Spectral properties of the spin-boson Hamiltonian

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Abstract. We consider a two level atom coupled to the radiation field. Using a Mourre type estimate, we provide a complete spectral characterization of the spin-boson Hamiltonian for sufficiently small, but nonzero coupling. In particular, the singular continuous spectrum is empty and the point spectrum consists only of the ground state energy. Technically we prove an extension of the Mourre estimate to a conjugate operator which is the generator of an isometry semigroup only. We illustrate such a technique for the Friedrichs model and apply it also to the rotating wave approximation of the spin-boson model.

1. Introduction

Atoms decay to their ground state through the emission of radiation. The energies involved in such a process are small compared to the rest energy of an electron. Thus to a high level of precision we may use nonrelativistic quantum mechanics as our theoretical description of an atom coupled to the radiation field. Since the coupling constant is in fact small, perturbation theory provides us with an accurate physical picture of the various radiation processes. To date atomic physics has pushed the theory to a high level of sophistication and we have nothing to add here except for a point of principle: such an everyday process as radiative decay should be understood theoretically on a *nonperturbative* level. Given that the problem is being posed since over sixty years, surprisingly little work has been done in this direction. In our paper we will make only a small step by treating a simplified atom with two energy levels. We hope that our methods eventually generalize to more realistic atoms.

Let us imagine that the electron is tightly bound to an infinitely heavy nucleus. We can then use the dipole approximation where the vector potential at the actual position of the electron is replaced by the one at the origin (the location of the nucleus). After a canonical transformation the Hamiltonian reads

$$H = \frac{1}{2m}p^2 + V(x) + \frac{\alpha^2}{2}\int d^3k|\rho(k)|^2 \sum_{i=1}^{2}(x \cdot e_i(k))^2 + \sum_{i=1}^{2}\int d^3k\omega(k)a^*(k,i)a(k,i)$$
$$+ \alpha\sum_{i=1}^{2}\int d^3k(\omega(k)/2)^{1/2}\rho(k)(e_i(k)\cdot x)a^*(k,i) + h.c.. \tag{1.1}$$

Here x, p are the position and momentum of the electron, V is an external potential, $a^*(k,i)$ and $a(k,i)$ are the creation and annihilation operators for the i-th transverse component of the vector potential with commutation relations $[a(k,i), a^*(k',i')] = \delta_{ii'}\delta(k-k')$, $\omega(k) = |k|$ is the photon dispersion relation, and $e_i(k)$ are the polarization vectors with $k/|k|, e_1(k), e_2(k)$ forming a left-handed dreibein. In order to have a well defined theory, we also introduced a cut-off function at high frequencies, $\rho(k)$. Now, to simplify matters, we take only two levels of the bare atom Hamiltonian, $p^2/2m + V(x)$, into account. They have an energy difference μ and eigenfunctions $\psi_1(x), \psi_2(x)$. Projecting H onto the subspace spanned by ψ_1, ψ_2 and under suitable symmetry conditions for ψ_1, ψ_2 we obtain the spin-boson Hamiltonian

$$H = \frac{1}{2}\mu\sigma_z + \int d^3k\omega(k)a^*(k)a(k) + \sigma_x\int d^3k(\lambda(k)a^*(k) + \lambda(k)^*a(k)) \tag{1.2}$$

acting on the Hilbert space $C^2 \otimes \mathcal{F}$ with $\mathcal{F}$ the symmetric Fock space over $L^2(R^3, d^3k)$. σ_x, σ_z are the Pauli spin 1/2 matrices. $\mu\sigma_z/2$ is the energy of the bare atom and σ_x corresponds to coupling its position. For notational simplicity the coupling constant α is absorbed into λ. The spin-boson Hamiltonian is also a reasonable model for various systems turning up in solid state physics [1].

We require that $\int d^3k|\lambda(k)|^2 < \infty$. By completing the square we obtain

$$H \geq -\frac{\mu}{2} - \int d^3k|\lambda(k)|^2/\omega(k). \tag{1.3}$$

To have the energy bounded from below we thus need $\int d^3k|\lambda(k)|^2/\omega(k) < \infty$. H is then self-adjoint on its natural domain and bounded from below. There is a more subtle point here which has been investigated in considerable detail [2,3]. It may happen that the physical ground state has an infinite number of bosons and therefore lies no longer in $\mathcal{F}$. H acting on $C^2 \otimes \mathcal{F}$ has then no ground state. If we strengthen to

$$\int d^3k|\lambda(k)|^2/\omega(k)^2 < \infty, \tag{1.4}$$

then, provided $\mu \neq 0$, H has a unique ground state $\psi_0 \in C^2 \otimes \mathcal{F}$.

To return to radiative decay, on physical grounds we expect that if initially the atom is in an excited state, then after a transient period there will be some photons travelling outwards away from the atom and the atom together with the radiation field is in its coupled ground state ψ_0. To verify such a picture one has to study the long time behaviour of the solution of the time-dependent Schrödinger equation. This is a problem in scattering theory which we discuss separately [4,5]. Here we investigate only spectral properties of H. Our ultimate goal is

Conjecture. *Let $\mu \neq 0, \lambda \neq 0, \omega(k) = |k|$, and $\int d^3k|\lambda(k)|^2 < \infty, \int d^3k|\lambda(k)|^2/\omega(k)^2 < \infty$. Let ψ_0 be the ground state of H with energy E_0. Then*

$$\sigma_{pp}(H) = \{E_0\}, \qquad \sigma_{sc}(H) = \emptyset, \qquad \sigma_{ac}(H) = [E_0, \infty). \tag{1.5}$$

Let us reintroduce the coupling constant as $\alpha\lambda(k)$. In this paper we will need a further assumption which in essence implies that the continuum edge is strictly above E_0. We then prove the conjecture provided $0 < \alpha < \alpha_0$ with a constant α_0 depending on μ and λ.

The plan of our paper is as follows: In Section 2 we state the main results. In Section 3 we prove a generalization of Mourre's theorem. Mourre considers the commutator $[H, iA]$ with the conjugate operator A being self-adjoint. We need here the generalization to the case where iA generates only a strongly continuous semigroup of isometries. To explain how the method works, we apply it to the Friedrichs model as a prototypical but simple example (Section 4). In Section 5 we provide the proofs for the spin-boson Hamiltonian. In the final Section 6 we point out that with our technique the spectrum of (1.2) in the rotating wave approximation can be handled fairly exhaustively. We also refer to [4], where we explain in detail related work on radiative decay, in particular scattering theory, the weak coupling limit, and analytic dilation.

2. Summary of results

In solid state physics applications of (1.2) ω is an effective dispersion relation. Therefore it is natural to keep ω and λ general. We refrain however from stating the minimal assumptions necessary for our mathematics. The spatial dimension, ν, of the Bose field plays no particular role and is left arbitrary. The formal Hamiltonian under investigation is then

$$H = \frac{1}{2}\mu\sigma_z \otimes I + I \otimes \int d^\nu k\omega(k)a^*(k)a(k) + \sigma_x \otimes \int d^\nu k(\lambda(k)a^*(k) + \lambda(k)^*a(k)) \tag{2.1}$$

acting on $C^2 \otimes \mathcal{F}$. $a^*(k), a(k)$ are a Bose field over R^ν with commutation relations $[a(k), a^*(k')] = \delta(k - k')$. I denotes the identity operator on Hilbert spaces. To have an explicit coupling constant we sometimes write $\alpha\lambda$ instead of λ. Note that one could substitute λ by $|\lambda|$ through the canonical gauge transformation $a(k) \mapsto [|\lambda(k)|^{-1}\lambda(k)]a(k)$. We first state our assumptions on the dispersion relation ω.

Assumption A1. $\omega : R^\nu \to R$ is spherically symmetric (only a function of $|k|$) with

$$\omega(k) > 0 \qquad \text{for} \qquad k \neq 0, \tag{2.2}$$

$$\lim_{|k| \to \infty} \omega(k) = \infty. \tag{2.3}$$

ω and ω' are absolutely continuous as functions of $|k|$, ω' satisfies a Lipschitz condition on every compact subset of R^ν, and

$$\omega'(|k|) > 0 \qquad \text{for} \qquad k \neq 0. \tag{2.4}$$

The most important consequence of Assumption A1 is that the level sets $\{\, k \in R^\nu \mid \omega(k) = \omega_0 \,\}$ have measure zero. We note that the relativistic dispersion $\omega(k) = \sqrt{k^2 + m^2}$ and its limiting cases $\omega(k) = |k|, \omega(k) = k^2/2m$ satisfy all conditions.

The coupling function λ satisfies

Assumption A2. $\lambda : R^\nu \to C$ with

$$\int d^\nu k |\lambda(k)|^2 < \infty, \qquad \int d^\nu k |\lambda(k)|^2/\omega(k) < \infty \tag{2.5}$$

and

$$\int d^\nu k |\lambda(k)|^2 \delta(\omega(k) - \mu) > 0. \tag{2.6}$$

In the notation of [6, p.302 and 309], let $H_B = \int d^\nu k \omega(k) a^*(k) a(k) = d\Gamma(\omega)$ on $\mathcal{F}$ with domain of self-adjointness $D(H_B)$. Then H is essentially self-adjoint on any core of $I \otimes H_B$ and self-adjoint on $C^2 \otimes D(H_B)$. For convenience of the reader we reproduce the well-known proof in Appendix I. For the Mourre estimate and the virial theorem below, we need a bound on the number of bosons in ψ for any finite energy state $\psi \in D(H)$. While this sounds like a technical requirement, the deeper reason is that one needs a control on the number of bosons uniformly in time. If bosons can have arbitrarily small energies, i.e. $\omega(0) = 0$, we simply do not know how to achieve such a bound. We distinguish two cases

i) excitation gap. We require that

$$\omega(0) > 0. \tag{2.7}$$

Bounded energy implies then a corresponding bound on the number $N_B = d\Gamma(I)$ of bosons. Also, in a functional integral representation of $e^{-\beta H}$, the effective interaction decays exponentially. This implies that H has a spectral gap [2].

ii) cut-off in N_B. Let $P_{\leq N} = P(N_B \leq N)$ be the projection onto the subspace of $\mathcal{F}$ with number of bosons $\leq N$. By a slight abuse of notation, we will denote $P_{\leq N}$ on $\mathcal{F}$ and $I \otimes P_{\leq N}$ on $C^n \otimes \mathcal{F}$ by the same symbol $P_{\leq N}$. We define then the cut-off Hamiltonian

$$H_N = P_{\leq N} H P_{\leq N}. \tag{2.8}$$

Sandwiching an operator between two equal projections and restricting it to the range of the projection is called a *compression*. We will use this suggestive notion (apparently due to Halmos [7, Chapter 23]) throughout. In the context of photons, the compressed H has the physically correct dispersion relation $\omega(k) = |k|$ but limits their maximal number to be N. We will prove in [5] that H_N has a spectral gap.

The Mourre estimate below employs the conjugate operator

$$D = \frac{1}{2}\left(\frac{1}{|\nabla_k \omega|^2}\nabla_k\omega \cdot \nabla_k + \nabla_k \cdot \nabla_k\omega \frac{1}{|\nabla_k\omega|^2}\right). \tag{2.9}$$

It corresponds to the radial derivative on momentum space, multiplied and symmetrized with the group velocity.

Assumption A3. The coupling function λ satisfies

$$\int d^\nu k |D\lambda(k)|^2 < \infty \qquad \text{and} \qquad \int d^\nu k |D^2\lambda(k)|^2 < \infty. \tag{2.10}$$

We state our main results in the form of three theorems.

