial_1^{n_1}\partial_2^{n_2}G_\alpha(e,e')\right)^*=\partial_1^{n_2}\partial_2^{n_1}G_\alpha(e',e), \tag{32}$$

for any $n_{1,2}\geq 0$, $n_1+n_2\leq n$, where * is the adjoint on $\mathcal{B}(\mathfrak{H})$. Similar statements hold for $G_\alpha(E,e)$, $G_\alpha(e,E)$.

The interaction is required to satisfy the following three conditions:

(A1) Infrared and ultraviolet behaviour of the form factors: for any fixed $\Sigma\in S^2$, $g_\alpha(\cdot,\Sigma)\in C^4(\mathbb{R}_+)$, and there are two constants $0<k_1,k_2<\infty$, s.t. if $\omega<k_1$, then

$$|\partial_\omega^j g_\alpha(\omega,\Sigma)|<k_2\omega^{p-j},\quad \text{for some } p>2, \tag{33}$$

uniformly in α, $j=0,\dots,4$ and $\Sigma\in S^2$. Similarly, there are two constants $0<K_1,K_2<\infty$, s.t. if $\omega>K_1$, then

$$|\partial_\omega^j g_\alpha(\omega,\Sigma)|<K_2\omega^{-q-j},\quad \text{for some } q>7/2. \tag{34}$$

(A2) The map $(e,e')\mapsto G_\alpha(e,e')$ is $C^3(\mathbb{R}_+\times\mathbb{R}_+,\mathcal{B}(\mathfrak{H}))$, and we have

$$\int_{\mathbb{R}_+} de\,\left\|e^{-m_1}\partial_1^{m_2}G_\alpha(e,E)\right\|_{\mathfrak{H}}^2<\infty, \tag{35}$$

$$\int_{\mathbb{R}_+} de\int_{\mathbb{R}_+} de'\,\left\|e^{-m_1}(e')^{-m_1'}\partial_1^{m_2}\partial_2^{m_2'}G_\alpha(e,e')\right\|_{\mathcal{B}(\mathfrak{H})}^2<\infty, \tag{36}$$

for all integers $m_{1,2}, m'_{1,2} \geq 0$, s.t. $m_1 + m'_1 + m_2 + m'_2 = 0, 1, 2, 3$. Moreover,

$$\int_{\mathbb{R}_+} de \int_{\mathbb{R}_+} de' \, \| e \, G_\alpha(e, e') \|^2_{\mathcal{B}(\mathfrak{H})} < \infty. \tag{37}$$

(A3) The Fermi Golden Rule Condition. Define a family of bounded operators on $\mathcal{H}_p$ by

$$F(\omega, \Sigma) = \sum_\alpha g_\alpha(\omega, \Sigma) G_\alpha. \tag{38}$$

There is an $\epsilon_0 > 0$, s.t. for $0 < \epsilon < \epsilon_0$, we have that

$$\int_{-E}^{\infty} d\omega \int_{S^2} d\Sigma \; \frac{\omega^2}{e^{\beta\omega} - 1} p_0 F(\omega, \Sigma) \frac{\overline{p}_0 \; \epsilon}{(H_p - E - \omega)^2 + \epsilon^2} F(\omega, \Sigma)^* p_0 \geq \gamma p_0, \tag{39}$$

for some strictly positive constant $\gamma > 0$. Here, p_0 is the orthogonal projection onto the eigenspace $\mathbb{C}$ of H_p (see (26), (27)), and $\overline{p}_0 = \mathbb{1} - p_0$ is the projection onto $L^2(\mathbb{R}_+, de; \mathfrak{H})$.

Remarks. 1) Since $E < 0$ we have that $\gamma \sim e^{\beta E}$ decays exponentially in β, for large β.

2) Recalling that $G_\alpha(E, e)$ is identified with $\Gamma_\alpha(e) \in \mathfrak{H}_e$, see Remark 1) after (31) above, we can rewrite the l.h.s. of (39) as

$$\int_{(-E,\infty)\times S^2} d\omega \; d\Sigma \int_{\mathbb{R}_+} de \; \frac{\omega^2}{e^{\beta\omega} - 1} \frac{\epsilon}{(e - E - \omega)^2 + \epsilon^2} \times \sum_{\alpha,\alpha'} \overline{g}_\alpha(\omega, \Sigma) \, \langle \Gamma_\alpha(e), \Gamma_{\alpha'}(e) \rangle_{\mathfrak{H}} \, g_{\alpha'}(\omega, \Sigma),$$

and this expression has the limit

$$\int_{(-E,\infty)\times S^2} d\omega \; d\Sigma \;\; \frac{\omega^2}{e^{\beta\omega} - 1} \sum_{\alpha,\alpha'} \overline{g}_\alpha(\omega, \Sigma) \, \langle \Gamma_\alpha(E + \omega), \Gamma_{\alpha'}(E + \omega) \rangle_{\mathfrak{H}} \, g_{\alpha'}(\omega, \Sigma),$$

as $\epsilon \to 0$, because $\Gamma_\alpha(e)$ is continuous in e. Consequently, (39) is satisfied if this integral is strictly positive.

2.1.3 The reference state $\omega_{\rho_0,\beta}$

Let ρ_0 be a strictly positive density matrix on $\mathcal{H}_p$, i.e., $\rho_0 > 0$, $\mathrm{tr}\rho_0 = 1$, and denote by $\omega^p_{\rho_0}$ the state on $\mathfrak{A}_p$ given by $A \mapsto \mathrm{tr}\rho_0 A$. Let ω^f_β be the (α^f_t, β)-KMS state on $\mathfrak{A}_f$ and define the reference state

$$\omega_{\rho_0,\beta} = \omega^p_{\rho_0} \otimes \omega^f_\beta.$$

The GNS representation $(\mathcal{H}, \pi_\beta, \Omega_{\rho_0})$ corresponding to $(\mathfrak{A}, \omega_{\rho_0,\beta})$ is explicitly known. It has first been described in [AW]; (we follow [JP] in its presentation). The representation Hilbert space is

$$\mathcal{H} = \mathcal{H}_p \otimes \mathcal{H}_p \otimes \mathcal{F}, \tag{40}$$

where $\mathcal{F}$ is a shorthand for the Fock space

$$\mathcal{F} = \mathcal{F}\left((L^2(\mathbb{R} \times S^2,\ du \times d\Sigma)\right), \tag{41}$$

du being the Lebesgue measure on $\mathbb{R}$, and $d\Sigma$ the uniform measure on S^2. $\mathcal{F}(X)$ denotes the bosonic Fock space over a (normed vector) space X:

$$\mathcal{F}(X) := \mathbb{C} \oplus \bigoplus_{n\geq 1} \left(\mathcal{S}X^{\otimes n}\right), \tag{42}$$

where $\mathcal{S}$ is the projection onto the symmetric subspace of the tensor product. We adopt standard notation, e.g. Ω is the vacuum vector, $[\psi]_n$ is the n-particle component of $\psi \in \mathcal{F}(X)$, $\mathrm{d}\Gamma(A)$ is the second quantization of the operator A on X, $N = \mathrm{d}\Gamma(\mathbb{1})$ is the number operator.

The representation map $\pi_\beta : \mathfrak{A} \to \mathcal{B}(\mathcal{H})$ is the product

$$\pi_\beta = \pi_p \otimes \pi^\beta_f,$$

where the $*$homomorphism $\pi_p : \mathfrak{A}_p \to \mathcal{B}(\mathcal{H}_p \otimes \mathcal{H}_p)$ is given by

$$\pi_p(A) = A \otimes \mathbb{1}_p.$$

The representation map $\pi^\beta_f : \mathfrak{A}_f \to \mathcal{B}(\mathcal{F})$ is determined by the representation map of the Weyl algebra, $\pi^\beta_{\mathfrak{W}} : \mathfrak{W} \to \mathcal{B}(\mathcal{F})$, according to (24). To describe

$\pi^{\beta}_{\mathfrak{W}}$, we point out that $L^2(\mathbb{R}_+ \times S^2) \oplus L^2(\mathbb{R}_+ \times S^2)$ is isometrically isomorphic to $L^2(\mathbb{R} \times S^2)$ via the map

$$(f, g) \mapsto h, \quad h(u, \Sigma) = \begin{cases} u\ f(u, \Sigma), & u > 0, \\ u\ g(-u, \Sigma), & u < 0. \end{cases} \tag{43}$$

The representation map $\pi^{\beta}_{\mathfrak{W}}$ is given by

$$\pi^{\beta}_{\mathfrak{W}} = \pi_{\text{Fock}} \circ \mathcal{T}_{\beta},$$

where the Bogoliubov transformation $\mathcal{T}_{\beta} : \mathfrak{W}(L^2_0) \to \mathfrak{W}(L^2(\mathbb{R} \times S^2))$ acts as $W(f) \mapsto W(\tau_{\beta} f)$, with $\tau_{\beta} : L^2(\mathbb{R}_+ \times S^2) \to L^2(\mathbb{R} \times S^2)$ given by

$$(\tau_{\beta} f)(u, \Sigma) = \sqrt{\frac{u}{1 - e^{-\beta u}}} \begin{cases} \sqrt{u}\ f(u, \Sigma), & u > 0, \\ -\sqrt{-u}\ \overline{f}(-u, \Sigma), & u < 0. \end{cases} \tag{44}$$

Remarks. 1) It is easily verified that $\operatorname{Im} \langle \tau_{\beta} f, \tau_{\beta} g \rangle_{L^2(\mathbb{R} \times S^2)} = \operatorname{Im} \langle f, g \rangle_{L^2(\mathbb{R}_+ \times S^2)}$, for all $f, g \in L^2_0$, so the CCR (19) are preserved under the map τ_{β}.

2) In the limit $\beta \to \infty$, the r.h.s. of (44) tends to

$$\begin{cases} u\ f(u, \Sigma), & u > 0, \\ 0, & u < 0, \end{cases}$$

which is identified, via (43), with $f \in L^2_0$. Thus, $\mathcal{T}_{\beta}$ reduces to the identity (an imbedding), $\pi^{\beta}_{\mathfrak{W}}$ becomes the Fock representation of $\mathfrak{W}(L^2_0)$, as $\beta \to \infty$, and we recover the zero temperature situation.

It is useful to introduce the following notation. For $f \in L^2(\mathbb{R} \times S^2)$, we define unitary operators, $\widehat{W}(f)$, on the Hilbert space (40), by

$$\widehat{W}(f) = e^{i\varphi(f)}, \quad f \in L^2(\mathbb{R} \times S^2),$$

where $\varphi(f)$ is the selfadjoint operator on $\mathcal{F}$ given by

$$\varphi(f) = \frac{a^*(f) + a(f)}{\sqrt{2}}, \tag{45}$$

and $a^*(f)$, $a(f)$ are the creation- and annihilation operators on $\mathcal{F}$, smeared out with f. One easily verifies that

$$\pi^{\beta}_{\mathfrak{W}}(W(f)) = \widehat{W}(\tau_{\beta} f).$$

The cyclic GNS vector is given by

$$\Omega_{\rho_0} = \Omega_p^{\rho_0} \otimes \Omega,$$

where Ω is the vacuum in $\mathcal{F}$, and

$$\Omega_p^{\rho_0} = \sum_{n \geq 0} k_n \varphi_n \otimes \mathcal{C}_p \varphi_n \in \mathcal{H}_p \otimes \mathcal{H}_p. \tag{46}$$

Here, $\{k_n^2\}_{n=0}^{\infty}$ is the spectrum of ρ_0, $\{\varphi_n\}$ is an orthogonal basis of eigenvectors of ρ_0, and $\mathcal{C}_p$ is an antilinear involution on $\mathcal{H}_p$. The origin of $\mathcal{C}_p$ lies in the identification of $l^2(\mathcal{H}_p)$ (Hilbert-Schmitt operators on $\mathcal{H}_p$) with $\mathcal{H}_p \otimes \mathcal{H}_p$, via $|\varphi\rangle\langle\psi| \mapsto \varphi \otimes \mathcal{C}_p \psi$. We fix a convenient choice for $\mathcal{C}_p$: it is the antilinear involution on $\mathcal{H}_p$ that has the effect of taking complex conjugates of components of vectors, in the basis in which the Hamiltonian H_p is diagonal, i.e.,

$$(\mathcal{C}_p \psi)(e) = \begin{cases} \overline{\psi(e)} \in \mathbb{C}, & e = E, \\ \overline{\psi(e)} \in \mathfrak{H}, & e \in [0, \infty). \end{cases}$$

By $\overline{\psi(e)} \in \mathfrak{H}$ for $e \in [0, \infty)$, we understand the element in $\mathfrak{H}$ obtained by complex conjugation of the components of $\psi(e) \in \mathfrak{H}$, in an arbitrary, but fixed, orthonormal basis of $\mathfrak{H}$. This $\mathcal{C}_p$ is also called the time reversal operator, and we have

$$\mathcal{C}_p H_p \mathcal{C}_p = H_p.$$

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

Let $\mathfrak{M}_\beta$ be the von Neumann algebra obtained by taking the weak closure (or equivalently, the double commutant) of $\pi_\beta(\mathfrak{A})$ in $\mathcal{B}(\mathcal{H})$:

$$\mathfrak{M}_\beta = \mathcal{B}(\mathcal{H}_p) \otimes \mathbb{1}_p \otimes \pi_f^\beta(\mathfrak{A}_f)'' \subset \mathcal{B}(\mathcal{H}).$$

Since ρ_0 is strictly positive, $\Omega_p^{\rho_0}$ is cyclic and separating for the von Neumann algebra $\pi_p(\mathfrak{A}_p)'' = \mathcal{B}(\mathcal{H}_p) \otimes \mathbb{1}_p$. Similarly, Ω is cyclic and separating for $\pi_f^\beta(\mathfrak{A}_f)''$, since it is the GNS vector of a KMS state (see e.g. [BRII]). Consequently, Ω_{ρ_0} is cyclic and separating for $\mathfrak{M}_\beta$. Let J be the modular conjugation operator associated to $(\mathfrak{M}_\beta, \Omega_{\rho_0})$. It is given by

$$J = J_p \otimes J_f, \tag{47}$$

where, for $\varphi, \psi \in \mathcal{H}_p$,

$$J_p\left(\varphi \otimes \mathcal{C}_p \psi\right) = \psi \otimes \mathcal{C}_p \varphi,$$

and, for $\psi = \{[\psi]_n\}_{n\geq 0} \in \mathcal{F}$,

$$\begin{aligned} [J_f\psi]_n(u_1,\ldots,u_n) &= \overline{[\psi]_n(-u_1,\ldots,-u_n)}, \quad \text{for } n\geq 1, \\ [J_f\psi]_0 &= \overline{[J_f\psi]_0} \in \mathbb{C}. \end{aligned}$$

Clearly, $J\Omega_{\rho_0} = \Omega_{\rho_0}$, and one verifies that

$$J_p \pi_p(A) J_p = \mathbb{1}_p \otimes \mathcal{C}_p A \mathcal{C}_p, \tag{48}$$

$$J_f \pi^\beta_{\mathfrak{W}}(W(f)) J_f = \widehat{W}(-e^{-\beta u/2}\tau_\beta(f)) = \widehat{W}(e^{-\beta u/2}\tau_\beta(f))^*, \tag{49}$$

for $f \in L^2_0$. More generally, for $f \in L^2(\mathbb{R}\times S^2)$, $J_f \widehat{W}(f) J_f = \widehat{W}(\overline{f(-u,\Sigma)})$.

