

# Regularity of Bound States

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## Abstract

We study regularity of bound states pertaining to embedded eigenvalues of a self-adjoint operator  $H$ , with respect to an auxiliary operator  $A$  that is conjugate to  $H$  in the sense of Mourre. We work within the framework of singular Mourre theory which enables us to deal with confined massless Pauli-Fierz models, our primary example, and many-body AC-Stark Hamiltonians. In the simpler context of regular Mourre theory our results boil down to an improvement of results obtained recently in [Ca, CGH].

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# Contents

<b>1</b>	<b>Introduction</b>	<b>2</b>
1.1	Singular Mourre Theory . . . . .	4
1.2	The Nelson Model . . . . .	7
1.3	The AC–Stark model . . . . .	12
<b>2</b>	<b>Assumptions and Statement of Regularity Results</b>	<b>14</b>
<b>3</b>	<b>Preliminaries</b>	<b>17</b>
3.1	Improved Smoothness for Operators of Class $C^1(A)$ . . . . .	17
3.2	Iterated commutators with $N^{1/2}$ . . . . .	20
3.3	Approximating $A$ by Regular Bounded Operators . . . . .	22
<b>4</b>	<b>Proof of the Abstract Results</b>	<b>25</b>
4.1	Proof of Theorem 2.7 . . . . .	25
4.2	Proof of Theorem 2.10 . . . . .	32
4.3	Theorem on more $N$ –Regularity . . . . .	33
<b>5</b>	<b>A Class of Massless Linearly Coupled Models</b>	<b>37</b>
5.1	The Model and the Result . . . . .	37
5.2	Application to the Nelson Model . . . . .	40
5.3	Expanded Objects . . . . .	42
5.4	Mourre Estimates . . . . .	44
5.5	Checking the Abstract Assumptions . . . . .	50
<b>6</b>	<b>AC–Stark type models</b>	<b>55</b>
6.1	The Model and the Result . . . . .	55
6.2	Regularity of Non-threshold Bound States . . . . .	57
6.3	Regularity of Non-threshold Atomic Type Bound States . . . . .	60

## 1 Introduction

This paper is the first in a series of two dealing with embedded eigenvalues and their bound states. Our arguments in both papers revolve around local positive commutator methods originating from Mourre's seminal paper [Mo]. In fact, some of the central ideas employed in the present paper can be traced back to [FH] by Froese and Herbst, where exponential decay of eigenfunctions for many-body Schrödinger operators were first extracted from a positive commutator estimate. See also [FHH2O] for a precursor pertaining to two-body operators.

In contrast to the above mentioned works we do not here study decay of bound states of a self-adjoint operator  $H$  in position space, but rather decay in the spectral representation for an auxiliary operator  $A$  conjugate to  $H$  in the sense of Mourre. More precisely, given a bound state  $\psi$  of  $H$ , we address the question

**Q( $k$ ):** For a given  $k \in \mathbb{N}$ , under what conditions on the pair of operators  $H$  and  $A$  does it hold true that  $\psi$  is in the domain of  $A^k$ .

It is a question that arises naturally in the context of second order perturbation theory for embedded eigenvalues because together with the Limiting Absorption Principle from [Mo], an affirmative answer allows one to construct and analyze the so called Fermi Golden Rule operator describing level shifts to second order in perturbation theory. In [HuSi] Fermi's golden rule was formulated and verified in an abstract setup under the condition that  $\psi \in \mathcal{D}(A^2)$ , following ideas from [AHS]. See also [BFSS, DJ1, FMS, MS]. For many-body Schrödinger operators the conjugate operator is usually taken to be the generator of dilation and here the condition  $\psi \in \mathcal{D}(A^2)$  is fulfilled by the Froese-Herbst exponential bound. In other contexts however, it is a non-trivial question to answer. The first results in an abstract setup are due to Cattaneo [Ca, CGH], and the setting is regular Mourre theory. The adjective *regular* refers to setups where multiple commutators between  $H$  and  $A$ , in particular  $[H, A]$ , are suitably controlled by resolvents of  $H$ . Results in this category range from Mourre's original work [Mo] to the results relying on the  $C^k(A)$  type conditions introduced by Amrein, Boutet de Monvel and Georgescu [ABG]. See also [AHS, BFSS, DG, FGSi, GJ, HuSi].

In this paper we address the question of regularity of bound states with respect to a conjugate operator  $A$  in the context of singular Mourre theory. In the second paper [FMS] the results obtained here are used to do second order perturbation theory of embedded eigenvalues, in particular we establish the validity of Fermi's golden rule for an abstract class of Hamiltonians. By *singular* Mourre theory we refer to the situation where the first commutator  $[H, A]$  is *not* controlled by the Hamiltonian itself, as in [DJ1, Go, GGM1, GGM2, MS, Sk]. Regular Mourre theory is a special case of the singular setup considered here, and our results thus extend those of [Ca, CGH]. Roughly speaking, our answer to the question Q( $k$ ) is that control of  $k + 1$  commutators suffices. We stress that even within regular Mourre theory we extend [Ca, CGH] in that we reduce by one, from  $k + 2$  to  $k + 1$ , the number of commutators one needs to control in order to answer the question in the affirmative. Our result is optimal in terms of integer numbers of commutators, cf. Example 1.1 below. See also [MW] where the regular Mourre theory analysis is extracted from this paper and conditions are established under which bound states become analytic vectors for  $A$ .

Our main motivation is applications to massless models from quantum field theory. In particular our results apply to the massless confined Nelson model at arbitrary coupling strength. We can deal with infrared singularities that are slightly weaker than the physical one, that is we can handle singularities of the form  $|k|^{-\frac{1}{2}+\epsilon}$ , for some  $\epsilon > 0$ . As a by-product

of our methods we also establish that all bound states are in the domain of the number operator.

In Section 5 we in fact deal with a larger class of quantum field theory models, sometimes called Pauli-Fierz models, which includes the Nelson model. For simplicity and concreteness we present our results in the introduction in the context of the Nelson model. This is done in Subsection 1.2 below. The reader can also consult [GGM2, Subsection 2.3] for a discussion of the field theory models considered in this paper and its sequel.

In Section 6 we apply the abstract results of this paper to many-body AC-Stark Hamiltonians where we obtain a new regularity result. See Subsection 1.3 below for a formulation of the model and the result.

The following example illustrates that if one desires bound states to be in the domain of the  $k$ 'th power of a conjugate operator, one needs at least control of  $k + 1$  commutators.

**Example 1.1.** Consider the one-dimensional Schrödinger operator  $H = -\Delta + V$  on  $\mathcal{H} = L^2(\mathbb{R})$ , where  $V$  is a rank-one potential  $V = |\phi\rangle\langle\phi|$ . Here  $\phi \in \mathcal{H}$  is constructed as follows: Let  $k_0 \in \mathbb{N}$  and  $\epsilon \in (0, 1/2)$ . In momentum space we write  $\phi$  as a sum of two functions  $\hat{\phi} = \hat{\phi}_1 + \hat{\phi}_2$ , where we choose  $\phi_2$ , or rather its Fourier transform, to be

$$\hat{\phi}_2(\xi) = \begin{cases} 0, & |\xi| \leq 1 \\ (\xi^2 - 1)^{k_0 + \frac{1}{2} + \epsilon} e^{-\xi^2}, & |\xi| > 1 \end{cases}.$$

Having fixed  $\phi_2$ , we choose  $\phi_1$ , such that

$$\hat{\phi}_1 \in C_0^\infty(-\frac{1}{2}, \frac{1}{2}), \quad \text{and} \quad \int_{\mathbb{R}} |\hat{\phi}(\xi)|^2 (\xi^2 - 1)^{-1} d\xi = -1. \quad (1.1)$$

The key to the example is the singular behaviour of  $\hat{\phi}$  near  $\xi^2 = 1$ . We have  $\phi \in C^\infty(\mathbb{R})$  and

$$\begin{aligned} \left| \frac{d^\ell \phi}{dx^\ell}(x) \right| &\leq C_\ell (1 + |x|)^{-k_0 - \frac{3}{2} - \epsilon}, \quad \text{for all } \ell \geq 0, \\ x^k \frac{d^\ell \phi}{dx^\ell} &\in L^2(\mathbb{R}) \Leftrightarrow k \leq k_0 + 1. \end{aligned} \quad (1.2)$$

Furthermore, the normalization in (1.1) ensures that  $H$  has  $\lambda = 1$  as an embedded eigenvalue with eigenfunction  $\psi = (-\Delta - 1)^{-1} \phi$ . Note that  $(\xi^2 - 1)^{-1} \hat{\phi}$  decays faster than any polynomial. We have  $\psi \in C^\infty(\mathbb{R})$  and

$$x^k \frac{d^\ell \psi}{dx^\ell} \in L^2(\mathbb{R}) \Leftrightarrow k \leq k_0. \quad (1.3)$$

Let  $A$  denote the generator of dilations  $A = \frac{1}{2i}(x \frac{d}{dx} + \frac{d}{dx} x)$ . Introducing the notation  $\text{ad}_A^k(H) = [\text{ad}_A^{k-1}(H), A]$  and  $\text{ad}_A^0(H) = H$  we formally compute

$$i^k \text{ad}_A^k(H) = -2^k \Delta + i^k \text{ad}_A^k(V).$$

Due to (1.2), the iterated commutator  $\text{ad}_A^k(V)$  is bounded, hence compact, if and only if  $k \leq k_0 + 1$ . Adding resolvents of  $H$  does not help. Furthermore  $i[H, A]$  obviously satisfies a Mourre estimate with compact error at positive energies: For any  $E > 0$

$$\mathbb{1}_{[H \geq E]} i[H, A] \mathbb{1}_{[H \geq E]} \geq E \mathbb{1}_{[H \geq E]} - K,$$

where  $K$  is compact and  $\mathbb{1}_{[H \geq E]}$  is the spectral projection for  $H$  associated with the Borel set  $[E, \infty)$ . That is, we are within the scope of [Ca, CGH]. We have the first  $k_0 + 1$

commutators all  $H$ -bounded, with the  $(k_0+2)$ 'nd commutator not controlled by any power of resolvents of  $H$ . Appealing to (1.3), we see that the bound state  $\psi$  is in the domain of  $A^{k_0}$ , but not in the domain of  $A^{k_0+1}$ . That  $\psi \in \mathcal{D}(A^{k_0})$  is a conclusion one cannot reach using [Ca, CGH]. It is however attainable by the abstract result of the present paper. See Section 2. The additional information that  $\psi \notin \mathcal{D}(A^{k_0+1})$  demonstrates that our result is optimal.

As a last observation, more geared towards our second paper [FMS], let us perturb  $H$  by adding a small multiple of  $V$  to obtain  $H_\sigma = H + (1 + \sigma)V$ , with  $|\sigma|$  being small. First note that the operator  $H_\sigma$  can have at most one eigenvalue. Repeating some of the analysis from above, and appealing to the implicit function theorem, one can verify the following statements: There exists  $\delta > 0$  and a function  $\lambda: (-\delta, 0] \rightarrow \mathbb{R}$  such that

$$\begin{aligned} \forall \sigma \in (0, \delta) : \quad \sigma_{\text{pp}}(H_\sigma) &= \emptyset, \\ \forall \sigma \in (-\delta, 0] : \quad \sigma_{\text{pp}}(H_\sigma) &= \{\lambda(\sigma)\}. \end{aligned}$$

The function  $\lambda$  satisfies that  $\lambda(0) = 1$ ,

$$\begin{aligned} \lambda &\text{ is real analytic in } (-\delta, 0), \\ \lambda &\in C^{k_0+1}((-\delta, 0]) \quad \text{and} \quad \lambda \notin C^{k_0+2}((-\delta, 0]). \end{aligned}$$

This establishes a natural limit on what one should expect from a perturbation theory for embedded eigenvalues. Indeed, it indicates that control of two commutators (corresponding to  $k_0 = 1$ ) may suffice for second order perturbation theory and this is in fact accomplished in [FMS, Section 5.1]. The strongest results, cf. [FMS, Section 5.2], require control of 3 commutators, since they rely on the condition  $\psi \in \mathcal{D}(A^2)$ .

## 1.1 Singular Mourre Theory

Before we formulate our results more precisely, we pause to discuss on a more heuristic level the origin of conjugate operators, and how we are led naturally to singular Mourre theory.

Consider the operator  $M_\omega$  of multiplication in momentum space  $L^2(\mathbb{R}^d)$  by a dispersion relation  $\omega$  assumed to be locally Lipschitz. The connection between dynamics and structure of the spectrum of a self-adjoint operator is fairly well understood, starting from Kato-smoothness and the RAGE theorem [RS]. When looking for a conjugate operator, one should study the dynamics of the operator  $M_\omega$ . It is natural to identify what states have (at least) ballistic motion, that is find states  $\psi_0$  satisfying

$$\langle x^2 \rangle_{\psi_t} \geq ct^2,$$

for some  $c > 0$ . Here  $\psi_t = \exp(-itM_\omega)\psi_0$ . The position operator  $x$  is equal to  $i\nabla_k$ . We can compute this quantity explicitly and we get

$$\begin{aligned} \langle x^2 \rangle_{\psi_t} &= \langle x^2 \rangle_{\psi_0} + \int_0^t \langle x \cdot \nabla \omega + \nabla \omega \cdot x \rangle_{\psi_s} ds \\ &= \langle x^2 \rangle_{\psi_0} + t \langle x \cdot \nabla \omega + \nabla \omega \cdot x \rangle_{\psi_0} + t^2 \langle |\nabla \omega|^2 \rangle_{\psi_0}. \end{aligned}$$

We observe that if  $\psi_0$  has support away from zeroes of  $\nabla \omega$ , then the motion is at least ballistic. More precisely this is the case if  $\text{essinf}_{k \in \text{supp } \psi_0} |\nabla \omega(k)| \geq c > 0$ .

If  $\omega = k^2$ , the standard non-relativistic dispersion relation, we find that  $\psi_0$  should be localized away from 0 in momentum space. Since  $|\nabla \omega|^2 = 4\omega$ , the requirement on

$\psi_0$  can also be expressed as  $\psi_0 \in E_{M_\omega}([c/4, \infty))L^2(\mathbb{R}^d)$ , where  $E_{M_\omega}$  denotes the spectral resolution associated with the self-adjoint operator  $M_\omega$ . We observe that the energy 0 has a special significance for the case  $\omega = k^2$  and is called a threshold, in the sense that states localized in energy near a threshold may not have strict ballistic motion.

A second example is  $\omega = |k|$ . Here we observe that  $|\nabla\omega| = 1$ , and hence all states  $\psi_0$  will exhibit ballistic motion. In other words this dispersion relation does not have thresholds. This of course reflects the constant (momentum independent) speed of light. See [GGM1, Subsection 1.2] for a discussion of general dispersion relations.

When picking a conjugate operator in Mourre theory, one is precisely looking for an observable  $a$  with at least ballistic growth. The choice often used is the Heisenberg derivative of  $x^2$ , where  $x$  is some suitably chosen position observable. That is, one would naturally be lead to consider

$$a = \frac{1}{2}(x \cdot \nabla\omega + \nabla\omega \cdot x).$$

This is for example the case for the  $N$ -body problem, see e.g. [AHS, Ca, CGH, HuSi], and in the case of field theory see [DG, DJ1, FGSch1, FGSch2, GGM2, Sk], where the position is the Newton-Wigner position  $d\Gamma(x)$ . The free energy is  $d\Gamma(M_\omega)$ , and we get as conjugate operator  $A = d\Gamma(a)$ , where  $a$  is as above. Here  $d\Gamma(b)$  denotes the second quantization of a one-body operator  $b$ , cf. the following subsection on Nelson's model.

It is often advantageous to modify the so obtained conjugate operator, to simplify proofs, or circumvent some technical issues. In this paper we need the modified generator of translations  $A_\delta$  from [GGM2] in order to deal with the confined massless Nelson model, and more generally confined massless Pauli-Fierz models.

There are two issues that come up naturally when following the above guidelines for massless field theory models, like the Nelson model. One is already apparent in the one-particle setup discussed above. If  $\omega(k) = |k|$ , the resulting conjugate operator  $a$ , the generator of radial translations, does not have a self-adjoint realization. This appears to be a purely technical complication, that becomes a serious issue when one is in need of localizations in the operator  $a$ . The operator is not normal, so we do not have spectral calculus at hand, only resolvents. This has so far not been a serious issue when dealing with the limiting absorption principle [DJ1, GGM2, HüSp, HuSi, Sk], and perturbation theory around an uncoupled system [DJ1, Go]. It does however become an obstacle when one tries to apply the conjugate operator  $a$  in the context of scattering theory [Gé].

In the present paper, non-self-adjointness of  $a$  is also a serious obstacle, which we overcome, as in [Gé], by passing to a so called expanded Hamiltonian. The idea is to write  $L^2(\mathbb{R}^d) \sim L^2(\mathbb{R}_+) \otimes L^2(S^{d-1})$  and double the Hilbert space to  $L^2(\mathbb{R}) \otimes L^2(S^{d-1})$ . The dispersion relation in polar coordinates is just multiplication by  $r$ , which when extended linearly to negative  $r$  gives rise to the self-adjoint conjugate operator  $i\partial/\partial r \otimes \mathbb{1}$ . We thus work with an expanded Hamiltonian, and in the end pull our results back to the physical Hamiltonian. The reader should keep this in mind when going through the abstract conditions in the following section.

However passing to an expanded Hamiltonian is not a silver bullet, it comes with a price. The operator of multiplication by  $r$  is no longer bounded from below, making it hard to utilize energy localizations. For this reason we have to develop an abstract theory which does not demand that any naturally occurring object can be controlled by the (expanded) Hamiltonian.

The second feature we want to discuss does not occur on the one-particle level, but only after second quantization. The free commutator becomes

$$i[d\Gamma(|k|), A] = \mathcal{N},$$

where  $\mathcal{N}$  is the number operator. In the standard (regular) commutator based methods, one typically has the commutator bounded at least as a form on  $\mathcal{D}(H)$ . (This is for example a consequence of a  $C^1(A)$  assumption.) This is not the case here and we call such a situation *singular*. One could of course avoid this issue by observing that the operators involved conserve particle number, and then rescale  $A$  by  $1/n$  on the  $n$ -particle sector. However, perturbations are typically expressed in terms of field operators, and straying from second quantized conjugate operators give rise to terms from the commutator with the perturbation, that have so far not been controllable.

The  $d\Gamma(|k|)$ -unboundedness of the number operator, has led authors to use a different conjugate operator instead, namely the second quantized generator of dilation given by  $d\Gamma((x \cdot k + k \cdot x)/2)$ , normally associated with the dispersion relation  $k^2$ . Here the commutator with  $d\Gamma(|k|)$  is  $d\Gamma(|k|)$  itself, so the issue disappears. However, this choice induces an artificial threshold at photon energy 0, which for a coupled system turns all eigenvalues of the atomic system into artificial thresholds. In order to circumvent this problem one can modify the generator of dilation by building the level shift from Fermi's golden rule into the conjugate operator. This was done in [BFSS] and gives rise to positive relatively bounded commutators, at weak coupling. There are however disadvantages to this approach. It does not cover situations where symmetries may cause embedded eigenvalues to persist to second order in perturbation theory. For the  $N$ -body problem in quantum mechanics one can for example show that the underlying spectrum is absolutely continuous without a priori imposing Fermi's golden rule, which can then subsequently be established [AHS, HuSi]. Works employing this choice of conjugate operator has, so far, not been able to address what happens outside the regime of weak coupling, which may be an issue since coupling constants typically are explicitly given numbers. In electron-photon models, the coupling constant involve the feinstrucure constant  $1/137$  and in electron-phonon models from solid state physics, the coupling constants occurring may even be of the order 1. Effective coupling constants may also depend on an ultraviolet cutoff, thus imposing apparently artificial limitations on the size of the cutoff. Finally the restriction on the size of the coupling constant is always locally uniform in energy. That is, all statements of this type holds only below a fixed  $E_0$ . Papers employing the generator of dilation include [BFS, BFSS, FGSi].

We remark that in [Go], the author modifies the generator of radial translation, as it was done in [BFSS] for the generator of dilations, in order to establish Fermi's golden rule. We have no need for this construction since we follow the strategy of [AHS, HuSi, MS].

Instead of viewing the unboundedness of the first commutator with respect to  $d\Gamma(|k|)$  as a technical problem, one can also adopt the point of view that it is a feature of the model which can be exploited. This is most obviously done for small coupling constants, where one gets a positive commutator globally in energy, modulo a compact error. This was done in [DJ1, FGSch2, Go, Sk]. In [GGM2] the extra positivity of the commutator is directly utilized to prove a Mourre estimate at arbitrary coupling constant, the first (and so far only) such result for massless models. Another piece of information one can extract is that the number operator has finite expectation in bound states. This was done in [Sk] for small coupling constants and generally in [GGM2]. A more subtle property is that one can obtain a stronger limiting absorption principle, see [GGM1, MS], which has so far not found an application. Here we prove in particular that bound states are in the domain of the number operator, not just in its form domain.

We have not discussed positive temperature models, where one has a similar situation, except that so far no positive commutator estimates at arbitrary coupling has been proven, regardless of choice of conjugate operator. See e.g. [DJ2, FM] and references therein.

## 1.2 The Nelson Model

The model describes a confined atomic system coupled to a massless scalar quantum field. The Hamiltonian  $K$  of the atomic system is

$$K = - \sum_{i=1}^P \frac{1}{2m_i} \Delta_i + \sum_{i<j} V_{ij}(x_i - x_j) + W(x_1, \dots, x_P) \quad (1.4)$$

acting on  $\mathcal{K} = L^2(\mathbb{R}^{3P})$ . Here  $m_i > 0$  denotes the mass of the  $i$ 'th particle located at  $x_i \in \mathbb{R}^3$ . We write  $x = (x_1, \dots, x_P) \in \mathbb{R}^{3P}$ . The external potential  $W$  is the confinement and must satisfy

**(W0)**  $W \in L^2_{\text{loc}}(\mathbb{R}^{3P})$  and there exist positive constants  $c_0, c_1$  and  $\alpha > 2$  such that  $W(x) \geq c_0|x|^{2\alpha} - c_1$ .

As for the pair potentials  $V_{ij}$ , they should satisfy

**(V0)** The  $V_{ij}$ 's are  $\Delta$ -bounded with relative bound 0.

The Hilbert space for the scalar bosons is the symmetric Fock-space  $\mathcal{F} = \Gamma(L^2(\mathbb{R}^3))$  and the kinetic energy for the massless bosons is  $d\Gamma(|k|)$ , the second quantization of the operator of multiplication with the massless dispersion relation  $|k|$ . The uncoupled Hamiltonian, describing the atomic system and the scalar field is  $K \otimes \mathbb{1}_{\mathcal{F}} + \mathbb{1}_{\mathcal{K}} \otimes d\Gamma(|k|)$ , as an operator on the full Hilbert space

$$\mathcal{H} = \mathcal{K} \otimes \mathcal{F}.$$

Our next task is to introduce a coupling of the form

$$I_\rho(x) = \sum_{i=1}^P \phi_\rho(x_i), \quad (1.5)$$

where  $\phi_\rho(y)$  is an ultraviolet and infrared regularized field operator

$$\phi_\rho(y) = \frac{1}{\sqrt{2}} \int_{\mathbb{R}^3} (\rho(k)e^{-ik \cdot y} a^*(k) + \overline{\rho(k)} e^{ik \cdot y} a(k)) dk.$$

We assume purely for simplicity that  $\rho$  only depends on  $k$  through its modulus. To conform with the notation used in [GGM2], we introduce

$$\tilde{\rho}(r) = r\rho(r, 0, 0), \quad \text{such that } |k|\rho(k) = \tilde{\rho}(|k|).$$

For the interacting Hamiltonian, indexed by the coupling function  $\rho$ ,

$$H_\rho^{\text{N}} = K \otimes \mathbb{1}_{\mathcal{F}} + \mathbb{1}_{\mathcal{K}} \otimes d\Gamma(|k|) + I_\rho(x) \quad (1.6)$$

to be essentially self-adjoint on  $\mathcal{D}(K) \otimes \Gamma_{\text{fin}}(C_0^\infty(\mathbb{R}^3))$ , we need the following basic assumption on  $\rho$ .

**(ρ1)**  $\int_0^\infty (1+r^{-1})|\tilde{\rho}(r)|^2 dr < \infty$ .

Here  $\Gamma_{\text{fin}}(V)$  denotes the subspace of  $\mathcal{F}$  consisting of elements  $\eta$  with only finitely many  $n$ -particle components  $\eta^{(n)}$  nonzero, and those that are nonzero lie in the  $n$ -fold algebraic tensor product of the subspace  $V \subseteq L^2(\mathbb{R}^3)$ . Note that  $\Gamma_{\text{fin}}(V)$  is dense in  $\mathcal{F}$  if  $V$  is dense in  $L^2(\mathbb{R}^3)$ .

In order to formulate the remaining assumption on  $\rho$  we introduce a function  $d \in C^\infty((0, \infty))$ , which measures the amount of infrared regularization carried by  $\rho$ . It should, for some  $C_d > 0$ , satisfy

$$d(r) = 1, \text{ for } r \geq 1, \quad -C_d \frac{d(r)}{r} \leq d'(r) < 0, \quad \lim_{r \rightarrow 0^+} d(r) = +\infty. \quad (1.7)$$

Note that the conditions above imply that  $1 \leq d(r) \leq r^{-C_d}$ , for  $r \in (0, 1]$ . In order to simplify some expressions below we make the additional assumption that

$$\forall r \in (0, 1] : \quad d(r) \leq C'_d r^{-\frac{1}{2}}, \quad (1.8)$$

for some  $C'_d > 0$ . In practice we want to construct a  $d$  with as weak a singularity as possible, so this extra assumption is no restriction. We formulate the remaining conditions on  $\rho$ , of which the two first also appeared in [GGM2].

$$(\rho 2) \quad \int_0^\infty (1 + r^{-1})d(r)^2[r^{-2}|\tilde{\rho}(r)|^2 + |\frac{d\tilde{\rho}}{dr}(r)|^2]dr < \infty.$$

$$(\rho 3) \quad \int_0^\infty |\frac{d^2\tilde{\rho}}{dr^2}(r)|^2 dr < \infty.$$

$$(\rho 4) \quad \int_0^\infty r^4|\tilde{\rho}(r)|^2 dr < \infty.$$

We remark that  $(\rho 2)$  and  $(\rho 4)$  implies  $(\rho 1)$ . A typical form of  $\rho$ , and hence  $\tilde{\rho}$ , would be

$$\rho(k) = e^{-\frac{|k|^2}{2\Lambda^2}}|k|^{-\frac{1}{2}+\epsilon}, \quad \tilde{\rho}(r) = e^{-\frac{r^2}{2\Lambda^2}}r^{\frac{1}{2}+\epsilon}. \quad (1.9)$$

One can construct a  $d$  by gluing together the functions 1 and  $r^{-\epsilon'}$ , with  $0 < \epsilon' < \min\{\epsilon, 1/2\}$ . The parameters  $\Lambda$  and  $\epsilon$  are the ultraviolet respectively infrared regularization parameters. Ideally we would like to have  $\Lambda = \infty$  and  $\epsilon = 0$ . For the conditions  $(\rho 1)$ – $(\rho 4)$  to be satisfied we must have  $0 < \Lambda < \infty$  and  $\epsilon > 1$ . Observe that it is the condition  $(\rho 3)$  on the second derivative of  $\tilde{\rho}$  that causes the strongest restriction on  $\epsilon$ .