Theorem 1. *Let Assumptions A1-A3 hold. Let the coupling function be of the form $\alpha\lambda$ and let $\mu \neq 0$. If $\omega(0) > 0$, then there exists an α_0 (depending on λ and μ) such that, for $0 < \alpha < \alpha_0$, H has only one eigenvector, the ground state, and otherwise purely absolutely continuous spectrum.*

Theorem 2. *Let Assumptions A1-A3 hold. Let the coupling function be of the form $\alpha\lambda$ and let $\mu \neq 0$. There exists an α_0 (depending only on λ and μ, but not on N) such that, for $0 < \alpha < \alpha_0$, $P_{\leq N} H P_{\leq N}$ has only one eigenvector, the ground state, and otherwise purely absolutely continuous spectrum.*

To our knowledge Theorems 1 and 2 constitute the first complete spectral characterization of a (simplified) atom coupled to the radiation field, regarding the dipole approximation with quadratic external potential [8,9] as an exception. If satisfied with a less ambitious result, namely a finite number of eigenvalues, we can prove a more general and explicit theorem. For this purpose we introduce an obvious generalization of the spin-boson Hamiltonian as

$$H = S \otimes I + I \otimes \int d^\nu k \omega(k) a^*(k) a(k) + K \otimes a^*(\lambda) + K^* \otimes a(\lambda) \tag{2.11}$$

acting on $C^n \otimes \mathcal{F}$. Here $S = S^*$, K are normal $n \times n$ matrices and we use the shorthand $a^*(\lambda) = \int d^\nu k \lambda(k) a^*(k)$.

Theorem 3. *Let Assumptions A1-A3 hold and let*

$$0 < n(1 - (D\lambda, D\lambda)||K||^2)^{-1} =: c_0 < \infty.$$

(i) If $\omega(0) > 0$, then H has no singular continuous spectrum and the number of eigenvalues is bounded by c_0.

(ii) $P_{\leq N}HP_{\leq N}$ *has no singular continuous spectrum and the number of eigenvalues is bounded by* c_0.

3. A generalization of Mourre's theorem

Let H be a self-adjoint operator on the Hilbert space $\mathcal{H}$ with inner product $\langle\cdot|\cdot\rangle$. Its spectral projection onto the open interval $(E-\delta, E+\delta)$ will be denoted by $P(E,\delta)$ and the projection operators onto the pure point (p.p.), absolutely continuous (a.c.), and singular continuous (s.c.) subspaces will be denoted by $P_{pp}\mathcal{H}$, $P_{ac}\mathcal{H}$ and $P_{sc}\mathcal{H}$, respectively. Those subspaces are mutually orthogonal and span the whole Hilbert space, i.e. $P_{pp}+P_{ac}+P_{sc}=1$.

We consider a strongly continuous one parameter semigroup $U(t)$ of isometries on the Hilbert space $\mathcal{H}$, i.e. $U:[0,\infty)\to B(\mathcal{H})$ is a map into the bounded linear operators on $\mathcal{H}$ such that

i) $U(0)=I$ and $U(s)U(t)=U(s+t)$, $\quad s,t\geq 0$ (semigroup property),

ii) $\lim_{t\downarrow 0}U(t)\psi=\psi$ for $\psi\in\mathcal{H}$ (right strong continuity at 0),

iii) $\langle U(t)\phi|U(t)\psi\rangle=\langle\phi|\psi\rangle$ equivalently $U(t)^*U(t)=1$ (isometry).

Such a semigroup has a closed and densely defined generator, which is denoted by $\tilde{A}$ throughout this paper, such that $U(t)=\exp(-\tilde{A}t), t\geq 0$. We remark that the symbol $\tilde{A}$ of the generator corresponds to (and was motivated by) Definition (4.18) in [10]. Note however that the operator $A=-i\tilde{A}$ will not be self-adjoint in general, unlike the situation in Chapter 4 of [10]. This is also reflected in the nonsurjectivity of $U(t)$ for $t>0$, a property of those isometry semigroups, which cannot be extended to unitary groups without enlarging the Hilbert space. Because of

$$||U^*(t)\phi-\phi||=||U^*(t)(\phi-U(t)\phi)||\leq||\phi-U(t)\phi|| \tag{3.1}$$

we have strong continuity of the adjoint semigroup and on $D(A)$ we have

$$\frac{U^*(t)\phi-\phi}{t}-U^*(t)A\phi=U^*(t)\Big(\frac{\phi-U(t)\phi}{t}-A\phi\Big)\to 0 \tag{3.2}$$

and $U^*(t)A\phi\to A\phi$. Therefore, if A^* denotes the generator of the adjoint semigroup $U^*(t)$, then $D(A)\subset D(A^*)$ and A^* extends $-A$.

If $\tilde{A}$ is an isometry semigroup generator such that $D(\tilde{A})\cap D(H)$ is dense in $\mathcal{H}$, then $[\tilde{A},H]$ denotes the sesquilinear form given by

$$\langle\phi|[\tilde{A},H]\psi\rangle=\langle\tilde{A}^*\phi|H\psi\rangle-\langle H\phi|\tilde{A}\psi\rangle,\quad \phi\in D(\tilde{A}^*)\cap D(H),\quad \psi\in D(\tilde{A})\cap D(H). \tag{3.3}$$

If this form is symmetric, bounded below and closable, then $[\tilde{A},H]^0$ denotes the self-adjoint operator associated to its closure.

Definition 4. The generator $\tilde{A}$ of an isometry semigroup is called a *conjugate operator* for H at a point $E\in R$ iff the following conditions hold:

a) $D(\tilde{A})\cap D(H)$ is a core for H.

b) $U(t)D(H)=\exp(-\tilde{A}t)D(H)\subset D(H)$, $U^*(t)D(H)\subset D(H)$ for $t>0$ and

$$\sup_{0\leq t\leq 1}||HU(t)\psi||<\infty,\quad \sup_{0\leq t\leq 1}||HU^*(t)\psi||<\infty,\quad \psi\in D(H). \tag{3.4}$$

c) The form $[\tilde{A}, H]$ is bounded below and closable. The domain of its self-adjoint closure $[\tilde{A}, H]^0$ contains $D(H)$.

d) The form defined on $D(\tilde{A}) \cap D(H)$ by $[\tilde{A}, [\tilde{A}, H]^0]$ is bounded as a map from $\mathcal{H}_{+2} := D(H)$ (with scalar product $\langle\phi|\psi\rangle + \langle H\phi|H\psi\rangle$) to its dual $\mathcal{H}_{-2}$.

e) There exist $\alpha, \delta > 0$ and a compact operator C such that

$$P(E, \delta)[\tilde{A}, H]^0 P(E, \delta) \geq \alpha P(E, \delta) - C. \tag{3.5}$$

An inequality as (3.5) is called a *Mourre estimate*. Starting from an estimate of this form, Mourre [11,12] proves spectral properties of H in the open set $(E - \delta, E + \delta)$. (For an introduction to Mourre techniques we refer to [10, Chapter 4].) His theorem makes the stronger assertions, the larger the interval around E. Because of this, we call an inequality of the form (3.5) with $\delta = +\infty$ a *strong Mourre estimate*. In the following sections, we will prove strong Mourre estimates yielding information about the global structure of the spectrum for several Hamiltonians, including (2.1).

Mourre required $\tilde{A}$ to generate a unitary group. This is too restrictive for our purposes and we have to generalize the Mourre theorem to generators of one-parameter isometry semigroups.

Theorem 5. *Let H be a self-adjoint operator which admits a conjugate operator at $E \in R$ with the estimate (3.5). Then:*

1. The point spectrum of H in $(E - \delta, E + \delta)$ is finite.

2. $\sigma_{sc}(H) = \emptyset$.

Our proof follows Mourre's paper [11]. We provide the details up to the virial theorem. The spectrum of a generator of a contraction semigroup is generally contained in a half plane, contrary to the unitary group case, where the spectrum of its generator is contained in the imaginary axis. Consequently, we can take resolvents only in the left half plane of the complex numbers, being always in the resolvent set of a contraction semigroup generator. This is the main additional ingredient of our proof as compared to [11]. Because of the geometric intuition behind the technical steps, we will emphasize the semigroup itself rather than its generator.

We divide the proof of Part 1 of Theorem 5 into four propositions and start to consider what happens if $D(\tilde{A}) \cap D(H)$ is not explicitly known. The first proposition states that an appropriate core suffices.

Proposition 6. *Let H be self-adjoint and $\tilde{A}$ be the generator of an isometry semigroup $U(t)$ satisfying conditions a),b) and the following conditions c').*

c') There exists a set $\mathcal{S} \subset D(\tilde{A}) \cap D(H)$ such that

i) $U(t)\mathcal{S} \subset \mathcal{S}$,

ii) $\mathcal{S}$ is a core for H,

iii) the form $[\tilde{A}, H]$ is bounded from below and closable, and the associated self-adjoint operator $[\tilde{A}, H]^0_{\mathcal{S}}$ satisfies

$$D([\tilde{A}, H]^0_{\mathcal{S}}) \supset D(H).$$

Then for all $\phi, \psi \in D(\tilde{A}) \cap D(H)$

$$\langle\phi|[\tilde{A}, H]\psi\rangle = \langle\phi|[\tilde{A}, H]^0_{\mathcal{S}}\psi\rangle.$$

Hence the form $[\tilde{A}, H]$ is closable and the associated self-adjoint operator satisfies

$$[\tilde{A}, H]^0 = [\tilde{A}, H]^0_{\mathcal{S}}.$$

Proof. We only need to check for $\phi, \psi \in D(\tilde{A}) \cap D(H)$

$$\langle \phi | [\tilde{A}, H] \psi \rangle = \langle \phi | [\tilde{A}, H]^0_{\mathcal{S}} \psi \rangle. \tag{3.6}$$

As a general fact (true on Banach spaces), the composition TB of a bounded and everywhere defined operator B and a closed operator T with $D(T) \subset \mathrm{range}(B)$ is closed and consequently, by the closed graph theorem, bounded. Thus, the operators $HU(t)(H+i)^{-1}$ are bounded by hypothesis b). For each $\psi \in \mathcal{H}$, we have by b) $\sup_{0 \le t \le 1} ||HU(t)(H+i)^{-1}\psi|| < \infty$ and by the uniform boundedness principle this operator family is uniformly bounded by some finite constant,

$$||HU(t)(H+i)^{-1}|| \le c_1, \qquad 0 \le t \le 1. \tag{3.7}$$

Consequently, for each $\phi, \psi \in D(\tilde{A}) \cap D(H)$ and $H(t) = U(t)^* HU(t)$,

$$\begin{aligned} \lim_{t \to 0} \langle \phi | (H(t) - H)\psi \rangle / t &= \lim_{t \to 0} \langle \phi | (U(t)^* - 1) HU(t) \psi \rangle / t + \langle \phi | H(U(t) - 1)\psi \rangle / t \\ &= \lim_{t \to 0} \langle \frac{1}{t}(U(t) - 1)\phi | HU(t)\psi \rangle + \langle H\phi | \frac{1}{t}(U(t) - 1)\psi \rangle \\ &= \langle \phi | [\tilde{A}, H] \psi \rangle. \end{aligned} \tag{3.8}$$

Here $HU(t)\psi$ is uniformly bounded in $0 \le t \le 1$, so this family of vectors converges weakly to $H\psi$ when $t \to 0$. For the first summand in the second line of (3.8) we used that the scalar product of a strongly convergent sequence with a weakly convergent sequence converges.