We now construct a unitary implementation of $\alpha^{(\epsilon)}_{t,\lambda}$ w.r.t. π_β. Recall that $\pi_\beta = \pi_p \otimes \pi^\beta_f$, where $\pi_p : \mathcal{B}(\mathcal{H}) \to \mathcal{B}(\mathcal{H}_p \otimes \mathcal{H}_p)$ is continuous w.r.t. the strong topologies and $\pi^\beta_f : \mathfrak{A}_f \to \mathcal{B}(\mathcal{F})$ is continuous w.r.t. the norm topologies (because it is a $*$ homomorphism). We thus have, for $A \in \mathfrak{A}$,

$$\begin{aligned} &\pi_\beta(\alpha^{(\epsilon)}_{t,\lambda}(A)) \\ &= \pi_\beta(\alpha_{t,0}(A)) + \sum_{n\geq 1} (i\lambda)^n \int_0^t dt_1 \cdots \int_0^{t_{n-1}} dt_n \Big[\pi_\beta(\alpha_{t_n,0}(V^{(\epsilon)})), \Big[\cdots \\ &\quad \cdots \Big[\pi_\beta(\alpha_{t_1,0}(V^{(\epsilon)})), \pi_\beta(\alpha_{t,0}(A))\Big]\cdots\Big]\Big]. \end{aligned} \tag{50}$$

Because

$$\pi_p(\alpha^p_t(A)) = e^{itH_p} A e^{-itH_p} \otimes \mathbb{1}_p = e^{it(H_p\otimes \mathbb{1}_p - \mathbb{1}_p \otimes H_p)} \pi_p(A) e^{-it(H_p\otimes \mathbb{1}_p - \mathbb{1}_p\otimes H_p)},$$

and

$$\begin{aligned} \pi^\beta_{\mathfrak{W}}(\alpha^{\mathfrak{W}}_t(W(f))) &= \pi^\beta_{\mathfrak{W}}(W(e^{i\omega t}f)) = \widehat{W}(e^{iut}\tau_\beta(f)) \\ &= e^{it\mathrm{d}\Gamma(u)} \widehat{W}(\tau_\beta(f)) e^{-it\mathrm{d}\Gamma(u)} = e^{it\mathrm{d}\Gamma(u)} \pi^\beta_{\mathfrak{W}}(W(f)) e^{-it\mathrm{d}\Gamma(u)}, \end{aligned}$$

so that

$$\pi^\beta_f(\alpha^f_t(a)) = e^{it\mathrm{d}\Gamma(u)} \pi^\beta_f(a) e^{-it\mathrm{d}\Gamma(u)}, \quad a \in \mathfrak{A}_f,$$

we find that

$$\sigma_{t,0}(\pi_\beta(A)) := \pi_\beta(\alpha_{t,0}(A)) = e^{itL_0}\pi_\beta(A)e^{-itL_0},$$

for all $A \in \mathfrak{A}$, where L_0 is the selfadjoint operator on $\mathcal{H}$, given by

$$L_0 = H_p \otimes \mathbb{1}_p - \mathbb{1}_p \otimes H_p + \mathrm{d}\Gamma(u), \tag{51}$$

commonly called the (non-interacting, standard) Liouvillian. One easily verifies that

$$Je^{itL_0} = e^{itL_0}J. \tag{52}$$

Remark. There are other selfadjoint operators generating unitary implementations of $\sigma_{t,0}$ on $\mathcal{H}$. Indeed, we may add to L_0 any selfadjoint operator L_0' affiliated with the commutant $\mathfrak{M}_\beta{}'$; then $L_0 + L_0'$ still generates a unitary implementation of $\sigma_{t,0}$ on $\mathcal{H}$. However, the additional condition (52) fixes L_0 uniquely, and the generator of this unitary group is called the *standard* Liouvillian for $\sigma_{t,0}$. This terminology has been used before in [DJP]. The importance of considering the standard Liouvillian (as opposed to other generators of the dynamics) lies in the fact that its spectrum is related to the dynamical properties of the system; see Theorem 2.2.

Notice that $\sigma_{t,0}$ is a group of $*$automorphisms of $\pi_\beta(\mathfrak{A})$, in particular, $e^{itL_0}\pi_\beta(\mathfrak{A})e^{-itL_0} = \pi_\beta(\mathfrak{A})$, $\forall t \in \mathbb{R}$. From Tomita-Takesaki theory, we know that $J\mathfrak{M}_\beta J = \mathfrak{M}_\beta{}'$ (the commutant), and since

$$\sigma_{t,0}\left(J\pi_\beta(V^{(\epsilon)})J\right) = J\sigma_{t,0}\left(\pi_\beta(V^{(\epsilon)})\right)J = J\pi_\beta(\alpha_{t,0}(V^{(\epsilon)}))J \in \mathfrak{M}_\beta{}',$$

we can write the multicommutator in (50) as

$$\Big[\sigma_{t_n,0}\left(\pi_\beta(V^{(\epsilon)}) - J\pi_\beta(V^{(\epsilon)})J\right), \Big[\cdots$$
$$\cdots\Big[\sigma_{t_1,0}\left(\pi_\beta(V^{(\epsilon)}) - J\pi_\beta(V^{(\epsilon)})J\right), \sigma_{t,0}(\pi_\beta(A))\Big]\cdots\Big]\Big].$$

It follows that the r.h.s. of (50) defines a $*$automorphism group of $\pi_\beta(\mathfrak{A})$, $\sigma_{t,\lambda}^{(\epsilon)}$, which is implemented unitarily by

$$\sigma_{t,\lambda}^{(\epsilon)}(\pi_\beta(A)) = \pi_\beta(\alpha_{t,\lambda}^{(\epsilon)}(A)) = e^{itL_\lambda^{(\epsilon)}}\pi_\beta(A)e^{-itL_\lambda^{(\epsilon)}},$$

with

$$L_\lambda^{(\epsilon)} = L_0 + \lambda\pi_\beta(V^{(\epsilon)}) - \lambda J\pi_\beta(V^{(\epsilon)})J.$$

It is not difficult to see (using Theorem 3.1) that the *regularized Liouvillian* $L_\lambda^{(\epsilon)}$ is essentially selfadjoint on

$$\mathcal{D} = C_0^\infty \otimes C_0^\infty \otimes (\mathcal{F}(C_0^\infty(\mathbb{R}\times S^2)) \cap \mathcal{F}_0) \subset \mathcal{H},$$

where $\mathcal{F}_0$ is the finite-particle subspace. Moreover, we have that $Je^{itL_\lambda^{(\epsilon)}} = e^{itL_\lambda^{(\epsilon)}}J$. We now explain how to remove the regularization ($\epsilon \to 0$), obtaining a weak$*$ continuous $*$automorphism group $\sigma_{t,\lambda}$ of the von Neumann algebra $\mathfrak{M}_\beta$. We recall that a $*$automorphism group τ_t on a von Neumann algebra $\mathfrak{M}$ is called *weak* continuous* iff $t \mapsto \omega(\tau_t(A))$ is continuous, for all $A \in \mathfrak{M}$ and for all normal states ω on $\mathfrak{M}$. From

$$\begin{aligned}
\pi_\beta(V^{(\epsilon)}) &= \sum_\alpha G_\alpha \otimes \mathbb{1}_p \otimes \frac{1}{2i\epsilon}\int_{\mathbb{R}} dt\ h_\epsilon(t)\left\{\widehat{W}(e^{iut}\epsilon\tau_\beta(g_\alpha)) - \right.\\
&\qquad \left.\widehat{W}(e^{iut}\epsilon\tau_\beta(g_\alpha))^*\right\}\\
J\pi_\beta(V^{(\epsilon)})J &= \sum_\alpha \mathbb{1}_p \otimes \mathcal{C}_p G_\alpha \mathcal{C}_p \otimes \frac{1}{2i\epsilon}\int_{\mathbb{R}} dt\ h_\epsilon(t)\left\{\widehat{W}(e^{iut}\epsilon e^{-\beta u/2}\tau_\beta(g_\alpha)) - \right.\\
&\qquad \left.\widehat{W}(e^{iut}\epsilon e^{-\beta u/2}\tau_\beta(g_\alpha))^*\right\},
\end{aligned}$$

where we recall that $h_\epsilon(t) = \frac{1}{\epsilon}e^{-t^2/\epsilon^2}$ approximates the Dirac delta distribution concentrated at zero, one verifies that, in the strong sense on $\mathcal{D}$,

$$\begin{aligned}
\lim_{\epsilon\to 0}\pi_\beta(V^{(\epsilon)}) &= \sum_\alpha G_\alpha \otimes \mathbb{1}_p \otimes \varphi(\tau_\beta(g_\alpha)),\\
\lim_{\epsilon\to 0} J\pi_\beta(V^{(\epsilon)})J &= \sum_\alpha \mathbb{1}_p \otimes \mathcal{C}_p G_\alpha \mathcal{C}_p \otimes \varphi(e^{-\beta u/2}\tau_\beta(g_\alpha)),
\end{aligned}$$

where the operator $\varphi(f)$ has been defined in (45). The symmetric operator L_λ, defined on $\mathcal{D}$ by

$$L_\lambda = L_0 + \lambda I, \tag{53}$$

with

$$I = \sum_\alpha G_\alpha \otimes \mathbb{1}_p \otimes \varphi(\tau_\beta(g_\alpha)) - \mathbb{1}_p \otimes \mathcal{C}_p G_\alpha \mathcal{C}_p \otimes \varphi(e^{-\beta u/2}\tau_\beta(g_\alpha)), \tag{54}$$

is essentially selfadjoint on $\mathcal{D}$, for any real value of λ; (this will be shown to be a consequence of Theorem 3.1). Using Theorem 5.1 on invariance of domains, the Duhamel formula gives

$$e^{itL_\lambda^{(\epsilon)}} = e^{itL_\lambda} - i\lambda \int_0^t e^{isL_\lambda} \left(I - \pi_\beta(V^{(\epsilon)}) + J\pi_\beta(V^{(\epsilon)})J \right) e^{-i(s-t)L_\lambda^{(\epsilon)}}$$

as operators defined on $\mathcal{D}$, from which it follows that $e^{itL_\lambda^{(\epsilon)}} \to e^{itL_\lambda}$, as $\epsilon \to 0$, in the strong sense on $\mathcal{H}$. Consequently, for $A \in \pi_\beta(\mathfrak{A})$, we have $\sigma_{t,\lambda}^{(\epsilon)}(A) \to \sigma_{t,\lambda}(A)$, in the σ-weak topology of $\mathcal{B}(\mathcal{H})$. Notice that for $A \in \pi_\beta(\mathfrak{A})$, we have $\sigma_{t,\lambda}(A) \in \mathfrak{M}_\beta$, because $\sigma_{t,\lambda}(A) = \text{w-}\lim_{\epsilon\to 0} \sigma_{t,\lambda}^{(\epsilon)}(A)$, $\sigma_{t,\lambda}^{(\epsilon)}(A) \in \pi_\beta(\mathfrak{A}) \subset \mathfrak{M}_\beta$, and $\mathfrak{M}_\beta$ is weakly closed. Clearly, $\sigma_{t,\lambda}$ is a σ-weakly continuous $*$automorphism group of $\mathcal{B}(\mathcal{H})$. If $A \in \mathfrak{M}_\beta$, there is a net $\{A_\alpha\}_{\alpha\in\mathcal{I}} \subset \pi_\beta(\mathfrak{A})$, s.t. $A_\alpha \to A$, in the weak operator topology. Thus, since $\sigma_{t,\lambda}$ is weakly continuous, we conclude that

$$\sigma_{t,\lambda}(A) = \text{w-}\lim_\alpha \sigma_{t,\lambda}(A_\alpha) \in \mathfrak{M}_\beta.$$

We summarize these considerations in a proposition.

Proposition 2.1 *$(\mathfrak{M}_\beta, \sigma_{t,\lambda})$ is a W^*-dynamical system, i.e. $\sigma_{t,\lambda}$ is a weak$*$ continuous group of $*$automorphisms of the von Neumann algebra $\mathfrak{M}_\beta$. Moreover, $\sigma_{t,\lambda}$ is unitarily implemented by e^{itL_λ}, where L_λ is given in (53), (54), and*

$$Je^{itL_\lambda} = e^{itL_\lambda}J, \quad \text{for all } t \in \mathbb{R}.$$

2.1.5 Kernel of L_λ and normal invariant states

Let $\mathcal{P}$ be the natural cone associated with $(\mathfrak{M}_\beta, \Omega_{\rho_0})$, i.e., $\mathcal{P}$ is the norm closure of the set

$$\{AJA\Omega_{\rho_0} \mid A \in \mathfrak{M}_\beta\} \subset \mathcal{H}.$$

The data $(\mathfrak{M}_\beta, \mathcal{H}, J, \mathcal{P})$ is called the *standard form* of the von Neumann algebra $\mathfrak{M}_\beta$. We have constructed J and $\mathcal{P}$ explicitly, starting from the cyclic and separating vector Ω_{ρ_0}. There is, however, a general theory of standard forms of von Neumann algebras; see [BRI], [Ara], [Con] for the case of σ-finite von Neumann algebras (as in our case), or [Haa] for the general case. Among the properties of standard forms, we mention here only the following:

(P) For every normal state ω on $\mathfrak{M}_\beta$, there exists a unique $\xi \in \mathcal{P}$, s.t. $\omega(A) = \langle \xi, A\xi \rangle$, $\forall A \in \mathfrak{M}_\beta$.

Recall that a state ω on $\mathfrak{M}_\beta \subset \mathcal{B}(\mathcal{H})$ is called normal iff it is σ-weakly continuous, or, equivalently, iff it is given by a density matrix $\rho \in l^1(\mathcal{H})$, as $\omega(A) = \mathrm{tr}\rho A$, for all $A \in \mathfrak{M}_\beta$. The uniqueness of the representing vector in the natural cone, according to (P), allows us to establish the following connection between the kernel of L_λ and the normal invariant states (see also e.g. [DJP]).

Theorem 2.2 *If L_λ does not have a zero eigenvalue, i.e., if* $\ker L_\lambda = \{0\}$, *then there does not exist any $\sigma_{t,\lambda}$-invariant normal state on $\mathfrak{M}_\beta$.*

Proof. We show below that, for all $t \in \mathbb{R}$,

$$e^{itL_\lambda}\mathcal{P} = \mathcal{P}. \tag{55}$$

If ω is a normal state on $\mathfrak{M}_\beta$, invariant under $\sigma_{t,\lambda}$, i.e., such that $\omega \circ \sigma_{t,\lambda} = \omega$, for all $t \in \mathbb{R}$, then, for a unique $\xi \in \mathcal{P}$,

$$\omega(A) = \langle \xi, A\xi \rangle = \omega(\sigma_{t,\lambda}(A)) = \left\langle e^{-itL_\lambda}\xi, Ae^{-itL_\lambda}\xi \right\rangle.$$

Since (55) holds, and due to the uniqueness of the vector in $\mathcal{P}$ representing a given state, we conclude that $e^{itL_\lambda}\xi = \xi$, for all $t \in \mathbb{R}$, i.e. L_λ has a zero eigenvalue with eigenvector ξ.

We now show (55). Notice that (55) is equivalent to $e^{itL_\lambda}\mathcal{P} \subseteq \mathcal{P}$. Since $\mathcal{P}$ is a closed set, it is enough to show that for all $A \in \mathfrak{M}_\beta$, $e^{itL_\lambda}AJA\Omega_{\rho_0} \in \mathcal{P}$. Since $e^{itL_\lambda}J = Je^{itL_\lambda}$, $e^{itL_\lambda}Ae^{-itL_\lambda} \in \mathfrak{M}_\beta$, for all $A \in \mathfrak{M}_\beta$, and $BJBJ\mathcal{P} \subset \mathcal{P}$, for all $B \in \mathfrak{M}_\beta$, we only need to prove that

$$e^{itL_\lambda}\Omega_{\rho_0} \in \mathcal{P}. \tag{56}$$

The Trotter product formula gives

$$e^{itL_\lambda}\Omega_{\rho_0} = \lim_{n\to\infty}\left(e^{i\frac{t}{n}\lambda I}e^{i\frac{t}{n}L_0}\right)^n \Omega_{\rho_0},$$

and, since $\mathcal{P}$ is closed, (56) holds provided the general term under the limit is in $\mathcal{P}$, for all $n \geq 1$. We show that $e^{isL_0}\mathcal{P} = \mathcal{P}$ and $e^{is\lambda I}\mathcal{P} = \mathcal{P}$, for all $s \in \mathbb{R}$. Remarking that

$$e^{isL_0}\Omega_{\rho_0} = \left(e^{isH_p} \otimes e^{-isH_p} \otimes e^{is\mathrm{d}\Gamma(u)}\right)\Omega_{\rho_0} = \left(e^{isH_p} \otimes \mathbb{1}_p\right) J \left(e^{isH_p} \otimes \mathbb{1}_p\right)\Omega_{\rho_0},$$

where we use that $J_p(e^{isH_p} \otimes \mathbb{1}_p)J_p = \mathbb{1}_p \otimes \mathcal{C}_p e^{isH_p}\mathcal{C}_p = \mathbb{1}_p \otimes e^{-isH_p}$, recalling that e^{isL_0} implements $\sigma_{t,0}$, and arguing as above, we see that $e^{itL_0}\mathcal{P} = \mathcal{P}$.