Observe that the set of  $\rho$ 's satisfying  $(\rho 1)$  –  $(\rho 4)$  is a complex vector space  $\mathcal{I}_N(d) \subseteq L^2(\mathbb{R}^3)$ , which can be equipped with a norm matching the four conditions. That is

$$\|\rho\|_N^2 := \int_0^\infty \left\{ (r^4 + d(r)^2 r^{-3})|\tilde{\rho}(r)|^2 + (1 + r^{-1})d(r)^2 \left| \frac{d\tilde{\rho}}{dr}(r) \right|^2 + \left| \frac{d^2\tilde{\rho}}{dr^2}(r) \right|^2 \right\} dr. \quad (1.10)$$

In order to formulate our main theorem, we need to introduce an operator conjugate to  $H_\rho^N$ . We use the one constructed in [GGM2], for which a Mourre estimate has been established under the assumptions above. Let  $\chi \in C_0^\infty(\mathbb{R})$ , with  $0 \leq \chi \leq 1$ ,  $\chi(r) = 1$  for  $|r| < 1/2$ , and  $\chi(r) = 0$  for  $|r| > 1$ . For  $0 < \delta \leq 1/2$  we define a function on  $(0, \infty)$  by

$$s_\delta(r) = \chi(r/\delta)d(\delta)r^{-1} + (1 - \chi)(r/\delta)d(r)r^{-1}.$$

Using this function we construct a vector-field by  $\vec{s}_\delta(k) = s_\delta(|k|)k$ , which equals  $k/|k|$  for  $|k| > 1$  and  $d(\delta)k/|k|$  for  $|k| < \delta/2$ . The conjugate operator on the one-particle sector is

$$a_\delta = \frac{1}{2}(\vec{s}_\delta \cdot i\nabla_k + i\nabla_k \cdot \vec{s}_\delta). \quad (1.11)$$

The operator is symmetric and closable on  $\{f \in C_0^\infty(\mathbb{R}^3) | f(0) = 0\}$ . We denote again by  $a_\delta$  its closure which is a maximally symmetric operator, but not self-adjoint. It is a modification, near  $k = 0$ , of the generator of radial translations  $a = (\frac{k}{|k|} \cdot i\nabla_k + i\nabla_k \cdot \frac{k}{|k|})/2$ . The conjugate operator is now the maximally symmetric operator

$$A_\delta = \mathbb{1}_{\mathcal{K}} \otimes d\Gamma(a_\delta).$$

The second quantization  $d\Gamma(a)$  of the generator of radial translations works as conjugate operator if one stays close to the uncoupled system. See [DJ1, Go, Sk]. It is not known if one really needs the modified generator of radial translations  $A_\delta$  in order to get a Mourre estimate at arbitrary coupling.

For an eigenvalue  $E \in \sigma_{\text{pp}}(H_\rho^{\text{N}})$  we write  $P_\rho$  for the associated eigenprojection. It is known from [GGM2] that  $P_\rho$  has finite dimensional range. Finally we need the number operator

$$\mathcal{N} = \mathbb{1}_{\mathcal{K}} \otimes d\Gamma(\mathbb{1}_{L^2(\mathbb{R}^3)}).$$

We will make use of the same notation for the (usual) number operator on  $\mathcal{F}$ . Our main result of this paper, formulated in terms of the Nelson model, is

**Theorem 1.2.** *Suppose **(W0)** and **(V0)**. Let  $E_0 \in \mathbb{R}$  and  $\rho_0 \in \mathcal{I}_{\text{N}}(d)$  be given. There exist  $0 < \delta \leq 1/2$ ,  $r > 0$  and  $C > 0$  such that for any  $\rho \in \mathcal{I}_{\text{N}}(d)$ , with  $\|\rho - \rho_0\|_{\text{N}} \leq r$ , and  $E \in \sigma_{\text{pp}}(H_\rho^{\text{N}}) \cap (-\infty, E_0]$  we have*

$$P_\rho : \mathcal{H} \rightarrow \mathcal{D}(\mathcal{N}^{\frac{1}{2}} A_\delta) \cap \mathcal{D}(A_\delta \mathcal{N}^{\frac{1}{2}}) \cap \mathcal{D}(\mathcal{N})$$

and

$$\|\mathcal{N}^{\frac{1}{2}} A_\delta P_\rho\| + \|A_\delta \mathcal{N}^{\frac{1}{2}} P_\rho\| + \|\mathcal{N} P_\rho\| \leq C.$$

We remark that for any  $\delta > 0$  small enough, one can find  $r$  and  $C$  such that the conclusion of the theorem holds. See Theorem 5.2. The above suffices for our purpose and is a cleaner statement.

We can implement a unitary transformation, the so-called Pauli-Fierz transform, which has the effect of smoothening the infrared singularity. Let  $U_\rho = \exp(-iP\phi_{i\rho/|k|}(0))$  be the unitary transformation with

$$U_\rho a(k) U_\rho^* = a(k) - \frac{P\rho(k)}{\sqrt{2}|k|} \quad \text{and} \quad U_\rho a^*(k) U_\rho^* = a^*(k) - \frac{P\overline{\rho(k)}}{\sqrt{2}|k|}.$$

For the transformation  $U_\rho$  to be well-defined we must require that  $\int_{\mathbb{R}^3} |k|^{-2} |\rho(k)|^2 dk < \infty$ . To achieve this we strengthen  $(\rho\mathbf{1})$  to read

$$(\rho\mathbf{1}^?) \quad \int_0^\infty (1 + r^{-2}) |\tilde{\rho}(r)|^2 dr < \infty.$$

We then get

$$H_\rho^{\text{N}'} = (\mathbb{1}_{\mathcal{K}} \otimes U_\rho) H_\rho^{\text{N}} (\mathbb{1}_{\mathcal{K}} \otimes U_\rho)^* = K_\rho \otimes \mathbb{1}_{\mathcal{F}} + \mathbb{1}_{\mathcal{K}} \otimes d\Gamma(|k|) + I_\rho(x) - I_\rho(0), \quad (1.12)$$

where

$$K_\rho = K - \sum_{i=1}^P v_\rho(x_i) + \frac{P^2}{2} \int_0^\infty r^{-1} |\tilde{\rho}(r)|^2 dr \mathbb{1}_{\mathcal{K}} \quad (1.13)$$

and

$$v_\rho(y) = P \int_{\mathbb{R}^3} \frac{|\rho(k)|^2}{|k|} \cos(k \cdot y) dk. \quad (1.14)$$

Observe that

$$\phi_\rho(y) - \phi_\rho(0) = \frac{1}{\sqrt{2}} \int_{\mathbb{R}^3} (\rho(k)(e^{-ik \cdot y} - 1)a^*(k) + \overline{\rho(k)}(e^{ik \cdot y} - 1)a(k)) dk.$$

The estimate

$$|e^{\pm ik \cdot y} - 1| \leq \max\{2, |k||y|\} \leq 2 \frac{|k|}{\langle k \rangle} \langle y \rangle, \quad (1.15)$$

with  $\langle \eta \rangle = (1 + |\eta|^2)^{1/2}$ , enables us to extract an extra infrared regularization using the decay in  $x$  supplied by the confinement condition **(W0)**. Keeping (1.8) and  $(\rho\mathbf{1}')$  in mind, the remaining two assumptions on  $\rho$  now weaken to

$$(\rho\mathbf{2}') \int_0^\infty \left| \frac{d\tilde{\rho}}{dr}(r) \right|^2 dr < \infty.$$

$$(\rho\mathbf{3}') \int_0^\infty r^2 \left| \frac{d^2\tilde{\rho}}{dr^2}(r) \right|^2 / (1 + r^2) dr < \infty.$$

The condition  $(\rho\mathbf{4})$ , being an ultraviolet condition, is unchanged. For the choice (1.9) to satisfy  $(\rho\mathbf{1}')$ – $(\rho\mathbf{3}')$  and  $(\rho\mathbf{4})$  we must have  $0 < \Lambda < \infty$  and  $\epsilon > 0$ . Here the first three conditions on  $\rho$  all require  $\epsilon > 0$ .

Observe again that the set of  $\rho$  satisfying  $(\rho\mathbf{1}')$ – $(\rho\mathbf{3}')$  and  $(\rho\mathbf{4})$  is a complex vector space  $\mathcal{I}'_{\mathbb{N}}(d)$ . We introduce the natural norm

$$\|\rho\|_{\mathbb{N}'}^2 := \int_0^\infty \left\{ (r^4 + r^{-2}) |\tilde{\rho}(r)|^2 + \left| \frac{d\tilde{\rho}}{dr}(r) \right|^2 + \frac{r^2}{1 + r^2} \left| \frac{d^2\tilde{\rho}}{dr^2}(r) \right|^2 \right\} dr.$$

Fix a  $\rho_0 \in \mathcal{I}'_{\mathbb{N}}(d)$ . There are now two avenues one can follow. Either one can continue as above, and for each  $\rho$  in a  $\|\cdot\|_{\mathbb{N}'}$ -ball around  $\rho_0$  we apply the transformation  $U_\rho$  to arrive at the more regular Hamiltonian  $H_\rho^{\mathbb{N}'}$  that we can fit into our class of Pauli-Fierz models. A second option would be to apply the same transformation  $U_{\rho_0}$  regardless of  $\rho$  chosen near  $\rho_0$ . The advantage of this is two-fold: Firstly, we would be working in the same coordinate system for all  $\rho$ 's, which in the context of perturbation theory, cf. [FMS], is the most natural. Secondly, in this way the Hamiltonian will have a linear dependence on the 'perturbation'  $\rho - \rho_0$ , which is a requirement in [FMS]. The drawback is that  $\rho - \rho_0$  has to be an element of  $\mathcal{I}'_{\mathbb{N}}(d)$ , and for example cannot be a small multiple of  $\rho_0$ .

To implement the latter approach, we now let  $\rho = \rho_0 + \rho_1$ , with  $\rho_1 \in \mathcal{I}'_{\mathbb{N}}(d)$ , the space of regular interactions. We then employ the transformation  $U_{\rho_0}$  which yields the transformed Hamiltonian

$$H_\rho^{\mathbb{N}''} = (\mathbb{1}_{\mathcal{K}} \otimes U_{\rho_0}) H_\rho^{\mathbb{N}} (\mathbb{1}_{\mathcal{K}} \otimes U_{\rho_0})^* = H_{\rho_0}^{\mathbb{N}'} + I_{\rho_1}(x) - \sum_{i=1}^P v_{\rho_0, \rho_1}(x_i), \quad (1.16)$$

where

$$v_{\rho_0, \rho_1}(y) = P \int_{\mathbb{R}^3} \operatorname{Re} \left\{ \frac{\rho_1(k) \overline{\rho_0(k)}}{|k|} e^{-ik \cdot y} \right\} dk. \quad (1.17)$$

For an eigenvalue  $E \in \sigma_{\text{pp}}(H_\rho^{\mathbb{N}})$  we write  $P'_\rho = (\mathbb{1}_{\mathcal{K}} \otimes U_\rho) P_\rho (\mathbb{1}_{\mathcal{K}} \otimes U_\rho)^*$  for the associated eigenprojection for  $H_\rho^{\mathbb{N}'}$ , and  $P''_\rho = (\mathbb{1}_{\mathcal{K}} \otimes U_{\rho_0}) P_\rho (\mathbb{1}_{\mathcal{K}} \otimes U_{\rho_0})^*$  for the associated eigenprojection for  $H_\rho^{\mathbb{N}''}$ . Again  $P'_\rho$  and  $P''_\rho$  have finite dimensional ranges. Theorem 5.2 can be applied to the transformed Hamiltonian and we arrive at the following theorem.

**Theorem 1.3.** *Suppose **(W0)** and **(V0)**. Let  $E_0 \in \mathbb{R}$  and  $\rho_0 \in \mathcal{I}'_{\mathbb{N}}(d)$  be given. There exist  $0 < \delta \leq 1/2$ ,  $r > 0$  and  $C > 0$  such that*

1) for any  $\rho \in \mathcal{I}'_{\mathbb{N}}(d)$  with  $\|\rho - \rho_0\|_{\mathbb{N}'} \leq r$  and  $E \in \sigma_{\text{pp}}(H_{\rho}^{\mathbb{N}}) \cap (-\infty, E_0]$  we have

$$P'_{\rho}: \mathcal{H} \rightarrow \mathcal{D}(\mathcal{N}^{\frac{1}{2}}A_{\delta}) \cap \mathcal{D}(A_{\delta}\mathcal{N}^{\frac{1}{2}}) \cap \mathcal{D}(\mathcal{N})$$

and

$$\|\mathcal{N}^{\frac{1}{2}}A_{\delta}P'_{\rho}\| + \|A_{\delta}\mathcal{N}^{\frac{1}{2}}P'_{\rho}\| + \|\mathcal{N}P'_{\rho}\| \leq C.$$

2) for any  $\rho_1 \in \mathcal{I}'_{\mathbb{N}}(d)$  with  $\|\rho_1\|_{\mathbb{N}} \leq r$  and  $E \in \sigma_{\text{pp}}(H_{\rho}^{\mathbb{N}}) \cap (-\infty, E_0]$ , where  $\rho = \rho_0 + \rho_1$ , we have

$$P''_{\rho}: \mathcal{H} \rightarrow \mathcal{D}(\mathcal{N}^{\frac{1}{2}}A_{\delta}) \cap \mathcal{D}(A_{\delta}\mathcal{N}^{\frac{1}{2}}) \cap \mathcal{D}(\mathcal{N})$$

and

$$\|\mathcal{N}^{\frac{1}{2}}A_{\delta}P''_{\rho}\| + \|A_{\delta}\mathcal{N}^{\frac{1}{2}}P''_{\rho}\| + \|\mathcal{N}P''_{\rho}\| \leq C.$$

Unfortunately the transformation  $U_{\rho}$ , with  $\rho \in \mathcal{I}'_{\mathbb{N}}(d)$ , is too singular to allow for a recovery of the full set of regularity results for the original Hamiltonian  $H_{\rho}^{\mathbb{N}}$ , as in Theorem 1.2. The only thing that remains after undoing the transformation is the following corollary to Theorem 1.3 1). The same argument using Theorem 1.3 2) would give a weaker result. Theorem 1.3 2) will however play a role in [FMS].

**Corollary 1.4.** *Suppose (W0) and (V0). Let  $E_0 \in \mathbb{R}$  and  $\rho_0 \in \mathcal{I}'_{\mathbb{N}}(d)$  be given. There exist  $0 < \delta \leq 1/2$ ,  $r > 0$  and  $C > 0$  such that for any  $\rho \in \mathcal{I}'_{\mathbb{N}}(d)$  with  $\|\rho - \rho_0\|_{\mathbb{N}'} \leq r$  and  $E \in \sigma_{\text{pp}}(H_{\rho}^{\mathbb{N}}) \cap (-\infty, E_0]$  we have*

$$P_{\rho}: \mathcal{H} \rightarrow \mathcal{D}(\mathcal{N}) \text{ and } \|\mathcal{N}P_{\rho}\| \leq C.$$

We make a number of remarks concerning the results above.

The domain of  $a_{\delta}$  is independent of  $\delta$ , and in fact equals the domain of the generator of radial translations. The same is (presumably) false for the second quantized versions. This is the reason for the somewhat unpleasant formulation of the theorems in terms of  $A_{\delta}$ . It should be read in the context of Mourre's commutator method, and in [FMS] we need the regularity formulated in terms of  $A_{\delta}$ .

The statement that bound states are in the domain of the number operator is new. Previously it was only known that bound states are in the domain of  $\mathcal{N}^{1/2}$ . See [GGM2].

The reader should first and foremost read the results above with  $\rho = \rho_0$ . In the sequel [FMS] we need the locally uniform version to deduce a Fermi golden rule under minimal assumptions. In traditional approaches to Fermi's golden rule, one typically require unperturbed bound states to be in the domain of the square of the conjugate operator. See [AHS, HuSi, MS]. In [FMS] we reduce the requirement to bound states  $\psi$  being in the domain of the conjugate operator itself, at the expense of a need for the norm  $\|A_{\delta}\psi\|$  to be bounded uniformly in  $\rho$  in a ball around the unperturbed coupling function  $\rho_0$  and uniformly in  $E$  running over eigenvalues of  $H_{\rho}$  in a fixed compact interval. This motivates the somewhat unorthodox formulation in Theorem 1.2.

The conditions  $(\rho\mathbf{3})$  and  $(\rho\mathbf{3}')$  come from a need of handling the double commutator  $[[H_{\rho}, A_{\delta}], A_{\delta}]$ . It is not a priori obvious that we should be able to place bound states in the domain of  $A_{\delta}$  with control of just two commutators. In the context of regular Mourre theory the question is addressed in [Ca, CGH] where the author(s) need three commutators to conclude a result of this type, which in view of Example 1.1 is not optimal. To deal effectively with the infrared singularity, it is crucial to minimize the number of commutators needed.

### 1.3 The AC–Stark model

The model describes a system of  $N$  charged particles in a nonzero time-periodic Stark-field with zero mean (AC-Stark field). The particles are here taken three-dimensional and we assume that the field is 1-periodic and, for simplicity, that it is continuous i.e. that  $\tilde{\mathcal{E}} \in C([0, 1]; \mathbb{R}^3)$ . The Hamiltonian is of the form

$$\tilde{h}(t) = \sum_{i=1}^N \left( \frac{p_i^2}{2m_i} - q_i \tilde{\mathcal{E}}(t) \cdot x_i \right) + V; \quad (1.18)$$

here  $x_i$ ,  $m_i$  and  $q_i$  are the position, the mass and the charge of the  $i$ 'th particle, respectively, and  $p_i = -i\nabla_{x_i}$  is its momentum. The potential is of the form

$$V = \sum_{1 \leq i < j \leq N} v_{ij}(x_i - x_j), \quad (1.19)$$

where the pair-potentials obey

**Conditions 1.5.** Let  $k_0 \in \mathbb{N}$  be given. For each pair  $(i, j)$  the pair-potential  $\mathbb{R}^3 \ni y \rightarrow v_{ij}(y) \in \mathbb{R}$  splits into a sum  $v_{ij} = v_{ij}^1 + v_{ij}^2$  where

- (1) Differentiability:  $v_{ij}^1 \in C^{k_0+1}(\mathbb{R}^3)$  and  $v_{ij}^2 \in C^{k_0+1}(\mathbb{R}^3 \setminus \{0\})$ .
- (2) Global bounds: For all  $\alpha$  with  $|\alpha| \leq k_0 + 1$  there are bounds  $|y|^{|\alpha|} |\partial_y^\alpha v_{ij}^1(y)| \leq C$ .
- (3) Decay at infinity:  $|v_{ij}^1(y)| + |y \cdot \nabla_y v_{ij}^1(y)| = o(1)$ .
- (4) Local singularity:  $v_{ij}^2$  is compactly supported and for all  $\alpha$  with  $|\alpha| \leq k_0 + 1$  there are bounds  $|y|^{|\alpha|+1} |\partial_y^\alpha v_{ij}^2(y)| \leq C$ ;  $y \neq 0$ .

In the above conditions, the letter  $\alpha$  denotes multiindices. Note that (1.18) and (1.19) with  $v_{ij}(y) = q_i q_j |y|^{-1}$  conform with Condition 1.5 for any  $k_0$ .

Introducing the inner product  $x \cdot y = \sum_i 2m_i x_i \cdot y_i$  for  $x = (x_1, \dots, x_N)$ ,  $y = (y_1, \dots, y_N) \in \mathbb{R}^{3N}$  we can split

$$\mathbb{R}^{3N} = X_{\text{CM}} \oplus X; \quad X_{\text{CM}} = \{x \in \mathbb{R}^{3N} \mid x_1 = \dots = x_N\}.$$

There is a corresponding splitting

$$\tilde{h}(t) = h_{\text{CM}}(t) \otimes I + I \otimes h(t), \quad \text{on } L^2(X_{\text{CM}}) \otimes L^2(X),$$

where

$$h_{\text{CM}}(t) = p_{\text{CM}}^2 - \mathcal{E}_{\text{CM}}(t) \cdot x, \quad \text{and } h(t) = p^2 - \mathcal{E}(t) \cdot x + V.$$

Here

$$\mathcal{E}_{\text{CM}} = \frac{Q}{2M} (\tilde{\mathcal{E}}, \dots, \tilde{\mathcal{E}}) \quad \text{and } \mathcal{E} = \left( \left( \frac{q_1}{2m_1} - \frac{Q}{2M} \right) \tilde{\mathcal{E}}, \dots, \left( \frac{q_N}{2m_N} - \frac{Q}{2M} \right) \tilde{\mathcal{E}} \right),$$

where  $Q = q_1 + \dots + q_N$  and  $M = m_1 + \dots + m_N$  are the total charge and mass of the system, respectively. In the special case where all the particles have identical charge to mass ratio, we see that the center of mass Hamiltonian is just an ordinary time-independent  $N$ -body Hamiltonian. Otherwise the Hamiltonian  $h(t)$  depends non-trivially on the time-variable

$t$ . We denote by  $\tilde{U}(t, s)$ ,  $U_{\text{CM}}(t, s)$  and  $U(t, s)$  the dynamics generated by  $\tilde{h}(t)$ ,  $h_{\text{CM}}(t)$  and  $h(t)$ , respectively, and observe that

$$\tilde{U}(t, s) = U_{\text{CM}}(t, s) \otimes U(t, s).$$

We shall address spectral properties of the *monodromy operator*  $U(1, 0)$ . Note that this is a unitary operator on  $L^2(X)$ . Let  $\mathcal{A}$  be the set of all cluster partitions  $a = \{C_1, \dots, C_{\#a}\}$ ,  $1 \leq \#a \leq N$ , each given by splitting the set of particles  $\{1, \dots, N\}$  into non-empty disjoint clusters  $C_i$ . The spaces  $X_a$ ,  $a \in \mathcal{A}$ , are the spaces of configurations of the  $\#a$  centers of mass of the clusters  $C_i$  (in the center of mass frame). The complement

$$X^a = X^{C_1} \oplus \dots \oplus X^{C_{\#a}}$$

is the space of relative configurations within each of the clusters  $C_i$ . More precisely

$$X^{C_i} = \{x \in X \mid x_j = 0, j \notin C_i\} \text{ and } X_a = \{x \in X \mid k, l \in C_i \Rightarrow x_k = x_l\}.$$

We will write  $x^a$  and  $x_a$  for the orthogonal projection of a vector  $x$  onto the subspace  $X^a$  and its orthogonal complement respectively. Notice the natural ordering on  $\mathcal{A}$ :  $a \subset b$  if and only if any cluster  $C \in a$  is contained in some cluster  $C' \in b$ . Clearly the minimal and maximal elements are  $a_{\min} = \{(1), \dots, (N)\}$  and  $a_{\max} = \{(1, \dots, N)\}$ , respectively. Any pair  $(i, j)$  defines an  $N - 1$  cluster decomposition  $(ij) \in \mathcal{A}$  by letting  $C = \{i, j\}$  constitute a cluster and all others being one-particle clusters.

For each  $a \neq a_{\max}$  the sub-Hamiltonian monodromy operator is  $U^a(1, 0)$ ; it is defined as the monodromy operator on  $\mathcal{H}^a = L^2(X^a)$  constructed for  $a \neq a_{\min}$  from  $h^a = (p^a)^2 - \mathcal{E}(t)^a \cdot x^a + V^a$ ,  $V^a = \sum_{(ij) \subset a} v_{ij}(x_i - x_j)$ . If  $a = a_{\min}$  we define  $U^a(1, 0) = \mathbb{1}$  (implying  $\sigma_{\text{pp}}(U^{a_{\min}}(1, 0)) = \{1\}$ ). The condition  $\int_0^1 \mathcal{E}(t) dt = 0$  leads to the existence of a unique 1-periodic function  $b$  such that

$$\frac{d}{dt} b(t) = \mathcal{E}(t) \text{ and } \int_0^1 b(t) dt = 0.$$

The set of *thresholds* is

$$\mathcal{F}(U(1, 0)) = \bigcup_{a \neq a_{\max}} e^{-i\alpha_a} \sigma_{\text{pp}}(U^a(1, 0)); \quad \alpha_a = \int_0^1 |b(t)_a|^2 dt. \quad (1.20)$$

We recall from [MS] that the set of thresholds is closed and countable, and non-threshold eigenvalues, i.e. points in  $\sigma_{\text{pp}}(U(1, 0)) \setminus \mathcal{F}(U(1, 0))$ , have finite multiplicity and can only accumulate at the set of thresholds. Moreover any corresponding bound state is exponentially decaying, the singular continuous spectrum  $\sigma_{\text{sc}}(U(1, 0)) = \emptyset$  and there are integral propagation estimates for states localized away from the set of eigenvalues and away from  $\mathcal{F}(U(1, 0))$ . These properties are known under Condition 1.5 with  $k_0 = 1$ . For completeness of presentation we mention that some of the results of [MS] hold under more general conditions, in particular the exponential decay result does not require that the Coulomb singularity of each pair-potential (if present) is located at the origin (this applies to Born-Oppenheimer molecules in an AC-Stark field).

Letting

$$A(t) = \frac{1}{2}(x \cdot (p - b(t)) + (p - b(t)) \cdot x), \quad (1.21)$$

and using a different frame, we prove in Section 6

**Theorem 1.6.** *Suppose Conditions 1.5, for some  $k_0 \in \mathbb{N}$ . Let  $\phi$  be a bound state for  $U(1,0)$  pertaining to an eigenvalue  $e^{-i\lambda} \notin \mathcal{F}(U(1,0))$ . Then*

- (1)  $\phi \in \mathcal{D}(A(1)^{k_0})$  where  $A(t)$  is given by (1.21).
- (2) If for all pairs  $(i, j)$  the term  $v_{ij}^2 = 0$  then  $\phi \in \mathcal{D}(|p|^{k_0+1})$ .

The result (1) is new for  $k_0 > 1$  while it is essentially contained in [MS] for  $k_0 = 1$ , see [MS, Proposition 8.7 (ii)]. We remark that the highest degree of smoothness known in general in the case  $v_{ij}^2 \neq 0$  is  $\phi \in \mathcal{D}(|p|)$ , cf. [MS, Theorem 1.8]. This holds without the non-threshold condition. The result (2) overlaps with [KY, Theorem 1.2], when  $N = 2$  and “ $k_0 = \infty$ ”.