$\mathcal{S}$ is a core for H. Thus there exist sequences $u_n, v_n \in \mathcal{S}$ for each $\phi \in \mathcal{H}, \psi \in D(H)$ such that

$$||u_n - \phi|| \to 0, ||(H + i)(v_n - \psi)|| \to 0. \tag{3.9}$$

By the uniform estimate (3.7)

$$\langle \phi | (H(t) - H)\psi \rangle / t = \lim_{n \to \infty} \langle u_n | (H(t) - H) v_n \rangle / t. \tag{3.10}$$

The derivative

$$\frac{d}{dt} \langle u_n | H(t) v_n \rangle = \langle u_n | U(t)^* [\tilde{A}, H]^0_{\mathcal{S}} U(t) v_n \rangle \tag{3.11}$$

exists for $0 \le t \le 1$ and the mean value theorem implies

$$\langle \phi | (H(t) - H)\psi \rangle / t = \lim_{n \to \infty} \langle u_n | U(t_n)^* [\tilde{A}, H]^0_{\mathcal{S}} U(t_n) v_n \rangle, \quad 0 \le t_n \le t. \tag{3.12}$$

Letting first $n \to \infty$ and then $t \downarrow 0$ leads to

$$||U(t_n)u_n - \phi|| \le ||U(t_n)(u_n - \phi)|| + ||U(t_n)\phi - \phi|| \to 0 \tag{3.13}$$

and

$$[\tilde{A},H]^0_{\mathcal{S}}U(t_n)v_n=[\tilde{A},H]^0_{\mathcal{S}}(H+i)^{-1}(H+i)U(t_n)(v_n-\psi)+[\tilde{A},H]^0_{\mathcal{S}}U(t_n)\psi \tag{3.14}$$

is uniformly bounded and converges weakly to $[\tilde{A},H]^0_{\mathcal{S}}\psi$, hence

$$\langle\phi|[\tilde{A},H]\psi\rangle=\lim_{t\to 0}\langle\phi|(H(t)-H)\psi\rangle/t=\langle\phi|[\tilde{A},H]^0_{\mathcal{S}}\psi\rangle. \qquad \square \tag{3.15}$$

Notice that we proved, as a byproduct

$$\lim_{t\to 0}\langle\phi|(H(t)-H)\psi\rangle/t=\langle\phi|[\tilde{A},H]^0\psi\rangle \qquad \phi\in\mathcal{H},\psi\in D(H) \tag{3.16}$$

Proposition 7. *Let $\tilde{A},H$ satisfy conditions a)-c). Then $U(t)$ acts as a strongly continuous semigroup of bounded operators on the Hilbert space $D(H)=\mathcal{H}_{+2}$ with the graph norm. $(H-z)^{-1}$ leaves $D(\tilde{A})$ invariant for all $z\notin\sigma(H)$.*

Proof. For this we need a much stronger version of (3.16), namely for every $\psi\in D(H)$

$$\lim_{t\to 0}||\frac{U(1-t)HU(t)-U(1)H}{t}\psi-U(1)[\tilde{A},H]^0\psi||=0. \tag{3.17}$$

(3.17) implies (3.16) by bracketing from the left with $\langle U(1)\phi|$ and applying isometry $U^*(1)U(1)=1$. Similarly as in Proposition 6, we have for $\phi,\psi\in D(A)\cap D(H)$

$$\begin{aligned}&\lim_{t\downarrow 0}\langle\phi|\frac{U(1-t)HU(t)-U(1)H}{t}\psi\rangle\\ =&\lim_{t\downarrow 0}\langle\frac{U^*(1-t)\phi-U^*(1)\phi}{t}|HU(t)\psi\rangle+\langle HU^*(1)\phi|\frac{U(t)\psi-\psi}{t}\rangle\\ =&\langle U^*(1)\phi|[\tilde{A},H]\psi\rangle.\end{aligned} \tag{3.18}$$

Additionally to above we used here Lemma (1.3) in [13] to evaluate the backwards differential quotient and the fact $U^*(t)D(A)\subset U^*(t)D(A^*)\subset D(A^*)$.

Let now $\psi_n\in D(\tilde{A})\cap D(H)$ so that $||(H+i)(\psi_n-\psi)||\to 0$ and $\phi\in D(\tilde{A})\cap D(H)$. Then for $t>0$

$$\frac{U(1-t)HU(t)-U(1)H}{t}\psi_n-U(1)[\tilde{A},H]^0\psi_n\to\frac{U(1-t)HU(t)-U(1)H}{t}\psi-U(1)[\tilde{A},H]^0\psi \tag{3.19}$$

and by the mean value theorem again

$$\langle\phi|\frac{U(1-t)HU(t)-U(1)H}{t}\psi_n\rangle=\langle\phi|U(1-t_{n,\phi})[\tilde{A},H]^0_{\mathcal{S}}U(t_{n,\phi})\psi_n\rangle, \quad 0\le t_{n,\phi}\le t\le 1. \tag{3.20}$$

This implies, first for ψ_n and, after taking limits, for ψ

$$||U(1-t)HU(t)\psi-U(1)H\psi||\le(c_1+1)t\ ||[\tilde{A},H]^0(H+i)^{-1}||\ ||(H+i)\psi||, \tag{3.21}$$

leading to strong continuity of the semigroup $U(t)$ on $D(H)$

$$||HU(t)\psi - H\psi|| \leq ||HU(t)\psi - U(t)H\psi|| + ||U(t)H\psi - \psi|| \to 0. \qquad (3.22)$$

Now (3.20) leads to

$$\begin{aligned}
&|\langle\phi|\frac{U(1-t)HU(t)-U(1)H}{t}\psi - U(1)[\tilde{A},H]^0\psi\rangle| \\
&\leq 2(c_1+1)||[\tilde{A},H]^0(H+i)^{-1}||\;||(H+i)(\psi_n-\psi)|| \\
&\qquad +|\langle\phi|U(1-t_{n,\phi})[\tilde{A},H]^0U(t_{n,\phi})\psi - U(1)[\tilde{A},H]^0\psi\rangle| \\
&\leq o(1)+\sup_{0\leq t'\leq t}||U(1-t')[\tilde{A},H]^0U(t')\psi - U(1)[\tilde{A},H]^0\psi|| \\
&\leq o(1)+\sup_{0\leq t'\leq t}||[\tilde{A},H]^0(U(t')\psi-\psi)|| + \sup_{0\leq t'\leq t}||(U(1-t')-U(1))[\tilde{A},H]^0\psi||.
\end{aligned} \qquad (3.23)$$

The first summand becomes arbitrarily small for large n, the second is small because of (3.22) and the third is small because of strong continuity, proving (3.17).

Let now $a \in D(\tilde{A})$, we prove that $U(t)(H-z)^{-1}a$ is differentiable. For this it is sufficient to prove that $(H-z)U(t)(H-z)^{-1}a$ is differentiable, for which in turn it is sufficient to prove that $((H-z)U(t)-U(t)(H-z))(H-z)^{-1}a$ is differentiable. (This is the only place where we use $a \in D(\tilde{A})$.) But $\psi = (H-z)^{-1}a \in D(H)$ and (3.17) implies

$$\lim_{t\to 0}||\frac{HU(t)-U(t)H}{t}\psi - U(t)[\tilde{A},H]^0\psi|| = 0. \qquad \square \qquad (3.24)$$

Proposition 8. *Let $\tilde{A}, H$ satisfy conditions a)-c). Then $(\tilde{A}+\lambda)^{-1}D(H) \subset D(H)$ for sufficiently large real λ. $(H+i)\lambda(\tilde{A}+\lambda)^{-1}(H+i)^{-1}$ converges strongly to I as $\lambda \to +\infty$.*

Proof. Equation (3.22) says that $U(t)$ acts as a strongly continuous semigroup on the Hilbert space $D(H) = \mathcal{H}_{+2}$ with its appropriate norm. Now standard semigroup theorems imply that $||U(t)||_{2,2} \leq Me^{at}$ for certain constants M, a and all $t \geq 0$. Then $(\tilde{A}+\lambda)^{-1}$ is a bounded, injective and closed operator from $\mathcal{H}_{+2}$ to itself for $\mathrm{Re}\lambda > a$ [13, Proposition 1.18 and Theorem 2.8]. For all $\phi \in D(\tilde{A}) \cap D(H)$, we have $(H+i)\lambda(\tilde{A}+\lambda)^{-1}\phi = (H+i)\phi - (H+i)(\tilde{A}+\lambda)^{-1}\tilde{A}\phi \to (H+i)\phi$ as $\lambda \to +\infty$ by the Hille-Yosida-Phillips theorem [13, Theorem 2.21]. By the same theorem $(H+i)\lambda(\tilde{A}+\lambda)^{-1}(H+i)^{-1}$ are uniformly bounded for large λ. This implies strong convergence of $(H+i)\lambda(\tilde{A}+\lambda)^{-1}(H+i)^{-1}$ to I on all of $\mathcal{H}$. $\square$

Proposition 9 (The Virial Theorem). *Let $\tilde{A}, H$ satisfy conditions a)-c). Then*

1. *For $\psi \in D(H)$*

$$[\tilde{A},H]^0\psi = \lim_{\lambda\to+\infty}[\tilde{A}\lambda(\tilde{A}+\lambda)^{-1},H]\psi.$$

2. *If ψ is an eigenvector of H, then*

$$\langle\psi|[\tilde{A},H]^0\psi\rangle = 0.$$

Proof. Part b) of Definition 4 implies that $U^*(t)$ acts as a semigroup of operators on $\mathcal{H}_{+2}$. By the same argument as in Proposition 6, $U^*(t)$ is uniformly bounded on compact t intervals. $U^*(t)$ is weakly continuous on $\mathcal{H}_{+2}$:

$$\begin{aligned}\lim_{t\downarrow 0}\langle (H+i)\phi|U^*(t)(H+i)\psi\rangle =&\lim_{t\downarrow 0}\langle U(t)(H+i)\phi|(H+i)\psi\rangle \\ =&\langle (H+i)\phi|(H+i)\psi\rangle, \quad \phi,\psi\in D(H).\end{aligned} \tag{3.25}$$

By a complicated argument involving the Krein-Smullyan theorem, $U^*(t)$ is then also strongly continuous on $\mathcal{H}_{+2}$ [13, Proposition 1.23]. This implies $(\tilde{A}^*+\lambda)^{-1}D(H)\subset D(H)$ for large λ and justifies, together with the foregoing Propositions, the following computation.