The Trotter product formula gives

$$\begin{aligned}
&\exp\left\{ is \sum_{\alpha=1}^{N} G_\alpha \otimes \mathbb{1}_p \otimes \varphi(\tau_\beta(g_\alpha)) - JG_\alpha \otimes \mathbb{1}_p \otimes \varphi(\tau_\beta(g_\alpha))J \right\} \xi = \\
&\quad \lim_{n_1 \to \infty} \left\{ \left(e^{i\frac{s}{n_1}G_1} \otimes \mathbb{1}_p \otimes \widehat{W}\left(\frac{s}{n_1}\tau_\beta(g_\alpha)\right)\right) J \left(e^{i\frac{s}{n_1}G_1} \otimes \mathbb{1}_p \otimes \widehat{W}\left(\frac{s}{n_1}\tau_\beta(g_\alpha)\right) J\right) \right. \\
&\quad \left. \times \exp\left[i\frac{s}{n_1} \sum_{\alpha=2}^{N} (G_\alpha \otimes \mathbb{1}_p \otimes \varphi(\tau_\beta(g_\alpha)) - JG_\alpha \otimes \mathbb{1}_p \otimes \varphi(\tau_\beta(g_\alpha))J) \right] \right\}^{n_1} \xi,
\end{aligned}$$

for all $\xi \in \mathcal{P}$, and we may apply Trotter's formula repeatedly to conclude that, since $AJAJ\mathcal{P} \subset \mathcal{P}$, for $A \in \mathfrak{M}_\beta$, and $\mathcal{P}$ is closed, we have that $e^{is\lambda I}\mathcal{P} = \mathcal{P}$, for all $s \in \mathbb{R}$. ■

Remark. The proof of Theorem 2.2 uses property (P), which is satisfied in our case, because Ω_{ρ_0} is cyclic and separating for $\mathfrak{M}_\beta$. This, in turn, is true because ρ_0 has been chosen to be strictly positive. One may start with any reference state of the form $\omega^p_\rho \otimes \omega^f_\beta$, where ρ is any density matrix on $\mathcal{H}_p$; it may be of finite rank. The resulting von Neumann algebra (obtained as the weak closure of $\mathfrak{A}$ when represented on the GNS Hilbert space corresponding to $(\mathfrak{A}, \omega^p_\rho \otimes \omega^f_\beta))$ is $*$isomorphic to $\mathfrak{M}_\beta$. This is the reason we have not added to $\mathfrak{M}_\beta$ an index for the density matrix ρ_0. More specifically, the GNS representation of $(\mathfrak{A}, \omega^p_\rho \otimes \omega^f_\beta)$ is given by $(\mathcal{H}_1, \pi_1, \Omega_1)$, where

$$\begin{aligned}
\mathcal{H}_1 &= \mathcal{H}_p \otimes \mathcal{K}_\rho \subseteq \mathcal{H}_p \otimes \mathcal{H}_p, \\
\pi_1(A \otimes (W(f))(h)) &= A \otimes \mathbb{1}_p \otimes \int_{\mathbb{R}} dt\ h(t)\widehat{W}(e^{iut}\tau_\beta(f)), \\
\Omega_1 &= \Omega^\rho_p \otimes \Omega.
\end{aligned}$$

Here, $\mathcal{K}_\rho$ is the closure of Ran ρ, Ω^ρ_p is given as in equation (46). Consequently,

$$\pi_1(\mathfrak{A})'' = \mathcal{B}(\mathcal{H}_p) \otimes \mathbb{1}_p \upharpoonright_{\mathcal{K}_\rho} \otimes \pi^\beta_f(\mathfrak{A}_f)'' \cong \mathfrak{M}_\beta.$$

In particular, $\pi_1(\mathfrak{A})''$ and $\mathfrak{M}_\beta$ have *the same set of normal states.* Thus, our particular choice for the reference state is immaterial when examining properties of normal states. One may express this in the following way: $(\mathfrak{M}_\beta, \mathcal{H}, J, \mathcal{P})$ is a standard form for all the von Neumann algebras obtained from any reference state $(\mathfrak{A}, \omega^p_\rho \otimes \omega^f_\beta)$.

2.2 Result on thermal ionization

Our main result in this paper is that the W^*-dynamical system $(\mathfrak{M}_\beta, \sigma_{t,\lambda})$ introduced above does not have any normal invariant states.

Theorem 2.3 *Assume conditions (A1)-(A3) hold. For any inverse temperature* $0 < \beta < \infty$ *there is a constant,* $\lambda_0(\beta) > 0$*, proportional to* γ *given in (39), such that the following holds. If* $0 < |\lambda| < \lambda_0$ *then the Liouvillian* L_λ *given in (53) and (54) does not have any eigenvalues.*

Remark. Since γ decays exponentially in β, for large β, Theorem 2.3 is a high temperature result (β has to be small for reasonable values of the coupling constant λ). From physics it is clear that thermal ionization takes place for *arbitrary positive temperatures* (but not at zero temperature, where the coupled system has a ground state).

Combining Theorems 2.3 and 2.2 yields our main result about thermal ionization.

Theorem 2.4 (Thermal ionization) *Under the assumptions of Theorem 2.3, there do not exist any normal* $\sigma_{t,\lambda}$*-invariant states on* $\mathfrak{M}_\beta$*.*

Remark. For $\lambda = 0$, the state ω_0, determined by the vector $\Omega^0_p \otimes \Omega$, where $\Omega^0_p = \varphi_0 \otimes \varphi_0 \in \mathcal{H}_p \otimes \mathcal{H}_p$, and φ_0 is the eigenvector of H_p, is a normal $\sigma_{t,0}$-invariant state on $\mathfrak{M}_\beta$. As we have explained in the introduction, the physical interpretation of Theorem 2.4 is that a single atom coupled to black-body radiation at a sufficiently high positive temperature will always end up being ionized.

The proof of Theorem 2.3 is based on a novel virial theorem.

3 Virial theorems and the positive commutator method

3.1 Two abstract virial theorems

Let $\mathcal{H}$ be a Hilbert space, $\mathcal{D} \subset \mathcal{H}$ a core for a selfadjoint operator $Y \geq \mathbb{1}$, and X a symmetric operator on $\mathcal{D}$. We say the triple $(X, Y, \mathcal{D})$ satisfies the *GJN (Glimm-Jaffe-Nelson) Condition*, or that $(X, Y, \mathcal{D})$ is a *GJN-triple*, if there is a constant $k < \infty$, s.t. for all $\psi \in \mathcal{D}$:

$$\begin{aligned} \|X\psi\| &\leq k\|Y\psi\| && (57) \\ \pm i \left\{ \langle X\psi, Y\psi \rangle - \langle Y\psi, X\psi \rangle \right\} &\leq k \langle \psi, Y\psi \rangle . && (58) \end{aligned}$$

Notice that if $(X_1, Y, \mathcal{D})$ and $(X_2, Y, \mathcal{D})$ are GJN triples, then so is $(X_1 + X_2, Y, \mathcal{D})$. Since $Y \geq \mathbb{1}$, inequality (57) is equivalent to

$$\|X\psi\| \leq k_1\|Y\psi\| + k_2\|\psi\|,$$

for some $k_1, k_2 < \infty$.

Theorem 3.1 (GJN commutator theorem) *If $(X, Y, \mathcal{D})$ satisfies the GJN Condition, then X determines a selfadjoint operator (again denoted by X), s.t. $\mathcal{D}(X) \supset \mathcal{D}(Y)$. Moreover, X is essentially selfadjoint on any core for Y, and (57) is valid for all $\psi \in \mathcal{D}(Y)$.*

Based on the GJN commutator theorem, we next describe the setting for a general *virial theorem*. Suppose one is given a selfadjoint operator $\Lambda \geq \mathbb{1}$ with core $\mathcal{D} \subset \mathcal{H}$, and operators L, A, N, D, C_n, $n = 0, 1, 2, 3$, all symmetric on $\mathcal{D}$, and satisfying

$$\begin{aligned} \langle \varphi, D\psi \rangle &= i \left\{ \langle L\varphi, N\psi \rangle - \langle N\varphi, L\psi \rangle \right\} && (59) \\ C_0 &= L && \\ \langle \varphi, C_n\psi \rangle &= i \left\{ \langle C_{n-1}\varphi, A\psi \rangle - \langle A\varphi, C_{n-1}\psi \rangle \right\}, \quad n = 1, 2, 3, && (60) \end{aligned}$$

where $\varphi, \psi \in \mathcal{D}$. We assume that

- $(X, \Lambda, \mathcal{D})$ satisfies the GJN Condition, for $X = L, N, D, C_n$. Consequently, all these operators determine selfadjoint operators, which we denote by the same letters.

- A is selfadjoint, $\mathcal{D} \subset \mathcal{D}(A)$, and e^{itA} leaves $\mathcal{D}(\Lambda)$ invariant.

Remarks. 1) From the invariance condition $e^{itA}\mathcal{D}(\Lambda) \subset \mathcal{D}(\Lambda)$, it follows that for some $0 \le k, k' < \infty$, and all $\psi \in \mathcal{D}(\Lambda)$,

$$\|\Lambda e^{itA}\psi\| \le k e^{k'|t|}\|\Lambda\psi\|. \tag{61}$$

A proof of this can be found in [ABG], Propositions 3.2.2 and 3.2.5.
2) Condition (57) is phrased equivalently as "$X \le kY$, in the sense of Kato on $\mathcal{D}$".
3) One can show that if $(A, \Lambda, \mathcal{D})$ satisfies conditions (57), (58), then the above assumption on A holds; see Theorem 5.1.

Theorem 3.2 (1$^{\text{st}}$ virial theorem) *Assume that, in addition to (59), (60), we have, in the sense of Kato on $\mathcal{D}$,*

$$\begin{aligned} D &\le kN^{1/2}, & (62)\\ e^{itA}C_1e^{-itA} &\le ke^{k'|t|}N^p, \quad \textit{some } 0 \le p < \infty, & (63)\\ e^{itA}C_3e^{-itA} &\le ke^{k'|t|}N^{1/2}, & (64) \end{aligned}$$

for some $0 \le k, k' < \infty$, and all $t \in \mathbb{R}$. Let ψ be an eigenvector of L. Then there is a one-parameter family $\{\psi_\alpha\} \subset \mathcal{D}(L) \cap \mathcal{D}(C_1)$, s.t. $\psi_\alpha \to \psi$, $\alpha \to 0$, and

$$\lim_{\alpha\to 0}\langle\psi_\alpha, C_1\psi_\alpha\rangle = 0. \tag{65}$$

Remarks. 1) A sufficient condition for (63) to hold (with $k' = 0$) is that N and e^{itA} commute, for all $t \in \mathbb{R}$, in the strong sense on $\mathcal{D}$, and $C_1 \le kN^p$. This condition will always be satisfied in our applications. A similar remark applies to (64).
2) In a heuristic way, we understand C_1 as the commutator $i[L, A] = i(LA - AL)$, and (65) as $\langle\psi, i[L, A]\psi\rangle = 0$, which is a standard way of stating the virial theorem, see e.g. [ABG], and [GG] for a comparison (and correction) of virial theorems encountered in the literature.

The result of the Virial Theorem is still valid if we add to the operator A a suitably small perturbation A_0:

Theorem 3.3 **($2^{\rm nd}$ virial theorem)** *Suppose that we are in the situation of Theorem 3.2 and that A_0 is a bounded operator on $\mathcal{H}$ s.t.* $\mathrm{Ran}\, A_0 \subset \mathcal{D}(L) \cap \mathrm{Ran}\, P(N \leq n_0)$*, for some $n_0 < \infty$. Then $i[L, A_0] = i(LA_0 - A_0L)$ is well defined in the strong sense on $\mathcal{D}(L)$, and we have, for the same family of approximating eigenvectors as in Theorem 3.2:*

$$\lim_{\alpha \to 0} \langle \psi_\alpha, (C_1 + i[L, A_0])\psi_\alpha \rangle = 0. \tag{66}$$

In conjunction with a positive commutator estimate, the virial theorem implies a certain regularity of eigenfunctions.

Theorem 3.4 **(Regularity of eigenfunctions)** *Suppose C is a symmetric operator on a domain $\mathcal{D}(C)$ s.t., in the sense of quadratic forms on $\mathcal{D}(C)$, we have that $C \geq \mathcal{P} - B$, where $\mathcal{P} \geq 0$ is a selfadjoint operator, and B is a bounded (everywhere defined) operator. Let ψ_α be a family of vectors in $\mathcal{D}(C)$, with $\psi_\alpha \to \psi$, as $\alpha \to 0$, and s.t.*

$$\lim_{\alpha \to 0} \langle \psi_\alpha, C\psi_\alpha \rangle = 0. \tag{67}$$

Then $\langle \psi, B\psi \rangle \geq 0$, $\psi \in \mathcal{D}(\mathcal{P}^{1/2})$, and

$$\|\mathcal{P}^{1/2}\psi\| \leq \langle \psi, B\psi \rangle^{1/2}. \tag{68}$$

Remark. Theorem 3.4 can be viewed as a consequence of an abstract Fatou Lemma, see [ABG], Proposition 2.1.1. We give a different, very short proof of (68) at the end of Section 6.

3.2 The positive commutator method

This method gives a conceptually very easy proof of absence of point spectrum. The subtlety of the method lies in the technical details, since one deals with unbounded operators.

Suppose we are in the setting of the virial theorems described in Section 3.1, and that the operator C_1 (or $C_1 + i[L, A_0]$) is *strictly positive*, i.e.

$$C_1 \geq \gamma, \tag{69}$$

for some $\gamma > 0$. Inequality (69) and the virial theorem immediately show that L cannot have any eigenvalues. Indeed, assuming ψ is an eigenfunction of L, we reach the contradiction

$$0 = \lim_{\alpha \to 0} \langle \psi_\alpha, C_1 \psi_\alpha \rangle \geq \gamma \lim_{\alpha \to 0} \langle \psi_\alpha, \psi_\alpha \rangle = \gamma \|\psi\|^2 > 0.$$

Although the *global PC estimate* (69) holds in our situation, often one manages to prove merely a *localized* version. Suppose $g \in C^\infty(J)$ is a smooth function with support in an interval $J \subseteq \mathbb{R}$, $g \upharpoonright J_1 = 1$, for some $J_1 \subset J$, s.t. $g(L)$ leaves the form domain of C_1 invariant. The same reasoning as above shows that if

$$g(L) C_1 g(L) \geq \gamma g^2(L),$$

for some $\gamma > 0$, then L has no eigenvalues in the interval J_1. The use of PC estimates for spectral analysis of Schrödinger operators has originated with Mourre [Mou], and had recent applications in [Ski], [BFSS], [DJ], [Mer].

4 Proof of Theorem 2.3

4.1 Strategy of the proof

As in [JP], [Mer], the starting point in the construction of a positive commutator is the adjoint operator $A_f = \mathrm{d}\Gamma(i\partial_u)$, the second quantized generator of translation in the radial variable of the glued Fock space $\mathcal{F}$, see (41). We formally have

$$i[L_0, A_f] = \mathrm{d}\Gamma(\mathbb{1}_f) = N \geq 0.$$

The kernel of this form is the *infinite dimensional* space $\mathcal{H}_p \otimes \mathcal{H}_p \otimes \mathrm{Ran}\, P_\Omega$. Following [Mer], one is led to try to add a suitable operator A_0 to A_f, where A_0 depends on the interaction λI, and is designed in such a way that $i[L_0 + \lambda I, A_f + A_0]$ is strictly positive (has trivial kernel). This method is applicable if the (imaginary part) of the so-called level shift operator is strictly positive, or equivalently, if (39) is satisfied, but where the finite-dimensional projection p_0 is replaced by the *infinite-dimensional* projection $\mathbb{1}_p$. Such a positivity condition does not hold for reasonable operators G_α and functions g_α.

In order to be able to carry out our program, we add to A_f a term $A_p \otimes \mathbb{1}_p - \mathbb{1}_p \otimes A_p$ that reduces the kernel of the commutator. A prime candidate for A_p would be the operator $i\partial_e$ acting on $\mathcal{H}_p$ (we write simply $i\partial_e$ instead of $0 \oplus i\partial_e$, c.f. (26)), since then

$$i[L_0, A_p \otimes \mathbb{1}_p - \mathbb{1}_p \otimes A_p + A_f] = P_+(H_p) \otimes \mathbb{1}_p + \mathbb{1}_p \otimes P_+(H_p) + N,$$

where $P_+(H_p) = \int_{\mathbb{R}_+}^{\oplus} de$ is the projection onto $L^2(\mathbb{R}_+, de; \mathcal{H})$. The above form has now a one-dimensional kernel, $\mathrm{Ran}\, p_0 \otimes p_0 \otimes P_\Omega$. By adding a suitable operator A_0, as described above, one can obtain a lower bound on the commutator (and in particular, reduce its kernel to $\{0\}$), provided (39) is satisfied.

However, the operator A_p chosen above has the inconvenience of not being selfadjoint, while our virial theorems require selfadjointness. We introduce a family of selfajoint operators A_p^a, $a > 0$, that approximate $i\partial_e$ in a certain sense ($a \to 0$). The idea of approximating a non-selfadjoint A by a selfadjoint sequence was also used in [Ski]. We now define A^a and then explain, in the remainder of this subsection, how to prove Theorem 2.3.

We define A_p^a as the generator of a unitary group on $L^2(\mathbb{R}_+, de; \mathcal{H})$, which is induced by a flow on $\mathbb{R}_+$. For the proof of the following proposition, and more information on unitary groups induced by flows, we refer to Section 7.