## 2 Assumptions and Statement of Regularity Results

For a self-adjoint operator  $A$  on a Hilbert space  $\mathcal{H}$ , we will make use of the  $C^1(A)$  class of operators. This class consists a priori of bounded operators  $B$  with the property that  $[B, A]$  extends from a form on  $\mathcal{D}(A)$  to a bounded form on  $\mathcal{H}$ . The class is (consistently) extended to self-adjoint operators  $H$ , by requiring that  $(H - z)^{-1}$  is of class  $C^1(A)$ , for some (and hence all)  $z \in \rho(H)$ , the resolvent set of  $H$ . We will use the notation  $H \in C^1(A)$  to indicate that an operator  $H$  is of class  $C^1(A)$ .

If  $H$  is of class  $C^1(A)$  then  $\mathcal{D}(H) \cap \mathcal{D}(A)$  is dense in  $\mathcal{D}(H)$  and the form  $[H, A]$  extends by continuity from the form domain  $\mathcal{D}(H) \cap \mathcal{D}(A)$  to a bounded form on  $\mathcal{D}(H)$ . The extension is denoted by  $[H, A]^0$ , and is also interpreted as an element of  $\mathcal{B}(\mathcal{D}(H), \mathcal{D}(H)^*)$ . If in addition  $[H, A]^0$  extends by continuity to an element of  $\mathcal{B}(\mathcal{D}(H), \mathcal{H})$ , then we say it is of class  $C_{\text{Mo}}^1(A)$ . Note that being of class  $C_{\text{Mo}}^1(A)$  is equivalent to having the conditions of Mourre [Mo] satisfied for the first commutator. See [GG].

**Conditions 2.1.** Let  $\mathcal{H}$  be a complex Hilbert space. Suppose there are given some self-adjoint operators  $H, A$  and  $N$  as well as a symmetric operator  $H'$  with  $\mathcal{D}(H') = \mathcal{D}(N)$ . Suppose  $N \geq \mathbb{1}$ . Let  $R(\eta) = (A - \eta)^{-1}$  for  $\eta \in \mathbb{C} \setminus \mathbb{R}$ .

- (1) The operator  $N$  is of class  $C_{\text{Mo}}^1(A)$ . We abbreviate  $N' = i[N, A]^0$ .
- (2) The operator  $N$  is of class  $C^1(H)$ , and there exists  $0 < \kappa \leq \frac{1}{2}$  such that the commutator obeys

$$i[N, H]^0 \in \mathcal{B}(N^{-\frac{1}{2}+\kappa}\mathcal{H}, N^{\frac{1}{2}-\kappa}\mathcal{H}). \quad (2.1)$$

- (3) There exists a (large)  $\sigma > 0$  such that for all  $\eta \in \mathbb{C}$  with  $|\text{Im} \eta| \geq \sigma$  we have as a form on  $\mathcal{D}(H) \cap \mathcal{D}(N^{1/2})$

$$i[H, R(\eta)] = -R(\eta)H'R(\eta). \quad (2.2)$$

(Here it should be noticed that  $N^{-1/2}H'N^{-1/2}$  and  $N^{\mp 1/2}R(\eta)N^{\pm 1/2}$  are bounded if  $\sigma$  is large enough, cf. Remark 2.4 1.)

- (4) The commutator form  $i[H', A]$  defined on  $\mathcal{D}(A) \cap \mathcal{D}(N)$  extends to a bounded operator

$$H'' := i[H', A]^0 \in \mathcal{B}(N^{-\frac{1}{2}}\mathcal{H}, N^{\frac{1}{2}}\mathcal{H}). \quad (2.3)$$

**Condition 2.2.** There are constants  $C_1, C_2, C_3 \in \mathbb{R}$  such that as a form on  $\mathcal{D}(H) \cap \mathcal{D}(N^{1/2})$

$$N \leq C_1 H + C_2 H' + C_3 \mathbb{1}. \quad (2.4)$$

**Condition 2.3.** For a given  $\lambda \in \mathbb{R}$  there exist  $c_0 > 0$ ,  $C_4 \in \mathbb{R}$ ,  $f_\lambda \in C_c^\infty(\mathbb{R})$  with  $0 \leq f_\lambda \leq 1$  and  $f_\lambda = 1$  in a neighborhood of  $\lambda$ , and a compact operator  $K_0$  on  $\mathcal{H}$  such that as a form on  $\mathcal{D}(H) \cap \mathcal{D}(N^{1/2})$

$$H' \geq c_0 \mathbb{1} - C_4 f_\lambda^\perp(H)^2 \langle H \rangle - K_0. \quad (2.5)$$

Here  $f_\lambda^\perp := 1 - f_\lambda$ .

**Remarks 2.4.** 1) It follows from Condition 2.1 (1) and an argument of Mourre [Mo, Proposition II.3], that there exists  $\sigma > 0$  such that for  $|\operatorname{Im} \eta| \geq \sigma$  we have  $(A - \eta)^{-1} : \mathcal{D}(N) \subseteq \mathcal{D}(N)$  and  $(A - \eta)^{-1} \mathcal{D}(N)$  is dense in  $\mathcal{D}(N)$ . By interpolation the same holds with  $N$  replaced by  $N^\alpha$ ,  $0 < \alpha < 1$ , cf. Lemma 3.4 below.

2) From Condition 2.1 (2) and Lemma 3.2 it follows that  $N^{1/2}$  is of class  $C_{\text{Mo}}^1(H)$ . In particular  $\mathcal{D}(H) \cap \mathcal{D}(N^{1/2})$  is dense in  $\mathcal{D}(N^{1/2})$ .

3) Combining the above two remarks with Condition 2.1 (3) and (3.14), we find that given  $H$ ,  $A$  and  $N$ , there can at most be one  $H'$  such that Condition 2.1 (1), (2), and (3) are satisfied.

4) We remark that in practice we work with the weaker commutator estimate

$$H' \geq c_0 \mathbb{1} - \operatorname{Re} \{B(H - \lambda)\} - K_0, \quad (2.6)$$

where  $B = B(\lambda)$  is a bounded operator, with  $B\mathcal{D}(N^{1/2}) \cup B^*\mathcal{D}(N^{1/2}) \subseteq \mathcal{D}(N^{1/2})$ . The one in Condition 2.3 is however more standard. To see that Condition 2.3 implies the above bound choose  $B = C_4 f_\lambda^\perp(H)^2 \langle H \rangle (H - \lambda)^{-1}$  which under our Condition 2.1 satisfies the requirements on  $B$  by Lemma 3.3.

We call  $H'$  the *first derivative* of  $H$ . Similarly  $H''$  is the *second derivative* of  $H$ . The estimate (2.4) is called the *virial estimate*, while (2.5) is the *Mourre estimate* at  $\lambda$ .

**Theorem 2.5.** *Suppose Conditions 2.1, 2.2 and 2.3, and let  $\psi$  be a bound state,  $(H - \lambda)\psi = 0$  (with  $\lambda$  as in Condition 2.3), obeying*

$$\psi \in \mathcal{D}(N^{\frac{1}{2}}). \quad (2.7)$$

*Then  $\psi \in \mathcal{D}(A)$  and  $A\psi \in \mathcal{D}(N^{1/2})$ .*

By imposing assumptions on higher-order commutators between  $H$  and  $A$  we obtain a higher-order regularity result. For this we need the following condition, which coincides with Condition 2.1 (4) if  $k_0 = 1$ , but for  $k_0 \geq 2$  it is stronger.

**Condition 2.6.** There exists  $k_0 \in \mathbb{N}$  such that the commutator forms  $i^\ell \operatorname{ad}_A^\ell(H')$  defined on  $\mathcal{D}(A) \cap \mathcal{D}(N)$ ,  $\ell = 0, \dots, k_0$ , extend to bounded operators

$$i^\ell \operatorname{ad}_A^\ell(H') \in \mathcal{B}(N^{-1} \mathcal{H}, \mathcal{H}); \quad \ell = 0, \dots, k_0 - 1. \quad (2.8)$$

$$i^{k_0} \operatorname{ad}_A^{k_0}(H') \in \mathcal{B}(N^{-\frac{1}{2}} \mathcal{H}, N^{\frac{1}{2}} \mathcal{H}). \quad (2.9)$$

We have the following extension of Theorem 2.5 to include higher orders

**Theorem 2.7.** *Suppose Conditions 2.1–2.3 and Condition 2.6, and let  $\psi$  be a bound state,  $(H - \lambda)\psi = 0$  (with  $\lambda$  as in Condition 2.3), obeying (2.7). Let  $k_0$  be given as in Condition 2.6. Then  $\psi \in \mathcal{D}(A^{k_0})$ , and for  $k = 1, \dots, k_0$  the states  $A^k \psi \in \mathcal{D}(N^{1/2})$ .*

It should be noted that under the assumptions imposed in Theorem 2.5 and Theorem 2.7, it is crucial that  $N^{1/2}$  is applied *after* the powers of  $A$ . The following result requires an additional assumption, and allows for arbitrary placement of  $N^{1/2}$  amongst the at most  $k_0$  powers of  $A$ . The new condition (2.10) below is a generalization of Condition 2.1 (1).

**Condition 2.8.** Let  $N'$  be given as in Condition 2.1 (1). There exists  $k_0 \in \mathbb{N}$  such that the commutator forms  $i^\ell \text{ad}_A^\ell(N')$  defined on  $\mathcal{D}(A) \cap \mathcal{D}(N)$ ,  $\ell = 0, \dots, k_0 - 1$ , extend to bounded operators

$$i^\ell \text{ad}_A^\ell(N') \in \mathcal{B}(N^{-1}\mathcal{H}, \mathcal{H}); \ell = 0, \dots, k_0 - 1. \quad (2.10)$$

Moreover there exists  $\kappa_1 > 0$  such that the commutators (initially defined as forms on  $\mathcal{D}(N)$ )

$$i \text{ad}_N(i^\ell \text{ad}_A^\ell(N')) \in \mathcal{B}(N^{-1}\mathcal{H}, N^{1-\kappa_1}\mathcal{H}); \ell = 0, \dots, k_0 - 1. \quad (2.11)$$

We have

**Corollary 2.9.** *Suppose Conditions 2.1–2.3, 2.6 and 2.8 (with the same  $k_0$  in Conditions 2.6 and 2.8). Let  $\psi \in \mathcal{D}(N^{1/2})$  be a bound state,  $(H - \lambda)\psi = 0$  (with  $\lambda$  as in Condition 2.3). For any  $k, \ell \geq 0$ , with  $k + \ell \leq k_0$ , we have  $\psi \in \mathcal{D}(A^k N^{1/2} A^\ell)$ .*

We end with the following improvement of Theorem 2.5, which concludes in addition that bound states are in the domain of  $N$ . It requires the added assumption (2.11), with  $k_0 = 1$ .

**Theorem 2.10.** *Suppose Conditions 2.1–2.3 and (2.11) for  $k_0 = 1$ , and let  $\psi \in \mathcal{D}(N^{1/2})$  be a bound state  $(H - \lambda)\psi = 0$  (with  $\lambda$  as in Condition 2.3). Then  $\psi \in \mathcal{D}(N)$ , the states  $\psi, N^{1/2}\psi \in \mathcal{D}(A)$  and  $A\psi \in \mathcal{D}(N^{1/2})$ .*

In Subsection 4.3 we in fact prove an extension of the above theorem, to include higher order estimates in  $N$ . These are applied in Section 6 to many-body AC-Stark Hamiltonians.

**Remarks 2.11.** 1) The condition that  $N \geq \mathbb{1}$  is imposed partly for convenience of formulation. Obviously one can obtain a version of the above results upon imposing only that  $N$  is bounded from below (upon “translating”  $N \rightarrow N + C \geq \mathbb{1}$  at various points in the above conditions).

2) The ‘standard’ or ‘regular’ Mourre theory, considered for example in [CGH], fits in the semi-bounded case into the above scheme so that Theorem 2.7 holds. In fact (assuming here for simplicity that  $H$  is bounded from below) we have  $N := H + C \geq \mathbb{1}$  for a sufficiently large constant  $C$ . Use this  $N$  and the same ‘conjugate operator’  $A$  in Conditions 2.1 – 2.3, 2.6 and 2.8. Note also that the standard Mourre estimate at energy  $\lambda$  reads

$$f_\lambda(H) i[H, A]^0 f_\lambda(H) \geq c'_0 f_\lambda^2(H) - K'_0; \quad c'_0 > 0, \quad K'_0 \text{ compact}. \quad (2.12)$$

From (2.12) we readily conclude (2.5) with  $c_0 = c'_0/2$ ,  $K_0 = K'_0$  an a suitable constant  $C_4 \geq 0$ .

Although we shall not elaborate we also remark that the method of proof of Theorem 2.7 essentially can be adapted under the conditions of the standard Mourre theory, in fact only a simplified version is needed. Whence although we can not literately conclude from Theorem 2.7 in the general non-semi-bounded case the result  $\psi \in \mathcal{D}(A^{k_0})$  is still valid given standard conditions on repeated commutators  $i^k \text{ad}_A^k(H)$  for  $k \leq k_0 + 1$ .

- 3) Theorem 2.7 does *not* hold with one less commutator in Condition 2.6. Alternatively, under the conditions of Theorem 2.7 it is in general *false* that the bound state  $\psi \in \mathcal{D}(A^{k_0+1})$ . Based on considerations for discrete eigenvalues this statement may at a first thought appear surprising. See Example 1.1. Compared to [CGH] our method works with one less commutator, cf. 2), although the overall scheme of ours and the one of [CGH] are similar.
- 4) The proofs of Theorems 2.5 and 2.7, Corollary 2.9 and Theorem 2.10 are constructive in that they yield explicit bounds. Precisely, if we have a positive lower bound of the constant  $c_0$  in (2.5) that is uniform in  $\lambda$  belonging to some fixed compact interval  $I$  as well as uniform bounds of the absolute value of the constants  $C_1, \dots, C_4$  of (2.4) and (2.5) (uniform in the same sense) and similarly for all possible operator norms related to Conditions 2.1, 2.6 and 2.8 (and the  $B(\lambda)$  in Remark 2.4 if it is used) then there are bounds of the form, for example,

$$\|N^{\frac{1}{2}}A^k\psi\| \leq C\|N^{\frac{1}{2}}\psi\|; \quad C = C(k, I, K_0);$$

here  $K_0 = K_0(\lambda)$  is the compact operator of (2.5) and  $k \leq k_0$ . Similar bounds are valid for the states  $A^k N^{1/2} A^\ell \psi$  of Corollary 2.9 and for the state  $N\psi$  of Theorem 2.10. In the context of perturbation theory typically  $I$  will be a small interval centered at some (unperturbed) embedded eigenvalue  $\lambda_0$  and  $K_0 = K_0(\lambda_0)$ . Whence the constant will depend only on the interval. For various models one can verify the condition (2.7) for all bound states  $\psi$  by a ‘virial argument’, cf. [GGM2, MS, Sk], along with a similar bound

$$\|N^{\frac{1}{2}}\psi\| \leq C(I)\|\psi\|.$$

This virial argument is in a concrete situation related to the virial estimate (2.4). Clearly the above bounds can be used in combination, and this is precisely how we in Section 5 arrive at the Theorems 1.2 and 1.3. In [MW] the case of regular Mourre theory is considered where the derivation of the bounds is simpler, and care is taken to derive good explicit bounds, which in particular are independent of any proof technical constructions. The bounds are good enough to formulate a reasonable condition on the growth of norms of multiple commutators which ensures that bound states are analytic vectors with respect to  $A$ .

### 3 Preliminaries

In this section we establish basic consequences of Conditions 2.1, and introduce a calculus of almost analytic extensions tailored to avoid issues with  $(A - \eta)^{-1}$ , when  $|\operatorname{Im} \eta|$  is small.

#### 3.1 Improved Smoothness for Operators of Class $C^1(A)$

For an operator  $N$  of class  $C^1(A)$  not much in the way of regularity can be expected, beyond the  $C^1(A)$  property itself, and its equivalent formulations. See [ABG, GGM1]. Often one requires some additional smoothness properties to manipulate and estimate expressions in the two operators. The typical way of achieving improved smoothness is to impose conditions on  $i[N, A]^0$  stronger than what is implied by the  $C^1(A)$  property itself. This is what is done in Condition 2.1 (1) and (2).

This subsection is devoted primarily to the extraction of improved smoothness properties of the pair of operators  $N, H$ , afforded to us by Conditions 2.1.

**Lemma 3.1.** *Let  $N \geq \mathbb{1}$  be of class  $C^1(H)$  with*

$$[N, H]^0 \in \mathcal{B}(N^{-1/2}\mathcal{H}, N^{1/2}\mathcal{H}).$$

*For any  $\alpha \in ]0, 1[$ , the operator  $N^\alpha$  is of class  $C^1(H)$ .*

*Proof.* Let  $0 < \alpha < 1$ . It suffices to check for one  $\eta \in \rho(N^\alpha)$  that  $(N^\alpha - \eta)^{-1}$  is of class  $C^1(H)$ . To this end we pick  $\eta = 0$ , and use the representation formula

$$N^{-\alpha} = c_\alpha \int_0^\infty t^{-\alpha} (N+t)^{-1} dt, \quad c_\alpha = \frac{\sin(\alpha\pi)}{\pi}. \quad (3.1)$$

Since  $N \in C^1(H)$  we have for all  $t > 0$  that the operator  $(N+t)^{-1}$  preserves  $\mathcal{D}(H)$ . In fact

$$[H, (N+t)^{-1}]\phi = (N+t)^{-1}[N, H]^0(N+t)^{-1}\phi; \quad \phi \in \mathcal{D}(H). \quad (3.2)$$

By combining (3.1) and (3.2) we can compute  $[N^{-\alpha}, H]$  considered as a form on  $\mathcal{D}(H)$  as

$$[N^{-\alpha}, H] = c_\alpha \int_0^\infty t^{-\alpha} (N+t)^{-1} [N, H]^0 (N+t)^{-1} dt. \quad (3.3)$$

Notice that the integral is absolutely convergent for any  $0 < \alpha < 1$ . This completes the proof.  $\square$

**Lemma 3.2.** *Assume  $N \geq \mathbb{1}$  and  $H$  satisfy Condition 2.1 (2) and let  $\alpha \in ]0, 1[$ . Then  $N^\alpha \in C^1(H)$  and for  $\tau_1, \tau_2 \geq 0$ , with*

$$\max\{0, \frac{1}{2} - \kappa - \tau_1\} + \max\{0, \frac{1}{2} - \kappa - \tau_2\} < 1 - \alpha,$$

*we have  $[N^\alpha, H]^0 \in \mathcal{B}(N^{-\tau_1}\mathcal{H}, N^{\tau_2}\mathcal{H})$ . In particular  $N^{1/2}$  is of class  $C_{\text{Mo}}^1(H)$ .*

*Proof.* That  $N^\alpha \in C^1(H)$  follows from Lemma 3.1. We compute as a form on  $\mathcal{D}(N^\alpha) \cap \mathcal{D}(H)$

$$[N^\alpha, H] = c_\alpha \int_0^\infty t^\alpha (N+t)^{-1} [N, H]^0 (N+t)^{-1} dt, \quad (3.4)$$

where we have used the strongly convergent integral representation formula

$$N^\alpha = c_\alpha \int_0^\infty t^\alpha (t^{-1} - (N+t)^{-1}) dt, \quad (3.5)$$

which follows from (3.1). We thus get for  $\tau_1, \tau_2 \geq 0$

$$\begin{aligned} |\langle \psi, [N^\alpha, H]\varphi \rangle| &\leq C \int_0^\infty t^\alpha \|(N+t)^{-1} N^{\frac{1}{2}-\kappa-\tau_1}\| \|(N+t)^{-1} N^{\frac{1}{2}-\kappa-\tau_2}\| dt \\ &\quad \times \|N^{\tau_1}\psi\| \|N^{\tau_2}\varphi\|. \end{aligned}$$

The integrand is of the order  $O(t^{\alpha-2+\theta})$ , with  $\theta = \max\{0, \frac{1}{2} - \kappa - \tau_1\} + \max\{0, \frac{1}{2} - \kappa - \tau_2\}$ . It is integrable provided  $\theta < 1 - \alpha$ , which proves the lemma.  $\square$

We shall need a boundedness result:

**Lemma 3.3.** *Assume  $N \geq \mathbb{1}$  and  $H$  satisfy Condition 2.1 (2) and let  $\alpha \in ]0, 1/2 + \kappa[$ . Suppose  $f \in C^\infty(\mathbb{R})$  is given such that*

$$\frac{d^k}{dt^k} f(t) = O(\langle t \rangle^{-k}); \quad k = 0, 1, \dots$$

*Then*

$$N^\alpha f(H) N^{-\alpha} \in \mathcal{B}(\mathcal{H}). \quad (3.6)$$

*Proof.* Let  $\rho \in ]0, 1/2 + \kappa[$ , where  $0 < \kappa \leq 1/2$  comes from Condition 2.1 (2). From Lemma 3.2 applied with  $\tau_1 = \max\{0, \rho - \kappa\}$  and  $\tau_2 = 0$ , we get

$$[N^\rho, H]^0 \in \mathcal{B}(N^{-\max\{0, \rho - \kappa\}} \mathcal{H}, \mathcal{H}). \quad (3.7)$$

We recall from [Mo, Proposition II.3] that if an operator  $\tilde{N}$  is of class  $C_{\text{Mo}}^1(H)$ , then

$$\begin{aligned} \exists \sigma > 0 : |\text{Im } \eta| \geq \sigma &\Rightarrow (H - \eta)^{-1} \text{ preserves } \mathcal{D}(\tilde{N}) \text{ and} \\ \tilde{N}(H - \eta)^{-1} \psi &= (H - \eta)^{-1} \tilde{N} \psi \\ + i(H - \eta)^{-1} i[\tilde{N}, H]^0 (H - \eta)^{-1} \psi &\text{ for all } \psi \in \mathcal{D}(\tilde{N}). \end{aligned} \quad (3.8)$$

We apply this to  $\tilde{N} = N^\rho$ ,  $0 < \rho < 1/2 + \kappa$ . The assumption is satisfied by (3.7).

We shall show a representation formula for the special case  $f(x) = f_\eta(x) = (x - \eta)^{-1}$  with  $v = \text{Im } \eta \neq 0$ . Now fix  $\alpha \in ]0, 1/2 + \kappa[$ . Using (3.7) and (3.8), multiple times with  $\rho = \alpha - j\kappa$ , we obtain for  $|\text{Im } \eta|$  sufficiently large and for all  $\psi \in \mathcal{D}(N^\alpha)$

$$\begin{aligned} N^\alpha (H - \eta)^{-1} \psi - (H - \eta)^{-1} N^\alpha \psi \\ = \sum_{j=1}^n ((H - \eta)^{-1} B_1) \cdots ((H - \eta)^{-1} B_j) (H - \eta)^{-1} N^{\alpha - j\kappa} \psi \\ + ((H - \eta)^{-1} B_1) \cdots ((H - \eta)^{-1} B_n) ((H - \eta)^{-1} B_{n+1}) (H - \eta)^{-1} \psi, \end{aligned} \quad (3.9)$$

where  $n$  is the biggest natural number for which  $\alpha - n\kappa > 0$  and the  $B_j$ 's are bounded and independent of  $\eta$ . Next by analytic continuation we conclude that (3.9) is valid for all  $\eta \in \mathbb{C} \setminus \mathbb{R}$ . Hence we have verified the adjoint version of (3.6) for  $f = f_\eta$ ;  $v \neq 0$ .

We shall now show (3.6) in general. Define a new function by  $h(t) = f(t)(t + i)^{-1}$ , and let  $\tilde{h}$  denote an almost analytic extension of  $h$  such that (using the notation  $\eta = u + iv$ )

$$\forall n \in \mathbb{N} : |\partial \tilde{h}(\eta)| \leq C_n \langle \eta \rangle^{-n-2} |v|^n.$$

We shall use the representation

$$\begin{aligned} f(H) &= \frac{1}{\pi} \int_{\mathbb{C}} (\partial \tilde{h})(\eta) (H - \eta)^{-1} (H + i) du dv \\ &= \frac{1}{\pi} \int_{\mathbb{C}} (\partial \tilde{h})(\eta) (\mathbb{1} + (\eta + i)(H - \eta)^{-1}) du dv, \end{aligned} \quad (3.10)$$

which should be read as a strong integral on  $\mathcal{D}(H)$ . We multiply by  $N^\alpha$  and  $N^{-\alpha}$  from the left and from the right, respectively. Inserting (3.9) we conclude the lemma. Observe that  $N^{-\alpha}$  being  $C^1(H)$  preserves  $\mathcal{D}(H)$ .  $\square$

It will be important to work with the following ‘regularization’ operators, cf. [Mo]: Let for any given self-adjoint operator  $\tilde{A}$  and any positive operator  $\tilde{N}$

$$I_n(\tilde{A}) = -in(\tilde{A} - in)^{-1} \text{ and } I_{in}(\tilde{N}) = n(\tilde{N} + n)^{-1}; \quad n \in \mathbb{N}. \quad (3.11)$$

In particular we shall use  $I_n(A)$  in conjunction with (2.2),  $I_n(H)$  in conjunction with (2.2), (2.4) and (2.5), while  $I_{in}(N)$  will be used in conjunction with (2.1).

**Lemma 3.4.** *Assume the pairs  $N, A$  and  $N, H$  satisfy Conditions 2.1 (1) and (2) respectively. Then*

$$s\text{-}\lim_{n \rightarrow \infty} N^{\frac{1}{2}} I_n(H) N^{-\frac{1}{2}} = \mathbb{1} \quad (3.12)$$

$$s\text{-}\lim_{n \rightarrow \infty} N I_n(A) N^{-1} = \mathbb{1} \quad (3.13)$$

$$s\text{-}\lim_{n \rightarrow \infty} N^{\frac{1}{2}} I_n(A) N^{-\frac{1}{2}} = \mathbb{1}. \quad (3.14)$$

*Proof.* Observe first that  $s\text{-}\lim I_n(A) = \mathbb{1}$  and  $s\text{-}\lim A(A - in)^{-1} = 0$ , and similarly with  $A$  replaced by  $H$ . The statements (3.12) and (3.13) now follows from (3.8) and boundedness of the operators  $[N^{1/2}, H]^0 N^{-1/2}$  and  $[N, A]^0 N^{-1}$ . This argument appears also in [Mo].