Let $\phi\in D(\tilde{A})\cap D(H)$ and $\psi\in D(H)$. For large λ

$$\begin{aligned}&\langle\phi|[\tilde{A}\lambda(\tilde{A}+\lambda)^{-1},H]\psi\rangle = \langle\phi|\{\tilde{A}\lambda(\tilde{A}+\lambda)^{-1}H - H\tilde{A}\lambda(\tilde{A}+\lambda)^{-1}\}\psi\rangle\\ &=\langle\phi|(\tilde{A}H-H\tilde{A})\lambda(\tilde{A}+\lambda)^{-1}\psi\rangle + \langle\tilde{A}^*\phi|\lambda(\tilde{A}+\lambda)^{-1}H - H\lambda(\tilde{A}+\lambda)^{-1}\psi\rangle\\ &=\langle\phi|[\tilde{A},H]\lambda(\tilde{A}+\lambda)^{-1}\psi\rangle + \langle\tilde{A}^*\phi|(\tilde{A}+\lambda)^{-1}H(\tilde{A}+\lambda)\lambda(\tilde{A}+\lambda)^{-1}\psi\rangle\\ &\quad - \langle(\tilde{A}^*+\lambda)(\tilde{A}^*+\lambda)^{-1}\tilde{A}^*\phi|H\lambda(\tilde{A}+\lambda)^{-1}\psi\rangle\\ &=\langle\phi|[\tilde{A},H]\lambda(\tilde{A}+\lambda)^{-1}\psi\rangle + \langle H(\tilde{A}^*+\lambda)^{-1}\tilde{A}^*\phi|(\tilde{A}+\lambda)\lambda(\tilde{A}+\lambda)^{-1}\psi\rangle\\ &\quad - \langle(\tilde{A}^*+\lambda)(\tilde{A}^*+\lambda)^{-1}\tilde{A}^*\phi|H\lambda(\tilde{A}+\lambda)^{-1}\psi\rangle\\ &=\langle\phi|[\tilde{A},H]\lambda(\tilde{A}+\lambda)^{-1}\psi\rangle - \langle(\tilde{A}^*+\lambda)^{-1}\tilde{A}^*\phi|[\tilde{A},H]\lambda(\tilde{A}+\lambda)^{-1}\psi\rangle\\ &=\langle\phi|\lambda(\tilde{A}+\lambda)^{-1}[\tilde{A},H]^0\lambda(\tilde{A}+\lambda)^{-1}\psi\rangle.\end{aligned} \tag{3.26}$$

Since the commutator is H-bounded, the operator converges strongly to $[\tilde{A},H]^0$ on $D(H)$, which can be seen by factoring the operator as

$$\lambda(\tilde{A}+\lambda)^{-1}\cdot[\tilde{A},H]^0(H+i)^{-1}\cdot(H+i)\lambda(\tilde{A}+\lambda)^{-1}(H+i)^{-1}\cdot(H+i). \tag{3.27}$$

Now, if ψ is an eigenvector of H, then $\psi\in D(H)$ and $H\psi=E\psi$ and we obtain the virial theorem,

$$\langle\psi|[\tilde{A},H]^0\psi\rangle = \lim_{\lambda\to+\infty}\langle\psi|[\tilde{A}\lambda(\tilde{A}+\lambda)^{-1},H]\psi\rangle = 0. \qquad \square \tag{3.28}$$

Lemma 10. *Let the assumptions of Proposition 9 hold. In addition, let the commutator be bounded from below as a quadratic form,*

$$[\tilde{A},H]^0 \geq \alpha I - C, \tag{3.29}$$

with $\alpha>0$ and C a positive self-adjoint operator of trace class. Then

$$\mathrm{dim}P_{pp}\leq\alpha^{-1}\mathrm{tr}C.$$

(dimP_{pp} *equals the number of eigenvalues, counted with their multiplicity.)*

Proof. We use the virial theorem which states that

$$\langle\psi|[\tilde{A},H]^0\psi\rangle = 0$$

for every eigenvector of H. Then

$$0 = \mathrm{tr}P_{pp}[\tilde{A},H]^0 \geq \mathrm{tr}P_{pp}(\alpha I - C) \geq \alpha\mathrm{dim}P_{pp} - \mathrm{tr}C. \qquad \square \tag{3.30}$$

We return to the

Proof of Part 1 of Theorem 5. Let the Hamiltonian H and the conjugate operator $\tilde{A}$ obey conditions a)-c) and e) at the energy E. Suppose that the point spectrum in $(E-\delta,E+\delta)$ is infinite. There exists then an orthonormal sequence of eigenvectors (ψ_n) with $H\psi_n = E\psi_n$. By the Virial Theorem

$$0 = \langle\psi_n|[\tilde{A},H]^0\psi_n\rangle \geq \alpha\langle\psi_n|\psi_n\rangle - \langle\psi_n|C\psi_n\rangle. \tag{3.31}$$

The orthonormal sequence (ψ_n) converges weakly to zero. Since C is compact, $(C\psi_n)$ converges strongly to zero, which is in contradiction to $\alpha > 0$. $\square$

Since the details in the proof of Part 2 of Theorem 5 are analogous to [11], we omit them. We only mention that Proposition II.5 in [11] easily generalizes to nonself-adjoint C in the following sense. Let H be a self-adjoint operator B', B, C be bounded operators with $B'^*B' \leq B^*B$. Then

1. $H - z - i\epsilon B^*B$ is invertible if $\mathrm{Im}z$ and ϵ have the same sign.
2. If $\mathrm{Im}z$ and ϵ have the same sign, let $G_z(\epsilon) = (H - z - i\epsilon B^*B)^{-1}$. Then

$$||B'G_z(\epsilon)C|| \leq \frac{1}{\sqrt{\epsilon}}||C^*G_z(\epsilon)C||. \tag{3.32}$$

In the proof of Part 2 one takes $C = (1+\tilde{A})^{-1}$ and $C^* = (1+\tilde{A}^*)^{-1}$.

4. Mourre estimate for the Friedrichs model

Friedrichs introduced his model with the goal to understand the coupling of a discrete state to the continuum [14]. Such a toy model reappeared second quantized in quantum field theory and is usually called Lee model [15,16]. The spectral properties of the Friedrichs model are well understood [14]. Here we only want to explain how within the context of this model one sets up a Mourre type estimate and how to extract information on the number of eigenvalues out of it. Our estimate will be poorer than the complete treatment in [14]. However the method generalizes to more difficult problems, as the spin-boson Hamiltonian. From now on both the Hermitian form $[\tilde{A},H]$ and its associated self-adjoint operator $[\tilde{A},H]^0$ will be denoted by $[\tilde{A},H]$.

The Hamiltonian H of the Friedrichs model is given by

$$H\begin{pmatrix} c \\ \psi \end{pmatrix} = \begin{pmatrix} \mu & (\lambda,\cdot) \\ \lambda & \omega \end{pmatrix}\begin{pmatrix} c \\ \psi \end{pmatrix} = \begin{pmatrix} \mu c + (\lambda,\psi) \\ c\lambda + \omega\psi \end{pmatrix} \tag{4.1}$$

acting on $\mathcal{H} = C \oplus L^2(R^\nu)$. ω, λ satisfy Assumptions A1-A3. An even simpler version would be

$$H = \begin{pmatrix} \mu & (\lambda, \cdot) \\ \lambda & x \end{pmatrix} \tag{4.2}$$

acting on $\mathcal{H} = C \oplus L^2(R_+, dx)$ with $\int_0^\infty dx|\lambda(x)|^2 < \infty$. The obvious choice for the conjugate operator is then

$$\tilde{A} = \begin{pmatrix} 0 & 0 \\ 0 & \partial/\partial x \end{pmatrix}.$$

Formally, $[\partial/\partial x, x] = 1$. Clearly $\exp(-\tilde{A}t), t \geq 0$, acts as a right shift by t and is an isometry semigroup which however cannot be extended to a unitary group in $\mathcal{H}$.

Returning to the Hamiltonian in (4.1) the analogue of $\partial/\partial x$ is given by the "normalized" radial derivative D of (2.9). Formally it satisfies $[D, \omega] = 1$. Such a choice of a conjugate operator is by no means original and appears already in [17, p.21] as a formal time operator. The more popular choice is the operator $D_0 = (v \cdot x + x \cdot v)/2 = (\nabla_k \omega \cdot \nabla_k + \nabla_k \cdot \nabla_k \omega)/2$ which becomes the dilation operator in the case $\omega(k) = k^2/2$. Their common feature is that the semigroup is induced by a radial outward flow in momentum space. If we want to estimate the number of eigenvalues, we need that $[D, \omega] \geq \alpha I$. The vector field defining the flow and thereby D is then by necessity singular at $k = 0$. Thus, at best, $\exp(-Dt), t \geq 0$, is an isometry semigroup. For this reason we made in Section 3 the effort to extend Mourre estimates to isometry semigroups.

Let us study the semigroup $\exp(-Dt), t \geq 0$, in somewhat more detail. We define the radial flow $k \mapsto k_t$ as the solution of

$$\frac{d}{dt} k_t = \frac{1}{\omega'(k_t)} \frac{k_t}{|k_t|}, \qquad k_t \in R^\nu \setminus \{0\}, \qquad k_0 = k. \tag{4.3}$$

(4.3) is solved implicitely by $\omega(k_t) = \omega(k) + t$ such that $k_t/|k_t| = k/|k|$. We extend the solution of (4.3) to $t < 0$ and set $k_t = 0$ for $t \leq -\omega(k)$. Let us define the flow $T_t : R^\nu \to R^\nu$ by $T_t k = k_t, k \neq 0$. We have then, for $t \geq 0$,

$$(e^{-Dt}\psi)(k) = \begin{cases} (\frac{|T_{-t}k|}{|k|})^{(d-1)/2} \exp[-\frac{1}{2}\int_0^t ds \frac{\omega''}{\omega'^2}(|T_{-s}k|)]\psi(T_{-t}k), & \text{if } T_{-t}k \neq 0, \\ 0, & \text{if } T_{-t}k = 0. \end{cases} \tag{4.4}$$

e^{-Dt} is a strongly continuous semigroup on $L^2(R^\nu)$. Actually, this is a general fact for (semi)groups on L^p spaces with $1 \leq p < \infty$, which are induced by a pullback of a differentiable (semi)flow on a differentiable manifold (with boundary). Our explicit representation allows us to handle the domain conditions listed in Definition 4.

As conjugate operator for the Friedrichs model we first try

$$\tilde{A} = \begin{pmatrix} 0 & 0 \\ 0 & D \end{pmatrix}. \tag{4.5}$$

In the sense of quadratic forms on the smooth functions with compact support not containing $0 \in R^\nu$, the commutator is worked out easily as

$$[\tilde{A}, H] = \begin{pmatrix} 0 & (D\lambda, \cdot) \\ D\lambda & 1 \end{pmatrix} \geq I - \frac{1}{2}(1 + \sqrt{1 + 4(D\lambda, D\lambda)})|a\rangle\langle a|. \tag{4.6}$$

Here we estimated the rank two perturbation of I from below by its unique negative eigenvalue with corresponding projection $|a\rangle\langle a|$. If we can verify that the technical conditions a) to e) in Definition 4 are satisfied, then the Friedrichs Hamiltonian obeys a strong Mourre estimate in the form (3.29) with $\alpha = 1$ and the positive rank one perturbation

$$C = \frac{1}{2}(1 + \sqrt{1 + 4(D\lambda, D\lambda)})|a\rangle\langle a|. \tag{4.7}$$

ad a) By (4.4) $e^{-\tilde{A}t}$ is a strongly continuous semigroup. The domain $D(\tilde{A})$ consists of pairs (c, ψ) with $c \in C$ and ψ absolutely continuous in the radial direction, $\psi(0) = 0$, and $D\psi \in L^2(R^\nu)$. By [13, Lemma 1.5] $\tilde{A}$ on $D(\tilde{A})$ is closed. H is densely defined and closable since $\lambda \in L^2(R^\nu)$ and $D(H)$ consists of ordered pairs (c, ψ) with $c \in C$ and functions $\psi \in L^2(R^\nu)$ with $||\omega\psi||^2 = \int d^\nu k \omega^2 |\psi|^2 < \infty$. $D(\tilde{A}) \cap D(H)$ is a core for H.
ad b) Let $U(t) = \exp(-\tilde{A}t)$ and $V(t) = \exp(-Dt)$. $U(t), U^*(t)$ leave the form domain $Q(H)$ invariant, since by (4.4)

$$(V(t)\psi, \omega V(t)\psi) = \int d^\nu k (\omega(|k|) + t)|\psi(k)|^2 = (\psi, \omega\psi) + t(\psi, \psi). \tag{4.8}$$

Similarly for the operator domain $D(H)$ we use

$$||\omega V(t)\psi||^2 = \int d^\nu k (\omega(|k|) + t)^2 |\psi(k)|^2 = ||\omega\psi||^2 + 2t(\psi, \omega\psi) + t^2(\psi, \psi). \tag{4.9}$$

ad c) Since $D\lambda \in L^2(R^\nu)$, the self-adjoint operator $[\tilde{A}, H]^0$ is bounded.
ad d) The second commutator equals, as a quadratic form,

$$[\tilde{A}, [\tilde{A}, H]] = \begin{pmatrix} 0 & (D^2\lambda, \cdot) \\ D^2\lambda & 0 \end{pmatrix}, \tag{4.10}$$

hence is bounded with norm $||D^2\lambda||$, closable, and has self-adjoint closure. (This is the only instance where we invoke $D^2\lambda \in L^2(R^\nu)$.)
ad e) We can satisfy (3.29) with $\alpha = 1$ and C of (4.7), yielding a strong Mourre estimate.