Proposition 4.1 *Let $\xi : \mathbb{R}_+ \to \mathbb{R}_+$ be a bounded, smooth vector field, s.t. $\xi(0) = 0$, $\xi(e) \to 1$, as $e \to \infty$, and $\|(1+e)\xi'\|_\infty < \infty$. Then ξ generates a global flow, and this flow induces a continuous unitary group on $L^2(\mathbb{R}_+, de; \mathfrak{H})$. The generator A_p of this group is essentially selfadjoint on C_0^∞, and it acts on C_0^∞ as*

$$A_p = i\left(\frac{1}{2}\xi'(e) + \xi(e)\partial_e\right), \tag{70}$$

where $\xi'(e)$ and $\xi(e)$ are multiplication operators. Given $a > 0$, $\xi_a(e) = \xi(e/a)$ is a vector field on $\mathbb{R}_+$, and $\lim_{a\to 0} \xi_a = 1$, pointwise (except at zero). The generator A_p^a of the unitary group induced by ξ_a is given on its core, C_0^∞, by

$$A_p^a = i\left(\frac{1}{2}\frac{1}{a}\xi'(e/a) + \xi(e/a)\partial_e\right). \tag{71}$$

We define the selfadjoint operator

$$A^a = A_p^a \otimes \mathbb{1}_p \otimes \mathbb{1}_f - \mathbb{1}_p \otimes A_p^a \otimes \mathbb{1}_f + A_f, \tag{72}$$

and calculate the commutator C_1^a of iL with A^a (in the sense given in (60), see also Subsection 4.2):

$$C_1^a = \int_{\mathbb{R}_+}^{\oplus} \xi_a(e) de \otimes 1\!\!1_p + 1\!\!1_p \otimes \int_{\mathbb{R}_+}^{\oplus} \xi_a(e) de + N + \lambda I_1^a, \tag{73}$$

where I_1^a is $N^{1/2}$-bounded. In Section 4.3, we show that $C_1^a + i[L, A_0] \geq M_a$, where M_a is a bounded operator. We will see that $\text{s-}\lim_{a \to 0_+} M_a = M$ (see Proposition 4.6), where M is a bounded, strictly positive operator (see Proposition 4.8). Since M_a, M are bounded, we obtain from the virial theorem

$$0 = \lim_{\alpha \to 0} \langle \psi_\alpha, (C_1^a + i[L, A_0])\psi_\alpha \rangle \geq \langle \psi, (M_a - M)\psi \rangle + \langle \psi, M\psi \rangle \,, \tag{74}$$

for any eigenfunction ψ of L. Taking $a \to 0_+$ and using strict positivity of M (for small, but nonzero λ, see Proposition 4.8), gives a contradiction, and this will prove Theorem 2.3.

4.2 Concrete setting for the virial theorems

The Hilbert space is the GNS representation space (40), and we set

$$\mathcal{D} = C_0^\infty \otimes C_0^\infty \otimes \mathcal{D}_f, \tag{75}$$

where

$$\mathcal{D}_f = \mathcal{F}\left(C_0^\infty(\mathbb{R} \times S^2)\right) \cap \mathcal{F}_0,$$

and $\mathcal{F}_0$ denotes the finite-particle subspace of Fock space. The operator Λ is given by

$$\begin{aligned} \Lambda &= \Lambda_p \otimes 1\!\!1_p + 1\!\!1_p \otimes \Lambda_p + \Lambda_f, & (76)\\ \Lambda_p &= \int_{\mathbb{R}_+}^{\oplus} e \; de + 1\!\!1_p = H_p P_+(H_p) + 1\!\!1_p, & (77)\\ \Lambda_f &= \mathrm{d}\Gamma(u^2 + 1) + 1\!\!1_f. & (78)\end{aligned}$$

In (77), we have introduced $P_+(H_p)$, the projection onto the spectral interval $\mathbb{R}_+$ of H_p. It is clear that Λ is essentially selfadjoint on $\mathcal{D}$, and $\Lambda \geq 1\!\!1$. The operator L is the interacting Liouvillian (53), and

$$N = \mathrm{d}\Gamma(1\!\!1) \tag{79}$$

is the particle number operator in $\mathcal{F} \equiv \mathcal{F}(L^2(\mathbb{R} \times S^2))$. Clearly, $X = L, N$ are symmetric operators on $\mathcal{D}$, and the symmetric operator D on $\mathcal{D}$ (see (59)) is given by

$$\begin{aligned} D &= \frac{i\lambda}{\sqrt{2}} \sum_\alpha \big\{ G_\alpha \otimes \mathbb{1}_p \otimes (-a^*(\tau_\beta(g_\alpha)) + a(\tau_\beta(g_\alpha))) \\ &\quad -\mathbb{1}_p \otimes \mathcal{C}_p G_\alpha \mathcal{C}_p \otimes \left(-a^*(e^{-\beta u/2}\tau_\beta(g_\alpha)) + a(e^{-\beta u/2}\tau_\beta(g_\alpha))\right) \big\}. \end{aligned} \quad (80)$$

The operator A is given by A^a defined in (72). Notice that A_p^a leaves C_0^∞ invariant, A_f leaves $\mathcal{D}_f$ invariant, so A^a maps $\mathcal{D}$ into $\mathcal{D}(L)$. Furthermore, it is easy to see that L maps $\mathcal{D}$ into $\mathcal{D}(A^a)$, hence the commutator of L with A^a is well defined in the strong sense on $\mathcal{D}$. The same is true for the multiple commutators of L with A^a. Setting $\xi_a'(e) = \xi'(e/a)$, $\xi_a''(e) = \xi''(e/a)$, we obtain

$$C_1^a = \int_{\mathbb{R}_+}^\oplus \xi_a(e) de \otimes \mathbb{1}_p + \mathbb{1}_p \otimes \int_{\mathbb{R}_+}^\oplus \xi_a(e) de + N + \lambda I_1^a, \quad (81)$$

$$C_2^a = \frac{1}{a} \int_{\mathbb{R}_+}^\oplus \xi_a'(e)\xi_a(e) de \otimes \mathbb{1}_p - \mathbb{1}_p \otimes \frac{1}{a} \int_{\mathbb{R}_+}^\oplus \xi_a'(e)\xi_a(e) de + \lambda I_2^a \quad (82)$$

$$\begin{aligned} C_3^a &= \frac{1}{a^2} \int_{\mathbb{R}_+}^\oplus \left(\xi_a''(e)\xi_a(e)^2 + \xi_a'(e)^2\xi_a(e)\right) de \otimes \mathbb{1}_p \\ &\quad + \mathbb{1}_p \otimes \frac{1}{a^2} \int_{\mathbb{R}_+}^\oplus \left(\xi_a''(e)\xi_a(e)^2 + \xi_a'(e)^2\xi_a(e)\right) de + \lambda I_3^a, \end{aligned} \quad (83)$$

where

$$\begin{aligned} I_n^a &= i^n \sum_{j=0}^n \binom{n}{k} \sum_\alpha \Big\{ \mathrm{ad}_{A_p^a}^{(j)}(G_\alpha) \otimes \mathbb{1}_p \otimes \mathrm{ad}_{A_f}^{(n-j)}\left(\varphi(\tau_\beta(g_\alpha))\right) \\ &\quad + (-1)^j \mathbb{1}_p \otimes \mathrm{ad}_{A_p^a}^{(j)}(\mathcal{C}_p G_\alpha \mathcal{C}_p) \otimes \mathrm{ad}_{A_f}^{(n-j)}\left(\varphi(e^{\beta u/2}\tau_\beta(g_\alpha))\right) \Big\}, \end{aligned} \quad (84)$$

for $n = 1, 2, 3$.

We define the bounded selfadjoint operator A_0 on $\mathcal{H}$ by

$$A_0 = i\theta\lambda(\Pi I R_\epsilon^2 \overline{\Pi} - \overline{\Pi} R_\epsilon^2 I \Pi), \quad (85)$$

with

$$R_\epsilon^2 = (L_0^2 + \epsilon^2)^{-1}. \tag{86}$$

Here, θ and ϵ are positive parameters, and Π is the projection onto the zero eigenspace of L_0:

$$\begin{aligned} \Pi &= P_0 \otimes P_\Omega, & (87)\\ P_0 &= p_0 \otimes p_0, & (88)\\ \overline{\Pi} &= \mathbb{1} - \Pi, & (89) \end{aligned}$$

where p_0 is the projection in $\mathcal{B}(\mathcal{H}_p)$ projecting onto the eigenspace corresponding to the eigenvalue E of H_p, i.e. $p_0\psi = \psi(E) \in \mathbb{C}$, and P_Ω is the projection in $\mathcal{B}(\mathcal{F})$ projecting onto $\mathbb{C}\Omega$. We also introduce the notation

$$\overline{R}_\epsilon = \overline{\Pi} R_\epsilon.$$

Notice that the operator A_0 satisfies the conditions given in Theorem 3.3 with $n_0 = 1$. Moreover, $[L, A_0] = LA_0 - A_0 L$ extends to a bounded operator on the entire Hilbert space, and

$$\|[L, A_0]\| \leq k \left(\frac{\theta\lambda}{\epsilon} + \frac{\theta\lambda^2}{\epsilon^2} \right). \tag{90}$$

This choice for the operator A_0 was initially introduced in [BFSS] for the spectral analysis of Pauli-Fierz Hamiltonians (zero temperature systems), and was adopted in [Mer] to show return to equilibrium (positive temperature systems). The key feature of A_0 is that $i\Pi[L, A_0]\Pi = 2\theta\lambda^2 \Pi I \overline{R}_\epsilon^2 I \Pi$ is a *non-negative* operator. Assuming the Fermi Golden Rule Condition (39), it is a *strictly positive operator*, as shows

Proposition 4.2 *Assume Condition (A3). For $0 < \epsilon < \epsilon_0$, we have*

$$\Pi I \overline{R}_\epsilon^2 I \Pi \geq \frac{\gamma}{\epsilon} \Pi. \tag{91}$$

The proof is given in Section 8.

We are now ready to verify that the virial theorems are applicable.

Proposition 4.3 *The unitary group e^{itA^a} leaves $\mathcal{D}(\Lambda)$ invariant ($a > 0, t \in \mathbb{R}$), and, for $\psi \in \mathcal{D}(\Lambda)$,*

$$\|\Lambda e^{itA^a}\psi\| \leq k e^{k'|t|/a} \|\Lambda\psi\|, \tag{92}$$

where $k, k' < \infty$ are independent of a.

The proof is given in Section 8.

Next, we verify the GJN conditions, and the bounds (62), (64), (63). The following result is useful.

Proposition 4.4 *Under conditions (35), (36), the multiple commutators of G_α with A_p^a are well defined in the strong sense on C_0^∞, and, for any $\psi \in C_0^\infty$, we have that*

$$\|\mathrm{ad}_{A_p^a}^{(n)}(G_\alpha)\psi\| \leq k\|\psi\|, \tag{93}$$

for $n = 1, 2, 3$, and uniformly in $a > 0$.

The proofs of this and the next proposition are given in Section 8.

Proposition 4.5 *The virial theorems, Theorem 3.2 and Theorem 3.3, apply in the concrete situation described above, with the following identifications: the domain $\mathcal{D}$ of section 3.1 is given in (75), the operators L, N, D, Λ, A_0 appearing in Theorems 3.2, 3.3 are chosen in (53), (79), (80), (76), (85), and the operator A is given by A^a in (72).*

4.3 A lower bound on $C_1^a + i[L, A_0]$ uniform in a

In order to estimate $C_1^a + i[L, A_0]$ from below, we start with the following observation: in the sense of forms on $\mathcal{D}$,

$$\pm\lambda I_1^a \leq \frac{1}{10} N\overline{P}_\Omega + k\lambda^2, \tag{94}$$

for some k independent of $a > 0$. This estimate follows in a standard way from the explicit expression for I_1^a, equation (84), and the bound in (93). We conclude from (94), (81) that

$$C_1^a + i[L, A_0] \geq M_a, \tag{95}$$

where

$$M_a = \int_{\mathbb{R}_+}^{\oplus} \xi_a(e)de \otimes \mathbb{1}_p + \mathbb{1}_p \otimes \int_{\mathbb{R}_+}^{\oplus} \xi_a(e)de + \frac{9}{10}\overline{P}_\Omega - k\lambda^2 + i[L, A_0]. \tag{96}$$

The constant k on the r.h.s. is independent of a. Recalling that $\xi_a \to 1$ a.e., we are led to define the bounded limiting operator

$$M = P_+(H_p) \otimes \mathbb{1}_p + \mathbb{1}_p \otimes P_+(H_p) + \frac{9}{10}\overline{P}_\Omega - k\lambda^2 + i[L, A_0], \tag{97}$$

where k is the same constant as in (96). Using Dominated Convergence, one readily verifies that $\int_{\mathbb{R}_+}^{\oplus} \xi_a(e)de \to P_+(H_p)$, in the strong sense on $\mathcal{H}_p$.

Proposition 4.6 *$\lim_{a\to 0_+} M_a = M$, strongly on $\mathcal{H}$.*

Our next task is to show that M is strictly positive.

4.4 The Feshbach method and strict positivity of M

Recall that $\Pi = P_0 \otimes P_\Omega$ is the rank-one projection onto the zero eigenspace of L_0, see (87). We apply the Feshbach method to analyze the operator M, with the decomposition

$$\mathcal{H} = \mathrm{Ran}\,\Pi \oplus \mathrm{Ran}\,\overline{\Pi}.$$

First, we note that

$$\begin{aligned} \overline{\Pi}M\overline{\Pi} \ \geq\ & \overline{P}_0 \otimes P_\Omega \left(P_+(H_p) \otimes \mathbb{1}_p + \mathbb{1}_p \otimes P_+(H_p) - k\lambda^2 \right) \\ & +(9/10 - k\lambda^2)\overline{P}_\Omega + i\overline{\Pi}[L, A_0]\overline{\Pi}. \end{aligned} \tag{98}$$

Recalling the definitions of P_0 and A_0, (88) and (85), one easily sees that

$$\begin{aligned} \overline{P}_0(P_+(H_p) \otimes \mathbb{1}_p + \mathbb{1}_p \otimes P_+(H_p)) &\geq \overline{P}_0, \\ i\overline{\Pi}[L, A_0]\overline{\Pi} &= -\theta\lambda^2(\overline{\Pi}I\Pi I\overline{R}_\epsilon^2 + \overline{R}_\epsilon^2 I\Pi I\overline{\Pi}), \end{aligned}$$

in particular, $\|i\overline{\Pi}[L, A_0]\overline{\Pi}\| \leq k\theta\lambda^2/\epsilon^2$. Together with (98), this shows that there is a constant $\lambda_1 > 0$ (independent of $\lambda, \theta, \epsilon$ and of $\beta \geq \beta_0$, for any $\beta_0 > 0$ fixed), s.t.

$$\overline{M} := \overline{\Pi}M\overline{\Pi} \upharpoonright \mathrm{Ran}\,\overline{\Pi} > \frac{1}{2}\overline{\Pi}, \tag{99}$$

provided

$$|\lambda|, \frac{\theta\lambda^2}{\epsilon^2} < \lambda_1. \tag{100}$$

It follows from equation (99) that the resolvent set of $\overline{M}$, $\rho(\overline{M})$, contains the interval $(-\infty, 1/2)$, and for $m < 1/2$:

$$\|(\overline{M} - m\overline{\Pi})^{-1}\| < (1/2 - m)^{-1}. \tag{101}$$

For $m \in \rho(\overline{M})$, we define the *Feshbach map* $F_{\Pi,m}$ applied to M by

$$F_{\Pi,m}(M) = \Pi \left(M - M\overline{\Pi}(\overline{M} - m\overline{\Pi})^{-1}\overline{\Pi}M \right) \Pi. \tag{102}$$

The operator $F_{\Pi,m}(M)$ acts on the space $\operatorname{Ran}\Pi$. In our specific case, $\operatorname{Ran}\Pi \cong \mathbb{C}$, hence $F_{\Pi,m}(M)$ is a number. (If $\operatorname{Ran}\Pi$ had dimension n, then $F_{\Pi,m}(M)$ would be represented by an $n \times n$ matrix.) The following crucial property is called the *isospectrality of the Feshbach map* (see e.g. [BFS], [DJ]):

$$m \in \rho(\overline{M}) \cap \sigma(M) \Longleftrightarrow m \in \rho(\overline{M}) \cap \sigma(F_{\Pi,m}(M)), \tag{103}$$

where $\sigma(\cdot)$ denotes the spectrum. Hence by examining the spectrum of the operator $F_{\Pi,m}(M)$, one obtains information about the spectrum of M. The idea is, of course, that it is easier to examine the former operator, since it acts on a smaller space.