As for (3.14) we observe first that  $N(I_n(A) - \mathbb{1})N^{-1}$  is bounded uniformly in  $n$ . By interpolation the same holds true for  $N^{1/2}(I_n(A) - \mathbb{1})N^{-1/2}$ . The result now follows from observing that the result holds true strongly on the dense set  $\mathcal{D}(N^{1/2})$  by (3.13).  $\square$

We end with a small technical remark

**Remark 3.5.** Suppose  $N$  and  $H$  are as in Lemma 3.1 and  $0 \leq \alpha < 1$ . Then  $\mathcal{D}(H) \cap \mathcal{D}(N)$  is dense in  $\mathcal{D}(H) \cap \mathcal{D}(N^\alpha)$  in the intersection topology.

To see this let  $\psi \in \mathcal{D}(H) \cap \mathcal{D}(N^\alpha)$ . Then  $\psi_n = I_{in}(N)\psi \in \mathcal{D}(H) \cap \mathcal{D}(N)$  since  $N$  is of class  $C^1(H)$ . We claim that  $\psi_n \rightarrow \psi$  in  $\mathcal{D}(H) \cap \mathcal{D}(N^\alpha)$ . Obviously  $N^\alpha \psi_n \rightarrow N^\alpha \psi$ , so it remains to consider

$$H\psi_n = I_{in}(N)H\psi + \sqrt{\frac{N}{n}}I_{in}(N)(N^{-\frac{1}{2}}[N, H]^0 N^{-\frac{1}{2}})\sqrt{\frac{N}{n}}I_{in}(N)\psi.$$

As in the proof above, the last term goes to zero and the first term converges to  $H\psi$  proving the claim.

### 3.2 Iterated commutators with $N^{1/2}$

We address here the following question. Supposing Condition 2.1 (1) and (2.10) is satisfied for some  $k_0 \geq 1$ . One could reasonably assume that  $N^{1/2}$  is also of class  $C_{\text{Mo}}^1(A)$  and admits  $k_0$  iterated  $N^{1/2}$ -bounded commutators. We have however not been able to establish this, but making the additional assumption (2.11) we answer the question in the affirmative below. This permits us to deduce Corollary 2.9 from Theorem 2.7. The reader primarily interested in Theorem 2.7 may skip this subsection.

We begin with a technical lemma. Let  $q \in \mathbb{N}$  and  $\underline{\ell} \in (\mathbb{N} \cap \{0\})^q$ , with  $0 \leq \ell_j < k_0$  for all  $j = 1, \dots, q$ . We abbreviate  $N'_m = i^m \text{ad}_A^m(N')$ , which is the iteratively defined  $N$ -bounded operator from (2.10). Let for  $t \geq 0$  and  $q, \underline{\ell}$  as above

$$4B_q^{\underline{\ell}}(t) = t^{\frac{1}{2}} \left( \prod_{j=1}^q (N+t)^{-1} N'_{\ell_j} \right) (N+t)^{-1}. \quad (3.15)$$

Observe that  $B_q^{\underline{\ell}}(t)$  is bounded for all  $t$ . Indeed it satisfies the bound  $B_q^{\underline{\ell}}(t) = O(t^{-1/2})$  and is thus not norm integrable. However if  $\varphi \in \mathcal{D}(N)$  we have  $B_q^{\underline{\ell}}(t)\varphi = O(t^{-3/2})$ . The extra assumption (2.11) allows us to prove

**Lemma 3.6.** *Suppose Condition 2.1 (1) and Condition 2.8. For any  $q \in \mathbb{N}$ ,  $\underline{\ell} \in (\mathbb{N} \cup \{0\})^q$  (with  $0 \leq \ell_j < k_0$  as above) and  $\varphi \in \mathcal{D}(N)$  the map  $t \rightarrow B_q^{\underline{\ell}}(t)\varphi$  is integrable and there exist constants  $C_q^{\underline{\ell}}$  such that*

$$\left\| \int_0^\infty B_q^{\underline{\ell}}(t)\varphi dt \right\| \leq C_q^{\underline{\ell}} \|N^{\frac{1}{2}}\varphi\|.$$

*Proof.* We only have to prove the bound on the strong integral, since we already discussed strong integrability. We begin by analyzing the leftmost factors in  $B_q^{\underline{\ell}}(t)$ , namely the  $N$ -bounded operator  $(N+t)^{-1}N'_{\ell_1}$ .

We compute strongly on  $\mathcal{D}(N)$

$$\begin{aligned} (N+t)^{-1}N'_{\ell_1} &= (N'_{\ell_1}N^{-1})N(N+t)^{-1} \\ &\quad - (N+t)^{-1}N(N^{-1}[N, N'_{\ell_1}]N^{-1+\kappa_1})N^{1-\kappa_1}(N+t)^{-1} \\ &= (N'_{\ell_1}N^{-1})N(N+t)^{-1} + O(t^{-\kappa_1}). \end{aligned} \quad (3.16)$$

The contribution to the integral  $\int_0^\infty B_q^\ell(t)N^{-1/2}dt$  coming from the last term is  $O(t^{-1-\kappa_1})$  and hence norm-integrable.

If  $q = 1$  we can now finish the argument because the contribution to the integral coming from the first term on the right-hand side of (3.16) is

$$(N'_{\ell_1}N^{-1})t^{\frac{1}{2}}(N+t)^{-2}N,$$

which on the domain of  $N$  integrates to the  $N^{1/2}$ -bounded operator  $cN'_{\ell_1}N^{-1/2}$ , for some  $c \in \mathbb{R}$ .

If  $q > 1$  we write  $N(N+t)^{-1} = \mathbb{1} - t(N+t)^{-1}$ . We can now bring out the next term  $N'_{\ell_2}$ , and again the commutators with  $(N+t)^{-1}$  give norm-integrable contributions. Repeating this procedure successively until all the terms  $N'_{\ell_j}$  are brought out to the left yields the formula

$$B_q^\ell(t) = \left( \prod_{j=1}^q N'_{\ell_j}N^{-1} \right) t^{\frac{1}{2}} (\mathbb{1} - t(N+t)^{-1})^{q-1} (N+t)^{-2}N + O(t^{-1-\kappa_1})N^{\frac{1}{2}}.$$

We compute, by a change of variables,

$$\int_0^\infty t^{\frac{1}{2}} (\mathbb{1} - t(N+t)^{-1})^{q-1} (N+t)^{-2} dt = c'N^{-\frac{1}{2}},$$

for some  $c' \in \mathbb{R}$ . This implies the lemma.  $\square$

**Proposition 3.7.** *Assume Condition 2.1 (1) and Condition 2.8. Then  $N^{1/2}$  is of class  $C_{\text{Mo}}^1(A)$  and the iterated commutators  $i^p \text{ad}_A^p(N^{1/2})$ ,  $p \leq k_0$ , extends from  $\mathcal{D}(A) \cap \mathcal{D}(N^{1/2})$  to  $N^{1/2}$ -bounded operators.*

*Proof.* We already know from Lemma 3.1 that  $N^{1/2}$  is of class  $C^1(A)$ . Hence we only need to establish that the iterated commutator forms extend to  $N^{1/2}$ -bounded operators. Recall also that  $\mathcal{D}(A) \cap \mathcal{D}(N)$  is dense in  $\mathcal{D}(A) \cap \mathcal{D}(N^{1/2})$ , cf. Remark 3.5, which implies that it suffices to show that the iterated commutator forms extend from  $\mathcal{D}(A) \cap \mathcal{D}(N)$  to  $N^{1/2}$ -bounded operators.

By Lemma 3.6 and the above remark it suffices to prove, iteratively, the following representation formula

$$i^p \text{ad}_A^p(N^{\frac{1}{2}})\varphi = \sum_{q=1}^p \sum_{\ell_1+\dots+\ell_q=p-q} \alpha_{\underline{\ell}}^{p,q} \int_0^\infty B_q^\ell(t)\varphi dt, \quad (3.17)$$

for  $\varphi \in \mathcal{D}(N)$ . Note that the integrals are absolutely convergent. Here  $B_q^\ell(t)$  are defined in (3.15).

For  $p = 1$  we compute using (3.5)

$$i[A_n, N^{\frac{1}{2}}]\varphi = c_{\frac{1}{2}} \int_0^\infty B_{1,n}^0(t)\varphi dt,$$

where the extra subscript  $n$  indicates that  $N'_0 = N'$  has been replaced by  $I_n(A)N'I_n(A)$ . By (3.22) the integrand is  $O(t^{-3/2})$  uniformly in large  $n$ , and by (3.13) and Lebesgue's theorem on dominated convergence we can thus compute

$$\lim_{n \rightarrow \infty} i[A_n, N^{\frac{1}{2}}]\varphi = c_{\frac{1}{2}} \int_0^\infty B_1^0(t)\varphi dt.$$

Obviously this together with Lemma 3.6 implies that the form  $i \operatorname{ad}_A(N^{1/2})$  extends from  $\mathcal{D}(A) \cap \mathcal{D}(N)$  to an  $N^{1/2}$ -bounded operator represented on  $\mathcal{D}(N)$  by the strongly convergent integral above.

We can now proceed by induction, assuming that the iterated commutator  $i^{p-1} \operatorname{ad}_A^{p-1}(N^{1/2})$  exists as an  $N^{1/2}$ -bounded operator and is represented on  $\mathcal{D}(N)$  by (3.17). Compute first the commutator  $i[A_n, i^{p-1} \operatorname{ad}_A^{p-1}(N^{1/2})]$  strongly on  $\mathcal{D}(N)$  using that

$$i[A_n, N'_\ell] = -I_n(A)N'_{\ell+1}I_n(A) \text{ and } i[A_n, (N+t)^{-1}] = (N+t)^{-1}N'(N+t)^{-1}.$$

Subsequently take the limit  $n \rightarrow \infty$  as above and appeal to Lemma 3.6 to conclude that the so computed limit in fact is an  $N^{1/2}$ -bounded extension of the form  $i[A, i^{p-1} \operatorname{ad}_A^{p-1}(N^{1/2})]$  from  $\mathcal{D}(A) \cap \mathcal{D}(N)$  and represented on  $\mathcal{D}(N)$  as in (3.17).  $\square$

*Proof of Corollary 2.9:* We can now argue that Corollary 2.9 is indeed a direct corollary of Theorem 2.7.

Note that  $\psi \in \mathcal{D}(N^{1/2}A^k)$  for all  $k \leq k_0$  due to Theorem 2.7. We can now repeatedly use the fact that  $\mathcal{D}(A) \cap \mathcal{D}(N^{1/2})$  is dense in  $\mathcal{D}(A)$  and Proposition 3.7 to compute for  $\varphi \in \mathcal{D}(A^p)$ , with  $p+k \leq k_0$ ,

$$\langle A^p \varphi, N^{\frac{1}{2}} A^k \psi \rangle = \sum_{q=0}^p \beta_q \langle \varphi, (\operatorname{ad}_A^{p-q}(N^{\frac{1}{2}})N^{-\frac{1}{2}})N^{\frac{1}{2}}A^{q+k}\psi \rangle,$$

with  $\beta_q$  some real combinatorial factors. This completes the proof since the norm of the right-hand side is bounded by  $C\|\varphi\|$ .  $\square$

### 3.3 Approximating $A$ by Regular Bounded Operators

We recall now a construction from [MS] (see [MS, p. 203]). Consider an odd real-valued function  $g \in C^\infty(\mathbb{R})$  obeying  $g' \geq 0$ , that the function  $\mathbb{R} \ni t \rightarrow tg'(t)/g(t)$  has a smooth square root, that the function  $]0, \infty[ \ni t \rightarrow g(t)$  is concave and the properties

$$g(t) = \begin{cases} 2 & \text{for } t > 3 \\ t & \text{for } |t| < 1 \\ -2 & \text{for } t < -3 \end{cases}.$$

Let  $h(t) = g(t)/t$ . We pick an almost analytic extension of  $h$ , denoted by  $\tilde{h}$ , such that for some  $\rho > 0$  (and using again the notation  $\eta = u + iv$ )

$$\forall N : |\bar{\partial} \tilde{h}(\eta)| \leq C_N \langle \eta \rangle^{-N-2} |v|^N, \quad (3.18)$$

$$\tilde{h}(\eta) = \begin{cases} 2/\eta & \text{for } u > 6, |v| < \rho(u-6) \\ -2/\eta & \text{for } u < -6, |v| < \rho(6-u) \end{cases}.$$

We can choose  $\tilde{h}$  such that  $\overline{\tilde{h}(\eta)} = \tilde{h}(\bar{\eta})$ .

This gives the representation

$$g(t) = \frac{1}{\pi} \int_{\mathbb{C}} (\bar{\partial}\tilde{h})(\eta)t(t-\eta)^{-1} du dv. \quad (3.19)$$

Let  $g_m(t) = mg(t/m)$ , for  $m \geq 1$ . Using the properties of  $g$  one verifies that for all  $t \in \mathbb{R}$  the function

$$m \rightarrow g_m(t)^2 \text{ is increasing.} \quad (3.20)$$

We recall that there exists  $\sigma > 0$  such that for  $|v| \geq \sigma/m$  the operator

$$R_m(\eta) := \left( \frac{A}{m} - \eta \right)^{-1} \quad (3.21)$$

preserves  $\mathcal{D}(N)$ . See (3.8). Moreover we have uniformly in  $\alpha \in [0, 1]$ ,  $m \in \mathbb{N}$  and  $\eta$  that

$$\|N^\alpha R_m(\eta) N^{-\alpha}\| \leq C|v|^{-1}; \quad \eta \in V_m^>, \quad (3.22)$$

where

$$V_m^> := \{u + iv \in \mathbb{C} : |v| \geq \sigma/m\} \quad \text{and} \quad V_m^< := \{u + iv \in \mathbb{C} : |v| < \sigma/m\}.$$

This motivates the decomposition into smooth bounded real-valued functions  $g_m = g_{1m} + g_{2m}$ , where

$$g_{1m}(t) = \frac{m}{\pi} \int_{V_m^>} (\bar{\partial}\tilde{h})(\eta) \left( 1 + \eta \left( \frac{t}{m} - \eta \right)^{-1} \right) du dv + C_m, \quad (3.23)$$

$$g_{2m}(t) = \frac{m}{\pi} \int_{V_m^<} (\bar{\partial}\tilde{h})(\eta) \eta \left( \frac{t}{m} - \eta \right)^{-1} du dv; \quad (3.24)$$

$$C_m = \frac{m}{\pi} \int_{V_m^<} \bar{\partial}\tilde{h}(\eta) du dv.$$

Note that the integral in the expression for  $g_{2m}$  is over a compact set (decreasing with  $m$ ). This implies the property

$$\sup_{m \in \mathbb{N}, t \in \mathbb{R}} m^n \langle t \rangle^{k+1} |g_{2m}^{(k)}(t)| \leq C_{n,k} < \infty \text{ for } n, k \in \mathbb{N} \cup \{0\}. \quad (3.25)$$

Since  $g_m$  and  $g_{2m}$  are bounded functions, we conclude the same for  $g_{1m}$ .

At a key point in the proof we will need a smooth square root of the function  $tg'g$ . We pick

$$\hat{g} = pg \in C_0^\infty(\mathbb{R}), \quad (3.26)$$

where  $p(t) = \sqrt{tg'(t)/g(t)}$ , which was assumed smooth. Clearly  $\hat{g}^2 = tg'g$ . Let  $\tilde{p} \in C_0^\infty(\mathbb{C})$  be an almost analytic extension of  $p$ . It satisfies

$$\forall N : |\bar{\partial}\tilde{p}(\eta)| \leq C_N |v|^N. \quad (3.27)$$

As above we put  $p_m(t) = p(t/m)$  and make the splitting  $p_m = p_{1m} + p_{2m}$ , where

$$p_{1m}(t) = \frac{1}{\pi} \int_{V_m^>} (\bar{\partial}\tilde{p})(\eta) \left( \frac{t}{m} - \eta \right)^{-1} du dv, \quad (3.28)$$

$$p_{2m}(t) = \frac{1}{\pi} \int_{V_m^<} (\bar{\partial}\tilde{p})(\eta) \left( \frac{t}{m} - \eta \right)^{-1} du dv. \quad (3.29)$$

Let  $\hat{g}_m = p_m g_m$  and split  $\hat{g}_m = \hat{g}_{1m} + \hat{g}_{2m}$  by

$$\hat{g}_{1m} = p_{1m} g_{1m} \quad \text{and} \quad \hat{g}_{2m} = p_m g_{2m} + p_{2m} g_{1m}. \quad (3.30)$$

Clearly we can choose  $C_{n,k}$  in (3.25) possibly larger such that  $\hat{g}_{2m}$  satisfies the same estimates. Since  $p_m$  and  $p_{2m}$  are uniformly bounded in  $m$  we get

$$P := \sup_{m \in \mathbb{N}} \sup_{t \in \mathbb{R}} |p_{1m}(t)| < \infty. \quad (3.31)$$

We observe that the operators  $g_{2m}(A)$  and  $p_{1m}(A)$ ,  $p_{2m}(A)$  are given by norm convergent integrals, whereas  $g_m(A)$  and  $g_{1m}(A)$  are given on the domain of  $\langle A \rangle^s$ , for any  $s > 0$ , as strongly convergent integrals.

From (3.20) and Lebesgue's theorem on monotone convergence, we observe that  $\psi \in \mathcal{D}(A^k)$  is equivalent to  $\sup_m \|g_m(A)^k \psi\| < \infty$ . Combining this with (3.25) we find that for  $k \geq 1$

$$\psi \in \mathcal{D}(A^k) \Leftrightarrow \psi \in \mathcal{D}(A^{k-1}) \quad \text{and} \quad \sup_m \|g_{1m}(A)^k \psi\| < \infty. \quad (3.32)$$

It will be convenient in the following when dealing with  $g_{1m}$  to abbreviate

$$d\lambda(\eta) = \frac{1}{\pi} (\bar{\partial} \tilde{h})(\eta) du dv.$$

This is however not a complex measure, just a notation. Similarly we will on one occasion write  $d\lambda_p(\eta) = \frac{1}{\pi} (\bar{\partial} \tilde{p})(\eta) du dv$ , which is in fact a complex measure.

We have the following

**Lemma 3.8.** *As a result of the above constructions we have for any  $m \geq 1$  and  $0 \leq \alpha \leq 1$  that the bounded operators  $g_{1m}(A)$ ,  $g'_{1m}(A)$ ,  $p_{1m}(A)$  and  $Ag'_{1m}(A)$  preserve  $\mathcal{D}(N^\alpha)$ .*

*Proof.* Let  $\psi \in \mathcal{D}(N)$  and  $\varphi \in \mathcal{D}(A)$ . Observe that  $N^{-1}\varphi \in \mathcal{D}(A)$ , by the  $C^1(A)$  property of  $N$ , cf. Condition 2.1 (1). We can thus compute using the strongly convergent integral representation for  $g_{1m}(A)$ , and the notation introduced in (3.21),

$$\begin{aligned} & \langle N\psi, g_{1m}(A)N^{-1}\varphi \rangle & (3.33) \\ &= m \int_{V_m^>} \langle N\psi, (1 + \eta R_m(\eta)) N^{-1}\varphi \rangle d\lambda(\eta) + C_m \langle \psi, \varphi \rangle \\ &= \langle \psi, g_{1m}(A)\varphi \rangle + i \int_{V_m^>} \eta \langle \psi, R_m(\eta) N' R_m(\eta) N^{-1}\varphi \rangle d\lambda(\eta). \end{aligned}$$

By Condition 2.1 (1), (3.18) and (3.22) we find that for some constant  $K_m$  we have

$$|\langle N\psi, g_{1m}(A)N^{-1}\varphi \rangle| \leq K_m \|\psi\| \|\varphi\|. \quad (3.34)$$

This together with an interpolation argument concludes the proof.

The cases  $g'_{1m}(A)$  and  $p_{1m}(A)$  are done the same way. As for  $Ag'_{1m}(A)$  we write  $A_j = AI_j(A)$  and compute

$$NA_j g'_{1m}(A) N^{-1} = A_j N g'_{1m}(A) N^{-1} - i I_j(A) N' N^{-1} N I_j(A) g'_{1m}(A) N^{-1}.$$

To complete the proof by taking  $j \rightarrow \infty$  we need to argue that

$$N g'_{1m}(A) \mathcal{D}(N) \subseteq \mathcal{D}(A).$$

To achieve this we repeat the computation (3.33), with  $\psi$  replaced by  $A\psi$ ,  $\psi \in \mathcal{D}(A)$ , and  $g_{1m}$  replaced by  $g'_{1m}$ . We get

$$\begin{aligned} \langle A\psi, Ng'_{1m}(A)N^{-1}\varphi \rangle &= \langle \psi, Ag'_{1m}(A)\varphi \rangle \\ &+ \int_{V_m^>} \eta \left\langle \frac{A}{m}\psi, \{R_m(\eta)N'R_m(\eta)^2 + R_m(\eta)^2N'R_m(\eta)\}N^{-1}\varphi \right\rangle d\lambda(\eta). \end{aligned}$$

The result now follows from writing  $\frac{A}{m}R_m(\eta) = \mathbb{1} + \eta R_m(\eta)$  and appealing to (3.18) and (3.22) as above.  $\square$

## 4 Proof of the Abstract Results

In this section we prove the abstract theorems formulated in Section 2 as well as an extended version of Theorem 2.10. The proofs are given in separate subsections.

### 4.1 Proof of Theorem 2.7

Let

$$\mathcal{D}_k = \{\varphi \in \mathcal{D}(A^k) \mid \forall 0 \leq j \leq k : A^j\varphi \in \mathcal{D}(N^{\frac{1}{2}})\}.$$

Using Conditions 2.1 – 2.3 and 2.6 we shall prove Theorem 2.7 by induction in  $k = 0, \dots, k_0$  that  $\psi \in \mathcal{D}_k$ . We can assume without loss of generality that  $\lambda = 0$ .

The proof relies on three estimates which we state first in the form of three propositions. After giving the proof of Theorem 2.7, we then proceed to verify the propositions.

We begin with some abbreviations and a definition. For a state  $\psi$  we introduce the notation

$$\psi_m = g_{1m}(A)^k\psi, \quad \text{and} \quad \hat{\psi}_m = \hat{g}_{1m}(A)g_{1m}(A)^{k-1}\psi = p_{1m}(A)\psi_m.$$

Let  $\sigma > 0$  be fixed as in Remark 2.4 1), applied with  $N^{1/2}$  in place of  $N$ .

**Definition 4.1.** Let  $k \geq 1$ . A family of forms  $\{R_m\}_{m=1}^\infty$  on  $\mathcal{D}_{k-1}$  will be called a  $k$ -remainder if for all  $\epsilon > 0$  there exists  $C_\epsilon > 0$  such that

$$|\langle \psi, R_m\psi \rangle| \leq \epsilon \|N^{\frac{1}{2}}\psi_m\|^2 + C_\epsilon \|N^{\frac{1}{2}}(A - i\sigma)^{k-1}\psi\|^2, \quad (4.1)$$

for any  $\psi \in \mathcal{D}_{k-1}$  and  $m \in \mathbb{N}$ .

Lemma 3.8 is repeatedly used below, mostly without comment, to justify manipulations. The first proposition is a virial result, to be proved by a symmetrization of a commutator between  $H$  and a regularized version of  $A^{2k+1}$ .

**Proposition 4.2.** Let  $0 < k \leq k_0$  and  $\psi \in \mathcal{D}_{k-1}$  be a bound state for  $H$ . There exists a  $k$ -remainder  $R_m$ , such that

$$\langle \psi_m, H'\psi_m \rangle + 2k\langle \hat{\psi}_m, H'\hat{\psi}_m \rangle = \langle \psi, R_m\psi \rangle.$$

The second result is an implementation of the virial bound (2.4) in Condition 2.2, which together with Proposition 4.2 makes it possible to deal with  $N^{1/2}\psi_m$ . This is reminiscent of what was done in the proof of [MS, Proposition 8.2]. The constant  $C_2$  appearing in the proposition comes from Condition 2.2.

**Proposition 4.3.** *Let  $\psi \in \mathcal{D}_{k-1}$  be a bound state. There exists  $C$  independent of  $m$  such that*

$$\|N^{\frac{1}{2}}\psi_m\|^2 \leq 2C_2\langle\psi_m, H'\psi_m\rangle + C(\|\psi_m\|^2 + \|N^{\frac{1}{2}}(A - i\sigma)^{k-1}\psi\|^2)$$

and

$$\|N^{\frac{1}{2}}\hat{\psi}_m\|^2 \leq 2C_2\langle\hat{\psi}_m, H'\hat{\psi}_m\rangle + C(\|\hat{\psi}_m\|^2 + \|N^{\frac{1}{2}}(A - i\sigma)^{k-1}\psi\|^2).$$

The third and final input is an implementation of the positive commutator estimate in Condition 2.3. The constant  $c_0$  and the compact operator  $K_0$  appearing in the proposition come from Condition 2.3.

**Proposition 4.4.** *Let  $\psi \in \mathcal{D}_{k-1}$  be a bound state. There exist constants  $C, \tilde{C} > 0$  independent of  $m$  such that*

$$\langle\psi_m, H'\psi_m\rangle \geq \frac{c_0}{2}\|\psi_m\|^2 - \tilde{C}\langle\psi_m, K_0\psi_m\rangle - C\|N^{\frac{1}{2}}(A - i\sigma)^{k-1}\psi\|^2$$

and

$$\langle\hat{\psi}_m, H'\hat{\psi}_m\rangle \geq \frac{c_0}{2}\|\hat{\psi}_m\|^2 - \tilde{C}\langle\hat{\psi}_m, K_0\hat{\psi}_m\rangle - C\|N^{\frac{1}{2}}(A - i\sigma)^{k-1}\psi\|^2.$$

*Proof of Theorem 2.7:* Let  $\psi$  be the bound state, which we take to be normalized. By assumption  $\psi \in \mathcal{D}_0$ . Assume by induction that  $\psi \in \mathcal{D}_{k-1}$ , for some  $k \leq k_0$ . We proceed to show that  $\psi \in \mathcal{D}_k$ :

From Proposition 4.2 we get the existence of a  $k$ -remainder  $R_m$  such that

$$\langle\psi_m H'\psi_m\rangle + 2k\langle\hat{\psi}_m, H'\hat{\psi}_m\rangle = \langle\psi, R_m\psi\rangle.$$

Estimating the right-hand side using (4.1) and Proposition 4.3 we find a  $C > 0$  such that

$$\langle\psi_m, H'\psi_m\rangle + 2k\langle\hat{\psi}_m, H'\hat{\psi}_m\rangle \leq \frac{c_0}{4}\|\psi_m\|^2 + C\|N^{\frac{1}{2}}(A - i\sigma)^{k-1}\psi\|^2.$$

Finally, we appeal to Proposition 4.4 to derive the bound

$$\frac{c_0}{4}\|\psi_m\|^2 \leq C\|N^{\frac{1}{2}}(A - i\sigma)^{k-1}\psi\|^2 + \tilde{C}\langle\psi_m, K_0\psi_m\rangle + 2k\tilde{C}\langle\hat{\psi}_m, K_0\hat{\psi}_m\rangle. \quad (4.2)$$

Pick  $\Lambda > 0$  large enough such that

$$2\tilde{C}\|K_0\mathbb{1}_{[|A|>\Lambda]}\| \leq \frac{c_0}{12(1 + 2kP^2)},$$

where  $P$  is given by (3.31). Write  $\mathbb{1}_{[|A|\leq\Lambda]}\psi_m = [\mathbb{1}_{[|A|\leq\Lambda]}(g_m(A) - g_{2m}(A))]^k\psi$  and estimate using (3.25)

$$\begin{aligned} 2\tilde{C}|\langle\mathbb{1}_{[|A|\leq\Lambda]}\psi_m, K_0\psi_m\rangle| &\leq 2\tilde{C}(\Lambda + C_{0,0})^k\|K_0\|\|\psi\|\|\psi_m\| \\ &\leq \frac{c_0}{12}\|\psi_m\|^2 + \frac{12\tilde{C}^2(\Lambda + C_{0,0})^{2k}\|K_0\|^2}{c_0}\|\psi\|^2 \end{aligned}$$

and similarly

$$2\tilde{C}|\langle\mathbb{1}_{[|A|\leq\Lambda]}\hat{\psi}_m, K_0\hat{\psi}_m\rangle| \leq \frac{c_0}{24k}\|\psi_m\|^2 + \frac{24k\tilde{C}^2(\Lambda + C_{0,0})^{2k}\|K_0\|^2P^4}{c_0}\|\psi\|^2.$$

Inserting  $\mathbb{1} = \mathbb{1}_{[|A|\leq\Lambda]} + \mathbb{1}_{[|A|>\Lambda]}$  ahead of the  $K_0$ 's in (4.2) and appealing to the bounds above we get

$$\frac{c_0}{8}\|\psi_m\|^2 \leq C(\|N^{\frac{1}{2}}(A - i\sigma)^{k-1}\psi\|^2 + \|\psi\|^2),$$

for a suitable  $m$ -independent  $C$ . Recalling (3.32) we conclude that  $\psi \in \mathcal{D}(A^k)$ .