¿From Lemma 10 we can conclude that $\dim P_{pp} \leq (1 + \sqrt{1 + 4(D\lambda, D\lambda)})/2$, which is a poor estimate in several respects. One knows that $\dim P_{pp} \leq 1$ always and $\dim P_{pp} = 0$ precisely if $\mu - \omega(0) \geq \int d^\nu k |\lambda(k)|^2/(\omega(k) - \omega(0))$ [14]. To capture some of these features, we improve $\tilde{A}$ by off-diagonal elements as

$$\tilde{A}_1 = \begin{pmatrix} 0 & (f, \cdot) \\ -f & D \end{pmatrix}, \qquad f \in D(\omega). \tag{4.11}$$

Then, with the shorthand $g = D\lambda + \omega_1 f, \omega_1 = \omega - \mu$,

$$\begin{aligned} [\tilde{A}_1, H] &= \begin{pmatrix} (\lambda, f) + (f, \lambda) & (g, \cdot) \\ g & 1 - f(\lambda, \cdot) - \lambda(f, \cdot) \end{pmatrix} \\ &\geq \begin{pmatrix} (\lambda, f) + (f, \lambda) & (g, \cdot) \\ g & 1 - ||\lambda||\,||f|| - |(\lambda, f)| \end{pmatrix}. \end{aligned} \tag{4.12}$$

Absence of eigenvalues is implied by $[\tilde{A}_1, H] > 0$, i.e. by

$$(\lambda, f) + (f, \lambda) > 0 \quad \text{and} \quad ((\lambda, f) + (f, \lambda))(1 - ||\lambda||\,||f|| - |(\lambda, f)|) - (g, g) > 0. \qquad (4.13)$$

For sufficiently small coupling (4.13) can be satisfied by a suitable choice of f, which we take as

$$f_\epsilon = \frac{1}{(\omega - \mu)^2 + \epsilon}(\lambda - (\omega - \mu)D\lambda). \qquad (4.14)$$

Since similar variational problems will reappear in Section 5, we skip a more explicit discussion here. However, we still have to verify a) to e) of Definition 4 for the improved $\tilde{A}_1$. $\tilde{A}_1$ is a bounded perturbation of $\tilde{A}$ by the term

$$\tilde{A}_1 - \tilde{A} = \begin{pmatrix} 0 & (f_\epsilon, \cdot) \\ -f_\epsilon & 0 \end{pmatrix} \qquad (4.15)$$

with the norm $||f_\epsilon|| < \infty$. Hence by [13, Theorem 3.1] $\tilde{A}_1$ is the generator of a one-parameter semigroup with the same domain as $\tilde{A}$. $\tilde{A}_1 - \tilde{A}$ generates a unitary group. It follows then from the Trotter product formula [13, Theorem 3.30] that $\tilde{A}_1$ generates an isometry semigroup. Thereby we prove a). $\tilde{A}$ is a semigroup generator on the Hilbert space $C \oplus D(\omega)$, because of (4.9). On this Hilbert space the perturbation $\tilde{A}_1 - \tilde{A}$ is bounded, since $\omega f_\epsilon \in L^2(R^\nu)$. Thus we can again apply [13, Theorem 3.1] to prove b). c) holds because $[\tilde{A}_1, H]$ differs from $[\tilde{A}, H]$ by bounded terms only. $[\tilde{A}_1, [\tilde{A}_1, H]]$ has in addition to $[\tilde{A}, [\tilde{A}, H]]$ terms which depend linearly on $D\lambda, Df_\epsilon, Dg_\epsilon$ and are explicitly given by

$$\begin{aligned} Df_\epsilon &= [D, \frac{1}{(\omega - \mu)^2 + \epsilon}](\lambda - (\omega - \mu)D\lambda) + \frac{1}{(\omega - \mu)^2 + \epsilon}(D\lambda - D(\omega - \mu)D\lambda) \\ &= -\frac{2(\omega - \mu)}{((\omega - \mu)^2 + \epsilon)^2}(\lambda - (\omega - \mu)D\lambda) - \frac{1}{(\omega - \mu)^2 + \epsilon}(\omega - \mu)D^2\lambda \end{aligned} \qquad (4.16)$$

and

$$Dg_\epsilon = D^2\lambda + D(\omega - \mu)f_\epsilon = D^2\lambda + f_\epsilon + (\omega - \mu)Df_\epsilon.$$

To show d), we observe that $D\lambda, Df_\epsilon, Dg_\epsilon$ are in $L^2(R^\nu)$. Hence $[\tilde{A}, [\tilde{A}, H]]$ is bounded, closable and has a self-adjoint closure. (4.12), (4.13) are then a strong Mourre estimate in the form (3.29) with $C = 0$ and α equal to the minimum of the two numbers in (4.13), which proves e).

5. Mourre estimate for the spin-boson Hamiltonian

Motivated by the Friedrichs model, we choose for $\tilde{A}$ the second quantization of D on the one boson momentum space $L^2(R^\nu, d^\nu k)$,

$$\tilde{A} = I \otimes d\Gamma(D) \qquad \text{on } C^n \otimes \mathcal{F}. \qquad (5.1)$$

It is well known that the second quantization of bounded operators acts as a functor which respects the commutator (Lie algebra) structure,

$$[d\Gamma(F), d\Gamma(G)] = d\Gamma([F, G]).$$

We define the creation operators to be linear in the test function, $a^*(f) = \int d^\nu k f(k) a^*(k)$. The annihilation operator is the adjoint of the creation operator, $a(f) = (a^*(f))^*$, and consequently semilinear. For the commutators of $d\Gamma(G)$ with a creation, resp. an annihilation operator we have in the strong sense on dense subspaces

$$[d\Gamma(G), a^*(f)] = a^*(Gf) \qquad \text{and} \qquad [d\Gamma(G), a(f)] = -a(G^*f).$$

With these preliminaries, we are ready for the

Proof of Theorem 3. (i) First we consider the case $\omega(0) > 0$. We compute the formal commutator of $\tilde{A}$ with the Hamiltonian H of (2.11). Let $T = \exp[K \otimes a^*(D\lambda) - K^* \otimes a(D\lambda)]$. Then T is unitary and because $[K, K^*] = 0$ by assumption, $TI \otimes a^*(D\lambda)T^* = I \otimes a^*(D\lambda) - K^* \otimes (D\lambda, D\lambda)I$ and $TK \otimes IT^* = K \otimes I$. We have the lower bound

$$\begin{aligned}
[\tilde{A}, H] &= I \otimes N_B + K \otimes a^*(D\lambda) + K^* \otimes a(D\lambda) \\
T[\tilde{A}, H]T^* &= I \otimes N_B - K^*K \otimes (D\lambda, D\lambda)I \\
&\geq I \otimes I - I \otimes |vac\rangle\langle vac| - (D\lambda, D\lambda)K^*K \otimes I \\
&\geq (1 - (D\lambda, D\lambda)||K||^2)I \otimes I - I \otimes |vac\rangle\langle vac|.
\end{aligned} \tag{5.2}$$

For $(D\lambda, D\lambda)||K||^2 < 1$, this is a strong Mourre estimate with $\alpha = 1 - (D\lambda, D\lambda)||K||^2$ and $TCT^* = I \otimes |vac\rangle\langle vac|$. We apply now Lemma 10 which yields

$$\dim P_{pp} \leq n(1 - (D\lambda, D\lambda)||K||^2)^{-1}. \tag{5.3}$$

We have to show the validity of conditions a)-d). The smooth functions with bounded N_B which have compact support on momentum space and vanish at $k = 0$ are in $D(\tilde{A}) \cap D(H)$, dense in $C^n \otimes \mathcal{F}$, and invariant under the semigroup $U(t)$. They build a core $\mathcal{S}$ of H. We apply Proposition 6, thereby justifying the formal computation of the commutator. In the sense of quadratic forms, we have on $Q(H_B)$

$$\omega(0)N_B \leq H_B.$$

Since N_B, H_B commute, we can take the square on $D(H_B)$, showing that N_B is H_B-bounded. The first commutator $[\tilde{A}, H]$ differs from $I \otimes N_B$ by a perturbation of relative $I \otimes N_B$-bound 0, hence H-bound 0. This and evaluating the second commutator in the sense of forms,

$$[\tilde{A}, [\tilde{A}, H]] = K \otimes a^*(D^2\lambda) + K^* \otimes a(D^2\lambda), \tag{5.4}$$

prove c) and d). For condition b), we compute on the form domain $Q(H_B) \subset Q(N_B) \subset \mathcal{F}$,

$$\begin{aligned}
\langle \Gamma(V(t))\psi | H_B \Gamma(V(t))\psi \rangle =& \langle \Gamma(V(t))\psi | d\Gamma(\omega)\Gamma(V(t))\psi \rangle = \langle \psi | d\Gamma(\omega + t)\psi \rangle \\
=& \langle \psi | H_B \psi \rangle + t\langle \psi | N_B \psi \rangle,
\end{aligned} \tag{5.5}$$

compare with (4.8), and on operator domains,

$$||H_B\Gamma(V(t))\psi||^2 = ||d\Gamma(\omega + t)\psi||^2 = ||H_B\psi||^2 + 2t\langle N_B\psi | H_B\psi \rangle + t^2||N_B\psi||^2, \tag{5.6}$$

compare with (4.9). (By a similar binomial expansion, it is easily seen that $\Gamma(V(t))$ leaves invariant every element $\mathcal{H}_l = D(H_B^{l/2})$ of the usual scale of Hilbert spaces and acts on them as a strongly continuous semigroup.)