Proposition 4.7 *Assume condition (A3) and let* $0 < \epsilon < \epsilon_0$*. Then*

$$F_{\Pi,m}(M) \geq 2\frac{\theta\lambda^2}{\epsilon}\gamma \left(1 - k\theta \left(1 + \frac{|\lambda|}{\epsilon} \right)^2 - k\frac{\epsilon}{\gamma\theta} \right) \Pi, \tag{104}$$

uniformly in $m < 1/4$.

Proof. Recall the structure of $F_{\Pi,m}(M)$, given in (102). We show that $-\Pi M\overline{\Pi}(\overline{M} - m\overline{\Pi})^{-1}\overline{\Pi}M\Pi$ is small, as compared to $\Pi M \Pi$, and that the latter is strictly positive. Estimate (101) gives

$$-\Pi M\overline{\Pi}(\overline{M} - m\overline{\Pi})^{-1}\overline{\Pi}M\Pi \geq -4\Pi M\overline{\Pi}M\Pi, \tag{105}$$

for $m < 1/4$. An easy calculation shows that

$$\overline{\Pi}M\Pi = \overline{\Pi}i[L, A_0]\Pi = \theta\lambda\overline{\Pi}L\overline{R}_\epsilon^2 I\Pi = \theta\lambda\overline{\Pi} \left(L_0\overline{R}_\epsilon^2 I + \lambda I\overline{R}_\epsilon^2 I \right) \Pi,$$

and using that $\|L_0 R_\epsilon\| \leq 1$, $\|R_\epsilon\| \leq 1/\epsilon$, we obtain the bound

$$\|\overline{\Pi}M\Pi\psi\| \leq \left(\theta|\lambda| + k\frac{\theta\lambda^2}{\epsilon} \right) \|\overline{R}_\epsilon I\Pi\psi\|, \tag{106}$$

for any $\psi \in \mathcal{H}$, where we have used that $\operatorname{Ran}\overline{R}_\epsilon^2 I\Pi \subset \operatorname{Ran} P(N \leq 1)$, and $\|IP(N \leq 1)\| \leq k$. Combining (106) with (105) yields

$$-\Pi M\overline{\Pi}(\overline{M} - m\overline{\Pi})^{-1}\overline{\Pi}M\Pi \geq -k\theta^2\lambda^2(1 + |\lambda|/\epsilon)^2\Pi I\overline{R}_\epsilon^2 I\Pi.$$

Furthermore, we have that

$$\Pi M \Pi = \Pi i[L, A_0]\Pi - k\lambda^2\Pi = 2\theta\lambda^2 \Pi I \overline{R}_\epsilon^2 I \Pi - k\lambda^2\Pi.$$

These observations and the definition of the Feshbach map, (102), show that

$$F_{\Pi,m}(M) \geq 2\theta\lambda^2(1 - k\theta(1 + |\lambda|/\epsilon)^2)\Pi I \overline{R}_\epsilon^2 I \Pi - k\lambda^2\Pi,$$

which, by Proposition 4.2, yields (104). ■

Estimate (104) tells us that there is a $\lambda_2 > 0$ s.t.

$$F_{\Pi,m}(M) \geq \frac{\theta\lambda^2}{\epsilon}\gamma\Pi, \tag{107}$$

provided conditions (100) hold, and

$$\theta\left(1 + \frac{|\lambda|}{\epsilon}\right)^2 + \frac{\epsilon}{\gamma\theta} < \lambda_2, \quad 0 < \epsilon < \epsilon_0. \tag{108}$$

Notice that all these estimates are independent of $m < 1/4$. Using the isospectrality property of the Feshbach map, (103), we conclude that if the bounds (100) and (108) are imposed on the parameters, and if $m < 1/4$ and $m \in \sigma(M)$, then $m > \frac{\theta\lambda^2}{\epsilon}\gamma$. Consequently,

$$M \geq \min\left\{\frac{1}{4}, \frac{\theta\lambda^2}{\epsilon}\gamma\right\} = \frac{\theta\lambda^2}{\epsilon}\gamma.$$

Fix a $\theta < \lambda_2/4$ and an $\epsilon < \min\{\epsilon_0, \gamma\theta\lambda_2\}$. Then, defining

$$\lambda_0 = \min\left\{\lambda_1, \frac{\epsilon\sqrt{\lambda_1}}{\sqrt{\theta}}, \epsilon\right\},$$

(100) and (108) are satisfied for $|\lambda| < \lambda_0$.

Proposition 4.8 *There is a choice of the parameters θ and ϵ, and of $\lambda_0 > 0$ (depending on θ, ϵ, β) s.t. if $|\lambda| < \lambda_0$ then*

$$M > \frac{\theta\lambda^2}{\epsilon}\gamma. \tag{109}$$

We have $\lambda_0 \leq k\gamma$, for some k independent of $\beta \geq \beta_0$ (for any $\beta_0 > 0$ fixed), i.e., $\lambda_0 \sim e^{\beta E}$ is exponentially small in β, as $\beta \to \infty$ (see remark 1) after (39)).

Proposition 4.8 completes the proof of Theorem 2.3, according to the argument given in (74).

5 Some functional analysis

The following two theorems are useful in our analysis. Their proofs can be found in [Frö].

Theorem 5.1 (invariance of domain, [Frö]) *Suppose $(X, Y, \mathcal{D})$ satisfies the GJN Condition, (57), (58). Then the unitary group, e^{itX}, generated by the selfadjoint operator X leaves $\mathcal{D}(Y)$ invariant, and*

$$\|Ye^{itX}\psi\| \leq e^{k|t|}\|Y\psi\|, \tag{110}$$

for some $k \geq 0$, and all $\psi \in \mathcal{D}(Y)$.

Theorem 5.2 (commutator expansion, [Frö]) *Suppose $\mathcal{D}$ is a core for the selfadjoint operator $Y \geq \mathbb{1}$. Let $X, Z, \mathrm{ad}_X^{(n)}(Z)$ be symmetric operators on $\mathcal{D}$, where*

$$\begin{aligned} \mathrm{ad}_X^{(0)}(Z) &= Z, \\ \left\langle \psi, \mathrm{ad}_X^{(n)}(Z)\psi \right\rangle &= i\left\{ \left\langle \mathrm{ad}_X^{(n-1)}(Z)\psi, X\psi \right\rangle - \left\langle X\psi, \mathrm{ad}_X^{(n-1)}(Z)\psi \right\rangle \right\}, \end{aligned}$$

for all $\psi \in \mathcal{D}$, $n = 1, \ldots, M$. We suppose that the triples $(\mathrm{ad}_X^{(n)}(Z), Y, \mathcal{D})$, $n = 0, 1, \ldots, M$, satisfy the GJN Condition (57), (58), and that X is selfadjoint, with $\mathcal{D} \subset \mathcal{D}(X)$, e^{itX} leaves $\mathcal{D}(Y)$ invariant, and (110) holds. Then

$$\begin{aligned} e^{itX} Z e^{-itX} &= Z - \sum_{n=1}^{M-1} \frac{t^n}{n!} \mathrm{ad}_X^{(n)}(Z) \\ &\quad - \int_0^t dt_1 \cdots \int_0^{t_{M-1}} dt_M e^{it_M X} \mathrm{ad}_X^{(M)}(Z) e^{-it_M X}, \end{aligned} \tag{111}$$

as operators on $\mathcal{D}(Y)$.

Remark. This theorem is proved in [Frö], under the assumption that $(X, Y, \mathcal{D})$ satisfies (57), (58). However, [Frö]'s proof only requires the properties of the group e^{itX} indicated in our Theorem 5.2.

An easy, but useful result follows from (110).

Proposition 5.3 *Suppose that the unitary group e^{itX} leaves $\mathcal{D}(Y)$ invariant, for some operator Y, and that estimate (110) holds. For a function χ on $\mathbb{R}$ with Fourier transform $\widehat{\chi} \in L^1(\mathbb{R})$, we define $\chi(X) = \int_{\mathbb{R}} \widehat{\chi}(s) e^{isX} ds$. If $\widehat{\chi}$ has compact support, then $\chi(X)$ leaves $\mathcal{D}(Y)$ invariant, and, for $\psi \in \mathcal{D}(Y)$,*

$$\|Y\chi(X)\psi\| \leq e^{kR} \|\widehat{\chi}\|_{L^1(\mathbb{R})} \, \|Y\psi\|, \tag{112}$$

for any R s.t. $\mathrm{supp}\widehat{\chi} \subset [-R, R]$.

The proof is obvious. Proposition 5.4 states a similar result, but for a function whose Fourier transform is not necessarily of compact support.

Proposition 5.4 *Suppose $(X, Y, \mathcal{D})$ satisfies the GJN Condition, and so do the triples $(\mathrm{ad}_X^{(n)}(Y), Y, \mathcal{D})$, for $n = 1, \ldots, M$, and for some $M \geq 1$. Moreover, assume that, in the sense of Kato on $\mathcal{D}(Y)$, $\pm \mathrm{ad}_X^{(M)}(Y) \leq kX$, for some $k \geq 0$. For $\chi \in C_0^\infty(\mathbb{R})$, a smooth function with compact support, define $\chi(X) = \int \widehat{\chi}(s) e^{isX}$, where $\widehat{\chi}$ is the Fourier transform of χ. Then $\chi(X)$ leaves $\mathcal{D}(Y)$ invariant.*

Proof. For $R > 0$, set $\chi_R(X) = \int_{-R}^{R} \widehat{\chi}(s) e^{isX}$, then $\chi_R(X) \to \chi(X)$ in operator norm, as $R \to \infty$. From the invariance of domain theorem, we see that $\chi_R(X)$ leaves $\mathcal{D}(Y)$ invariant. Let $\psi \in \mathcal{D}(Y)$, then using the commutator expansion theorem above, we have

$$\begin{aligned}
&Y\chi_R(X)\psi \\
&= \chi_R(X) Y\psi + \int_{-R}^{R} \widehat{\chi}(s) e^{isX} \left(e^{-isX} Y e^{isX} - Y \right) \psi \\
&= \chi_R(X) Y\psi - \int_{-R}^{R} \widehat{\chi}(s) e^{isX} \left(\sum_{n=1}^{M-1} \frac{(-s)^n}{n!} \mathrm{ad}_X^{(n)}(Y) \right. \\
&\quad \left. + (-1)^M \int_0^s ds_1 \cdots \int_0^{s_{M-1}} ds_M e^{-is_M X} \mathrm{ad}_X^{(M)}(Y) e^{is_M X} \right) \psi. \qquad (113)
\end{aligned}$$

The integrand of the s-integration in (113) is bounded in norm by

$$k(|s|^M + 1) \left(\|Y\psi\| + \|X\psi\| \right) \leq k(|s|^M + 1) \|Y\psi\|,$$

where we have used that $\|\mathrm{ad}_X^{(M)}(Y) e^{is_M X}\psi\| \leq \|X e^{is_M X}\psi\| \leq \|X\psi\|$. Since $\widehat{\chi}$ is of rapid decrease, it can be integrated against any power of $|s|$, and we conclude that the r.h.s. of (113) has a limit as $R \to \infty$. Since Y is a closed operator, it follows that $\chi(X)\psi \in \mathcal{D}(Y)$. ∎

Proposition 5.5 *Let* $\chi \in C_0^\infty(\mathbb{R})$*,* $\chi = F^2 \geq 0$*. Suppose* $(X, Y, \mathcal{D})$ *satisfies the GJN condition. Suppose* $F(X)$ *leaves* $\mathcal{D}(Y)$ *invariant. Let* Z *be a symmetric operator on* $\mathcal{D}$ *s.t., for some* $M \geq 1$*, and* $n = 0, 1, \ldots, M$*, the triples* $(\mathrm{ad}_X^{(n)}(Z), Y, \mathcal{D})$ *satisfy the GJN condition. Moreover, we assume that the multiple commutators, for* $n = 1, \ldots, M$*, are relatively* X^{2p}*-bounded in the sense of Kato on* $\mathcal{D}$*, for some* $p \geq 0$*. In other words, there is some* $k < \infty$*, s.t.* $\forall \psi \in \mathcal{D}$*,*

$$\|\mathrm{ad}_X^{(n)}(Z)\psi\| \leq k \left(\|\psi\| + \|X^{2p}\psi\| \right), \qquad n = 1, \ldots, M.$$

Then the commutator $[\chi(X), Z] = \chi(X)Z - Z\chi(X)$ *is well defined on* $\mathcal{D}$ *and extends to a bounded operator.*

Proof. We write F, χ instead of $F(X), \chi(X)$. Since F leaves $\mathcal{D}(Y)$ invariant, we have that

$$[\chi, Z] = F[F, Z] + [F, Z]F,$$

as operators on $\mathcal{D}(Y)$. We expand the commutator

$$\begin{aligned} [F, Z] &= \int \widehat{F}(s) e^{isX} \left(Z - e^{-isX} Z e^{isX} \right) \\ &= \int \widehat{F}(s) e^{isX} \left\{ \sum_{n=1}^{M-1} \frac{s^n}{n!} \mathrm{ad}_X^{(n)}(Z) \right. \\ &\qquad \left. + \int_0^s ds_1 \cdots \int_0^{s_{M-1}} ds_M e^{-is_M X} \mathrm{ad}_X^{(M)}(Z) e^{is_M X} \right\}. \end{aligned} \tag{114}$$

Multiplying this equation from the right with F (and noticing that F commutes with $e^{is_M X}$), we see immediately that $[F, Z]F$ is bounded, and hence $F[F, Z] = -([F, Z]F)^*$ is bounded, too. ■

Proposition 5.6 *Suppose* $(X, Y, \mathcal{D})$ *is a GJN triple. Then the resolvent* $(X - z)^{-1}$ *leaves* $\mathcal{D}(Y)$ *invariant, for all* $z \in \{\mathbb{C} | \, |\mathrm{Im} z| > k\}$*, for some* $k > 0$*.*

Proof. Suppose $\mathrm{Im} z < 0$ (the case $\mathrm{Im} z > 0$ is dealt with similarly). We write the resolvent as

$$(X - z)^{-1} = i \int_0^\infty dt \; e^{i(X-z)t},$$

and it follows from Theorem 5.1 that for $\psi \in \mathcal{D}(Y)$,

$$\|Y(X-z)^{-1}\psi\| \leq \|Y\psi\| \int_0^\infty dt\ e^{(\mathrm{Im} z + k)t} < \infty,$$

provided $\mathrm{Im} z < -k$. ■

6 Proof of the virial theorems and the regularity theorem

Proof of Theorem 3.2. We start by introducing some cutoff operators, and the regularized (cutoff, approximate) eigenfunction.

Let $g_1 \in C_0^\infty((-1,1))$ be a real valued function, s.t. $g_1(0) = 1$, and set $g = g_1^2 \in C_0^\infty((-1,1))$, $g(0) = 1$. Pick a real valued function f on $\mathbb{R}$ with the properties that $f(0) = 1$ and $\widehat{f} \in C_0^\infty(\mathbb{R})$ (Fourier transform). We set

$$f_1(x) = \int_{-\infty}^{x} f^2(y)dy,$$

so that $f_1'(x) = f^2(x)$. Since $\widehat{f_1'}\,(s) = is\widehat{f_1}(s) = (2\pi)^{-1/2}\widehat{f} * \widehat{f}(s)$, it follows that $\widehat{f_1}$ has compact support, and is smooth except at $s = 0$, where it behaves like s^{-1}. We have $\widehat{f_1^{(n)}} = (is)^n \widehat{f_1} \in C_0^\infty$, for $n \geq 1$. Let $\alpha, \nu > 0$ be two parameters and define the cutoff-operators

$$\begin{aligned} g_{1,\nu} &= g_1(\nu N) = \int_{\mathbb{R}} \widehat{g_1}(s) e^{is\nu N} ds, \\ g_\nu &= g_{1,\nu}^2 \\ f_\alpha &= f(\alpha A) = \int_{\mathbb{R}} \widehat{f}(s) e^{is\alpha A} ds, \end{aligned}$$

For $\eta > 0$, define

$$f_{1,\alpha}^\eta = \frac{1}{\alpha} \int_{\mathbb{R}\setminus(-\eta,\eta)} ds \widehat{f_1}(s) e^{is\alpha A} = (f_{1,\alpha}^\eta)^*.$$

$f_{1,\alpha}^\eta$ leaves $\mathcal{D}(\Lambda)$ invariant, and $\|f_{1,\alpha}^\eta\| \leq k/\alpha$, where k is a constant independent of η; this can be seen by noticing that $\|f_1\|_\infty < \infty$.