It remains to prove that  $A^k\psi \in \mathcal{D}(N^{1/2})$ .

Note that what we just established implies that  $\psi_m \rightarrow A^k\psi$  in norm, cf. (3.20) and (3.25). We can now compute

$$\langle A^k\psi, NI_{in}(N)A^k\psi \rangle = \lim_{m \rightarrow \infty} \langle \psi_m, NI_{in}(N)\psi_m \rangle.$$

But by Propositions 4.2 and 4.3 we have

$$\begin{aligned} \langle \psi_m, NI_{in}(N)\psi_m \rangle &\leq \|N^{\frac{1}{2}}\psi_m\|^2 \\ &\leq \|N^{\frac{1}{2}}\psi_m\|^2 + 2k\|N^{\frac{1}{2}}\hat{\psi}_m\|^2 \\ &\leq 2C_2(\langle \psi_m, H'\psi_m \rangle + 2k\langle \hat{\psi}_m, H'\hat{\psi}_m \rangle) + C \\ &= \langle \psi, R_m\psi \rangle + C, \end{aligned}$$

where  $C > 0$  is constant independent of  $m$ . The result now follows from (4.1) by first taking the limit  $m \rightarrow \infty$ , and subsequently  $n \rightarrow \infty$ . Notice that Lebesgue's theorem on monotone convergence applies, since  $I_{in}(N) = n(N+n)^{-1} \rightarrow \mathbb{1}$  monotonously.  $\square$

The rest of the section is devoted to establishing Propositions 4.2–4.4.

We begin with a definition and a series of lemmata. The  $\sigma$  in the definition below is the same  $\sigma$  that entered into Definition 4.1.

**Definition 4.5.** Let  $E_m^l$  and  $E_m^r$  be families of forms on  $\mathcal{D}_{k-1} \times \mathcal{D}(N^{1/2})$  and  $\mathcal{D}(N^{1/2}) \times \mathcal{D}_{k-1}$  respectively. We say that  $E_m^l$  is a left-error if

$$|\langle \psi, E_m^l\varphi \rangle| \leq C\|N^{\frac{1}{2}}(A - i\sigma)^{k-1}\psi\|\|N^{\frac{1}{2}}\varphi\|.$$

We say that  $E_m^r$  is a right-error if

$$|\langle \psi, E_m^r\varphi \rangle| \leq C\|N^{\frac{1}{2}}\psi\|\|N^{\frac{1}{2}}(A - i\sigma)^{k-1}\varphi\|.$$

**Remark 4.6.** An example of a right-error that we will encounter below are forms

$$N^{1/2}B_mN^{1/2}g_{1m}(A)^\ell(A - i\sigma)^{-j},$$

with  $\ell - j \leq k - 1$  and  $\sup_m \|B_m\| < \infty$ . To see that this is a right-error observe that it suffices to prove that  $Ng_{1m}(A)^\ell(A - i\sigma)^{-j-k+1}N^{-1}$  is uniformly bounded in  $m$ . The result then follows from interpolation. Since  $j + k - 1 \geq \ell$ , recalling that  $\sigma$  was chosen according to (3.8), we reduce the problem to showing that  $Ng_{1m}(A)(A - i\sigma)^{-1}N^{-1}$  is bounded uniformly in  $m$ . But this follows by a computation similar to (3.33), where the extra resolvent produces a bound which is uniform in  $m$  compared with the point wise bound (3.34).

We introduce the notation

$$H_n := HI_n(H) = in(I_n(H) - \mathbb{1}), \quad (4.3)$$

which plays the role of a regularized Hamiltonian. See (3.11) for the definition of  $I_n(H)$ .

**Lemma 4.7.** *We have the following limit in the sense of forms on  $\mathcal{D}(N^{1/2})$*

$$\lim_{n \rightarrow \infty} i[H_n, g_{1m}(A)] = - \int_{V_m^>} \eta R_m(\eta) H' R_m(\eta) d\lambda(\eta).$$

*Proof.* Observe first that the integral on the right-hand side in the lemma is norm convergent.

Compute as a form on  $\mathcal{D}(A)$  using that the integral representation for  $g_{1m}(A)$  is strongly convergent on  $\mathcal{D}(A)$

$$i[H_n, g_{1m}(A)] = \int_{V_m^>} \eta i[H_n, R_m(\eta)] d\lambda(\eta).$$

Recalling (4.3) we arrive at

$$\begin{aligned} i[H_n, g_{1m}(A)] &= in \int_{V_m^>} \eta i[I_n(H), R_m(\eta)] d\lambda(\eta) \\ &= \int_{V_m^>} \eta I_n(H) i[H, R_m(\eta)] I_n(H) d\lambda(\eta). \end{aligned}$$

Finally we employ Condition 2.1 3) to conclude that for each  $n$ , the following holds as a form identity on  $\mathcal{D}(A) \cap \mathcal{D}(N^{1/2})$

$$i[H_n, g_{1m}(A)] = - \int_{V_m^>} \eta I_n(H) R_m(\eta) H' R_m(\eta) I_n(H) d\lambda(\eta).$$

The integral on the right-hand side of the above identity is absolutely convergent in  $\mathcal{B}(N^{-1/2}\mathcal{H}; N^{1/2}\mathcal{H})$ . By density of  $\mathcal{D}(A) \cap \mathcal{D}(N^{1/2})$  in  $\mathcal{D}(N^{1/2})$ , see Remark 2.4 2), the identity therefore extends to a form identity on  $\mathcal{D}(N^{1/2})$ . The lemma now follows from (3.12).  $\square$

**Lemma 4.8.** *Let  $1 \leq k \leq k_0$ .*

(1) *There exist right-errors  $E_m^r, \hat{E}_m^r$  such that, as forms on  $\mathcal{D}(N^{1/2}) \times \mathcal{D}_{k-1}$ ,*

$$\begin{aligned} \lim_{n \rightarrow \infty} i[H_n, g_{1m}(A)^k] &= E_m^r \\ \lim_{n \rightarrow \infty} i[H_n, \hat{g}_{1m}(A) g_{1m}(A)^{k-1}] &= \hat{E}_m^r. \end{aligned}$$

(2) *There exist a left-error  $E_m^l$  and a right-error  $E_m^r$  such that, as forms on  $\mathcal{D}_{k-1} \times \mathcal{D}(N^{1/2})$  and  $\mathcal{D}(N^{1/2}) \times \mathcal{D}_{k-1}$  respectively,*

$$\begin{aligned} \lim_{j \rightarrow \infty} \lim_{n \rightarrow \infty} i[H_n, g_{1m}(A)^k] A_j &= k g_{1m}(A)^{k-1} A g'_{1m}(A) H' + E_m^l \\ \lim_{j \rightarrow \infty} \lim_{n \rightarrow \infty} A_j i[H_n, g_{1m}(A)^k] &= k H' A g'_{1m}(A) g_{1m}(A)^{k-1} + E_m^r. \end{aligned}$$

*Proof.* (1) also holds if we take the limit in the sense of forms on  $\mathcal{D}_{k-1} \times \mathcal{D}(N^{1/2})$  and replace the right-error by a left-error. We will however not need that statement. One does however need its proof for the left-error part of (2).

In the proof we will only work with right-errors. The other case is similar. We begin with (1) and prove only the first statement leaving the second to the reader.

We first compute as a form on  $\mathcal{D}(N^{1/2})$ .

$$\begin{aligned} i[H_n, g_{1m}(A)^k] &= ki[H_n, g_{1m}(A)] g_{1m}(A)^{k-1} \\ &\quad + \sum_{\ell=2}^k (-1)^{\ell+1} \binom{k}{\ell} i \operatorname{ad}_{g_{1m}(A)}^\ell (H_n) g_{1m}(A)^{k-\ell}. \end{aligned} \quad (4.4)$$

We now analyze the large  $n$  limit. The first term on the right-hand side of (4.4) can be dealt with using Lemma 4.7 directly, observing that by Lemma 3.8  $g_{1m}(A)$  preserves the domain of  $N^{1/2}$ . As for the terms involving higher order commutators, we again use Lemma 4.7 to compute

$$\lim_{n \rightarrow \infty} \text{i ad}_{g_{1m}(A)}^\ell(H_n) = - \int_{V_m^\geq} \eta R_m(\eta) \text{ad}_{g_{1m}(A)}^{\ell-1}(H') R_m(\eta) d\lambda(\eta)$$

in the sense of forms on  $\mathcal{D}(N^{1/2})$ .

We can now employ Condition 2.6 to compute as forms on  $\mathcal{D}(N^{1/2})$

$$\lim_{n \rightarrow \infty} \text{i ad}_{g_{1m}(A)}^\ell(H_n) = (-1)^\ell N^{\frac{1}{2}} B_m^{(\ell)} N^{\frac{1}{2}}, \quad (4.5)$$

where  $B_m^{(\ell)}$  is a family of bounded operators with  $\sup_m \|B_m^{(\ell)}\| < \infty$ , for all  $\ell$ . They are given by

$$\begin{aligned} B_m^{(\ell)} &= \int_{(V_m^\geq)^\ell} \eta_1 \cdots \eta_\ell N^{-\frac{1}{2}} R_m(\eta_1) \cdots R_m(\eta_\ell) \text{ad}_A^{\ell-1}(H') \\ &\quad \times R_m(\eta_\ell) \cdots R_m(\eta_1) N^{-\frac{1}{2}} d\lambda(\eta_1) \cdots d\lambda(\eta_\ell). \end{aligned} \quad (4.6)$$

From (4.4), (4.5) and Lemma 4.7 we thus obtain

$$\begin{aligned} \lim_{n \rightarrow \infty} \text{i}[H_n, g_{1m}(A)^k] &= -k \int_{V_m^\geq} \eta R_m(\eta) H' R_m(\eta) d\lambda(\eta) g_{1m}(A)^{k-1} \\ &\quad - \sum_{\ell=2}^k \binom{k}{\ell} N^{\frac{1}{2}} B_m^{(\ell)} N^{\frac{1}{2}} g_{1m}(A)^{k-\ell}. \end{aligned} \quad (4.7)$$

Combining this computation with Remark 4.6 yields (1).

We now turn to part (2) of the lemma. In view of (4.7) we begin by computing as a form on  $\mathcal{D}(N^{1/2})$ , using Condition 2.1 (4)

$$\begin{aligned} &-k \int_{V_m^\geq} \eta R_m(\eta) H' R_m(\eta) d\lambda(\eta) \\ &= k H' g'_{1m}(A) - \frac{\text{i}k}{m} \int_{V_m^\geq} \eta R_m(\eta) H'' R_m(\eta)^2 d\lambda(\eta). \end{aligned} \quad (4.8)$$

We remark that the identity  $\text{i}[H', R_m(\eta)] = -m^{-1} R_m(\eta) H'' R_m(\eta)$  holds a priori as a form identity on  $\mathcal{D}(N)$ . It extends by continuity to a form identity on  $\mathcal{D}(N^{1/2})$ , which is what is used in the above computation. Note that the integral on the right-hand side is convergent as a form on  $\mathcal{D}(N^{1/2})$ .

From (4.7), (4.8) and Remark 4.6 we find that

$$\lim_{n \rightarrow \infty} \text{i}[H_n, g_{1m}(A)^k] A_j = (k H' g'_{1m}(A) A g_{1m}(A)^{k-1} + E_m^r) I_j(A)$$

and hence by (3.14) we conclude the following identity as forms on  $\mathcal{D}(N^{1/2})$

$$\lim_{j \rightarrow \infty} \lim_{n \rightarrow \infty} \text{i}[H_n, g_{1m}(A)^k] A_j = k H' g'_{1m}(A) A g_{1m}(A)^{k-1} + E_m^r.$$

To prove the second statement in (2) it remains to show that the commutator between  $A_j$  and  $\text{i}[H_n, g_{1m}(A)^k]$  converges to a right-error.

From (4.8) we get, as a form on  $\mathcal{D}(N^{1/2})$ ,

$$\begin{aligned} & \left[ -k \int_{V_m^{\geq}} \eta R_m(\eta) H' R_m(\eta) d\lambda(\eta), A_j \right] \\ &= k I_j(A) H'' I_j(A) g'_{1m}(A) - \frac{ik}{m} \int_{V_m^{\geq}} \eta R_m(\eta) (H'' A_j - A_j H'') R_m(\eta)^2 d\lambda(\eta). \end{aligned}$$

We can now take the limit  $j \rightarrow \infty$  and obtain

$$\lim_{j \rightarrow \infty} \left[ -k \int_{V_m^{\geq}} \eta R_m(\eta) H' R_m(\eta) d\lambda(\eta), A_j \right] = N^{\frac{1}{2}} B_m^{(1)} N^{\frac{1}{2}}, \quad (4.9)$$

where  $B_m^{(1)}$ , is a family of bounded operators with  $\sup_m \|B_m^{(1)}\| < \infty$ . It is given by

$$B_m^{(1)} = k N^{-\frac{1}{2}} \left\{ H'' g'_{1m}(A) - i \int_{V_m^{\geq}} \eta (R_m(\eta) H'' - H'' R_m(\eta)) R_m(\eta) d\lambda(\eta) \right\} N^{-\frac{1}{2}}.$$

Here we used (3.14), that  $A_j R_m(\eta) = R_m(\eta) A_j = m(\mathbb{1} + \eta R_m(\eta)) I_j(A)$ , as well as Lebesgue's theorem on dominated convergence.

For the commutator between  $A_j$  and the second term on the right-hand side of (4.7) we compute

$$[N^{\frac{1}{2}} B_m^{(\ell)} N^{\frac{1}{2}}, A_j] = I_j(A) N^{\frac{1}{2}} \tilde{B}_m^{(\ell)} N^{\frac{1}{2}} I_j(A),$$

where  $\tilde{B}_m^{(\ell)}$  are bounded operators with  $\sup_{m \in \mathbb{N}} \|B_m^{(\ell)}\| < \infty$ , for all  $\ell$ . They are given by

$$\begin{aligned} \tilde{B}_m^{(\ell)} &= \int_{(V_m^{\geq})^\ell} N^{-\frac{1}{2}} R_m(\eta_1) \cdots R_m(\eta_\ell) \text{ad}_A^\ell(H') \\ &\quad \times R_m(\eta_\ell) \cdots R_m(\eta_1) N^{-\frac{1}{2}} d\lambda(\eta_1) \cdots d\lambda(\eta_\ell). \end{aligned}$$

We can now take the limit  $j \rightarrow \infty$  using (3.14), and the resulting expression together with (4.9), the formula (4.7) and Remark 4.6 yields that

$$\lim_{j \rightarrow \infty} \lim_{n \rightarrow \infty} [i[H_n, g_{1m}(A)^k], A_j] = E_m^r.$$

□

**Lemma 4.9.** *There exists a  $k$ -remainder  $R_m$  such that*

$$\begin{aligned} & \lim_{j \rightarrow \infty} \lim_{n \rightarrow \infty} i[H_n, g_{1m}(A)^k A_j g_{1m}(A)^k] \\ &= g_{1m}(A)^k H' g_{1m}(A)^k + 2k \text{Re} \{ g_{1m}(A)^{k-1} A g'_{1m}(A) H' g_{1m}(A)^k \} + R_m, \end{aligned}$$

in the sense of forms on  $\mathcal{D}_{k-1}$ .

*Proof.* We compute as a form on  $\mathcal{D}_{k-1}$

$$\begin{aligned} i[H_n, g_{1m}(A)^k A_j g_{1m}(A)^k] &= i[H_n, g_{1m}(A)^k] A_j g_{1m}(A)^k \\ &\quad + g_{1m}(A)^k i[H_n, A_j] g_{1m}(A)^k + g_{1m}(A)^k A_j i[H_n, g_{1m}(A)^k]. \end{aligned}$$

Using that  $\lim_{n \rightarrow \infty} i[H_n, A_j] = I_j(A) H' I_j(A)$ ,  $\lim_{j \rightarrow \infty} I_j(A) H' I_j(A) = H'$  (in the sense of forms on  $\mathcal{D}(N^{1/2})$ ), and Lemma 4.8 (2), we conclude the result, with

$$R_m = E_m^l g_{1m}(A)^k + g_{1m}(A)^k E_m^r.$$

Note that  $R_m$  is a  $k$ -remainder, in the sense of Definition 4.1. □

We now symmetrize the form  $g_{1m}(A)^{k-1}Ag'_{1m}(A)H'g_{1m}(A)^k$ , defined on  $\mathcal{D}(N^{1/2})$ .

**Lemma 4.10.** *There exists a  $k$ -remainder  $R_m$  such that*

$$\begin{aligned} & \operatorname{Re} \{g_{1m}(A)^{k-1}Ag'_{1m}(A)H'g_{1m}(A)^k\} \\ &= g_{1m}(A)^k p_{1m}(A)H'p_{1m}(A)g_{1m}(A)^k + R_m, \end{aligned}$$

in the sense of forms on  $\mathcal{D}_{k-1}$ .

*Proof. Step I:* From the proof of Lemma 3.8 it follows that

$$[N, Ag'_{1m}(A)]N^{-1}, \quad [N, p_{1m}^2(A)g_{1m}(A)]N^{-1}, \quad (4.10)$$

$$\text{and } N^{-1}p_{1m}(A)N \quad (4.11)$$

extend as forms from  $\mathcal{D}(N)$  to bounded operators with norm bounded uniformly in  $m$ .

**Step II:** Boundedness of the forms in (4.10), together with the observation that  $\|tg'_{1m} - p_{1m}^2g_{1m}\|_\infty$  is bounded uniformly in  $m$ , implies after an interpolation argument that

$$N^{\frac{1}{2}}(Ag'_{1m}(A) - p_{1m}(A)^2g_{1m}(A))N^{-\frac{1}{2}}$$

is bounded uniformly in  $m$ . Hence

$$\begin{aligned} & \operatorname{Re} \{g_{1m}(A)^{k-1}Ag'_{1m}(A)H'g_{1m}(A)^k\} \\ &= g_{1m}(A)^k \operatorname{Re} \{p_{1m}(A)^2H'\}g_{1m}(A)^k + R_m^{(1)}, \end{aligned}$$

where  $R_m^{(1)}$  is a  $k$ -remainder.

**Step III:** We compute as a form on  $\mathcal{D}(N^{1/2})$

$$(A + i\sigma)[p_{1m}(A), H'] = -i \int_{V_m^\geq} \frac{A + i\sigma}{m} R_m(\eta)H''R_m(\eta) d\lambda_p(\eta),$$

which is bounded uniformly in  $m$  as a form on  $\mathcal{D}(N^{1/2})$ . This together with (4.11) and a interpolation argument as in step II, shows that

$$g_{1m}(A)^k \operatorname{Re} \{p_{1m}(A)^2H'\}g_{1m}(A)^k = g_{1m}(A)^k p_{1m}(A)H'p_{1m}(A)g_{1m}(A)^k + R_m^{(2)},$$

where  $R_m^{(2)}$  is a  $k$ -remainder. Here we used again Remark 4.6. This proves the lemma with  $R_m = R_m^{(1)} + R_m^{(2)}$ .  $\square$

*Proof of Proposition 4.2.* Combine Lemmas 4.9 and 4.10.  $\square$

*Proof of Proposition 4.3.* We only prove the first estimate. The second is verified the same way. We can assume that  $\lambda = 0$ .

We estimate using Condition 2.2

$$\begin{aligned} \|N^{\frac{1}{2}}I_n(H)\psi_m\|^2 &\leq C_1 \langle I_n(H)\psi_m, HI_n(H)\psi_m \rangle \\ &\quad + C_2 \langle I_n(H)\psi_m, H'I_n(H)\psi_m \rangle + C_3 \|I_n(H)\psi_m\|^2. \end{aligned} \quad (4.12)$$

Note that  $HI_n(H)\psi_m = H_n\psi_m = [H_n, g_{1m}(A)^k]\psi$ .

By Lemma 4.8 (1) we find that for any  $\varphi \in \mathcal{D}(N^{1/2})$  we have

$$\lim_{n \rightarrow \infty} \langle \varphi, H_n \psi_m \rangle = \langle \varphi, E_m^r \psi \rangle. \quad (4.13)$$

By this observation and the uniform boundedness principle there exists  $C = C(m)$  such that  $|\langle \varphi, H_n \psi_m \rangle| \leq C \|N^{1/2} \varphi\|$  uniformly in  $n$ , for  $\varphi \in \mathcal{D}(N^{1/2})$ . Applying this to  $\varphi = (I_n(H) - I)\psi_m$ , together with (4.13), now applied with  $\varphi = \psi_m$ , we get

$$\lim_{n \rightarrow \infty} \langle I_n(H) \psi_m, H I_n(H) \psi_m \rangle = \langle \psi_m, E_m^r \psi \rangle. \quad (4.14)$$

Here  $E_m^r$  is a right-error.

We can now take the limit  $n \rightarrow \infty$  in (4.12), and the result follows from Definition 4.5.  $\square$

*Proof of Proposition 4.4.* As above we assume  $\lambda = 0$  and prove only the first bound.

By Remark 2.4 4) it suffices to estimate using the bound (2.6) instead of the one in Condition 2.3. We get

$$\begin{aligned} \langle I_n(H) \psi_m, H' I_n(H) \psi_m \rangle &\geq c_0 \|I_n(H) \psi_m\|^2 \\ &+ \operatorname{Re} \langle I_n(H) \psi_m, B H I_n(H) \psi_m \rangle - \langle I_n(H) \psi_m, K_0 I_n(H) \psi_m \rangle. \end{aligned} \quad (4.15)$$

Arguing as in the part of the proof of Proposition 4.3 pertaining to (4.14), we find that

$$\lim_{n \rightarrow \infty} \operatorname{Re} \langle I_n(H) \psi_m, B H I_n(H) \psi_m \rangle = \operatorname{Re} \langle \psi_m, E_m^r \psi \rangle.$$

where  $E_m^r$  is a right-error. Here (4.13) was used (twice) with  $\varphi$  replaced by  $B\varphi$  and  $B^*\varphi$ , where we used the assumption on  $B$  in Remark 2.4 4) to argue that  $B\varphi, B^*\varphi \in \mathcal{D}(N^{1/2})$  in (4.13).

Inserting this limit into (4.15) yields

$$\begin{aligned} \langle \psi_m, H' \psi_m \rangle &= \lim_{n \rightarrow \infty} \langle I_n(H) \psi_m, H' I_n(H) \psi_m \rangle \\ &\geq c_0 \|\psi_m\|^2 - \langle \psi_m, K_0 \psi_m \rangle + \operatorname{Re} \langle \psi_m, E_m^r \psi \rangle, \end{aligned}$$

with  $E_m^r$  being a right-error. Using Definition 4.5 and Proposition 4.3 we conclude the first estimate.  $\square$

## 4.2 Proof of Theorem 2.10

We shall show Theorem 2.10, which is an extension of Corollary 2.9 under the minimal condition  $k_0 = 1$ .

*Proof of Theorem 2.10:* We can without loss of generality take  $\lambda = 0$ . Due to Corollary 2.9 only the first statement needs elaboration. The idea of the proof is to apply a virial argument for the commutator  $i[H, A]$  and the state  $N^{1/2}\psi$ . We divide the proof into three steps. Let  $N_n^{(1/2)} = N^{1/2} I_n(N)$ .

**Step I:** Due to Lemma 3.1 we have  $N_n^{(1/2)} \psi \in \mathcal{D}(H)$ . We shall show that

$$\sup_{n \in \mathbb{N}} \|H N_n^{(1/2)} \psi\| < \infty. \quad (4.16)$$

We can use the representation formula (3.5) with  $\alpha = 1/2$  and commute  $H$  through  $N^{1/2}$ , cf. (3.4). Whence it suffices to bound

$$\int_0^\infty t^{\frac{1}{2}}(N+t)^{-1}[H, N]^0(N+t)^{-1}I_{in}(N)N^{-\frac{1}{2}}dt$$

independently of  $n$ . (Note that the contribution from commuting through the second factor  $I_{in}(N)$  indeed is bounded independently of  $n$ .) By (2.1) we have

$$[H, N]^0 = N^{\frac{1}{2}-\kappa}BN^{\frac{1}{2}-\kappa} \text{ for } B \text{ bounded,}$$

and we can estimate

$$\|(N+t)^{-1}i[H, N]^0(N+t)^{-1}I_{in}(N)N^{-\frac{1}{2}}\| \leq \|B\|\langle t \rangle^{-\frac{3}{2}-\kappa} \text{ uniformly in } n.$$

Hence the integrand is  $O(t^{-1-\kappa})$  uniformly in  $n$ , and (4.16) follows.

**Step II:** We shall show that

$$\sup_{n \in \mathbb{N}} \|AN_n^{(1/2)}\psi\| < \infty. \quad (4.17)$$

Since  $\phi := N^{1/2}\psi \in \mathcal{D}(A)$  due to Corollary 2.9 it suffices to bound the state  $[A, I_{in}(N)]\phi$  independently of  $n$ . This is obvious from the representation

$$[A, I_{in}(N)]\phi = -i(N+n)^{-1}N'I_{in}(N)\phi,$$

and whence (4.17) follows.