(ii) We consider the compression $P_{\leq N} H P_{\leq N}$ of H with $P_{\leq N} = P(N_B \leq N)$. As conjugate operator we use

$$\tilde{A} = I \otimes P_{\leq N} d\Gamma(D) P_{\leq N}. \tag{5.7}$$

Then

$$[\tilde{A}, P_{\leq N} H P_{\leq N}] = P_{\leq N}[\tilde{A}, H] P_{\leq N}. \tag{5.8}$$

By the Courant min-max principle, the spectrum of an operator cannot decrease during compression on a subspace. Hence the computational part of the proof follows from (i). The commutator and the double commutator are bounded once compressed to $P_{\leq N} C^n \otimes \mathcal{F}$, which shows c) and d). The image $P_{\leq N}\mathcal{S}$ of the core $\mathcal{S}$ from Part (i) provides an appropriate core, yielding a). b) follows because of (5.6) and $[\Gamma(V(t)), P_{\leq N}] = 0$. □

Remark. Since the bound (5.3) does not depend on $\omega(0)$, it is tempting to extend the reasoning in (i) to the case $\omega(0) = 0$. Unfortunately, then the conditions b),c) cannot be justified anymore. N_B is not H_B-bounded and the semigroups $\Gamma(V(t))$ and $U(t)$ lead vectors in $D(H_B)$ with many infrared bosons out of $D(H_B)$. In fact for our application it would suffice to know that any eigenvector of H is in $D(N_B)$, which can be seen as follows. $U(t)$ commutes with $I \otimes N_B$ and, from (5.6), $U(t)$ acts strongly continuous on $C^n \otimes D(N_B) \cap C^n \otimes D(H_B)$. Hence on such states holds s-lim$(H+i)\lambda(\tilde{A}+\lambda)^{-1} = (H+i)$. Every line in (3.26) and (3.27) makes sense and strong convergence of $(I \otimes N_B)(\tilde{A}+\lambda)^{-1}$ is trivial because of $[U(t), I \otimes N_B] = 0$.

Let us return to the standard spin boson model with $S = \mu\sigma_z/2$ and $K = \sigma_x$. We first observe that the "particle" number $(1+\sigma_z)/2 \otimes I + I \otimes N_B$ can change only in steps of two units. This means that the parity, P, of the particle number is conserved,

$$P = \sigma_z \otimes (-1)^{N_B} \qquad \text{and} \qquad [P, H] = 0. \tag{5.9}$$

Let $P_\pm$ be the two eigenprojections of P, $P = P_+ - P_-$. We apply the canonical transformation

$$U = \exp(i\pi \frac{1-\sigma_x}{2} \otimes N_B) = U^* = U^{-1} \tag{5.10}$$

to P, H and obtain

$$\begin{aligned} &U\sigma_z \otimes (-1)^{N_B} U = \sigma_z, \\ &\qquad UHU = \frac{\mu}{2}\sigma_z \otimes (-1)^{N_B} + I \otimes H_B + I \otimes (a^*(\lambda) + a(\lambda)). \end{aligned} \tag{5.11}$$

Therefore $P_\pm H$ on $P_\pm \mathcal{H}$ is unitarily equivalent to

$$H_{+,-} = \mp\frac{\mu}{2}(-1)^{N_B} + \int dk\omega(k) a^*(k) a(k) + a^*(\lambda) + a(\lambda) \tag{5.12}$$

on $\mathcal{F}$.

Corollary 11. *Let Assumptions A1-A3 hold, $\mu, \omega(0) > 0$, and $(D\lambda, D\lambda) < \frac{1}{2}$. Then H_+ has a unique ground state and the rest of the spectrum is purely absolutely continuous.*

Proof. The ground state properties follow from [2]. The remainder is an immediate consequence of the proof of Theorem 3, Part i). The commutator to be considered is now

$$\begin{aligned} [\tilde{A}, H_+] &= N_B + a^*(D\lambda) + a(D\lambda) \\ T[\tilde{A}, H_+]T^* &= N_B - (D\lambda, D\lambda)I \geq (1 - (D\lambda, D\lambda))I - |vac\rangle\langle vac|, \end{aligned} \tag{5.13}$$

with $T = \exp[a^*(D\lambda) - a(D\lambda)]$, yielding a strong Mourre estimate for $(D\lambda, D\lambda) < 1$. We bound the number of eigenvalues using Lemma 10. □

A comment is in order concerning the commutator $[\tilde{A}, N_B]$ which is used in $[\tilde{A}, (-1)^{N_B}]$ and comes up again when considering the double commutator $[\tilde{A}, [\tilde{A}, H]]$. Let us always take $t \geq 0$. On the one-particle space $(e^{-Dt})^* e^{-Dt} = 1$, but $e^{-Dt}(e^{-Dt})^* \neq 1$ because the flow T_{-t} is absorbing at $k = 0$, compare with (4.3), (4.4). This property is also reflected by D having different defect indices, which implies that D has no self-adjoint extensions. On Fock space the semigroups $U(t) = e^{-\tilde{A}t}$ and $U^*(t)$ leave the subspaces with fixed boson number invariant but, by lifting from the one-particle space, we have $U(t)^* N_B U(t) = N_B$ whereas $U(t) N_B U(t)^* \neq N_B$. The formal commutator is $[\tilde{A}, N_B] = 0$ in both cases and the difference between outward and inward flow in k-space is hidden in domains. It is of crucial importance to use always the outward shift.

Corollary 12. *Let Assumptions A1-A3 hold, $\mu > 0$ and $(D\lambda, D\lambda) < \frac{1}{2}$. Then $P_{\leq N} H_+ P_{\leq N}$ has purely absolutely continuous spectrum apart from the unique ground state.*

Proof. The proof of Theorem 3, Part ii) extends straightforwardly to the present case. □

The P_- sector is more difficult if one aims for the best possible result, namely purely absolutely continuous spectrum. Guided by the Friedrichs model, we improve the conjugate operator to

$$\tilde{A} = d\Gamma(D) + a(f) - a^*(f). \tag{5.14}$$

Here $f \in D(\omega)$ and we will optimize f at the end. Of course the commutator is now more complicated,

$$\begin{aligned} [\tilde{A}, H_-] = N_B &+ a(D\lambda + (\omega - \mu)f) + a^*(D\lambda + (\omega - \mu)f) \\ &+ (\lambda, f) + (f, \lambda) + (1 - (-1)^{N_B}) a(\mu f) + a^*(\mu f)(1 - (-1)^{N_B}). \end{aligned} \tag{5.15}$$

In this expression, we have subtracted $a(\mu f)$, resp. $a^*(\mu f)$, in the first line and added it in the second line, so as to achieve an appearance similar to (4.12) - once more the Friedrichs model serves as a source of inspiration. We would like to choose f such that the commutator (5.15) becomes positive. The strategy is to divide $[\tilde{A}, H]$ in two parts and work them out separately. More precisely, we divide the boson number into two positive summands $(1 - r)N_B$ and rN_B with $r \in (0, 1)$. Let us first state

Proposition 13. *Let Assumptions A1-A3 hold, and let $\mu, \omega(0) > 0$. There exists a coupling constant α_0 depending on μ and λ such that for $0 < \alpha < \alpha_0$ the spectrum of H_- is purely absolutely continuous.*

Proof. We discuss first the term

$$C_1 := (1-r)N_B + (\lambda, f) + (f, \lambda) + a(D\lambda + (\omega-\mu)f) + a^*(D\lambda + (\omega-\mu)f). \tag{5.16}$$

Shifting the mode $D\lambda + (\omega - \mu)f$ shows that in the sense of quadratic forms

$$C_1 \geq [(\lambda, f) + (f, \lambda) - \frac{1}{1-r}(D\lambda + (\omega-\mu)f, D\lambda + (\omega-\mu)f)]I. \tag{5.17}$$

We have to search for the supremum of the square bracket over $f \in L^2(R^\nu)$. If the function f makes the expression (5.17) positive, then so does αf for the coupling function $\alpha\lambda$. In this sense, our optimization problem is homogeneous and independent of a linear coupling constant. Formal maximization in (5.17) leads to

$$f = \frac{1}{(\omega-\mu)^2}(1-r)\lambda - (\omega-\mu)D\lambda, \tag{5.18}$$

which is highly singular in the vicinity of μ. We regularize f by taking instead

$$f_\epsilon = \frac{1}{(\omega-\mu)^2+\epsilon}(\lambda - (\omega-\mu)D\lambda), \qquad \epsilon > 0, \tag{5.19}$$

as we did already in (4.14) above. We define $\omega_1 = \omega - \mu$ and

$$g_\epsilon = D\lambda + \omega_1 f_\epsilon = \frac{1}{\omega_1^2+\epsilon}(\omega_1\lambda + \epsilon D\lambda). \tag{5.20}$$

With this choice we compute

$$\begin{aligned}(\lambda, f_\epsilon) + (f_\epsilon, \lambda) &= 2(\lambda, \frac{1}{\omega_1^2+\epsilon}\lambda) - (\lambda, \frac{\omega_1}{\omega_1^2+\epsilon}D\lambda) - (\frac{\omega_1}{\omega_1^2+\epsilon}D\lambda, \lambda) \\ &= 2(\lambda, \frac{1}{\omega_1^2+\epsilon}\lambda) - (\lambda, \frac{\omega_1}{\omega_1^2+\epsilon}D\lambda) + (\lambda, D\frac{\omega_1}{\omega_1^2+\epsilon}\lambda) \\ &= 2(\lambda, \frac{1}{\omega_1^2+\epsilon}\lambda) + (\lambda, [D, \frac{\omega_1}{\omega_1^2+\epsilon}]\lambda) \\ &= \int d^\nu k \frac{(\omega_1^2+3\epsilon)}{(\omega_1^2+\epsilon)^2}|\lambda|^2\end{aligned} \tag{5.21}$$

and

$$\begin{aligned}(g_\epsilon, g_\epsilon) &= (\frac{\omega_1}{\omega_1^2+\epsilon}\lambda, \frac{\omega_1}{\omega_1^2+\epsilon}\lambda) - \epsilon(\lambda, [D, \frac{\omega_1}{(\omega_1^2+\epsilon)^2}]\lambda) + \epsilon^2(\frac{1}{\omega_1^2+\epsilon}D\lambda, \frac{1}{\omega_1^2+\epsilon}D\lambda) \\ &= \int d^\nu k \left(\frac{\omega_1^2}{(\omega_1^2+\epsilon)^2} + \frac{3\epsilon\omega_1^2 - \epsilon^2}{(\omega_1^2+\epsilon)^3}\right)|\lambda|^2 + \epsilon^2 \int d^\nu k \frac{|D\lambda|^2}{(\omega_1^2+\epsilon)^2}.\end{aligned} \tag{5.22}$$

Their difference equals

$$(\lambda, f_\epsilon) + (f_\epsilon, \lambda) - (g_\epsilon, g_\epsilon) = 4\epsilon^2 \int d^\nu k \frac{|\lambda|^2}{(\omega_1^2 + \epsilon)^3} - \epsilon^2 \int d^\nu k \frac{|D\lambda|^2}{(\omega_1^2 + \epsilon)^2}. \tag{5.23}$$

By rescaling the integrands, we see that the first summand behaves as $\epsilon^2 \epsilon^{-5/2} = \epsilon^{-1/2}$ since $\int d^\nu k |\lambda|^2 \delta(\omega(k) - \mu) > 0$ by Assumption A2. The second summand behaves as $\epsilon^2 \epsilon^{-3/2} = \epsilon^{1/2}$ if $(D\lambda)(k) \neq 0$ on the level set $\{ k \in R^\nu \mid \omega(k) = \mu \}$ and is even smaller if $(D\lambda)(k)$ vanishes on that set. Thus we can make the difference positive by choosing ϵ sufficiently small. Therefore also $(1 - r)((\lambda, f_\epsilon) + (f_\epsilon, \lambda)) - (g_\epsilon, g_\epsilon) > 0$ provided r is sufficiently small.