Suppose that ψ is an eigenfunction of L with eigenvalue e: $L\psi = e\psi$. Since $\psi \in \mathcal{D}(L)$, then $\psi = (L+i)^{-1}\varphi$, for some $\varphi \in \mathcal{H}$. Let $\{\varphi_n\} \subset \mathcal{D}(\Lambda)$ be a sequence of vectors converging to φ. Then

$$\psi_n := (L+i)^{-1}\varphi_n \to \psi, \quad n \to \infty, \tag{115}$$

and moreover, $\psi_n \in \mathcal{D}(\Lambda)$. The latter follows because the resolvent $(L+i)^{-1}$ leaves $\mathcal{D}(\Lambda)$ invariant, see Proposition 5.6; without loss of generality, we assume that $k=1$. Moreover, by Proposition 5.3, we know that f_α leaves $\mathcal{D}(\Lambda)$ invariant (see also (61)), and g_ν leaves $\mathcal{D}(\Lambda)$ invariant (Λ commutes with N in the strong sense on $\mathcal{D}$). Hence, the regularized eigenfunction

$$\psi_{\alpha,\nu,n} = f_\alpha g_\nu \psi_n$$

satisfies $\psi_{\alpha,\nu,n} \in \mathcal{D}(\Lambda)$, $\psi_{\alpha,\nu,n} \to \psi$, as $\alpha,\nu \to 0$, $n \to \infty$.

Notice that in the definition of ψ_n, we introduced the resolvent of L, so that we have $(L-e)\psi_n \to 0$, as $n \to \infty$, which we write as

$$(L-e)\psi_n = o(n). \tag{116}$$

We now prove the estimate

$$\left| \left\langle i f_{1,\alpha}^\eta (L-e) \right\rangle_{g_\nu \psi_n} \right| \le k \frac{1}{\alpha} \left(\sqrt{\nu} + o(n) \right), \tag{117}$$

where k is some constant independent of η, α, ν, n. This estimate follows from the bound

$$\|(L-e) g_\nu \psi_n\| \le k \left(\sqrt{\nu} + o(n) \right), \tag{118}$$

which is proven as follows. We have that

$$\begin{aligned} (L-e) g_\nu \psi_n \;&=\; g_\nu (L-e)\psi_n & (119)\\ &\quad + g_{1,\nu}[L, g_{1,\nu}]\psi_n & (120)\\ &\quad + [L, g_{1,\nu}] g_{1,\nu}\psi_n, & (121) \end{aligned}$$

and the r.h.s. of (119) is $o(n)$, by (116). Let us show that both (120) and (121) are bounded above by $k\sqrt{\nu}$, uniformly in n. The commutator expansion of Theorem 5.2 (see also (114)) yields

$$g_{1,\nu}[L, g_{1,\nu}] = \nu \int_{\mathbb{R}} ds\ \widehat{g_1}(s) e^{is\nu N} \int_0^s ds_1 e^{-is_1\nu N} g_{1,\nu} D e^{is_1\nu N}, \tag{122}$$

as operators on $\mathcal{D}(\Lambda)$, where D is given in (80). We use that $g_{1,\nu}$ commutes with $e^{is\nu N}$. From (62), we see that for any $\phi \in \mathcal{D}(\Lambda)$,

$$
\begin{aligned}
\|g_{1,\nu} D e^{is_1\nu N}\phi\| &= \sup_{\varphi\in\mathcal{D},\varphi\neq 0} \frac{\left|\left\langle \varphi, g_{1,\nu} D e^{is_1\nu N}\phi\right\rangle\right|}{\|\varphi\|} \\
&\leq \sup_{\varphi\in\mathcal{D},\varphi\neq 0} \frac{\|D g_{1,\nu}\varphi\|\ \|\phi\|}{\|\varphi\|} \leq k \sup_{\varphi\in\mathcal{D},\varphi\neq 0} \frac{\|N^{1/2} g_{1,\nu}\varphi\|}{\|\varphi\|}\ \|\phi\| \leq k\frac{1}{\sqrt{\nu}}\|\phi\|,
\end{aligned}
$$

and consequently,

$$
\begin{aligned}
\|g_{1,\nu}[L, g_{1,\nu}]\phi\| &\leq \nu \int_{\mathbb{R}} ds |\widehat{g_1}(s)| \int_0^s ds_1\, \|g_{1,\nu} D e^{is_1\nu N}\phi\| \\
&\leq k\sqrt{\nu} \int_{\mathbb{R}} ds\, |s\widehat{g_1}(s)|\ \|\phi\|. \qquad (123)
\end{aligned}
$$

Thus, the desired bound for (120) is proven, and the same bound is established for (121) by proceeding in a similar way. This proves (118).

Next, since $f_{1,\alpha}^{\eta}$ leaves $\mathcal{D}(\Lambda)$ invariant, the commutator $[f_{1,\alpha}^{\eta}, L]$ is defined in the strong sense on $\mathcal{D}(\Lambda)$, and Theorem 5.2 yields

$$
\begin{aligned}
&[f_{1,\alpha}^{\eta}, L] \\
&= \int_{\mathbb{R}\setminus(-\eta,\eta)} ds \widehat{f_1}(s) e^{is\alpha A}\left(sC_1 + \alpha\frac{s^2}{2}C_2\right) \\
&\quad +\alpha^2 \int_{\mathbb{R}\setminus(-\eta,\eta)} ds \widehat{f_1}(s) e^{is\alpha A} \int_0^s ds_1 \int_0^{s_1} ds_2 \int_0^{s_2} ds_3\ e^{-is_3\alpha A} C_3 e^{is_3\alpha A}. \qquad (124)
\end{aligned}
$$

For $n \geq 1$, we have

$$
f_1^{(n)}(\alpha A) = \int_{\mathbb{R}} ds (is)^n \widehat{f_1}(s) e^{is\alpha A} = \int_{\mathbb{R}\setminus(-\eta,\eta)} ds (is)^n \widehat{f_1}(s) e^{is\alpha A} - \mathcal{R}_{\eta,n},
$$

where the remainder term

$$
\mathcal{R}_{\eta,n} = -\int_{-\eta}^{\eta} ds\ (is)^n \widehat{f_1}(s) e^{is\alpha A}
$$

satisfies $\mathcal{R}_{\eta,n} = (\mathcal{R}_{\eta,n})^*$, and $\|\mathcal{R}_{\eta,n}\| \leq k_n\eta$, with a constant k_n that does not depend on α, η. We obtain from (124)

$$
\begin{aligned}
[f_{1,\alpha}^\eta, L] &= -i\left(f_1'(\alpha A) + \mathcal{R}_{\eta,1}\right) C_1 - \frac{\alpha}{2}\left(f_1''(\alpha A) + \mathcal{R}_{\eta,2}\right) C_2 \\
&\quad +\alpha^2 \int_{\mathbb{R}\setminus(-\eta,\eta)} ds \widehat{f}_1(s) e^{is\alpha A} \int_0^s ds_1 \int_0^{s_1} ds_2 \int_0^{s_2} ds_3\ e^{-is_3\alpha A} C_3 e^{is_3\alpha A}.
\end{aligned}
\tag{125}
$$

Recalling that $f_1'(\alpha A) = f^2(\alpha A) = f_\alpha^2$, we write

$$
\begin{aligned}
-if_\alpha^2 C_1 &= -if_\alpha C_1 f_\alpha \\
&\quad -if_\alpha \int_{\mathbb{R}} ds \widehat{f}(s) e^{is\alpha A} \left(\alpha s C_2 + \alpha^2 \int_0^s ds_1 \int_0^{s_1} ds_2 e^{-is_2\alpha A} C_3 e^{is_2\alpha A}\right) \\
&= -if_\alpha C_1 f_\alpha - \alpha f_\alpha f_\alpha' C_2 \\
&\quad -i\alpha^2 f_\alpha \int_{\mathbb{R}} ds \widehat{f}(s) e^{is\alpha A} \int_0^s ds_1 \int_0^{s_1} ds_2 e^{-is_2\alpha A} C_3 e^{is_2\alpha A},
\end{aligned}
\tag{126}
$$

where $f_\alpha' = f'(\alpha A)$. Remarking that $f_\alpha f_\alpha' = \frac{1}{2}(f^2)'(\alpha A) = \frac{1}{2} f_1''(\alpha A)$, we obtain from (125), (126):

$$
\begin{aligned}
[f_{1,\alpha}^\eta, L] &= -if_\alpha C_1 f_\alpha - \alpha f_1''(\alpha A) C_2 - i\mathcal{R}_{\eta,1} C_1 - \frac{\alpha}{2}\mathcal{R}_{\eta,2} C_2 \\
&\quad +\alpha^2 \int_{\mathbb{R}\setminus(-\eta,\eta)} ds \widehat{f}_1(s) e^{is\alpha A} \int_0^s ds_1 \int_0^{s_1} ds_2 \int_0^{s_2} ds_3\ e^{-is_3\alpha A} C_3 e^{is_3\alpha A} \\
&\quad -i\alpha^2 f_\alpha \int_{\mathbb{R}} ds \widehat{f}(s) e^{is\alpha A} \int_0^s ds_1 \int_0^{s_1} ds_2 e^{-is_2\alpha A} C_3 e^{is_2\alpha A}.
\end{aligned}
\tag{127}
$$

Consequently, taking into account estimate (64), we obtain that

$$
\begin{aligned}
\left\langle i[f_{1,\alpha}^\eta, L]\right\rangle_{g_\nu\psi_n} &= \langle C_1\rangle_{\psi_{\alpha,\nu,n}} - \mathrm{Re}\ i\alpha \left\langle f''(\alpha A) C_2\right\rangle_{g_\nu\psi_n} + \mathrm{Re}\left\langle \mathcal{R}_{\eta,1} C_1\right\rangle_{g_\nu\psi_n} \\
&\quad -\mathrm{Re}\ i\frac{\alpha}{2}\left\langle \mathcal{R}_{\eta,2} C_2\right\rangle_{g_\nu\psi_n} + O\left(\frac{\alpha^2}{\sqrt{\nu}}\right),
\end{aligned}
\tag{128}
$$

as we show next. We have taken the real part on the right side, since the left side is a real number. To estimate the remainder term, we use condition (64) to obtain

$$
\left\| e^{-is_3\alpha A} C_3 e^{is_3\alpha A} g_\nu\psi_n \right\| \leq k \frac{1}{\sqrt{\nu}} e^{\alpha k' |s_3|},
$$

uniformly in n, so the middle line in (127) is estimated from above by

$$k\frac{\alpha^2}{\sqrt{\nu}}\int_{\mathbb{R}} ds\ |\widehat{f}_1(s)|\ |s|^3 e^{\alpha k'|s|} \le k\frac{\alpha^2}{\sqrt{\nu}} e^{\alpha k' K}\int_{\mathbb{R}} ds\ |\widehat{f}_1(s)|\ |s|^3,$$

where $K<\infty$ is such that $\mathrm{supp}\widehat{f}_1 \subset [-K,K]$. The exponential is bounded uniformly in $0\le\alpha<1$, hence the r.h.s. is $\le k\frac{\alpha^2}{\sqrt{\nu}}$. The last line in (127) is analyzed in the same way and (128) follows.

Finally, we observe that

$$\begin{aligned}
-\mathrm{Re}\,\langle i\alpha f''(\alpha A)C_2\rangle_{g_\nu\psi_n} &= -\frac{\alpha}{2}\,\langle i[f''(\alpha A),C_2]\rangle_{g_\nu\psi_n} \\
= \quad -\frac{\alpha^2}{2}\left\langle \int_{\mathbb{R}} ds\ \widehat{f''}(s)e^{is\alpha A}\int_0^s ds_1\ e^{-is_1\alpha A}C_3 e^{is_1\alpha A}\right\rangle_{g_\nu\psi_n} &= O\left(\frac{\alpha^2}{\sqrt{\nu}}\right),
\end{aligned}$$

where we use (64) again, as above. A similar estimate yields

$$\mathrm{Re}\ i\frac{\alpha}{2}\,\langle \mathcal{R}_{\eta,2}C_2\rangle_{g_\nu\psi_n} = -i\frac{\alpha}{4}\,\langle[\mathcal{R}_{\eta,2},C_2]\rangle_{g_\nu\psi_n} = O\left(\frac{\alpha^2\eta}{\sqrt{\nu}}\right),$$

and using the bound (63), we have that

$$\langle \mathcal{R}_{\eta,1}C_1\rangle_{g_\nu\psi_n} = O\left(\frac{\eta}{\nu^p}\right).$$

Combining this with (128) and (117) shows that

$$\left|\langle C_1\rangle_{\psi_{\alpha,\nu,n}}\right| \le k\left(\frac{\sqrt{\nu}+o(n)}{\alpha}+\frac{\alpha^2}{\sqrt{\nu}}+\frac{\eta}{\nu^p}\right). \tag{129}$$

Notice that

$$C_1\psi_{\alpha,\nu,n} = \int ds\ \widehat{f}(s)C_1 e^{is\alpha A}g_\nu\psi_n \to C_1\psi_{\alpha,\nu},$$

as $n\to\infty$, where $\psi_{\alpha,\nu} := f_\alpha g_\nu\psi$. This follows from the boundedness condition (63) and from $\psi_n\to\psi$, $n\to\infty$, see (115). Consequently we obtain by taking the limit $n\to\infty$ in (129)

$$\left|\langle C_1\rangle_{\psi_{\alpha,\nu}}\right| \le k\left(\frac{\sqrt{\nu}}{\alpha}+\frac{\alpha^2}{\sqrt{\nu}}+\frac{\eta}{\nu^p}\right).$$

Choose for instance $\nu = \alpha^3$, $\eta = \alpha^{3p+\delta}$, for any $\delta > 0$, then

$$\lim_{\alpha \to 0} \langle C_1 \rangle_{\psi_{\alpha,\alpha^3}} = 0.$$

This concludes the proof of the theorem. ■

Proof of Theorem 3.3. We adopt the definitions and notation introduced in the proof of Theorem 3.2. It suffices to prove

$$\lim_{\alpha \to 0} \langle \psi_\alpha, i[L, A_0]\psi_\alpha \rangle = 0,$$

where we set $\psi_\alpha = \psi_{\alpha,\nu}|_{\nu=\alpha^3}$; see in the proof of Theorem 3.2. The scalar product can be estimated by

$$\begin{aligned} |\langle \psi_\alpha, i[L, A_0]\psi_\alpha \rangle| &\leq 2\,|\langle (L-e)\psi_\alpha, A_0\psi_\alpha \rangle| \\ &\leq 2\|P(N \leq n_0)(L-e)\psi_\alpha\|\ \|A_0\psi_\alpha\|. \end{aligned}$$

We have

$$\begin{aligned} P(N \leq n_0)(L-e)\psi_{\alpha,\nu} &= \lim_{n\to\infty} P(N \leq n_0)[L, f_\alpha]g_\nu\psi_n && (130) \\ &\quad + \lim_{n\to\infty} P(N \leq n_0) f_\alpha [L, g_\nu]\psi_n. && (131) \end{aligned}$$

Using condition (63), we easily find (expanding the commutator $[L, f_\alpha]$) that $\|P(N \leq n_0)[L, f_\alpha]g_\nu\psi_n\| \leq k_{n_0}\alpha$. Similarly, using (62), we find that $\|P(N \leq n_0) f_\alpha[L, g_\nu]\psi_n\| \leq k\sqrt{\nu}$. It follows that $\|P(N \leq n_0)(L-e)\psi_\alpha\| \leq k_{n_0}\alpha$. ■

Proof of Theorem 3.4. The inequality $C \geq \mathcal{P} - B$, the continuity of B, and (67) imply that for any $\epsilon > 0$, there is an $\alpha_0(\epsilon)$, s.t. if $\alpha < \alpha_0(\epsilon)$ then

$$\langle \psi_\alpha, \mathcal{P}\psi_\alpha \rangle \leq \langle \psi, B\psi \rangle + \epsilon. \tag{132}$$

Let μ_ϕ be the spectral measure of $\mathcal{P}$ corresponding to some $\phi \in \mathcal{H}$. Then

$$\langle \psi_\alpha, \mathcal{P}\psi_\alpha \rangle = \int_{\mathbb{R}_+} p\, d\mu_{\psi_\alpha}(p) = \lim_{R\to\infty} \int_{\mathbb{R}_+} p\chi(p \leq R)\, d\mu_{\psi_\alpha}(p),$$

where $\chi(p \leq R)$ is the indicator of $[0, R]$. We obtain from (132)

$$\lim_{R\to\infty} \langle \psi_\alpha, \chi(\mathcal{P} \leq R)\mathcal{P}\psi_\alpha \rangle = \lim_{R\to\infty} \left\| \chi(\mathcal{P} \leq R)\mathcal{P}^{1/2}\psi_\alpha \right\|^2 \leq \langle \psi, B\psi \rangle + \epsilon \equiv k.$$

We have $\left\|\chi(\mathcal{P} \leq R)\mathcal{P}^{1/2}\psi\right\| \leq R^{1/2}\|\psi - \psi_\alpha\| + \sqrt{k}$, and taking $\alpha \to 0$ gives $\|\chi(\mathcal{P} \leq R)\mathcal{P}^{1/2}\psi\| \leq \sqrt{k}$, uniformly in R, so $\lim_{R\to\infty} \int_0^R p d\mu_\psi(p)$ exists and is finite, by the monotone convergence theorem. Since $\mathcal{D}(\mathcal{P}^{1/2}) = \left\{\psi \,\middle|\, \int_0^\infty p d\mu_\psi(p) < \infty\right\}$, we have that $\psi \in \mathcal{D}(\mathcal{P}^{1/2})$, and $\|\mathcal{P}^{1/2}\psi\| \leq \langle\psi, B\psi\rangle$. ■

7 Flows and induced unitary groups

Let $R \subseteq \mathbb{R}^n$ be a Borel set of $\mathbb{R}^n$ (with non-empty interior), let X be a vector field on $\mathbb{R}^n$, and consider the initial value problem for $x \in R$:

$$\begin{aligned} \frac{d}{dt}x_t &= X(x_t), \\ x_t|_{t=0} &= x. \end{aligned} \tag{133}$$

We assume that X has the property that, for any initial condition $x \in R$, there is a unique, global (for all $t \in \mathbb{R}$) solution $x_t \in R$ to (133). Let Φ_t denote the corresponding flow and assume Φ_t is a diffeomorphism of R into R, for all $t \in \mathbb{R}$. The following properties of the flow will be needed: $\Phi_{s+t} = \Phi_s \circ \Phi_t$, $\Phi_t^{-1} = \Phi_{-t}$, $\Phi_0 = \mathbb{1}$. The Jacobian determinant of $\Phi_t(x)$ is given by

$$J_t(x) = \left|\det \Phi_t'(x)\right|, \tag{134}$$

where $\Phi_t'(x)$ is the matrix $\left(\frac{\partial(\Phi_t)_i}{\partial x_j}(x)\right)$.