**Step III:** We look at

$$\langle i[H, A] \rangle_{N_n^{(1/2)}\psi} = -2\text{Re} \langle iHN_n^{(1/2)}\psi, AN_n^{(1/2)}\psi \rangle.$$

Due to (4.16) and (4.17) the right hand side is bounded independently of  $n$ . We compute using Condition 2.1 (1) and (3)

$$\langle i[H, A] \rangle_{N_n^{(1/2)}\psi} = \lim_{\tilde{n} \rightarrow \infty} \langle i[H, A\tilde{I}_{\tilde{n}}(A)] \rangle_{N_n^{(1/2)}\psi} = \langle H' \rangle_{N_n^{(1/2)}\psi}.$$

Whence using the virial estimate Condition 2.2 (and also Step I again) we conclude that

$$\langle N \rangle_{N_n^{(1/2)}\psi} \leq C \text{ uniformly in } n.$$

Taking  $n \rightarrow \infty$  we obtain that indeed  $\psi \in \mathcal{D}(N)$ . □

### 4.3 Theorem on more $N$ -Regularity

We formulate and prove an extended version of Theorem 2.10.

Notice that under Condition 2.1 (1) and (2), and the additional condition (2.11) for  $k_0 = 1$ ,

$$N^{\frac{1}{2}} \in C_{\text{Mo}}^1(A) \cap C_{\text{Mo}}^1(H), \quad (4.18)$$

cf. Lemma 3.2 and Proposition 3.7.

We impose the conditions of Corollary 2.9 and aim at an improvement of Corollary 2.9 and Theorem 2.10 in the case  $k_0 \geq 2$ . Let  $M_0 = i[N^{1/2}, A]^0$ . Then, cf. Proposition 3.7,

$$i^m \text{ad}_A^m(M_0) \text{ is } N^{\frac{1}{2}}\text{-bounded for } m = 0, \dots, k_0 - 1. \quad (4.19)$$

Here the commutators are defined iteratively as extensions of forms on  $\mathcal{D}(N^{1/2}) \cap \mathcal{D}(A)$  and they are considered as symmetric  $N^{1/2}$ -bounded operators. We introduce the following  $N^{1/2}$ -bounded operators:

$$M_1 = i[N^{\frac{1}{2}}, H]^0 = c_{\frac{1}{2}} \int_0^\infty t^{\frac{1}{2}} (N+t)^{-1} i[N, H]^0 (N+t)^{-1} dt,$$

$$M_2 = H' N^{-\frac{1}{2}} \quad \text{and} \quad M_3 = N^{-\frac{1}{2}} H'.$$

Notice that

$$M_3 \subseteq M_2^* \quad \text{and} \quad M_2 \subseteq M_3^*. \quad (4.20)$$

We need to consider repeated commutation of  $M_j$ ,  $j = 1, \dots, 3$ , with factors of  $T = A$  or  $T = N^{1/2}$ .

**Condition 4.11.** For all  $j = 1, \dots, 3$ ,  $m = 1, \dots, k_0 - 1$  and all possible combinations of factors  $T_n \in \{A, N^{1/2}\}$  where  $n = 1, \dots, m$

$$i^m \text{ad}_{T_m} \cdots \text{ad}_{T_1}(M_j) \text{ is } N^{\frac{1}{2}}\text{-bounded.} \quad (4.21)$$

Notice that in (4.21) the commutators are defined iteratively as extensions of forms on  $\mathcal{D}(N^{1/2}) \cap \mathcal{D}(A)$  using (4.20) and the analogue properties for  $m \geq 2$

$$\begin{aligned} (-1)^{m-1} \text{ad}_{T_{m-1}} \cdots \text{ad}_{T_1}(M_3) &\subseteq (\text{ad}_{T_{m-1}} \cdots \text{ad}_{T_1}(M_2))^*, \\ (-1)^{m-1} \text{ad}_{T_{m-1}} \cdots \text{ad}_{T_1}(M_2) &\subseteq (\text{ad}_{T_{m-1}} \cdots \text{ad}_{T_1}(M_3))^*. \end{aligned}$$

We shall prove the following extension of Corollary 2.9 and Theorem 2.10.

**Theorem 4.12.** *Suppose the conditions of Corollary 2.9 and for  $k_0 \geq 2$  also Condition 4.11. Let  $\psi \in \mathcal{D}(N^{1/2})$  be a bound state  $(H - \lambda)\psi = 0$  (with  $\lambda$  as in Condition 2.3). Then  $\psi \in \mathcal{D}(T_{k_0+1} \cdots T_1)$  where  $T_n \in \{A, N^{1/2}, \mathbb{1}\}$  for  $n = 1, \dots, k_0 + 1$  and at least for one such  $n$ ,  $T_n \neq A$ .*

*Proof.* We proceed by induction in  $k_0$ . The case  $k_0 = 1$  is the content of Theorem 2.10. So suppose  $k_0 \geq 2$  and that the statement holds for  $k_0 \rightarrow k_0 - 1$ . Consider any product  $S = T_{k_0+1} \cdots T_1$  not all factors being given by  $A$ . We shall show that  $\psi \in \mathcal{D}(S)$ . By Corollary 2.9 and the induction hypothesis we can assume that the factors  $T_n \in \{A, N^{1/2}\}$  and that for at least two  $n$ 's  $T_n = N^{1/2}$ . By using (4.19) and the induction hypothesis we can assume that  $T_{k_0+1} = N^{1/2}$ . Whence we can assume  $S = N^{1/2} S_{k,\ell}^\alpha$  with  $k = k_0$  introducing here the following notation for  $k = 1, \dots, k_0$ ,  $\ell = 0, \dots, k$  and  $\alpha$  being a multiindex  $\alpha \in \{0, 1\}^k$  with  $\sum_{j \leq k} \alpha_j = \ell$ ,

$$S_{k,\ell}^\alpha = S_{\alpha_k} \cdots S_{\alpha_1} =: \prod_{j=1}^k S_{\alpha_j} \quad \text{where } S_0 = A \text{ and } S_1 = N^{\frac{1}{2}}.$$

Partly motivated by the above considerations we introduce the following quantity for  $n \in \mathbb{N}$  large and  $\epsilon \in ]0, 1[$  small

$$f(n, \epsilon) = \sum_{\ell=0}^{k_0} \epsilon^{-2\ell^2} g(n, \ell); \quad g(n, \ell) := \sum_{\substack{\alpha \in \{0,1\}^{k_0} \\ \alpha_1 + \cdots + \alpha_{k_0} = \ell}} \|N^{\frac{1}{2}} I_{in}(N) S_{k_0,\ell}^\alpha \psi\|^2.$$

We claim that for some constants  $K_1, K_2(\epsilon) > 0$  independent of  $n$

$$f(n, \epsilon) \leq \epsilon^2 K_1 f(n, \epsilon) + K_2(\epsilon). \quad (4.22)$$

The theorem follows from (4.22) by first choosing  $\epsilon$  so small that  $\epsilon^2 K_1 \leq 1/2$ , subtraction of the first term on the right-hand side and then letting  $n \rightarrow \infty$ . By Corollary 2.9 (or Theorem 2.7),  $\sup_n g(n, \ell = 0) < \infty$ , in agreement with (4.22).

To see how the factor  $\epsilon^2$  comes about let us note that

$$-2\ell^2 = -(\ell - 1)^2 - (\ell + 1)^2 + 2,$$

whence (to be used later) we can for  $\ell = 1, \dots, k_0 - 1$  bound the expression

$$\epsilon^{-2\ell^2} \sqrt{g(n, \ell - 1)} \sqrt{g(n, \ell + 1)} \leq \epsilon^2 f(n, \epsilon). \quad (4.23)$$

To show (4.22) we mimic the proof of Theorem 2.10. Again this is in three steps and we assume that  $\lambda = 0$ . We need to bound each term of  $g(n, \ell)$  for  $\ell \geq 1$ .

**Step I:** Bounding  $\|HI_{in}(N)S_{k_0, \ell}^\alpha \psi\|$ . We expand into terms; some can be bounded independently of  $n$  (using the induction hypothesis) while others will be estimated as  $C\sqrt{g(n, \ell + 1)}$  (assuming here that  $\ell \leq k_0 - 1$ ). We compute formally

$$i[H, I_{in}(N)S_{k_0, \ell}^\alpha] = i[H, I_{in}(N)]S_{k_0, \ell}^\alpha + I_{in}(N)i[H, \prod_{j=1}^{k_0} S_{\alpha_j}], \quad (4.24)$$

where the second commutator is expanded as

$$i[H, \prod_{j=1}^{k_0} S_{\alpha_j}] = \sum_{m=1}^{k_0} \left( \prod_{j=m+1}^{k_0} S_{\alpha_j} \right) i[H, S_{\alpha_m}] \left( \prod_{j=1}^{m-1} S_{\alpha_j} \right). \quad (4.25)$$

In turn we have the expressions

$$i[H, I_{in}(N)] = n^{-1} I_{in}(N) i[N, H]^0 I_{in}(N), \quad (4.26a)$$

$$i[H, S_{\alpha_m}] = -M_1 \quad \text{if } \alpha_m = 1, \quad (4.26b)$$

$$i[H, S_{\alpha_m}] = M_2 S_1 \quad \text{if } \alpha_m = 0. \quad (4.26c)$$

We plug (4.26a)–(4.26c) into (4.24) and (4.25) and look at each term separately. Before embarking on a such examination we need to “fix” the above formal computation. This is done in terms of multiple approximation somewhat similar to the one of the proof of Theorem 2.7. We replace  $H \rightarrow H_p$  and the factors  $A \rightarrow A_q$  and  $N^{1/2} \rightarrow N_{iq}^{1/2} = (N^{1/2})_{iq}$ . More precisely it is convenient to introduce  $k_0$  different  $q$ ’s, say  $q_1, \dots, q_{k_0}$ ; the  $q$  used for the  $j$ ’th factor  $S_{\alpha_j}$  is  $q_j$ . For fixed  $p$  and  $q$ ’s the product rule applies for computing the commutator of the product and the analogues of (4.24) and (4.25) hold true. Now we can take the limit  $p \rightarrow \infty$ . We can plug the modified expressions of (4.26a)–(4.26c) into (modified) (4.24) and (4.25). Actually (4.26a) is the same, but (4.26b) and (4.26c) are changed as

$$i[H, N_{iq_j}^{1/2}] = -I_{iq_j}(N^{1/2}) M_1 I_{iq_j}(N^{1/2}), \quad (4.27a)$$

$$i[H, A_{q_j}] = I_{q_j}(A) M_2 S_1 I_{q_j}(A). \quad (4.27b)$$

Of course we have a  $q$ -dependence of the various factors of either  $S_1 \rightarrow N_{iq_j}^{1/2}$  or  $S_0 \rightarrow A_{q_j}$ . Eventually we take the limits in the  $q$ ’s done in increasing order starting by taking  $q_1 \rightarrow \infty$

and ending by taking  $q_{k_0} \rightarrow \infty$ . Before taking these limits we need to do some further commutation using Condition 4.11. For simplicity of presentation we ignore below in this process commutation with the regularizing factors of  $I_{iq_j}(N^{1/2})$  or  $I_{q_j}(A)$  since in the limit they will disappear (a manifestation of this occurred also in the proof of Lemma 3.4). In other words we proceed now slightly formally using (4.24) and (4.25) with the plugged in expressions (4.26a)–(4.26c):

From (4.26a) we obtain that  $\|i[H, I_{in}(N)]\| \leq C$  so the contribution from the first term of (4.24) can be estimated (uniformly in  $n$ ) as

$$\|i[H, I_{in}(N)]S_{k_0, \ell}^\alpha \psi\| \leq C \|S_{k_0, \ell}^\alpha \psi\| \leq \tilde{C}. \quad (4.28)$$

As for the contribution from (4.26b) we compute

$$-I_{in}(N) \left( \prod_{j=m+1}^{k_0} S_{\alpha_j} \right) M_1 \left( \prod_{j=1}^{m-1} S_{\alpha_j} \right) = \tilde{T}_1 \left( N^{\frac{1}{2}} \prod_{\substack{1 \leq j \leq k_0 \\ j \neq m}} S_{\alpha_j} \right) + \tilde{T}_2,$$

where

$$\tilde{T}_1 = -I_{in}(N) M_1 N^{-\frac{1}{2}}.$$

Here  $\tilde{T}_2$  is given by repeated commutation using Condition 4.11. We apply this identity to the bound state  $\psi$ . Since  $\|\tilde{T}_1\| \leq C$  the induction hypothesis gives similar bounds as (4.28) for the contribution from (4.26b).

It remains to look at the contribution from (4.26c): We commute the factor  $M_2$  to the left and get similarly

$$\begin{aligned} I_{in}(N) \left( \prod_{j=m+1}^{k_0} S_{\alpha_j} \right) M_2 S_1 \left( \prod_{j=1}^{m-1} S_{\alpha_j} \right) \\ = \tilde{T}_1 N^{\frac{1}{2}} I_{in}(N) \left( \prod_{j=m+1}^{k_0} S_{\alpha_j} \right) S_1 \left( \prod_{j=1}^{m-1} S_{\alpha_j} \right) + \tilde{T}_2, \end{aligned}$$

where

$$\tilde{T}_1 = I_{in}(N) M_2 (N^{\frac{1}{2}} I_{in}(N))^{-1}.$$

As before  $\|\tilde{T}_1\| \leq C$  (here we use that  $H'$  is  $N$ -bounded) and the contribution from  $\tilde{T}_2$  is treated by using Condition 4.11 and the induction hypothesis. Consequently we get for  $\ell \leq k_0 - 1$  the total bound

$$\|HI_{in}(N)S_{k_0, \ell}^\alpha \psi\| \leq \tilde{C}_1 \sqrt{g(n, \ell + 1)} + \tilde{C}_2, \quad (4.29)$$

where  $\tilde{C}_1$  and  $\tilde{C}_2$  are independent of  $n$ , and for  $\ell = k_0$  this bound without the first term to the right.

**Step II:** Bounding  $\|AI_{in}(N)S_{k_0, \ell}^\alpha \psi\|$ . We claim that (recall  $\ell \geq 1$ )

$$\|AI_{in}(N)S_{k_0, \ell}^\alpha \psi\| \leq \tilde{C}_3 \sqrt{g(n, \ell - 1)} + \tilde{C}_4, \quad (4.30)$$

where  $\tilde{C}_3$  and  $\tilde{C}_4$  are independent of  $n$ .

To prove (4.30) we observe that it suffices by the induction hypothesis to bound  $\|I_{in}(N)AS_{k_0, \ell}^\alpha \psi\|$ . Since  $\ell \geq 1$  there is a nearest factor of  $N^{1/2}$  in the product  $S_{k_0, \ell}^\alpha$  that we move to the left in front of the factor  $A$ :

$$I_{in}(N)AS_{k_0, \ell}^\alpha = N^{\frac{1}{2}} I_{in}(N)AS_{k_0-1, \ell-1}^\beta + T.$$

We apply this identity to the bound state  $\psi$ . The contribution from  $T$  is treated by using (4.19) and the induction hypothesis. This proves (4.30).

**Step III:** We repeat Step III of the proof of Theorem 2.10 using now the proven estimates (4.29) and (4.30) to bound any term of  $g(n, \ell)$  for  $\ell \geq 1$ . In combination with (4.23) these bounds yield (4.22) with

$$K_1 = 2C_2 \tilde{C}_1 \tilde{C}_3 (2^{k_0} - 1) + 1;$$

here the constant  $C_2$  comes from (2.4) while  $\tilde{C}_1$  and  $\tilde{C}_3$  come from (4.29) and (4.30), respectively. Notice that the cardinality of set  $\{0, 1\}^{k_0}$  is  $2^{k_0}$ , so the factor  $2^{k_0} - 1$  arises by counting only those indices  $\alpha \in \{0, 1\}^{k_0}$  with  $\sum \alpha_j \geq 1$ .  $\square$

**Corollary 4.13.** *Suppose the conditions of Corollary 2.9 and for  $k_0 \geq 2$  also Condition 4.11. Let  $\psi \in \mathcal{D}(N^{1/2})$  be a bound state  $(H - \lambda)\psi = 0$  (with  $\lambda$  as in Condition 2.3). Then  $\psi \in \mathcal{D}(N^{(k_0+1)/2})$ .*

## 5 A Class of Massless Linearly Coupled Models

In this section we introduce a class of massless linearly coupled Hamiltonians, sometimes referred to as Pauli-Fierz Hamiltonians [BD, DG, DJ1, GGM2]. The bulk of this section is spent on checking that an expanded version of the Hamiltonian does indeed satisfy the abstract assumptions of Section 2. In Subsection 5.2 we verify that the Nelson model described in Subsection 1.2 is indeed an example of the type of models discussed here.

### 5.1 The Model and the Result

Consider the Hilbert space  $\mathcal{H}_{\text{PF}} = \mathcal{K} \otimes \Gamma(\mathfrak{h})$ , where  $\mathcal{K}$  is the Hilbert space for a “small” quantum system, and  $\Gamma(\mathfrak{h})$  is the symmetric Fock space over  $\mathfrak{h} = L^2(\mathbb{R}^d, dk)$ , describing a field of massless scalar bosons. The Pauli-Fierz Hamiltonian  $H_v^{\text{PF}}$  acting on  $\mathcal{H}_{\text{PF}}$  is defined by

$$H_v^{\text{PF}} = K \otimes \mathbb{1}_{\Gamma(\mathfrak{h})} + \mathbb{1}_{\mathcal{K}} \otimes d\Gamma(|k|) + \phi(v), \quad (5.1)$$

where  $K$  is a Hamiltonian on  $\mathcal{K}$  describing the dynamics of the small system. We assume that  $K$  is bounded from below, and for convenience we require furthermore that

$$K \geq 0.$$

The term  $d\Gamma(|k|)$  is the second quantization of the operator of multiplication by  $|k|$ , and  $\phi(v) = (a^*(v) + a(v))/\sqrt{2}$ . The form factor  $v$  is an operator from  $\mathcal{K}$  to  $\mathcal{K} \otimes \mathfrak{h}$ , and  $a^*(v)$ ,  $a(v)$  are the usual creation and annihilation operators associated to  $v$ . See [BD, GGM2]. The hypotheses we make are slightly stronger than the ones considered in [GGM2]. The first one, Hypothesis **(H0)**, expresses the assumption that the small system is confined:

**(H0)**  $(K + i)^{-1}$  is compact on  $\mathcal{K}$ .

Let  $0 \leq \tau < 1/2$  be fixed. We will introduce a class of interactions which increase with  $\tau$ . In order to formulate our assumption on the form factor  $v$  we introduce the subspace  $\mathcal{O}_\tau$  of  $\mathcal{B}(\mathcal{D}(K^\tau); \mathcal{K} \otimes \mathfrak{h})$  consisting of those operators which extend by continuity from  $\mathcal{D}(K^\tau)$  to an element of  $\mathcal{B}(\mathcal{K}; \mathcal{D}(K^\tau)^* \otimes \mathfrak{h})$ . In other words

$$\mathcal{O}_\tau := \left\{ v \in \mathcal{B}(\mathcal{D}(K^\tau); \mathcal{K} \otimes \mathfrak{h}) \mid \exists C > 0, \forall \psi \in \mathcal{D}(K^\tau) : \|[(K + 1)^{-\tau} \otimes \mathbb{1}_{\mathfrak{h}}]v\psi\|_{\mathcal{K} \otimes \mathfrak{h}} \leq C \|\psi\|_{\mathcal{K}} \right\}.$$

We also write  $v$  for the extension. It is natural to introduce a norm on  $\mathcal{O}_\tau$  by

$$\|v\|_\tau = \|v(K+1)^{-\tau}\|_{\mathcal{B}(\mathcal{K}; \mathcal{K} \otimes \mathfrak{h})} + \|[(K+1)^{-\tau} \otimes \mathbb{1}_{\mathfrak{h}}]v\|_{\mathcal{B}(\mathcal{K}; \mathcal{K} \otimes \mathfrak{h})}.$$

Our first assumption on the form factor interaction is the following:

**(I1)**  $v, [\mathbb{1}_{\mathcal{K}} \otimes |k|^{-1/2}]v \in \mathcal{O}_\tau$ .

It is proved in [GGM2] that if **(I1)** holds,  $H_v^{\text{PF}}$  is self-adjoint with domain  $\mathcal{D}(H_v^{\text{PF}}) = \mathcal{D}(K \otimes \mathbb{1}_{\Gamma(\mathfrak{h})} + \mathbb{1}_{\mathcal{K}} \otimes d\Gamma(|k|))$ .

The unitary operator  $T : L^2(\mathbb{R}^d) \rightarrow L^2(\mathbb{R}_+) \otimes L^2(S^{d-1}) =: \tilde{\mathfrak{h}}$  defined by  $(Tu)(\omega, \theta) = \omega^{(d-1)/2} u(\omega\theta)$  allows us to pass to polar coordinates. Lifting  $T$  to the full Hilbert space as  $\mathbb{1}_{\mathcal{K}} \otimes \Gamma(T)$  gives a unitary map from  $\mathcal{H}_{\text{PF}}$  to  $\tilde{\mathcal{H}}_{\text{PF}} := \mathcal{K} \otimes \Gamma(\tilde{\mathfrak{h}})$ . The Hamiltonian  $H_v^{\text{PF}}$  is unitarily equivalent to

$$\tilde{H}_v^{\text{PF}} := K \otimes \mathbb{1}_{\Gamma(\tilde{\mathfrak{h}})} + \mathbb{1}_{\mathcal{K}} \otimes d\Gamma(\omega) + \phi(\tilde{v}), \quad (5.2)$$

where  $\tilde{v} = [\mathbb{1}_{\mathcal{K}} \otimes T]v \in \mathcal{B}(\mathcal{K}; \mathcal{K} \otimes \tilde{\mathfrak{h}})$ .

In polar coordinates the space of couplings consists of operators of the form  $[\mathbb{1}_{\mathcal{K}} \otimes T]v : \mathcal{K} \rightarrow \mathcal{K} \otimes \tilde{\mathfrak{h}}$ , where  $v \in \mathcal{O}_\tau$ . We write  $\tilde{\mathcal{O}}_\tau = [\mathbb{1}_{\mathcal{K}} \otimes T]\mathcal{O}_\tau$  and equip it with the obvious norm  $\|\tilde{v}\|_\tau = \|[\mathbb{1}_{\mathcal{K}} \otimes T^*]\tilde{v}\|_\tau$ . Observe  $\|\tilde{v}\|_\tau = \|v\|_\tau$ , when  $\tilde{v} = [\mathbb{1}_{\mathcal{K}} \otimes T]v$ .

Let  $d$  be as in (1.7) and (1.8). We recall that  $d$  expresses the least amount of infrared regularization carried by a  $v$  satisfying **(I2)** below. The following further assumptions on the interaction are made:

**(I2)** The following holds

$$\begin{aligned} [\mathbb{1}_{\mathcal{K}} \otimes (1 + \omega^{-1/2})\omega^{-1}d(\omega) \otimes \mathbb{1}_{L^2(S^{d-1})}]\tilde{v} &\in \tilde{\mathcal{O}}_\tau, \\ [\mathbb{1}_{\mathcal{K}} \otimes (1 + \omega^{-1/2})d(\omega)\partial_\omega \otimes \mathbb{1}_{L^2(S^{d-1})}]\tilde{v} &\in \tilde{\mathcal{O}}_\tau, \end{aligned}$$

**(I3)**  $[\mathbb{1}_{\mathcal{K}} \otimes \partial_\omega^2 \otimes \mathbb{1}_{L^2(S^{d-1})}]\tilde{v} \in \mathcal{B}(\mathcal{D}(K^\tau); \mathcal{K} \otimes \tilde{\mathfrak{h}})$ .

In this paper we need an additional assumption compared to [GGM2]. For bounded  $K$ , it is implied by **(I1)**. Its presence is motivated by a desire to deal effectively with infrared singularities.

**(I4)** The form  $[K \otimes \mathbb{1}_{\tilde{\mathfrak{h}}}] \tilde{v} - \tilde{v}K$  extends from  $[\mathcal{D}(K) \otimes \tilde{\mathfrak{h}}] \times \mathcal{D}(K)$  to an element of  $\tilde{\mathcal{O}}_{\frac{1}{2}}$ .

Here  $\tilde{\mathcal{O}}_{\frac{1}{2}}$  is defined as  $\tilde{\mathcal{O}}_\tau$ . Supposing **(I1)**, the statement above is meaningful. See also Remark 5.14 below.

**Remark 5.1.** We remark that for separable Hilbert spaces  $\mathcal{K}_1$  and  $\mathcal{K}_2$  there are two natural subspaces of  $\mathcal{B}(\mathcal{K}_1; \mathcal{K}_2 \otimes \mathfrak{h})$ . Namely

$$\begin{aligned} L^2(\mathbb{R}^d; \mathcal{B}(\mathcal{K}_1; \mathcal{K}_2)) &= \left\{ v : \mathbb{R}^d \rightarrow \mathcal{B}(\mathcal{K}_1; \mathcal{K}_2) \mid \int_{\mathbb{R}^d} \|v(k)\|_{\mathcal{B}(\mathcal{K}_1; \mathcal{K}_2)}^2 dk < \infty \right\} \\ L_w^2(\mathbb{R}^d; \mathcal{B}(\mathcal{K}_1; \mathcal{K}_2)) &= \left\{ v : \mathbb{R}^d \rightarrow \mathcal{B}(\mathcal{K}_1; \mathcal{K}_2) \mid \sup_{\|\psi\|_1 \leq 1} \int_{\mathbb{R}^d} \|v(k)\psi\|_2^2 dk < \infty \right\}. \end{aligned}$$

The functions  $v$  should be weakly measurable, to ensure that  $\|v(k)\|_{\mathcal{B}(\mathcal{K}_1; \mathcal{K}_2)}$  and  $\|v(k)\psi\|_2$  are measurable. Here  $\|\cdot\|_j$  denotes the norm on  $\mathcal{K}_j$ . We have the obvious inclusions

$$L^2(\mathbb{R}^d; \mathcal{B}(\mathcal{K}_1; \mathcal{K}_2)) \subseteq L_w^2(\mathbb{R}^d; \mathcal{B}(\mathcal{K}_1; \mathcal{K}_2)) \subseteq \mathcal{B}(\mathcal{K}_1; \mathcal{K}_2 \otimes \mathfrak{h}).$$

The first inclusion is a contraction and the second an isometry. Both inclusions are strict as exemplified by choosing  $\mathcal{K}_1 = \mathcal{K}_2 = L^2(\mathbb{R}_x^3)$ ,  $\mathfrak{h} = L^2(\mathbb{R}_k^3)$  and  $v_1(k) = e^{-|x-k|}$  (read as a multiplication operator) for the first inclusion and  $v_2(k, x) = |x-k|^{-1}e^{-|x-k|}$  for the second. Here  $v_2$  induces the bounded operator  $v_2: L^2(\mathbb{R}_x^3) \rightarrow L^2(\mathbb{R}_k^3 \times \mathbb{R}_x^3)$  by the prescription  $(v_2\psi)(k, x) = v_2(k, x)\psi(x)$ . (In [DG, Subsection 2.16] and [GGM2, Subsection 3.4] the second inclusion is claimed to be an equality.)