We turn to the remainder term

$$C_2 := r N_B + (1 - (-1)^{N_B}) a(\mu f_\epsilon) + a^*(\mu f_\epsilon)(1 - (-1)^{N_B}) \tag{5.24}$$

in (5.15). Since

$$[\beta^{-1/2} a^*(\mu f_\epsilon) + \beta^{1/2}(1 - (-1)^{N_B})][\beta^{-1/2} a(\mu f_\epsilon) + \beta^{1/2}(1 - (-1)^{N_B})] \geq 0, \tag{5.25}$$

we have the lower bound

$$\begin{aligned} C_2 \geq & r N_B - \beta^{-1} a^*(\mu f_\epsilon) a(\mu f_\epsilon) - \beta(1 - (-1)^{N_B})^2 \\ \geq & (r - 4\beta) N_B - \beta^{-1} a^*(\mu f_\epsilon) a(\mu f_\epsilon) \end{aligned} \tag{5.26}$$

which is positive provided $r - 4\beta \geq \beta^{-1} \mu^2 (f_\epsilon, f_\epsilon)$. Optimizing with respect to β yields the condition

$$4\mu ||f_\epsilon|| \leq r. \tag{5.27}$$

(A more detailed analysis shows that $C_2 > 0$ is equivalent to $2\mu||f_\epsilon|| \leq r$.)

For given μ and coupling function $\alpha\lambda$ the positivity of $[\tilde{A}, H_-]$ is thus ensured by first choosing ϵ sufficiently small to make (5.23) positive, then choosing $0 < r < 1$ such that C_1 in (5.17) stays positive and finally choosing the coupling constant α small enough for $(f_\epsilon, f_\epsilon) \sim \alpha^2$ to satisfy (5.27).

We still have to verify the technical conditions of Definition 4. c) and d) are fulfilled by considerations completely analogous to those at the end of Section 4, since the double commutator is bounded as before. The operator $\tilde{A}$ of (5.14) is a semigroup generator. This be can seen by giving explicitly the action of the corresponding semigroup on the set of coherent states $\exp(a^*(h) - a(h))|vac\rangle, h \in L^2(R^\nu)$, which is a dense subset of $\mathcal{F}$. Indeed, the ansatz

$$U(t) \exp[a^*(h) - a(h)]|vac\rangle = \exp[a^*(h_t) - a(h_t)]|vac\rangle = |v(t)\rangle, \qquad t \geq 0 \tag{5.28}$$

solves formally

$$\frac{d}{dt}|v(t)\rangle = -\tilde{A}|v(t)\rangle, \qquad t \geq 0, \tag{5.29}$$

provided the single particle wave function h_t solves

$$\frac{dh_t}{dt} = -Dh_t + f, \qquad h_0 = h, \qquad t \geq 0. \tag{5.30}$$

For $h \in D(D)$ and with $V(t) = \exp(-Dt)$, Equation (5.30) has the explicit solution

$$h_t = V(t)h + \int_0^t V(t-\tau) f d\tau, \qquad t \geq 0. \tag{5.31}$$

The coherent shift operators $\exp[a^*(h) - a(h)]$ depend strongly continuously on the single particle function h and are unitary. Therefore $U(t)$ of (5.28) acts on the coherent states as a strongly continuous, isometric operator function on $\{t \geq 0\}$. By continuity, it can be extended to $\mathcal{F}$, preserving the semigroup property and isometry. The coherent states with $h \in D(D) \cap D(\omega)$ form a core for H, which shows a). b) follows by similar reasoning for coherent states in $D(H) = D(d\Gamma(\omega))$, since $h, f \in D(\omega)$, (4.9), and (5.31) imply $h_t \in D(\omega)$. $\square$

Proposition 14. *Let Assumptions A1-A3 hold. There is a coupling constant* α_0 *depending on* $\mu > 0$ *and* λ*, but not on* N*, such that for* $0 < \alpha < \alpha_0$ *the compression* $P_{\leq N} H_- P_{\leq N}$ *has purely absolutely continuous spectrum.*

Proof. As a conjugate operator, we use the compression of the conjugate operator in (5.14), i.e.

$$\tilde{A} = P_{\leq N}\{d\Gamma(D) + a(f) - a^*(f)\}P_{\leq N}. \tag{5.32}$$

The commutator equals, with $P_N = P(N_B = N)$,

$$\begin{aligned}[\tilde{A}, H] =& [P_{\leq N}\{d\Gamma(D) + a(f) - a^*(f)\}P_{\leq N}, P_{\leq N} H_- P_{\leq N}] \\ =& P_{\leq N}\{N_B + a(D\lambda + \omega f) + a^*(D\lambda + \omega f) - (-1)^{N_B} a(\mu f) - a^*(\mu f)(-1)^{N_B}\}P_{\leq N} \\ &+ \{(\lambda, f) + (f, \lambda)\}P_{\leq N-1} - \{a^*(\lambda)a(f) + a^*(f)a(\lambda)\}P_N.\end{aligned} \tag{5.33}$$

As in the proof of Proposition 13, we divide the commutator in two parts,

$$\begin{aligned} C_1 =& P_{\leq N}\{(1-r)N_B + a(D\lambda + (\omega - \mu)f) + a^*(D\lambda + (\omega - \mu)f) \\ &+ (\lambda, f) + (f, \lambda)\}P_{\leq N} \\ C_2 =& P_{\leq N}\{rN_B + (1 - (-1)^{N_B})a(\mu f) + a^*(\mu f)(1 - (-1)^{N_B})\}P_{\leq N} \\ &- \{(\lambda, f) + (f, \lambda) + a^*(\lambda)a(f) + a^*(f)a(\lambda)\}P_N.\end{aligned} \tag{5.34}$$

C_1 is the compression to a subspace of an operator which can be made positive definite by the appropriate f_ϵ. We refer to the proof of Proposition 13. For C_2 we use (5.26) with $\beta = \mu||f_\epsilon||/2$ and $||(a^*(\lambda)a(f) + a^*(f)a(\lambda))P_N|| \leq 2N||\lambda||\,||f||P_N$. Then

$$C_2 \geq [(r - 2\mu||f_\epsilon||)N_B - 2(\mu||f_\epsilon||)^{-1}a^*(\mu f_\epsilon)a(\mu f_\epsilon)]P_{\leq N} - 2(N+1)||\lambda||\,||f_\epsilon||P_N. \tag{5.35}$$

The lower bound is positive provided (5.27) holds and

$$2(1 + \frac{1}{N})||\lambda||\,||f_\epsilon|| \leq r - 4\mu||f_\epsilon||. \tag{5.36}$$

(5.36) can be easily fulfilled by choosing α sufficiently small. This proves the announced uniformity in the boson number cutoff.

Again we have to check the technical conditions of Definition 4. Since $P_{\leq N}N_B$ is bounded our arguments are analogous to those at the end of Section 4. $P_{\leq N}\{a(f_\epsilon) - a^*(f_\epsilon)\}P_{\leq N}$ has a norm bounded by $\leq 2\sqrt{N}||f_\epsilon||$. Therefore $\tilde{A}$ is a bounded perturbation of $P_{\leq N}d\Gamma(D)P_{\leq N}$ and we can again apply [13, Theorem 3.1]. By the Trotter product formula [13, Theorem 3.30] the semigroup generated by $\tilde{A}$ is indeed isometric. $P_{\leq N}\mathcal{S}$, with $\mathcal{S}$ defined below (5.3), is a core for $P_{\leq N}H_{-}P_{\leq N}$. b) follows now from (5.6), $\omega f \in L^2(R^\nu)$, and [13, Theorem 3.1]. $[\tilde{A}, H]$ is bounded and $[\tilde{A}, [\tilde{A}, H]]$ depends only on scalar products and on creation and annihilation operators in the modes $D\lambda, D^2\lambda, Df_\epsilon, Dg_\epsilon$ which are all bounded because of compression and Equation (4.16). This proves conditions c) and d) from Definition 4. $\square$

Proof of Theorem 1. The assertion follows from Corollary 11 and Proposition 13. $\square$

Proof of Theorem 2. The assertion follows from Corollary 12 and Proposition 14. $\square$

6. Rotating wave approximation

We introduce the spin raising and lowering operators by $\sigma^{\pm} = (\sigma_x \pm i\sigma_y)/2$. Then the interaction term for the spin-boson Hamiltonian reads $(\sigma^+ + \sigma^-) \otimes (a^*(\lambda) + a(\lambda))$. A standard approximation in quantum optics is to ignore the anti-resonant terms $\sigma^+ \otimes a^*, \sigma^- \otimes a$. If the effective frequency distribution $\rho(\omega) = \int d^\nu k |\lambda(k)|^2 \delta(\omega(k) - \omega)$ is sharply peaked at μ then the resonant terms $\sigma^- \otimes a^*, \sigma^+ \otimes a$ dominate the interaction. In this rotating wave approximation the spin-boson Hamiltonian is given by

$$H = \mu \frac{1+\sigma_z}{2} \otimes I + I \otimes \int d^\nu k \omega(k) a^*(k) a(k) + \sigma^- \otimes a^*(\lambda) + \sigma^+ \otimes a(\lambda). \tag{6.1}$$

To our knowledge, the spectral properties of H have not been determined so far, although the analogous Hamiltonian with *one* boson mode (Jaynes-Cummings Hamiltonian) was studied thoroughly.

H admits an additional conservation law as

$$N_P := \frac{1+\sigma_z}{2} + \int d^\nu k a^*(k) a(k) = \frac{1+\sigma_z}{2} + N_B. \tag{6.2}$$

We have $[H, N_P] = 0$ and N_P has the spectral representation $N_P = \sum_{l=0}^{\infty} l P_l$. We can then study $H_l = P_l H P_l$ as the restriction of H to the subspace $P_l(C^2 \otimes \mathcal{F})$. The subspace $P_0\mathcal{H}$ is one-dimensional and consists of the ground state vector $|\downarrow\rangle \otimes |vac\rangle$ with energy 0, where $|\uparrow\rangle, |\downarrow\rangle$ denote the eigenstates of σ_z. Note that, in contrast to the full spin-boson model, there is no vacuum polarization.

H_1 is isomorphic to the Friedrichs model. Thus if

$$\mu - \omega(0) > \int d^\nu k \lambda^2 / (\omega - \omega(0)), \tag{6.3}$$

the $l = 1$ sector has purely absolutely continuous spectrum. One would expect then that also in higher sectors there are no eigenvectors and that the continuum edge in the l-th sector is precisely $l\omega(0)$.

Theorem 15. *Let Assumptions A1-A3 hold. If $(D\lambda, D\lambda) < 1$, then H_l has purely absolutely continuous spectrum for every $l \geq 2$.*

Proof. It is easy to compute formally the commutator, with $\tilde{A} = I \otimes d\Gamma(D)$,

$$[\tilde{A}, H] = I \otimes N_B + \sigma^- \otimes a^*(D\lambda) + \sigma^+ \otimes a(D\lambda). \tag{6.4}$$

Since $\tilde{A}$ commutes with the particle number N_P, so does $[\tilde{A}, H]$. $[\tilde{A}, H]$ is bounded on every sector and can be represented as a matrix on the direct sum $|\uparrow\rangle \otimes P_{l-1}\mathcal{F} \oplus |\downarrow\rangle \otimes P_l\mathcal{F}$,

$$[\tilde{A}, H] = \begin{pmatrix} l-1 & a(D\lambda) \\ a^*(D\lambda) & l \end{pmatrix}. \tag{6.5}$$

This is a strong Mourre estimate with $C = 0$ provided

$$(D\lambda, D\lambda) < l - 1. \tag{6.6}$$

The technical conditions are verified as in Section 5. $\square$

The l-th sector contains approximate eigenstates, in which the spin is down (in the state $|\downarrow\rangle$) and l bosons with momenta $k_1, \ldots, k_l$ are far away from the spin in ν-dimensional configuration space. In approximation such states have the energy $\omega(k_1)+\cdots+\omega(k_l)$. Since there are no bound states, we expect that the spectrum of H_l equals the range of the boson kinetic energy. This guess is made precise in the next proposition.