Let $\mu : R \to \mathbb{R}_+$ be a continuous function which is C^1 on the interior of R and which is strictly positive except possibly on a set of measure zero. We write $d\mu$ for the absolutely continuous measure $\mu(x)dx$, where dx denotes Lebesgue measure on $\mathbb{R}^n$. Given a Hilbert space $\mathfrak{H}$, consider $L^2(R, d\mu; \mathfrak{H})$, the space of square integrable functions $\psi : R \to \mathfrak{H}$, equipped with the scalar product

$$\langle\psi, \phi\rangle = \int_R \langle\psi(x), \phi(x)\rangle_{\mathfrak{H}}\, d\mu(x).$$

On the Hilbert space $L^2(R, d\mu; \mathfrak{H})$, the flow Φ_t induces a strongly continuous unitary group, U_t, defined by

$$(U_t\psi)(x) = \sqrt{J_t(x)\frac{\mu(\Phi_t(x))}{\mu(x)}}\,\psi(\Phi_t(x)), \tag{135}$$

for $\psi \in L^2(R, d\mu; \mathfrak{H})$. To check that U_t preserves the norm, we make the change of variables $y = \Phi_t(x)$ to arrive at

$$\begin{aligned}\int_R |(U_t\psi)(x)|^2 \, d\mu(x) &= \int_R J_t(x)|\psi(\Phi_t(x))|^2 \mu(\Phi_t(x))dx \\ &= \int_R J_t(\Phi_t^{-1}(y))|\det(\Phi_t^{-1})'(y)| \; |\psi(y)|^2 \mu(y)dy.\end{aligned}$$

We observe that $J_t(\Phi_t^{-1}(y)) \; |\det(\Phi_t^{-1})'(y)| = |\det \mathbb{1}| = 1$, hence $\|U_t\psi\| = \|\psi\|$. Next, using that $\Phi_{t+s} = \Phi_t \circ \Phi_s$, one easily shows that $J_{t+s}(x) = J_t(\Phi_s(x))J_s(x)$, and that

$$\frac{\mu(\Phi_{t+s}(x))}{\mu(x)} = \frac{\mu(\Phi_t(\Phi_s(x)))}{\mu(\Phi_s(x))} \; \frac{\mu(\Phi_s(x))}{\mu(x)},$$

hence $t \mapsto U_t$ is a unitary group.

In order to see that the unitary group is strongly continuous and to calculate its generator, we impose some additional assumptions on μ and X.

1. X is C^∞ and bounded,
2. for any compact set $M \subset R$, there is a $k < \infty$ s.t. $\partial_t|_{t=0} J_t(x) \leq k$, uniformly in $x \in M$,
3. for any compact set $M \subset R$, there is a $k < \infty$ s.t. $\left\| \frac{X'(x)\nabla\mu(x)}{\mu(x)} \right\| \leq k$, uniformly in $x \in M$,
4. $t \mapsto \{J_t(x)\mu(\Phi_t(x))\}^{1/2}$ is C^1 in a neighbourhood $(-t_0, t_0)$ of zero, and for any compact set $M \subset R$, there is a $k < \infty$ s.t. we have the estimate $\left|\{J_t(x)\mu(\Phi_t(x))\}^{1/2}\right| < f(x)$, for $|t| < t_0$, where $f \in L^2_{\mathrm{loc}}(R, dx)$.

If X is C^∞ then so is $\Phi_t(x)$ (jointly in (t, x)), and using that

$$\begin{aligned}\Phi_t(x) &= x + \int_0^t X(\Phi_s(x))ds, \\ \Phi_t'(x) &= \mathbb{1} + \int_0^t X'(\Phi_s(x))\Phi_s'(x)ds, \qquad (136)\end{aligned}$$

it follows immediately that

$$\|\Phi_t(x)\| \leq \|x\| + |t| \, \|X\|_\infty, \qquad (137)$$

where the subscript $_\infty$ denotes the supremum norm over $x \in R$. In order to obtain an estimate on $\|\Phi_t'(x)\|$ (the operator norm on $\mathcal{B}(\mathbb{R}^n)$, i.e. the matrix norm, for x fixed), we recall Gronwall's Lemma. If $\mu : \mathbb{R} \to \mathbb{R}_+$ is continuous, and $\nu : \mathbb{R} \to \mathbb{R}_+$ is locally integrable, then the inequality

$$\mu(t) \leq c + \int_{t_0}^{t} \nu(s)\mu(s) ds,$$

where $c \geq 0$, and $t \geq t_0$, implies that

$$\mu(t) \leq c e^{\int_{t_0}^{t} \nu(s) ds}. \tag{138}$$

Equation (136) implies

$$\|\Phi_t'(x)\| \leq 1 + \|X'\|_\infty \int_0^t \|\Phi_s'(x)\| ds,$$

so Gronwall's Lemma yields the estimate

$$\|\Phi_t'(x)\| \leq \exp(\|X'\|_\infty t), \quad \forall t \geq 0.$$

A similar bound holds for $t < 0$, and hence

$$\|\Phi_t'(x)\| \leq \exp\left(\|X'\|_\infty |t|\right), \qquad t \in \mathbb{R}, \tag{139}$$

from which it follows that

$$J_t(x) \leq \exp\left(n\|X'\|_\infty |t|\right). \tag{140}$$

For $\psi \in C_0^\infty$,

$$\begin{aligned} -\frac{1}{i}\partial_t|_{t=0}(U_t\psi)(x) &= -\frac{1}{i}\left(\frac{1}{2}\partial_t|_{t=0}J_t(x) + \frac{1}{2}\frac{\nabla\mu(x)\cdot X(x)}{\mu(x)} + X(x)\cdot\nabla\right)\psi(x) \\ &= (A\psi)(x), \end{aligned} \tag{141}$$

which defines an operator A on C_0^∞. Notice that due to conditions 1, 2 and 3, A maps C_0^∞ into $L^2(R, d\mu; \mathfrak{H})$.

Proposition 7.1 *Assume conditions 1-4 hold. Then for any $\psi \in C_0^\infty$, in the strong sense on $L^2(R, d\mu; \mathfrak{H})$,*

$$-\frac{1}{i}\frac{U_t - \mathbb{1}}{t}\psi \longrightarrow A\psi, \quad t \to 0. \tag{142}$$

Consequently, C_0^∞ is in the domain of definition of the selfadjoint generator of the unitary group U_t, and on C_0^∞, this generator can be identified with the operator A of equation (141).

Proof. Invoking the dominated convergence theorem, it is enough to verify that

$$\left\| -\frac{1}{i}\frac{1}{t}(U_t - \mathbb{1})\psi(x) - (A\psi)(x) \right\|_{\mathfrak{H}}^2 \tag{143}$$

is bounded above by a $d\mu$-integrable function which is independent of t, for small t. We write

$$\begin{aligned}(143) \quad \leq \quad & \frac{1}{\mu(x)} \left| \frac{1}{t}\left(\sqrt{J_t(x)\mu(\Phi_t(x))} - \sqrt{\mu(x)} \right) \right|^2 \|\psi(\Phi_t(x)\|_{\mathfrak{H}}^2 & (144)\\ & + \frac{1}{t^2}\|\psi(\Phi_t(x)) - \psi(x)\|_{\mathfrak{H}}^2 & (145)\\ & + \|(A\psi)(x)\|_{\mathfrak{H}}^2. & (146)\end{aligned}$$

Clearly, (146) is integrable, and, using the continuity properties of ψ and Φ and the bound (139), one sees that (145) is bounded above by a t-independent function that is $d\mu$-integrable (use the mean value theorem). Next, if ψ has support in a ball of radius ρ in $R \subset \mathbb{R}^n$, then $\psi \circ \Phi_t$ has support in the ball of radius $\rho + |t|\, \|X\|_\infty \leq \rho + \|X\|_\infty$, for $|t| \leq 1$. This follows from (137). Let $\chi(x)$ denote the indicator function on the ball of radius $\rho + \|X\|_\infty$, then we have for $|t| < t_0$ with t_0 as in condition 4,

$$(144) \leq k\chi(x)\frac{1}{\mu(x)} \left| \frac{1}{t}\left(\sqrt{J_t(x)\mu(\Phi_t(x))} - \sqrt{\mu(x)} \right) \right|^2 \leq k\chi(x)\frac{1}{\mu(x)}|f(x)|^2,$$

where we have used the mean value theorem and condition 4. The latter function is $d\mu$-integrable. ■

Proof of Proposition 4.1. Since ξ is globally Lipshitz (with Lipshitz constant $\|\xi'\|_\infty$), we have existence and uniqueness of global solutions to the initial value problem (133). Due to uniqueness and the fact that $\mathbb{R} \ni t \mapsto e_t = 0$ is a solution (since $\xi(0) = 0$), we see that $\Phi_t(e) \in (0, \infty)$, for all $t \in \mathbb{R}, e \in (0, \infty)$, so Φ_t is a diffeomorphism in $\mathbb{R}_+$. It is not difficult to verify that conditions 1-4 above are satisfied. Consequently, it follows from Proposition 7.1 that $C_0^\infty \subset \mathcal{D}(A)$, and that A is given by (70) on C_0^∞. Since ξ is infinitely many times differentiable, A leaves C_0^∞ invariant. Hence C_0^∞ is a core for A. ■

8 Proofs of some propositions

Proof of Proposition 4.2. Since $\Pi I \Pi = 0$ and $\Pi I R_\epsilon^2(\overline{p}_0 \otimes \overline{p}_0) I \Pi = 0$, we have

$$\begin{aligned}\Pi I \overline{R}_\epsilon^2 I \Pi = \Pi I R_\epsilon^2 I \Pi &= \Pi I R_\epsilon^2(\overline{p}_0 \otimes p_0 + p_0 \otimes \overline{p}_0) I \Pi \\ &\quad + \Pi I R_\epsilon^2(p_0 \otimes p_0) I \Pi. \end{aligned} \tag{147}$$

It is not difficult to see that $\epsilon \Pi I R_\epsilon^2(p_0 \otimes p_0) I \Pi \to 0$, as $\epsilon \to 0$, so the last term in (147) does not contribute effectively to a lower bound in the limit $\epsilon \to 0$. Let J be the modular conjugation operator introduced in (47). Using the relations $J^2 = J$, $J p_0 \otimes \overline{p}_0 = \overline{p}_0 \otimes p_0 J$, $J R_\epsilon^2 = R_\epsilon^2 J$, $JI = -IJ$, and the invariance of $\varphi_0 \otimes \varphi_0 \otimes \Omega$ under J, one verifies easily that

$$\begin{aligned}&\Pi I R_\epsilon^2(p_0 \otimes \overline{p}_0) I \Pi = \Pi I R_\epsilon^2(\overline{p}_0 \otimes p_0) I \Pi \\ &= \sum_{\alpha,\alpha'} \Pi\big(G_\alpha \otimes \mathbb{1}_p \otimes a(\tau_\beta(g_\alpha))\big) \frac{\overline{p}_0 \otimes p_0}{(H_p \otimes \mathbb{1}_p - E + L_f)^2 + \epsilon^2} \\ &\qquad \times \big(G_{\alpha'} \otimes \mathbb{1}_p \otimes a^*(\tau_\beta(g_{\alpha'}))\big)\Pi,\end{aligned}$$

where $L_f = \mathrm{d}\Gamma(u)$ and where τ_β has been defined in (44). We pull the annihilation operator through the resolvent, using the pull through-formula (for $f \in L^2(\mathbb{R} \times S^2)$)

$$a(f) L_f = \int_{\mathbb{R} \times S^2} \overline{f}(u, \Sigma)(L_f + u) a(u, \Sigma),$$

and then contract it with the creation operator. This gives the bound

$$\begin{aligned}\Pi I \overline{R}_\epsilon^2 I \Pi &\geq \int_{-\infty}^{E} du \int_{S^2} d\Sigma \, \frac{u^2}{e^{-\beta u}-1} \\ &\times \left(p_0 F(-u,\Sigma) \frac{\overline{p}_0}{(H_p - E + u)^2 + \epsilon^2} F(-u,\Sigma)^* p_0 \right) \otimes p_0 \otimes P_\Omega,\end{aligned}$$

where we restricted the domain of integration over u to $(-\infty, E) \subset \mathbb{R}_-$ (as $\epsilon \to 0$, $\frac{\epsilon}{(H_p - E+u)^2+\epsilon^2}$ tends to the Dirac distribution $\delta(H_p - E + u)$, hence $u = -H_p + E \in (-\infty, E)$), and where we used (44). The desired result (91) now follows by making the change of variable $u \mapsto -u$ in the integral, and by remembering the definition of γ, (39). ■

Proof of Proposition 4.3. First, we prove a bound on $\Lambda_p e^{itA_p^a}\psi$, for $\psi \in C_0^\infty$. Let Φ_t^a denote the flow generated by the vector field ξ_a. Then, for each $e \in [0,\infty)$, $((\Lambda_p - \mathbb{1}_p)e^{itA_p^a}\psi)(e) = e\psi(\Phi_t^a(e))$, and

$$\begin{aligned}\left\|(\Lambda_p - \mathbb{1}_p)e^{itA_p^a}\psi\right\|^2 &= \int_{\mathbb{R}_+} e^2 \left\|\psi(\Phi_t^a(e))\right\|^2 de \\ &= \int_{\mathbb{R}_+} \left(\Phi_{-t}^a(y)\right)^2 \|\psi(y)\|^2 \left(\Phi_{-t}^a\right)'(y) dy, \qquad (148)\end{aligned}$$

where we make the change of variables $y = \Phi_t^a(e)$. Recall that $\Phi_t^a(y) = y + \int_0^t \xi(\Phi_s^a(y)/a) ds$, so

$$|\Phi_t^a(y)| \leq |y| + |t| \, \|\xi\|_\infty. \qquad (149)$$

Next $(\Phi_t^a)'(y) = 1 + \int_0^t \frac{1}{a}\xi'(\Phi_s^a(y)/a)\,(\Phi_s^a)'(y) ds$ yields

$$|(\Phi_t^a)'(y)| \leq 1 + \int_0^t \frac{1}{a}\|\xi'\|_\infty \, |(\Phi_s^a)'(y)| \, ds, \qquad (150)$$

and Gronwall's estimate, (138), implies that

$$|(\Phi_t^a)'(y)| \leq e^{\|\xi'\|_\infty |t|/a}. \qquad (151)$$

Using (151) and (149) in (148) yieds

$$\begin{aligned}\left\|(\Lambda_p - \mathbb{1}_p)e^{itA_p^a}\psi\right\|^2 &\leq e^{\|\xi'\|_\infty |t|/a} \int_{\mathbb{R}_+} (y + \|\xi\|_\infty |t|)^2 \, \|\psi(y)\|^2 dy \\ &\leq 2e^{\|\xi'\|_\infty |t|/a} \left(1 + \|\xi\|_\infty |t|\right)^2 \left(\|(\Lambda_p - \mathbb{1}_p)\psi\| + \|\psi\|\right)^2,\end{aligned}$$

from which it follows that

$$\begin{aligned}\left\|\Lambda_p e^{itA_p^a}\psi\right\| &\leq 4\sqrt{2}\,(1+\|\xi\|_\infty|t|)\,e^{\|\xi'\|_\infty|t|/a}\|\Lambda_p\psi\| \\ &\leq 4\sqrt{2}e^{(\|\xi'\|_\infty+\|\xi\|_\infty)|t|/a}\|\Lambda_p\psi\|. \end{aligned} \tag{152}$$

Estimate (152) holds for all $\psi \in C_0^\infty$, which is a core for Λ_p. Next, let $\psi \in \mathcal{D}(\Lambda_p)$, and let $\{\psi_n\} \subset C_0^\infty$ be a sequence, s.t. $\psi_n \to \psi$, $\Lambda_p\psi_n \to \Lambda_p\psi$, as $n \to \infty$. If χ_R denotes the cutoff function $\chi(\Lambda_p \leq R)$, for $R > 0$, we have

$$\begin{aligned}\left\|\chi_R\Lambda_p e^{itA_p^a}\psi\right\| &\leq \left\|\chi_R\Lambda_p e^{itA_p^a}\psi_n\right\| + R\|\psi-\psi_n\| \\ &\leq 4\sqrt{2}e^{(\|\xi'\|_\infty+\|\xi\|_\infty)|t|/a}\|\Lambda_p\psi_n\| + R\|\psi-\psi_n\|.\end{aligned}$$

Taking $n \to \infty$ yields

$$\left\|\chi_R\Lambda_p e^{itA_p^a}\psi\right\| \leq 4\sqrt{2}e^{(\|\xi'\|_\infty+\|\xi\|_\infty)|t|/a}\|\Lambda_p\psi\|,$$

uniformly in the cutoff parameter R. This shows that $e^{itA_p^a}\psi \in \mathcal{D}(\Lambda_p)$, and (152) is valid for all $\psi \in \mathcal{D}(\Lambda_p)$.