We denote by  $\mathcal{I}_{\text{PF}}(d)$  the vector space of interactions  $v$  satisfying **(I1)**–**(I4)** and turn it into a normed vector space by equipping it (in polar coordinates) with the norm

$$\begin{aligned} \|v\|_{\text{PF}} := & \left\| [\mathbb{1}_{\mathcal{K}} \otimes (1 + \omega^{-3/2}d(\omega)) \otimes \mathbb{1}_{L^2(S^{d-1})}] \tilde{v} \right\|_{\tau} \\ & + \left\| [\mathbb{1}_{\mathcal{K}} \otimes (1 + \omega^{-1}d(\omega)\partial_{\omega}) \otimes \mathbb{1}_{L^2(S^{d-1})}] \tilde{v} \right\|_{\tau} \\ & + \left\| [(K+1)^{-1/2} \otimes \partial_{\omega}^2 \otimes \mathbb{1}_{L^2(S^{d-1})}] \tilde{v} \right\|_{\mathcal{B}(\mathcal{K}; \mathcal{K} \otimes \mathfrak{h})} \\ & + \left\| [K \otimes \mathbb{1}_{\mathfrak{h}}] \tilde{v} - \tilde{v}K \right\|_{\frac{1}{2}}, \end{aligned} \quad (5.3)$$

For any  $v_0 \in \mathcal{I}_{\text{PF}}(d)$  and  $r > 0$  write

$$\mathcal{B}_r(v_0) = \{v \in \mathcal{I}_{\text{PF}}(d) \mid \|v - v_0\|_{\text{PF}} \leq r\} \quad (5.4)$$

for the closed ball in  $\mathcal{I}_{\text{PF}}(d)$  with radius  $r$  around  $v_0$ .

Let us recall the definition of the conjugate operator on  $\tilde{\mathcal{H}}_{\text{PF}}$  used in [GGM2]. Let  $\chi \in C_0^\infty([0, \infty))$  be such that  $\chi(\omega) = 0$  if  $\omega \geq 1$  and  $\chi(\omega) = 1$  if  $\omega \leq 1/2$ . For  $0 < \delta \leq 1/2$ , the function  $m_\delta \in C^\infty([0, \infty))$  is defined by

$$m_\delta(\omega) = \chi\left(\frac{\omega}{\delta}\right)d(\delta) + (1 - \chi)\left(\frac{\omega}{\delta}\right)d(\omega),$$

On  $\tilde{\mathfrak{h}}$ , the operator  $\tilde{a}_\delta$  is defined in the same way as in [GGM2], that is

$$\tilde{a}_\delta := im_\delta(\omega) \frac{\partial}{\partial \omega} + \frac{i}{2} \frac{dm_\delta}{d\omega}(\omega), \quad \mathcal{D}(\tilde{a}_\delta) = H_0^1(\mathbb{R}^+) \otimes L^2(S^{d-1}). \quad (5.5)$$

Its adjoint is given by

$$\tilde{a}_\delta^* := im_\delta(\omega) \frac{\partial}{\partial \omega} - \frac{i}{2} \frac{dm_\delta}{d\omega}(\omega), \quad \mathcal{D}(\tilde{a}_\delta^*) = H^1(\mathbb{R}^+) \otimes L^2(S^{d-1}). \quad (5.6)$$

We recall that  $H_0^1(\mathbb{R}^+)$  is the closure of  $C_0^\infty((0, \infty))$  in  $H^1(\mathbb{R}^+)$ . The conjugate operator  $\tilde{A}_\delta$  on  $\tilde{\mathcal{H}}_{\text{PF}}$  is defined by  $\tilde{A}_\delta := \mathbb{1}_{\mathcal{K}} \otimes d\Gamma(\tilde{a}_\delta)$ . Going back to  $\mathcal{H}_{\text{PF}}$  we get  $a_\delta = T^{-1}\tilde{a}_\delta T$  and

$$A_\delta = d\Gamma(a_\delta) = [\mathbb{1}_{\mathcal{K}} \otimes \Gamma(T^{-1})] \tilde{A}_\delta [\mathbb{1}_{\mathcal{K}} \otimes \Gamma(T)].$$

The operator  $a_\delta$  takes the form (1.11) when written in the original coordinates.

We write  $\mathcal{N}$  for the number operator  $\mathbb{1}_{\mathcal{K}} \otimes d\Gamma(\mathbb{1}_{\mathfrak{h}})$  on  $\mathcal{H}_{\text{PF}}$ . For  $E \in \sigma_{\text{pp}}(H_v^{\text{PF}})$ , we write  $P_v$  for the corresponding eigenprojection. Recall from [GGM2, Theorem 2.4] that the range of  $P_v$  is finite dimensional under the assumptions **(H0)**, **(I1)** and **(I2)**.

**Theorem 5.2.** *Suppose **(H0)**. Let  $v_0 \in \mathcal{I}_{\text{PF}}(d)$  and  $J \subseteq \mathbb{R}$  be a compact interval. There exists  $0 < \delta_0 \leq 1/2$  such that for all  $0 < \delta \leq \delta_0$  the following holds: There exist  $\gamma > 0$  and  $C > 0$  such that for any  $v \in \mathcal{B}_\gamma(v_0)$  and  $E \in \sigma_{\text{pp}}(H_v^{\text{PF}}) \cap J$  we have*

$$P_v : \mathcal{H}_{\text{PF}} \rightarrow \mathcal{D}(\mathcal{N}^{\frac{1}{2}}A_\delta) \cap \mathcal{D}(A_\delta\mathcal{N}^{\frac{1}{2}}) \cap \mathcal{D}(\mathcal{N})$$

and

$$\|\mathcal{N}^{\frac{1}{2}}A_\delta P_v\| + \|A_\delta\mathcal{N}^{\frac{1}{2}}P_v\| + \|\mathcal{N}P_v\| \leq C.$$

Unfortunately we cannot employ our theory directly to conclude the above theorem, due to  $A_\delta$  not being self-adjoint. Instead we use a trick of passing to an 'expanded' model, for which we can use our abstract theory. The theorem above will then be a consequence of a corresponding theorem in the expanded picture.

**Remark 5.3.** Under the hypotheses of Theorem 5.2, we also have that  $P_v : \mathcal{H}_{\text{PF}} \rightarrow \mathcal{D}(A_\delta^* \mathcal{N}^{1/2}) \cap \mathcal{D}(\mathcal{N}^{1/2} A_\delta^*)$ . This follows from  $A_\delta \subseteq A_\delta^*$ . In particular this implies that  $P_v A_\delta$  extends from  $\mathcal{D}(A_\delta)$  to a bounded operator on  $\mathcal{H}_{\text{PF}}$ . Similar statements hold also for  $P_v A_\delta \mathcal{N}^{1/2}$  and  $P_v \mathcal{N}^{1/2} A_\delta$ .

## 5.2 Application to the Nelson Model

In this subsection we check the conditions **(H0)** and **(I1)**–**(I4)** for the Nelson model introduced in the introduction. After possibly adding a constant to  $W$ , we can assume that  $K \geq 0$ . See (1.4) and **(W0)**.

We begin by remarking that it follows from **(W0)** and **(V0)** that

$$|x|^\alpha (K+1)^{-\frac{1}{2}} \in \mathcal{B}(\mathcal{K}) \quad (5.7)$$

$$|p|(K+1)^{-\frac{1}{2}} \in \mathcal{B}(\mathcal{K}). \quad (5.8)$$

Here  $\alpha > 2$  is coming from **(W0)**,  $|x| = |x_1| + \dots + |x_P|$  and  $|p| = |p_1| + \dots + |p_P|$ , where  $p_\ell = -i\nabla_{x_\ell}$ . These bounds imply in particular **(H0)**.

Let  $\Psi_N : \mathcal{I}_N(d) \rightarrow \mathcal{B}(\mathcal{K}; \mathcal{K} \otimes \mathfrak{h})$  be defined by

$$\Psi_N(\rho) = \sum_{\ell=1}^P e^{-ik \cdot x_\ell} \rho.$$

Clearly  $\Psi_N$  is a linear map and  $\phi(\Psi_N(\rho)) = I_\rho(x)$  such that

$$H_\rho^N = K \otimes \mathbb{1}_{\mathcal{F}} + \mathbb{1}_{\mathcal{K}} \otimes d\Gamma(|k|) + \phi(\Psi_N(\rho)),$$

is a Pauli-Fierz Hamiltonian, cf. (1.5) and (1.6). Verifying the conditions **(I1)**–**(I4)** will be achieved if we can show that  $\Psi_N$  is a bounded operator from  $\mathcal{I}_N(d)$  to  $\mathcal{I}_{\text{PF}}(d)$ . This also implies that results valid uniformly for  $v$  in a ball in  $\mathcal{I}_{\text{PF}}(d)$  will translate into results holding uniformly for  $\rho$  in a sufficiently small ball in  $\mathcal{I}_N(d)$ . See Remark 2.11 4).

That the terms in the norm  $\|\Psi_N(\rho)\|_{\text{PF}}$ , cf. (5.3), pertaining to the conditions **(I1)**–**(I3)** can be bounded by  $\|\cdot\|_N$  (or rather terms in  $\|\cdot\|_N$  pertaining to **(\rho1)**–**(\rho3)**), follows as in [GGM2] after we have checked that  $|x|^2(K+1)^{-\tau}$  is bounded for some positive  $\tau < 1/2$ .

To produce such a  $\tau$  we invoke Hadamard's three-line theorem. Consider the function  $z \rightarrow |x|^{-i\alpha z}(K+1)^{iz/2} \in \mathcal{B}(\mathcal{K})$ . Observe that this function is bounded when  $\text{Im } z = 0$  or  $\text{Im } z = 1$ , cf. (5.7). It now follows, cf. [RS], that  $|x|^{s\alpha}(K+1)^{-s/2}$  is bounded for  $0 \leq s \leq 1$ . Choosing  $s = 2/\alpha$  implies the desired bound with  $\tau = \alpha^{-1} < 1/2$ . This will be the  $\tau$  used in the conditions **(I1)**–**(I3)**.

It remains to verify **(I4)**. For this we compute

$$\begin{aligned}
[K \otimes \mathbb{1}_{\mathfrak{h}}]e^{-ik \cdot x_j} \rho - e^{-ik \cdot x_j} \rho K &= - \sum_{\ell=1}^P \left[ \frac{1}{2m_\ell} \Delta_\ell e^{-ik \cdot x_j} \rho - \rho e^{-ik \cdot x_j} \frac{1}{2m_\ell} \Delta_\ell \right] \\
&= - \left[ \frac{1}{2m_j} \Delta_j e^{-ik \cdot x_j} \rho - \rho e^{-ik \cdot x_j} \frac{1}{2m_j} \Delta_j \right] \\
&= \frac{e^{-ik \cdot x_j}}{2m_\ell} [-2k \cdot p_j + k^2] \rho \\
&= [-2k \cdot p_j - k^2] \rho \frac{e^{-ik \cdot x_j}}{2m_j}
\end{aligned} \tag{5.9}$$

From this computation and (5.8) we conclude that  $[K \otimes \mathbb{1}] \Psi_N(\rho) - \Psi_N(\rho) K \in \mathcal{O}_{1/2}$  as required by **(I4)** and the  $\|\cdot\|_{1/2}$ -norm of the difference is bounded by a constant times  $\|\rho\|_N$ . Here we need the term in  $\|\cdot\|_N$  coming from **(\rho4)**.

We can thus conclude Theorem 1.2 from Theorem 5.2.

It remains to discuss the Nelson model after a Pauli-Fierz transformation. We recall that we have two transformations to consider, one giving rise to  $H_\rho^{N'}$  and one to  $H_\rho^{N''}$ . See (1.12) and (1.16). To identify these Hamiltonians as Pauli-Fierz Hamiltonians, we introduce a linear map  $\Psi'_N : \mathcal{I}'_N(d) \rightarrow \mathcal{B}(\mathcal{K}; \mathcal{K} \otimes \mathfrak{h})$  by

$$\Psi'_N(\rho) = \sum_{\ell=1}^P (e^{-ik \cdot x_\ell} - 1) \rho.$$

With this notation we find for  $\rho \in \mathcal{I}'_N(d)$

$$H_\rho^{N'} = K_\rho \otimes \mathbb{1}_{\Gamma(\mathfrak{h})} + \mathbb{1}_{\mathcal{K}} \otimes d\Gamma(|k|) + \phi(\Psi'_N(\rho))$$

and, specializing to  $\rho = \rho_0 + \rho_1$  with  $\rho_0 \in \mathcal{I}'_N(d)$  and  $\rho_1 \in \mathcal{I}_N(d)$ ,

$$H_\rho^{N''} = (K_{\rho_0} - \sum_{\ell=1}^P v_{\rho_0, \rho_1}(x_\ell)) \otimes \mathbb{1}_{\Gamma(\mathfrak{h})} + \mathbb{1}_{\mathcal{K}} \otimes d\Gamma(|k|) + \phi(\Psi'_N(\rho_0) + \Psi_N(\rho_1)).$$

See (1.13) for  $K_\rho$  and (1.17) for  $v_{\rho_0, \rho_1}$ .

In order to apply Theorem 5.2 one should first observe that  $\Psi'_N$  is a bounded map from  $\mathcal{I}'_N(d)$  to  $\mathcal{I}_{\text{PF}}(d)$ . We leave it to the reader to establish this following the arguments in [GGM2], using the key estimate (1.15). As for **(I4)**, observe that the extra  $-\rho$  from  $(e^{-ik \cdot x_j} - 1)\rho$  drops out when repeating (5.9) for  $\Psi'_N(\rho)$ . In particular we do not need (1.15) for **(I4)**.

Observe that for both the transformed Hamiltonians, the Hamiltonian for the confined quantum system  $K$  is altered by the transformation, to obtain e.g.  $K_\rho$  in the case of  $H_\rho^{N'}$ . A priori the norm  $\|\cdot\|_{\text{PF}}$  is however defined in terms of the operator  $K$ , and this definition we retain.

However, when verifying the Mourre estimate in Subsection 5.4 and our abstract assumptions for Pauli-Fierz Hamiltonians in Subsection 5.5, we will naturally meet norms with the modified  $\rho$ -dependent  $K$ 's, and not the original  $K$ . We proceed to argue that the  $\|\cdot\|_{\text{PF}}$  norms arising in this way are equivalent, locally uniformly in  $\rho$ , with respect to the appropriate normed space. Let for  $\rho \in \mathcal{I}'_N(d)$

$$B'_\rho = K_\rho - K = - \sum_{\ell=1}^P v_\rho(x_\ell) + \frac{P^2}{2} \int_0^\infty r^{-1} |\tilde{\rho}(r)|^2 dr \mathbb{1}_{\mathcal{K}}$$

and for  $\rho = \rho_0 + \rho_1$  as above

$$B''_\rho = - \sum_{\ell=1}^P v_{\rho_0, \rho_1}(x_\ell) - \sum_{\ell=1}^P v_{\rho_0}(x_\ell) + \frac{P^2}{2} \int_0^\infty r^{-1} |\tilde{\rho}_0(r)|^2 dr \mathbb{1}_{\mathcal{K}}.$$

We observe the bounds

$$\|B'_\rho\| \leq C \|\rho\|_{\mathbb{N}}^2 \text{ and } \|B''_\rho\| \leq C (\|\rho_0\|_{\mathbb{N}}^2 + \|\rho_1\|_{\mathbb{N}}^2),$$

for some  $\rho$ -independent constant  $C$ . In particular both  $B'_\rho$  and  $B''_\rho$  can be bounded locally uniformly in  $\rho$ , with respect to the appropriate norm. By yet another interpolation argument this implies that we can pass between  $\|\cdot\|_{\text{PF}}$  norms defined with either  $K$ ,  $K_\rho$ , or  $K_{\rho_0} + B''_\rho$ , and still retain bounds that are locally uniform in  $\rho$ .

Finally we note that the above bounds also imply that by possibly adding to  $W$  a positive constant we still have  $K_\rho \geq 0$  and  $K_{\rho_0} + B''_\rho \geq 0$  locally in  $\rho$ . This ensures that **(H0)** is satisfied also for transformed Nelson Hamiltonians. In particular we still have e.g.  $|x|^2(K_\rho + 1)^{-\tau}$  bounded.

In conclusion, Theorem 1.3 also follows from Theorem 5.2.

### 5.3 Expanded Objects

Let us now define the expanded operator  $\widehat{H}_v^e$  on  $\widehat{\mathcal{H}}^e := \widetilde{\mathcal{H}}_{\text{PF}} \otimes \Gamma(\tilde{\mathfrak{h}})$  by

$$\widehat{H}_v^e := \widetilde{H}_v^{\text{PF}} \otimes \mathbb{1}_{\Gamma(\tilde{\mathfrak{h}})} - \mathbb{1}_{\widetilde{\mathcal{H}}_{\text{PF}}} \otimes d\Gamma(\hat{h}), \quad (5.10)$$

where  $\hat{h}$  is the operator of multiplication by

$$\hat{h}(\omega) = e^\omega - 1 - \frac{\omega^2}{2}. \quad (5.11)$$

From the bound  $\omega \leq \frac{1}{2} + \omega^2/2$  we find that for  $\omega \geq 0$

$$\frac{d}{d\omega} \hat{h}(\omega) \geq \hat{h}(\omega) + \frac{1}{2}. \quad (5.12)$$

Since  $L^2(\mathbb{R}^+) \oplus L^2(\mathbb{R}^+) \simeq L^2(\mathbb{R})$ , it is known (see e.g. [DJ1]) that there exists a unitary operator

$$\mathcal{U} : \Gamma(\tilde{\mathfrak{h}}) \otimes \Gamma(\tilde{\mathfrak{h}}) \rightarrow \Gamma(\mathfrak{h}^e), \quad (5.13)$$

where  $\mathfrak{h}^e := L^2(\mathbb{R}) \otimes L^2(S^{d-1})$ . On  $\mathcal{K} \otimes \Gamma(\tilde{\mathfrak{h}}) \otimes \Gamma(\tilde{\mathfrak{h}})$ , the unitary operator  $\mathbb{1}_{\mathcal{K}} \otimes \mathcal{U}$  is still denoted by  $\mathcal{U}$ . It maps into  $\mathcal{H}^e = \mathcal{K} \otimes \Gamma(\mathfrak{h}^e)$ . In this representation, the operator  $\widehat{H}_v^e$  is unitary equivalent to the ‘expanded Pauli-Fierz Hamiltonian’  $H_v^e$  defined as an operator on  $\mathcal{H}^e$  by

$$H_v^e := \mathcal{U} \widehat{H}_v^e \mathcal{U}^{-1} = K \otimes \mathbb{1}_{\Gamma(\mathfrak{h}^e)} + \mathbb{1}_{\mathcal{K}} \otimes d\Gamma(h) + \phi(v^e), \quad (5.14)$$

where  $v^e \in \mathcal{B}(\mathcal{K}, \mathcal{K} \otimes \mathfrak{h}^e)$ , and  $v^e$  and  $h$  are defined by

$$h(\omega) := \begin{cases} \omega & \text{if } \omega \geq 0, \\ -\hat{h}(-\omega) & \text{if } \omega \leq 0, \end{cases} \quad v^e(\omega) := \begin{cases} \tilde{v}(\omega) & \text{if } \omega \geq 0, \\ 0 & \text{if } \omega \leq 0. \end{cases} \quad (5.15)$$

Note that  $h \in C^2(\mathbb{R})$ . The idea of expanding the Hilbert space in the above fashion has been used previously in [DJ1, DJ2, Gé, JP1]. Our choice of expansion for the boson dispersion relation to the unphysical negative  $\omega$  appears to be new. Previous implementations of the expansion all used the obvious linear expansion  $h(\omega) = \omega$ .

We remark that if  $\mathcal{C}_K \subseteq \mathcal{K}$  is a core for  $K$ ,  $\mathcal{C} \subseteq \Gamma(\tilde{h})$  is a core for  $d\Gamma(\omega)$ , then the algebraic tensor product  $\mathcal{C}_K \otimes \mathcal{C}$  is a core for  $\tilde{H}_0^{\text{PF}}$ , hence for  $\tilde{H}_v^{\text{PF}}$ , and finally  $\mathcal{C}_K \otimes \mathcal{C} \otimes \mathcal{C}$  is a core for  $\hat{H}_v^e$  for any  $v \in \mathcal{I}_{\text{PF}}(d)$ . The domain  $\mathcal{D}(H_v^e)$  itself may however be  $v$  dependent. (The argument for the contrary in [DJ1, Section 5.2] seems wrong.) We have however set up our analysis such that knowledge of  $H_v^e$ 's domain is not needed. See also Lemma 5.15 where an intersection domain is computed.

**Remark 5.4.** We remark that if one is going for higher order results, i.e.  $\psi \in \mathcal{D}(A^{k_0})$  for  $k_0 \geq 2$ , one should use a different  $\hat{h}$ . The choice

$$\hat{h}_{k_0}(\omega) = e^\omega - 1 - \sum_{\ell=2}^{k_0+1} \frac{\omega^\ell}{\ell!}$$

will work since the corresponding  $h_{k_0}$  is in  $C^{k_0+1}(\mathbb{R})$  and the bound

$$\frac{d}{d\omega} \hat{h}_{k_0}(\omega) \geq \frac{\hat{h}_{k_0}(\omega)}{(k_0 - 1)!} + \frac{1}{2}$$

holds for  $\omega \geq 0$  and  $k_0 \geq 1$ . For  $k_0 = 1$  this reduces to (5.12).

Before introducing the conjugate operator on  $\mathcal{H}^e$  that we shall use, let  $m_\delta^e \in C^\infty(\mathbb{R})$  be defined by

$$m_\delta^e(\omega) := \begin{cases} m_\delta(\omega) & \text{if } \omega \geq 0, \\ d(\delta) & \text{if } \omega \leq 0. \end{cases}$$

We set

$$a_\delta^e := im_\delta^e(\omega) \frac{\partial}{\partial \omega} + \frac{i}{2} \frac{dm_\delta^e}{d\omega}(\omega), \quad \mathcal{D}(a_\delta^e) = H^1(\mathbb{R}) \otimes L^2(S^{d-1}), \quad (5.16)$$

and  $A_\delta^e := \mathbb{1}_{\mathcal{K}} \otimes d\Gamma(a_\delta^e)$  as an operator on  $\mathcal{H}^e$ . Note that both  $a_\delta^e$  and  $A_\delta^e$  are self-adjoint.

We can now formulate the expanded version of our regularity theorem

Let

$$\mathcal{N}^e = \mathbb{1}_{\mathcal{K}} \otimes d\Gamma(\mathbb{1}_{\mathfrak{h}^e}) = \mathcal{U}(\mathcal{N} \otimes \mathbb{1}_{\Gamma(\tilde{h})} + \mathbb{1}_{\tilde{\mathcal{H}}_{\text{PF}}} \otimes d\Gamma(\mathbb{1}_{\tilde{h}}))\mathcal{U}^{-1}$$

denote the expanded number operator. For  $E \in \sigma_{\text{pp}}(H_v^e)$  we write  $P_v^e$  for the associated eigenprojection.

**Theorem 5.5.** *Suppose (H0). Let  $v_0 \in \mathcal{I}_{\text{PF}}(d)$  and  $J \subseteq \mathbb{R}$  be a compact interval. There exists a  $0 < \delta_0 \leq 1/2$  such that for any  $0 < \delta \leq \delta_0$  the following holds: There exist  $\gamma > 0$  and  $C > 0$  such that for any  $v \in \mathcal{B}_\gamma(v_0)$  and  $E \in \sigma_{\text{pp}}(H_v^e) \cap J$  we have*

$$P_v^e : \mathcal{H}^e \rightarrow \mathcal{D}((\mathcal{N}^e)^{\frac{1}{2}} A_\delta^e) \cap \mathcal{D}((A_\delta^e (\mathcal{N}^e)^{\frac{1}{2}}) \cap \mathcal{D}(\mathcal{N}^e)$$

and

$$\|(\mathcal{N}^e)^{\frac{1}{2}} A_\delta^e P_v^e\| + \|A_\delta^e (\mathcal{N}^e)^{\frac{1}{2}} P_v^e\| + \|\mathcal{N}^e P_v^e\| \leq C.$$

In the next two subsections we verify that our abstract theory applies to the expanded model, but before doing so we pause to check that Theorem 5.2 does indeed follow from Theorem 5.5. For that we need a lemma.

Let  $W_{\delta,t}$ ,  $t \geq 0$ , denote the contraction semigroup on  $\tilde{\mathcal{H}}_{\text{PF}}$  generated by  $\tilde{A}_\delta$ .

**Lemma 5.6.** *For any state  $\varphi \in \tilde{\mathcal{H}}_{\text{PF}}$  we have for  $t \geq 0$*

$$e^{-itA_\delta^e} \mathcal{U}(\varphi \otimes \Omega) = \mathcal{U}(W_{\delta,t} \varphi \otimes \Omega).$$

*In particular,  $\varphi \in \mathcal{D}(\tilde{A}_\delta^k)$  if and only if  $\mathcal{U}(\varphi \otimes \Omega) \in \mathcal{D}((A_\delta^e)^k)$ .*

*Proof.* It suffices to check the identity on a dense set of  $\varphi$ 's. Let  $\varphi \in \mathcal{K} \otimes \Gamma_{\text{fin}}(H_0^1(\mathbb{R}^+) \otimes L^2(S^{d-1})) \subseteq \mathcal{D}(\tilde{A}_\delta)$ . Then  $\mathcal{U}(\varphi \otimes \Omega) \in \mathcal{K} \otimes \Gamma_{\text{fin}}(H^1(\mathbb{R}) \otimes L^2(S^{d-1})) \subseteq \mathcal{D}(A_\delta^e)$ . The identity now follows by differentiating both sides of the equation and observing they satisfy the same differential equation, with the same initial condition. Here we made use of the equality  $A_\delta^e \mathcal{U}(\varphi \otimes \Omega) = \mathcal{U}(\tilde{A}_\delta \varphi \otimes \Omega)$  valid for  $\varphi \in \mathcal{K} \otimes \Gamma_{\text{fin}}(H_0^1(\mathbb{R}^+) \otimes L^2(S^{d-1}))$ .  $\square$

*Proof of Theorem 5.2.* We only have to recall that bound states of  $H_v^e$  are precisely states on the form  $\mathcal{U}(\varphi \otimes \Omega)$ , where  $\varphi$  is a bound state for  $\tilde{H}_v^{\text{PF}}$ , with the same eigenvalue. This implies that eigenprojections for  $H_v^e$  are on the form  $\mathcal{U}[\tilde{P} \otimes |\Omega\rangle\langle\Omega|]\mathcal{U}^{-1}$  where  $\tilde{P}$  is an eigenprojection for  $\tilde{H}_v^{\text{PF}}$ . Theorem 5.5, together with Lemma 5.6, now implies Theorem 5.2.  $\square$

## 5.4 Mourre Estimates

We begin by establishing a Mourre estimate for  $H_v^{\text{PF}}$  and  $A_\delta$  in a form appropriate for use in this paper. At the end of the subsection we derive a Mourre estimate for  $H_v^e$  and  $A_\delta^e$ .