Proposition 16. *Let $E_l = \inf \sigma(H_l)$. If the inequality (6.3) holds, then $\sigma(H_l) = [E_l, \infty)$ with $E_l = l\omega(0)$ for $l \geq 1$.*

Proof. First we show $E_l \geq l\omega(0)$ by contradiction. Let us assume that there exists an $E \in \sigma(H_l)$ with $E < l\omega(0)$. We consider the approximate eigenvalue equation in the sector $l \geq 1$ for a unit vector $v \in P(H_l < l\omega(0) - \epsilon)$ with components $|\uparrow\rangle \otimes |f_{l-1}\rangle$, $|\downarrow\rangle \otimes |g_l\rangle$

$$||(H-E)v|| = ||(H-E)(|\uparrow\rangle \otimes |f_{l-1}\rangle + |\downarrow\rangle \otimes |g_l\rangle)|| = o(1), \quad E < l\omega(0) - \epsilon < l\omega(0). \tag{6.7}$$

where $o(1)$ is a nonnegative error which can be made arbitrarily small by an appropriate choice of v (and would vanish for v an eigenvector). Equating the components with $l-1$, resp. l, bosons leads to

$$\begin{aligned} (E - \mu - H_{B,l-1})|f_{l-1}\rangle &= a(\lambda)|g_l\rangle + o(1) \\ a^*(\lambda)|f_{l-1}\rangle &= (E - H_{B,l})|g_l\rangle + o(1). \end{aligned} \tag{6.8}$$

Eliminating $|g_l\rangle$ and bracketing with $\langle f_{l-1}|$ gives

$$\begin{aligned} \langle f_{l-1}|a(\lambda)(H_{B,l} - E)^{-1}a^*(\lambda)|f_{l-1}\rangle =& \langle f_{l-1}|(\mu + H_{B,l-1} - E|f_{l-1}\rangle + o(1) \\ &> (\mu - \omega(0))\langle f_{l-1}|f_{l-1}\rangle. \end{aligned} \tag{6.9}$$

Now the inequality (6.3) translates to

$$|\lambda\rangle\langle\lambda| \leq (\mu - \omega(0))(\omega - \omega(0)) \tag{6.10}$$

in first quantization and to

$$a^*(\lambda)a(\lambda) \leq (\mu - \omega(0))(H_B - \omega(0)N_B) \tag{6.11}$$

in second quantization. Restricted to the sector with boson number $N_B = l$, this leads to

$$a^*(\lambda)a(\lambda)|_l \leq (\mu - \omega(0))(H_{B,l} - l\omega(0)) \leq (\mu - \omega(0))(H_{B,l} - E) \tag{6.12}$$

and

$$(H_{B,l} - E)^{-\frac{1}{2}} a^*(\lambda)a(\lambda)|_l (H_{B,l} - E)^{-\frac{1}{2}} \leq \mu - \omega(0). \tag{6.13}$$

Using the property $||A^*A|| = ||AA^*||$ for the bounded operator $a(\lambda)|_l(H_{B,l} - E)^{-\frac{1}{2}}$ implies

$$a(\lambda)(H_{B,l} - E)^{-1} a^*(\lambda) \leq \mu - \omega(0), \tag{6.14}$$

which contradicts the inequality (6.9).

Secondly we have to show that $E_l \leq l\omega(0)$. This will be done by adding a low energy boson to an (approximate) ground state of H_{l-1}.

Our assertion holds for $l = 1$. By induction let us assume that $E_{l-1} = (l-1)\omega(0)$. We have to prove then $E_l \leq l\omega(0)$.

Let $\delta_i(k)$ be positive smooth functions on momentum space with $\int d^\nu k \delta_i = 1$ and $\delta_i(k) \to \delta(k)$ as distributions. The square root $\sqrt{\delta_i}$ defines a square integrable function of norm 1 with $\sqrt{\delta_i} \to 0$ and $\omega\sqrt{\delta_i} \to 0$ weakly. Furthermore, let $(|v_j\rangle)$ be an orthonormal sequence in $Q(H_{l-1})$ with $\langle v_j|H_{l-1}|v_j\rangle \downarrow E_{l-1}$, as $j \to \infty$. By the canonical commutation relations (CCR) and weak convergence, $a(\sqrt{\delta_i})$ and $a^*(\sqrt{\delta_i})$ for large i strongly commute with every $a(f), a^*(f)$ on the dense set of vectors with finite boson number. Now $(a^*(\sqrt{\delta_i})|v_j\rangle)$ is in the l-th sector, asymptotically orthonormal as a sequence in i for fixed j, and

$$\langle v_j|a(\sqrt{\delta_i})a^*(\sqrt{\delta_i})|v_j\rangle \to \langle v_j|v_j\rangle \tag{6.15}$$

as $i \to \infty$. By CCR we have, again in the strong sense on a dense subset of Fock space,

$$\begin{aligned} a(\sqrt{\delta_i})H_B a^*(\sqrt{\delta_i}) &= H_B a(\sqrt{\delta_i})a^*(\sqrt{\delta_i}) + a(\omega\sqrt{\delta_i})a^*(\sqrt{\delta_i}) \\ &= (\sqrt{\delta_i}, \sqrt{\delta_i})H_B + H_B a^*(\sqrt{\delta_i})a(\sqrt{\delta_i}) + (\sqrt{\delta_i}, \omega\sqrt{\delta_i}) + a^*(\sqrt{\delta_i})a(\omega\sqrt{\delta_i}). \end{aligned} \tag{6.16}$$

$a(\sqrt{\delta_i}), a^*(\sqrt{\delta_i})$ commute asymptotically with $a(\lambda)$ and $a^*(\lambda)$. Therefore

$$\langle v_j|a(\sqrt{\delta_i})H_{l-1}a^*(\sqrt{\delta_i})|v_j\rangle \to \langle v_j|H_{l-1}|v_j\rangle + \int d^\nu k \delta_i(k)\omega(k) \tag{6.17}$$

as $i \to \infty$. The integral converges to $\omega(0)$. The expectation value tends to E_{l-1} as $j \to \infty$, by assumption. Finally, to show $\sigma(H_l) = [E_l, +\infty)$, we repeat our argument with $\delta_i(k) \to \delta(k - k_0)$ as distributions for arbitrary $k_0 \in R^\nu$. □

We summarize our findings: For arbitrary coupling strength $\inf \sigma_{ess}(H_l) = E_{l-1} + \omega(0)$. If $(D\lambda, D\lambda) < 1$ and the inequality (6.3) holds, then the ground state is $|\downarrow\rangle \otimes |vac\rangle$ with energy 0. For $l \geq 1$ we have $\sigma(H_l) = \sigma_{ac}(H_l) = [l\omega(0), \infty)$.

Appendix I

Here we prove self-adjointness for general Hamiltonians of the spin-boson type. This was already shown in [18], where the proof is attributed to G.Raggio.

Lemma. *Let* $\omega : R^\nu \to R$ *be measurable with* $\operatorname{ess\,inf} \omega \geq 0$, $\lambda \in L^2(R^\nu)$, $S, K : C^n \to C^n$ *be matrices on the Hilbert space* C^n, *and* $S = S^*$. *Let either* $\operatorname{ess\,inf} \omega > 0$ *or* $\operatorname{ess\,inf} \omega = 0$ *and* $\int |\lambda|^2/\omega < \infty$. *Then the Hamiltonian*

$$H = S \otimes I + I \otimes \int d^\nu k \omega(k) a^*(k) a(k) + K \otimes a^*(\lambda) + K^* \otimes a(\lambda) \tag{A.1}$$

on $C^n \otimes \mathcal{F}$ *is essentially self-adjoint on any core of* $I \otimes H_B$, *self-adjoint on* $I \otimes D(H_B)$, *and bounded from below.*

Proof. If $\operatorname{ess\,inf} \omega > 0$, because C^n is finite dimensional, it is sufficient to show that $a(\lambda), a^*(\lambda)$ have operator bound 0 relative to H_B. With $N_B = d\Gamma(I)$ as before, we start with

$$\begin{aligned} a^*(\lambda) a(\lambda) &\leq (\lambda, \lambda) N_B \\ a(\lambda) a^*(\lambda) &\leq (\lambda, \lambda)(N_B + 1) \end{aligned} \tag{A.2}$$

on the form domain of N_B, which contains the operator domains of $a(\lambda), a^*(\lambda)$. By the Cauchy-Schwarz inequality for every $\epsilon > 0$ on the operator domain

$$||a(\lambda)\phi|| \leq ||\lambda||\, ||N_B \phi||^{1/2} ||\phi||^{1/2} \leq \frac{1}{2} ||\lambda|| (\epsilon ||N_B \phi|| + \epsilon^{-1} ||\phi||), \tag{A.3}$$

which suffices because of $(\operatorname{ess\,inf} \omega) N_B = (\operatorname{ess\,inf} \omega) d\Gamma(I) \leq d\Gamma(\omega) = H_B$ and similarly for $a^*(\lambda)$.

If $\operatorname{ess\,inf} \omega = 0$, then $\omega - c^{-1} |\lambda\rangle\langle\lambda| \geq 0$ as a quadratic form with $c = \int d^\nu k |\lambda(k)|^2/\omega(k)$. By second quantization this inequality reads

$$a^*(\lambda) a(\lambda) \leq c H_B \tag{A.4}$$

and one may proceed as before. □

Appendix II

It is somewhat cumbersome to establish the strictly positive lower bound on the commutator (5.15). An alternative strategy is to choose f such that $(f, g) = 0$ with $g = D\lambda + (\omega - \mu) f$. Then

$$C_1 = (g, g)^{-1} a^*(g) a(g) + (\lambda, f) + (f, \lambda) + a^*(g) + a(g) \geq (\lambda, f) + (f, \lambda) - (g, g) \tag{A.5}$$

and

$$C_2 = N_B - (g, g)^{-1} a^*(g) a(g) + (1 - (-1)^{N_B}) a(\mu f) + a^*(\mu f)(1 - (-1)^{N_B}). \tag{A.6}$$

$C_2 > 0$ provided $4\mu||f|| \leq 1$, cf. (5.27), which is achieved by taking α sufficiently small. To ensure $C_1 > 0$ we choose

$$f = (\mu - \omega)^{-1} \chi_\Lambda(\omega) D\lambda. \tag{A.7}$$

Here χ_Λ is the characteristic function of the closed set $\Lambda \subset R$ and we assume $\mu \notin \Lambda$. Note that $f \in L^2(R^\nu)$ and the bound (A.5) is homogeneous in α. Indeed $(f, g) = 0$. Following the lines in (5.21) we obtain $(\lambda, f) + (f, \lambda) = \int_\Lambda d\omega \rho'(\omega)(\mu - \omega)^{-1}$ with

$$\rho(\omega) = \int d^\nu k |\lambda(k)|^2 \delta(\omega(k) - \omega). \tag{A.8}$$

If $\rho'(\mu) < 0$, then we take $\Lambda = [\mu + \epsilon_1, \mu + \epsilon_2]$ with $0 < \epsilon_1 < \epsilon_2$. From (A.8) we conclude that $(\lambda, f) + (f, \lambda)$ diverges as $\log(\epsilon_2/\epsilon_1)$ and therefore dominates the negative contribution (g, g). Similarly, if $\rho'(\mu) > 0$, we take $\Lambda = [\mu - \epsilon_2, \mu - \epsilon_1]$. If $\rho'(\mu) = 0$, with the choice (A.7) the negative term cannot be compensated in general.

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