We complete the proof of the proposition by examining $\Lambda_f e^{itA_f}\psi$. Let $\psi \in \mathcal{D}_f$. Then one finds the following bound for the n-particle component:

$$\begin{aligned}\left\|\left[(\Lambda_f - \mathbb{1}_f)e^{itA_f}\psi\right]_n\right\|^2 &= \left\|\sum_{j=1}^n (u_j^2+1)\psi_n(u_1-t,\ldots,u_n-t)\right\|^2 \\ &= \left\|\sum_{j=1}^n \left((u_j+t)^2+1\right)\psi_n(u_1,\ldots,u_n)\right\|^2 \\ &\leq \left(2(1+t^2)\right)^2\left\|\sum_{j=1}^n (u_j^2+1)\psi_n(u_1,\ldots,u_n)\right\|^2.\end{aligned}$$

It follows that $\|(\Lambda_f - \mathbb{1}_f)e^{itA_f}\psi\| \leq 2(1+t^2)\|\Lambda_f\psi\|$, for all $\psi \in \mathcal{D}_f$, so that

$$\|\Lambda_f e^{itA_f}\psi\| \leq 2(1+t^2)\|\Lambda_f\psi\| + \|\psi\| \leq 3e^t\|\Lambda_f\psi\|,$$

for all $\psi \in \mathcal{D}_f$. A similar argument as above shows that this estimate extends to all $\psi \in \mathcal{D}(\Lambda_f)$. ■

Proof of Proposition 4.4. We denote the fiber of A_p^a by $A_p^a(e)$, i.e.

$$A_p^a(e) = i\left(\frac{1}{2}\frac{1}{a}\xi'(e/a) + \xi(e/a)\partial_e\right), \tag{153}$$

see also (71). For $\psi \in C_0^\infty$, we have

$$\begin{aligned}(A_p^a G_\alpha \psi)(e) &= A_p^a(e)(G_\alpha\psi)(e) \\ &= A_p^a(e)G_\alpha(e,E)\psi(E) + A_p^a(e)\int_{\mathbb{R}_+} G_\alpha(e,e')\psi(e')de'.\end{aligned}$$

Due to the regularity property (36), we can take the operator $A_p^a(e)$ inside the integral (Dominated Convergence Theorem), and obtain the estimate

$$\|A_p^a G_\alpha\psi\|^2 \leq |\psi(E)|^2 \int_{\mathbb{R}_+} \|A_p^a(e)G_\alpha(e,E)\|_{\mathfrak{H}}^2 de \tag{154}$$

$$+\int_{\mathbb{R}_+}\left[\int_{\mathbb{R}_+} \|A_p^a(e)G_\alpha(e,e')\psi(e')\|_{\mathfrak{H}} de'\right]^2 de. \tag{155}$$

Using (153) and the bound $|a^{-1}\xi'(e/a)| \leq e^{-1}\sup_{e\geq 0} e\xi'(e) \leq ke^{-1}$, it is easily seen that the integrand of (154) is bounded above by

$$k\left(\|e^{-1}G_\alpha(e,E)\|_{\mathfrak{H}}^2 + \|\partial_1 G_\alpha(e,E)\|_{\mathfrak{H}}^2\right),$$

which is integrable, due to (35). We estimate the integrand in (155) by

$$\begin{aligned}&\|A_p^a(e)G_\alpha(e,e')\psi(e')\|_{\mathfrak{H}} \\ &\quad\leq k\left(\|e^{-1}G_\alpha(e,e')\|_{\mathcal{B}(\mathfrak{H})} + \|\partial_1 G_\alpha(e,e')\|_{\mathcal{B}(\mathfrak{H})}\right)\|\psi(e')\|_{\mathfrak{H}},\end{aligned}$$

and using Hölder's inequality, we arrive at

$$\begin{aligned}(155) \leq\ & k\int_{\mathbb{R}_+}\|\psi(e)\|^2 de \\ &\times\int_{\mathbb{R}_+}\int_{\mathbb{R}_+}\left\{\|e^{-1}G_\alpha(e,e')\|_{\mathcal{B}(\mathfrak{H})}^2 + \|\partial_1 G_\alpha(e,e')\|_{\mathcal{B}(\mathfrak{H})}^2\right\} de de'.\end{aligned}$$

By condition (36), the double integral is finite. We conclude that

$$\|A_p^a G_\alpha\psi\| \leq k\|\psi\|. \tag{156}$$

One also finds that $\|G_\alpha A_p^a\psi\| \leq k\|\psi\|$, e.g. by noticing that $\|G_\alpha A_p^a\psi\| = \sup_{0\neq\phi\in C_0^\infty}\|\phi\|^{-1}|\left\langle \phi, G_\alpha A_p^a\psi\right\rangle| = \sup_{0\neq\phi\in C_0^\infty}\|\phi\|^{-1}|\left\langle A_p^a G_\alpha\phi, \psi\right\rangle|$ and using (156). Consequently, we have shown (93) for $n = 1$.

The proof for $n = 2, 3$ follows the above lines. For instance, in order to show boundedness of the third multi-commutator, a typical term to estimate is $\|A_p^a A_p^a G_\alpha A_p^a\psi\|$, for $\psi \in C_0^\infty$. We shall sketch the proof that this term is bounded, all other ones being treated similarly. We have

$$\|A_p^a A_p^a G_\alpha A_p^a\psi\| = \sup_{0\neq\phi\in C_0^\infty}\|\phi\|^{-1}\left|\left\langle \phi, A_p^a A_p^a G_\alpha A_p^a\psi\right\rangle\right|, \tag{157}$$

and the scalar product equals

$$\int_{\mathbb{R}_+}\int_{\mathbb{R}_+}\left\langle \phi(e), A_p^a(e)^2 G_\alpha(e,e')A_p^a(e')\psi(e')\right\rangle_{\mathfrak{H}} de\, de'. \tag{158}$$

Recalling (153), one can calculate the operator $A_p^2(e)^2 G_\alpha(e,e')$. It can be written as a sum of terms, involving multiplications by functions with argument e, and derivatives $\partial_1 G_\alpha(e,e')$, $\partial_1^2 G_\alpha(e,e')$. Using the formulas for the adjoints of derivatives of $\partial_1^{1,2}G_\alpha(e,e')$, see (32), we obtain $[A_p^a(e)^2 G_\alpha(e,e')]^*$, and (158) becomes

$$\int_{\mathbb{R}_+}\int_{\mathbb{R}_+}\left\langle A_p^a(e')[A_p^a(e)^2 G_\alpha(e,e')]^*\phi(e), \psi(e')\right\rangle_{\mathfrak{H}} de\, de', \tag{159}$$

due to selfadjointness of $A_p^a(e')$ on $\mathfrak{H}$, and the fact that for all $e \in \mathbb{R}_+$,

$$[A_p^a(e)^2 G_\alpha(e,e')]^*\phi(e) \in \mathcal{D}(A_p^a(e')),$$

which follows from condition (36). Moreover, the same condition allows us to estimate

$$\begin{aligned}
&|(159)| \\
&\leq \int_{\mathbb{R}_+}\int_{\mathbb{R}_+}\left\||A_p^a(e')[A_p^a(e)^2 G_\alpha(e,e')]^*\right\|_{\mathcal{B}(\mathfrak{H})}\|\phi(e)\|_{\mathfrak{H}}\|\psi(e')\|_{\mathfrak{H}} de\, de' \\
&\leq \|\phi\|\,\|\psi\|\left[\int_{\mathbb{R}_+}\int_{\mathbb{R}_+}\left\||A_p^a(e')[A_p^a(e)^2 G_\alpha(e,e')]^*\right\|^2_{\mathcal{B}(\mathfrak{H})} de\, de'\right]^{1/2} \\
&\leq k\|\phi\|\,\|\psi\|,
\end{aligned}$$

where we have used Hölder's inequality. This shows that (157) $\leq k\|\psi\|$. ■

Proof of Proposition 4.5. We have mentioned before (90) that A_0 satisfies the conditions of Theorem 3.3, so it suffices to verify the conditions of Theorem 3.2.

We need to check that $(X, \Lambda, \mathcal{D})$ is a GJN triple, for $X = L, N, D, C_n^a$, $n = 1, 2, 3$, and that (61), (62), (64),(63) are satisfied. Proposition 4.3 shows that (61) holds. The operator D, given in (80), is clearly $N^{1/2}$-bounded in the sense of Kato on $\mathcal{D}$, since G_α are bounded operators, and $\widetilde{g}_\alpha$, $e^{-\beta u/2}\widetilde{g}_\alpha$ are square-integrable. Hence (62) holds. Recalling Remark 1) after Theorem 3.2, and noticing that N commutes with e^{itA^a}, in the strong sense on $\mathcal{D}$, and that $C_3^a \leq kN^{1/2}$, in the sense of Kato on $\mathcal{D}$ (see (83)), we see that (64) is verified. Similarly, $C_1^a \leq kN$ in the sense of Kato on $\mathcal{D}$, see (81), so (63) holds.

It remains to show that the above mentioned triples satisfy the GJN properties. We first look at $(L, \Lambda, \mathcal{D})$. Clearly, $\|L\psi\| \leq k\|\Lambda\psi\|$, for $\psi \in \mathcal{D}$. Moreover, L_0 commutes with Λ in the strong sense on $\mathcal{D}$, so we need only consider the interaction term in the verification of (58). Due to condition (37), we have for all $\psi \in C_0^\infty$: $\|\Lambda_p G_\alpha \psi\| \leq k\|\psi\|$, $\|G_\alpha \Lambda_p \psi\| \leq k\|\psi\|$. Consequently, for $\psi \in \mathcal{D}$:

$$\begin{aligned}
&|\langle G_\alpha \otimes \mathbb{1}_p \otimes \varphi(\widetilde{g}_\alpha)\psi, \Lambda\psi\rangle - \langle \Lambda\psi, G_\alpha \otimes \mathbb{1}_p \otimes \varphi(\widetilde{g}_\alpha)\psi\rangle| \\
&\quad\leq\ k\|\psi\|\ \|\varphi(\widetilde{g}_\alpha)\psi\| \\
&\qquad + |\langle G_\alpha \otimes \mathbb{1}_p \otimes \varphi(\widetilde{g}_\alpha)\psi, \Lambda_f\psi\rangle - \langle \Lambda_f\psi, G_\alpha \otimes \mathbb{1}_p \otimes \varphi(\widetilde{g}_\alpha)\psi\rangle| \qquad (160)\\
&\quad\leq\ k\|\psi\|\ \|\varphi(\widetilde{g}_\alpha)\psi\| + k\|\psi\|\ \|\varphi((u^2+1)\widetilde{g}_\alpha)\psi\| \\
&\quad\leq\ k\|\psi\|\ \|\Lambda^{1/2}\psi\| \\
&\quad\leq\ k\left(\|\psi\|^2 + \|\Lambda^{1/2}\psi\|^2\right) \\
&\quad\leq\ k\,\langle\psi, (\Lambda + \mathbb{1})\psi\rangle \\
&\quad\leq\ 2k\,\langle\psi, \Lambda\psi\rangle\,.
\end{aligned}$$

We used in the third step that $\varphi(\widetilde{g}_\alpha)$ and $\varphi((u^2+1)\widetilde{g}_\alpha)$ are relatively $\Lambda_f^{1/2}$ bounded, in the sense of Kato on $\mathcal{D}$. This follows since $(u^2+1)\widetilde{g}_\alpha \in L^2(\mathbb{R} \times S^2, du \times d\Sigma)$, due to conditions (33) and (34). The same estimates hold for $\mathbb{1}_p \otimes \mathcal{C}_p G_\alpha \mathcal{C}_p \otimes \varphi(e^{-\beta u/2}\widetilde{g}_\alpha)$, hence we have shown that $(L, \Lambda, \mathcal{D})$ is a GJN triple.

It is clear that $N \leq \Lambda$ in the sense of Kato on $\mathcal{D}$, and since N commutes with Λ in the strong sense on $\mathcal{D}$, we see immediately that $(N, \Lambda, \mathcal{D})$ is a GJN triple.

Next, consider $(D, \Lambda, \mathcal{D})$. Since D has the same structure as I, c.f. (54) and (80), the proof that $(D, \Lambda, \mathcal{D})$ is a GJN triple goes as the one for $(L, \Lambda, \mathcal{D})$.

We examine $(C_n^a, \Lambda, \mathcal{D})$, $n = 1, 2, 3$, $a > 0$. Recall that the C_n^a are given in (81)-(83). Each C_n^a has a term that acts purely on the particle space. This term is a bounded multiplication operator that commutes with Λ, in the strong sense on $\mathcal{D}$. Therefore, we need only show that $(N + \lambda I_1^a, \Lambda, \mathcal{D})$, $(I_{2,3}^a, \Lambda, \mathcal{D})$ are GJN triples. Since we have shown it for $(N, \Lambda, \mathcal{D})$, it suffices to treat $(I_n^a, \Lambda, \mathcal{D})$, $n = 1, 2, 3$, $a > 0$. We take the general term in the sum of (84):

$$X := \mathrm{ad}_{A_p^a}^{(j)}(G_\alpha) \otimes \mathbb{1}_p \otimes \mathrm{ad}_{A_f}^{(n-j)}\left(\varphi(\widetilde{g}_\alpha)\right).$$

Since $\mathrm{ad}_{A_p^a}^{(j)}(G_\alpha)$ is bounded, $j = 1, 2, 3$ (see Proposition 4.4), and

$$\mathrm{ad}_{A_f}^{(n-j)}\left(\varphi(\widetilde{g}_\alpha)\right) = \varphi\left((i\partial_u)^{n-j}\widetilde{g}_\alpha\right)$$

is relatively $\Lambda_f^{1/2}$-bounded, in the sense of Kato on $\mathcal{D}$ (this follows from $\partial_u^k \widetilde{g}_\alpha \in L^2(\mathbb{R} \times S^2)$, $k = 1, 2, 3$, due to (33), (34)), then it is clear that $\|X\psi\| \leq k\|\Lambda\psi\|$, $\psi \in \mathcal{D}$. Next, we verify condition (58) as above in (160):

$$\begin{aligned} |\langle X\psi, \Lambda\psi\rangle - \langle \Lambda\psi, X\psi\rangle| &\leq k\|\psi\| \left\|\varphi\left((u^2+1)(i\partial)^{n-j}\widetilde{g}_\alpha\right)\psi\right\| \\ &\leq k\|\psi\| \, \|\Lambda^{1/2}\psi\|, \end{aligned}$$

since $(u^2+1)(\partial_u)^k \widetilde{g}_\alpha \in L^2(\mathbb{R} \times S^2)$, for $k = 1, 2, 3$, due to (33) and (34). ■

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