Let

$$M_\delta := \mathbb{1}_{\mathcal{K}} \otimes d\Gamma(m_\delta) \quad \text{and} \quad R_\delta = R_\delta(v) := -\phi(\text{ia}_\delta v)$$

as operators on  $\mathcal{H}_{\text{PF}}$ . Let  $H'$  be the closure of  $M_\delta + R_\delta$  with domain  $\mathcal{D}(H_v^{\text{PF}}) \cap \mathcal{D}(M_\delta)$ . Recall from [GGM2] that  $H' = [H_v^{\text{PF}}, \text{ia}_\delta]^0$ . Let  $f \in C_0^\infty(\mathbb{R})$  be such that  $0 \leq f \leq 1$ ,  $f(\lambda) = 1$  if  $|\lambda| \leq 1/2$  and  $f(\lambda) = 0$  if  $|\lambda| \geq 1$ . In addition we choose  $f$  to be monotonously decreasing away from 0, i.e.  $\lambda f'(\lambda) \leq 0$ . For  $E \in \mathbb{R}$  and  $\kappa > 0$  we set

$$f_{E,\kappa}(\lambda) := f\left(\frac{\lambda - E}{\kappa}\right).$$

The following ‘Mourre estimate’ for  $H_v^{\text{PF}}$  is proved in [GGM2]:

**Theorem 5.7.** [GGM2, Theorem 7.12] *Assume that Hypotheses (H0), (I1) and (I2) hold. Let  $E_0 \in \mathbb{R}$ . There exists  $\delta_0 \in ]0, 1/2]$  such that: For all  $E \leq E_0$ ,  $0 < \delta \leq \delta_0$  and  $\varepsilon_0 > 0$ , there exist  $C > 0$ ,  $\kappa > 0$ , and a compact operator  $K_0$  on  $\mathcal{H}_{\text{PF}}$  such that the estimate*

$$M_\delta + f_{E,\kappa}(H_v^{\text{PF}})R_\delta f_{E,\kappa}(H_v^{\text{PF}}) \geq (1 - \varepsilon_0)\mathbb{1}_{\mathcal{H}_{\text{PF}}} - C f_{E,\kappa}^\perp(H_v^{\text{PF}})^2 - K_0 \quad (5.17)$$

holds as a form on  $\mathcal{D}(\mathcal{N}^{1/2})$ .

The following lemma is just a reformulation of [GGM2, Proposition 4.1 i), Lemma 4.7 and Lemma 6.2 iv)]. We leave the proof to the reader.

**Lemma 5.8.** *Let  $v_0 \in \mathcal{I}_{\text{PF}}(d)$ . There exists  $c_0, c_1, c_2 > 0$ , depending on  $v_0$ , such that  $H_{v_0}^{\text{PF}} + c_0 \geq 0$  and the following holds: for all  $w \in \mathcal{I}_{\text{PF}}(d)$  and  $0 < \delta \leq 1/2$*

$$\pm\phi(w) \leq c_1 \|w\|_{\text{PF}}(H_{v_0}^{\text{PF}} + c_0) \quad \text{and} \quad \pm R_\delta(w) \leq c_1 \|w\|_{\text{PF}}(H_{v_0}^{\text{PF}} + c_0).$$

$$\|\phi(w)(H_{v_0}^{\text{PF}} + \text{i})^{-1}\| \leq c_2 \|w\|_{\text{PF}} \quad \text{and} \quad \|R_\delta(w)(H_{v_0}^{\text{PF}} + \text{i})^{-1}\| \leq c_2 \|w\|_{\text{PF}}.$$

The first step we take is to translate the commutator estimate above into the form used in this paper, see Condition 2.3. In anticipation of the need for local uniformity of constants, we need to already at this step ensure that  $B = C_B \mathbb{1}$  can be chosen uniformly in  $E \in J$ , where  $J$  is compact interval.

**Corollary 5.9.** *Let  $J \subseteq \mathbb{R}$  be a compact interval and  $v_0 \in \mathcal{I}_{\text{PF}}(d)$ . There exists  $\delta_0 \in ]0, 1/2]$  and  $C_B > 0$  such that for any  $E \in J$ ,  $\epsilon_0 > 0$  and  $0 < \delta < \delta_0$  the following holds. There exists  $\kappa > 0$ ,  $C_4 > 0$  and a compact operator  $K_0$  such that the form inequality*

$$M_\delta + R_\delta(v_0) \geq (1 - \epsilon_0)\mathbb{1}_{\mathcal{H}_{\text{PF}}} - C_4 f_{E,\kappa}^\perp(H_{v_0}^{\text{PF}})^2 - C_B(H_{v_0}^{\text{PF}} - E) - K_0 \quad (5.18)$$

holds on  $\mathcal{D}(\mathcal{N}^{1/2}) \cap \mathcal{D}(H_{v_0}^{\text{PF}})$ .

*Proof.* Let  $E_0$  be an upper bound for the interval  $J$  and take  $\delta_0$  to be the one coming from Theorem 5.7, applied with  $v = v_0$ .

Fix  $E \in J$ ,  $0 < \delta < \delta_0$  and  $\epsilon_0 > 0$ . Apply Theorem 5.7 with  $\epsilon_0/2$  in place of  $\epsilon_0$ .

Compute as a form on  $\mathcal{D}(H_{v_0}^{\text{PF}})$

$$\begin{aligned} R_\delta(v_0) &= f_{E,\kappa}(H_{v_0}^{\text{PF}})R_\delta(v_0)f_{E,\kappa}(H_{v_0}^{\text{PF}}) + f_{E,\kappa}^\perp(H_{v_0}^{\text{PF}})R_\delta(v_0)f_{E,\kappa}^\perp(H_{v_0}^{\text{PF}}) \\ &\quad + 2\text{Re}\{f_{E,\kappa}(H_{v_0}^{\text{PF}})R_\delta(v_0)f_{E,\kappa}^\perp(H_{v_0}^{\text{PF}})\}. \end{aligned}$$

Using Lemma 5.8 with  $w = v_0$  and abbreviating  $C_B = c_1\|v_0\|_{\text{PF}}$  we estimate

$$\begin{aligned} &f_{E,\kappa}^\perp(H_{v_0}^{\text{PF}})R_\delta(v_0)f_{E,\kappa}^\perp(H_{v_0}^{\text{PF}}) \\ &\geq -c_1\|v_0\|_{\text{PF}}(H_{v_0}^{\text{PF}} + c_0)f_{E,\kappa}^\perp(H_{v_0}^{\text{PF}})^2 \\ &= -C_B(H_{v_0}^{\text{PF}} - E)f_{E,\kappa}^\perp(H_{v_0}^{\text{PF}})^2 - C_B(c_0 + E)f_{E,\kappa}^\perp(H_{v_0}^{\text{PF}})^2 \\ &\geq -C_B(H_{v_0}^{\text{PF}} - E) - 3C_B\kappa - C_B(c_0 + E)f_{E,\kappa}^\perp(H_{v_0}^{\text{PF}})^2. \end{aligned}$$

Using Lemma 5.8 again we get

$$\begin{aligned} &2\text{Re}\{f_{E,\kappa}(H_{v_0}^{\text{PF}})R_\delta(v_0)f_{E,\kappa}^\perp(H_{v_0}^{\text{PF}})\} \\ &\geq -\frac{\epsilon_0}{4} - \frac{4}{\epsilon_0}\|R_\delta(v_0)f_{E,\kappa}(H_{v_0}^{\text{PF}})\|^2 f_{E,\kappa}^\perp(H_{v_0}^{\text{PF}})^2 \\ &\geq -\frac{\epsilon_0}{4} - \frac{4c_2^2\|v_0\|_{\text{PF}}^2(|E| + \kappa + 1)^2}{4\zeta} f_{E,\kappa}^\perp(H_{v_0}^{\text{PF}})^2. \end{aligned}$$

Combining the equations above with Theorem 5.7 yields (5.18) with  $C_B$  only depending on  $v_0$ .  $\square$

The above corollary suffices to prove Theorem 5.5 without local uniformity in  $v$  and  $E$ .

The following lemma is designed to deal with uniformity of estimates in a small ball of interactions  $v$  around a fixed (unperturbed) interaction  $v_0$ . Technically it replaces [GGM2, Lemma 6.2 iv)].

**Lemma 5.10.** *Let  $v_0 \in \mathcal{I}_{\text{PF}}(d)$ . There exists  $\gamma_0 > 0$ ,  $C'_B > 0$  and  $c'_0, c'_1, c'_2 > 0$ , only depending on  $v_0$ , such that*

- (1)  $\forall v \in \mathcal{B}_{\gamma_0}(v_0) : H_v^{\text{PF}} \geq -c'_0$ .
- (2)  $\forall v \in \mathcal{B}_{\gamma_0}(v_0) : \pm\phi(v) \leq c'_1(H_v^{\text{PF}} + c'_0)$  and  $\|\phi(v)(H_v^{\text{PF}} - i)^{-1}\| \leq c'_2$ .
- (3)  $\forall v \in \mathcal{B}_{\gamma_0}(v_0)$  and  $0 < \delta \leq 1/2$ :  $\pm R_\delta(v) \leq C'_B(H_v^{\text{PF}} + c'_0)$  and  $\|R_\delta(v)(H_v^{\text{PF}} - i)^{-1}\| \leq c'_2$ .

*Proof.* Let  $v_0 \in \mathcal{I}_{\text{PF}}(d)$  be given. Let  $C_1(r, v) = \|[\mathbb{1}_{\mathcal{K}} \otimes \omega^{-1/2}] \tilde{v}(K+r)^{-1/2}\|$ , for  $v \in \mathcal{I}_{\text{PF}}(d)$  and  $r > 0$ .

We begin with (1). Fix  $r = r(v_0) \geq 1$  such that  $\sqrt{2}C_1(r, v_0) \leq 1/3$ . This is possible due to **(I1)**. Using [GGM2, Proposition 4.1 i)] we get

$$\begin{aligned} H_v^{\text{PF}} &= H_0^{\text{PF}} + \phi(v) = H_0^{\text{PF}} + \phi(v_0) + \phi(v - v_0) \\ &\geq H_0^{\text{PF}} - \frac{1}{3}(H_0^{\text{PF}} + r) - \sqrt{2}C_1(1, v - v_0)(H_0^{\text{PF}} + 1) \\ &= \left(1 - \frac{1}{3} - \sqrt{2}C_1(1, v - v_0)\right)H_0^{\text{PF}} - \frac{r}{3} - \sqrt{2}C_1(1, v - v_0). \end{aligned}$$

Using that  $\omega^{-1/2} \leq 2/3 + \omega^{-3/2}/3 \leq 2/3(1 + \omega^{-3/2}d(\omega))$  we get  $C_1(r, v) \leq 2\|v\|_{\text{PF}}/3$  for any  $v \in \mathcal{I}_{\text{PF}}(d)$  and  $r \geq 1$ . This implies

$$H_v^{\text{PF}} \geq \left(\frac{2}{3} - \frac{2\sqrt{2}}{3}\|v - v_0\|_{\text{PF}}\right)H_0^{\text{PF}} - \frac{r}{3} - \frac{2\sqrt{2}}{3}\|v - v_0\|_{\text{PF}}.$$

Observe that the choice  $\gamma_0 = 1/(2\sqrt{2})$  ensures that we arrive at the bound

$$H_v^{\text{PF}} \geq -\frac{r+1}{3}.$$

Choose  $c'_0 = 1 + (r+1)/3$  such that  $H_v^{\text{PF}} + c'_0 \geq 1$ . This proves (1).

As for (2) we observe first that  $\phi(v) = H_v^{\text{PF}} - H_0^{\text{PF}} \leq H_v^{\text{PF}}$ . Next let  $r = r(v_0)$  and  $\gamma_0 = 1/(2\sqrt{2})$  be as in the proof of (1) and estimate

$$-\phi(v) = -\phi(v_0) + \phi(v_0 - v) \leq \frac{1}{3}(H_0^{\text{PF}} + r) + \frac{1}{3}(H_0^{\text{PF}} + 1) = \frac{2}{3}H_0^{\text{PF}} + \frac{r+1}{3}.$$

Writing  $H_0^{\text{PF}} = H_v^{\text{PF}} - \Phi(v)$  we arrive at

$$-\phi(v) \leq 2H_v^{\text{PF}} + r + 1.$$

Combining with the choice of  $c'_0$  in the proof of (1) now yields the first estimate in (2), for a sufficiently large  $c'_1$ .

As for the second part of (2) one can employ [GGM2, Proposition 4.1 ii)] in place of [GGM2, Proposition 4.1 i)] and argue as above. This gives a bound of the desired type for  $\gamma_0$  small enough. The choice  $\gamma_0 = 1/8$  works. Here one should observe that the constants  $C_j(r, v)$ ,  $j = 0, 1, 2$ , in [GGM2] are all related to the norm  $\|\cdot\|_{\text{PF}}$  by  $C_j(1, v) \leq 2\|v\|_{\text{PF}}/3$  as argued above for  $C_1$ .

The statement in (3) now follows by appealing to [GGM2, Proposition 4.1 i)] again

$$\begin{aligned} \pm R_\delta(v) &\leq \sqrt{2}C_1(1, [\mathbb{1}_{\mathcal{K}} \otimes a_\delta]v)(H_0^{\text{PF}} + 1) \\ &\leq \sqrt{2}C_1(1, [\mathbb{1}_{\mathcal{K}} \otimes a_\delta]v)((c'_1 + 1)H_v^{\text{PF}} + c'_1 c'_0 + 1). \end{aligned}$$

From (5.5) and (5.3) we conclude the existence of a  $C'_B$  for which the first estimate in (3) is satisfied.

Similarly for the second part of (3), where, as in the discussion of the second part of (2), one can make use of [GGM2, Proposition 4.1 ii)].  $\square$

We can now state and prove a commutator estimate that is uniform with respect to  $v$  from a small ball around  $v_0$ , and  $E$  in a compact interval. Given  $v_0$ , let  $\gamma_0$  denote the radius coming from Lemma 5.10.

**Corollary 5.11.** *Let  $J \subseteq \mathbb{R}$  be a compact interval,  $v_0 \in \mathcal{I}_{\text{PF}}(d)$ , and  $\epsilon_0 > 0$ . There exist a  $\delta_0 \in ]0, 1/2]$  such that for any  $0 < \delta < \delta_0$  the following holds. There exists  $0 < \gamma < \gamma_0$ ,  $\kappa > 0$ ,  $C_4 > 0$  and a compact operator  $K_0$ , with  $\gamma$  only depending on  $\delta, \epsilon_0, J$  and  $v_0$ , such that the form inequality*

$$M_\delta + R_\delta(v) \geq (1 - \epsilon_0)\mathbb{1}_{\mathcal{H}_{\text{PF}}} - C_4 f_{E, \kappa}^\perp (H_v^{\text{PF}})^2 \langle H_v^{\text{PF}} \rangle - K_0 \quad (5.19)$$

holds on  $\mathcal{D}(\mathcal{N}^{1/2}) \cap \mathcal{D}(H_v^{\text{PF}})$ , for all  $E \in J$  and  $v \in \mathcal{B}_\gamma(v_0)$ .

**Remark.** We note that the constant  $C_4$  in Corollary 5.9 can, on inspection of the proof of [GGM2, Theorem 7.12], be chosen uniformly in  $0 < \delta \leq \delta_0$ . Making use of this would allow us to choose  $\gamma$  independent of  $\delta \leq \delta_0$  here, which would slightly simplify the exposition. We however choose not to test the readers patience on this issue. See Step II in the proof below.

*Proof.* Given  $J, v_0$  and  $\epsilon_0$ , let  $\gamma_0$  be given by Lemma 5.10 and let  $C_B > 0, \delta_0 > 0$  be the constants coming from Corollary 5.9. For  $E \in J$  we apply Corollary 5.9, with  $\epsilon_0$  replaced by  $\epsilon_0/3$ , and get the form estimate

$$\begin{aligned} M_\delta + R_\delta(v_0) &\geq (1 - \epsilon_0/3)\mathbb{1}_{\mathcal{H}_{\text{PF}}} - C_4(v_0, E) f_{E, \kappa(v_0, E)}^\perp (H_{v_0}^{\text{PF}})^2 \\ &\quad - C_B(H_{v_0}^{\text{PF}} - E) - K_0(v_0, E). \end{aligned} \quad (5.20)$$

The constants  $C_4, \kappa$  and the operator  $K_0$  also depend on  $\delta$ , but this dependence does not concern us. We can assume that  $K_0 \geq 0$ . The key observation is that the constants  $C_4$  and  $\kappa$ , and the operator  $K_0$  above can be chosen independently of  $E \in J$  and  $v \in \mathcal{B}_\gamma(v_0)$ , for some sufficiently small  $\gamma$  which does not depend on  $\delta \leq \delta_0$ .

We divide the proof of the corollary into three steps, the two first establish the observation mentioned in the previous paragraph.

**Step I:** We begin by arguing that  $C_4, \kappa$  and  $K_0$  can be chosen independently of  $E \in J$ . By a covering argument it suffices to show that they can be chosen independently of  $E'$  in a small neighborhood of  $E \in J$ . For the compact error, we remark that one should replace  $K_0$  by a finite sum  $K_0(v_0) = K_0(v_0, E_1) + \dots + K_0(v_0, E_m)$  of non-negative compact operators, which is again compact.

Let  $E \in J$  be fixed. Pick  $\zeta_1 = \epsilon_0/(6C_B)$  such that for  $|E - E'| < \zeta_1$  we have

$$C_B E \geq C_B E' - \epsilon_0/6. \quad (5.21)$$

As for the term involving  $f_{E, \kappa}^\perp$  we observe that for any self-adjoint operator  $S$  we have

$$\begin{aligned} f_{E, \kappa}^\perp(S) - f_{E', \kappa}^\perp(S) &= f_{E', \kappa}(S) - f_{E, \kappa}(S) \\ &= \frac{1}{\pi} \int_{\mathbb{C}} (\bar{\partial} \tilde{f})(z) \left[ \left( \frac{S - E'}{\kappa} - z \right)^{-1} - \left( \frac{S - E}{\kappa} - z \right)^{-1} \right] du dv. \end{aligned}$$

Here  $z = u + iv$ . Estimating this we find that

$$\|f_{E, \kappa}^\perp(S) - f_{E', \kappa}^\perp(S)\| \leq C \frac{|E - E'|}{\kappa}.$$

Writing  $a^2 - b^2 = (a - b)(a + b)$  we observe a similar bound for  $f_{E, \kappa}^\perp(S)^2 - f_{E', \kappa}^\perp(S)^2$ . Again we conclude that for  $\zeta_2 = \kappa(v_0, E)\epsilon_0/(6CC_4(v_0, E))$  we find that for  $|E - E'| < \zeta_2$ :

$$-C_4 f_{E, \kappa}^\perp (H_{v_0}^{\text{PF}})^2 \geq -C_4(v_0, E) f_{E', \kappa}^\perp (H_{v_0}^{\text{PF}})^2 - \epsilon_0/6. \quad (5.22)$$

The estimates (5.21) and (5.22) plus the aforementioned covering argument implies the form estimate

$$\begin{aligned} M_\delta + R_\delta(v_0) &\geq (1 - 2\epsilon_0/3)\mathbb{1}_{\mathcal{H}_{\text{PF}}} - C_4(v_0)f_{E,\kappa(v_0)}^\perp(H_v^{\text{PF}})^2 \\ &\quad - C_B(H_v^{\text{PF}} - E) - K_0(v_0), \end{aligned} \quad (5.23)$$

for all  $E \in J$ .

**Step II:** Secondly we argue that one can use the same constants  $C_4$ ,  $\kappa$ , and compact operator  $K_0$  for  $v \in \mathcal{B}_\gamma(v_0)$ , if  $\gamma$  is small enough.

Using Lemma 5.10 we estimate

$$R_\delta(v_0) = R_\delta(v) + R_\delta(v_0 - v) \leq R_\delta(v) + C_1\|v - v_0\|_{\text{PF}}(H_v^{\text{PF}} + C_2).$$

Writing

$$C_1\|v - v_0\|_{\text{PF}}(H_v^{\text{PF}} + C_2) = C_1\|v - v_0\|_{\text{PF}}(H_v^{\text{PF}} - E) + C_1\|v - v_0\|_{\text{PF}}(C_2 + E),$$

We see that choosing  $\gamma_1 = \gamma_1(\epsilon_0, J, v_0)$  small enough we arrive at the following bound

$$R_\delta(v_0) \leq R_\delta(v) + C(H_v^{\text{PF}} - E) + \frac{\epsilon_0}{9}\mathbb{1}_{\mathcal{H}_{\text{PF}}}, \quad (5.24)$$

which holds for all  $v \in \mathcal{B}_{\gamma_1}(v_0)$  and  $E \in J$ .

For the  $f_{E,\kappa}^\perp$  contribution we compute

$$\begin{aligned} &f_{E,\kappa}(H_{v_0}^{\text{PF}}) - f_{E,\kappa}(H_v^{\text{PF}}) \\ &= \frac{1}{\pi} \int_{\mathbb{C}} (\bar{\partial}\tilde{f})(z) \left[ \left( \frac{H_{v_0}^{\text{PF}} - E}{\kappa} - z \right)^{-1} - \left( \frac{H_v^{\text{PF}} - E'}{\kappa} - z \right)^{-1} \right] dudv \\ &= \frac{1}{\kappa\pi} \int_{\mathbb{C}} (\bar{\partial}\tilde{f})(z) \left( \frac{H_v^{\text{PF}} - E}{\kappa} - z \right)^{-1} \phi(v - v_0) \left( \frac{H_{v_0}^{\text{PF}} - E'}{\kappa} - z \right)^{-1} dudv. \end{aligned}$$

From Lemma 5.8 and the representation formula above we find that

$$\|f_{E,\kappa}^\perp(H_{v_0}^{\text{PF}})^2 - f_{E,\kappa}^\perp(H_v^{\text{PF}})^2\| \leq C\|v - v_0\|_{\text{PF}}.$$

uniformly in  $E \in J$ . Arguing as above we thus find a  $\gamma_2 = \gamma_2(\epsilon_0, J, v_0, \delta) > 0$  such that

$$-C_4(v_0)f_{E,\kappa}^\perp(H_{v_0}^{\text{PF}})^2 \geq -C_4(v_0)f_{E,\kappa}^\perp(H_v^{\text{PF}})^2 - \frac{\epsilon_0}{9}\mathbb{1}_{\mathcal{H}_{\text{PF}}} \quad (5.25)$$

for all  $v \in \mathcal{B}_{\gamma_2}(v_0)$ . This is where the  $\delta$ -dependence enters into the choice of  $\gamma$  through  $C_4$ . See the remark to the corollary.

Using Lemma 5.10 we also get a  $\gamma_3 = \gamma_3(\epsilon_0, v_0) > 0$  such that

$$-C_B(H_{v_0}^{\text{PF}} - E) \geq -C_B(H_v^{\text{PF}} - E) - \frac{\epsilon_0}{9}\mathbb{1}_{\mathcal{H}_{\text{PF}}}, \quad (5.26)$$

for all  $v \in \mathcal{B}_{\gamma_3}(v_0)$ .

Combining (5.23) with (5.24)–(5.26) we conclude that the estimate (5.20) holds with the same  $C_4$ ,  $\kappa$  and  $K_0$ , for all  $E \in J$  and  $v \in \mathcal{B}_\gamma(v_0)$ , with  $\gamma = \min\{\gamma_1, \gamma_2, \gamma_3\}$  only depending on  $\epsilon_0, J, v_0$  and  $\delta$ .

**Step III:** To conclude the proof we let  $\gamma$ ,  $C_4$ ,  $\kappa$  and  $K_0$  be fixed by Steps I and II. Pick  $\kappa'$  smaller than  $\kappa$  such that  $\kappa' C_B(1 + \max_{E \in J} |E|) \leq \epsilon_0$ . The Corollary now follows from (5.20) and the estimate

$$-C_B(H_v^{\text{PF}} - E) \geq -C_B(1 + \max_{E \in J} |E|)f_{E,\kappa}^\perp(H_v^{\text{PF}})^2 \langle H_v^{\text{PF}} \rangle.$$

Observe that (5.20) holds with  $\kappa$  replaced by  $\kappa'$  as well.  $\square$

The corresponding objects in the expanded Hilbert space are defined as follows: We set

$$M_\delta^e := \mathbb{1}_{\mathcal{K}} \otimes d\Gamma(m_\delta^e h') \quad \text{and} \quad R_\delta^e = R_\delta^e(v) := -\phi(\text{ia}_\delta^e v^e).$$

Note that

$$\mathcal{U}^{-1} M_\delta^e \mathcal{U} = M_\delta \otimes \mathbb{1}_{\Gamma(\tilde{h})} + \mathbb{1}_{\mathcal{H}} \otimes \widehat{M}_\delta, \quad \mathcal{U}^{-1} R_\delta^e \mathcal{U} = R_\delta \otimes \mathbb{1}_{\Gamma(\tilde{h})}, \quad (5.27)$$

where  $\widehat{M}_\delta := d\Gamma(d(\delta)\hat{h}')$  as an operator on  $\Gamma(\tilde{h})$ . From (5.12), we get

$$\widehat{M}_\delta \geq d(\delta) \left[ d\Gamma(\hat{h}) + \frac{1}{2}\mathcal{N} \right], \quad (5.28)$$

The Mourre estimate for  $H_v^e$  is stated in the following theorem.

**Theorem 5.12.** *Assume that Hypotheses **(H0)**, **(I1)** and **(I2)** hold. Let  $v_0 \in \mathcal{I}_{\text{PF}}(d)$ ,  $J$  a compact interval, and  $\epsilon_0 > 0$ . There exists  $\delta_0 \in ]0, 1/2]$  such that for all  $0 < \delta \leq \delta_0$ , there exist  $0 < \gamma < \gamma_0$ ,  $C_4 > 0$ ,  $\kappa > 0$ , and a compact operator  $K_0$  on  $\mathcal{H}^e$  such that*

$$M_\delta^e + R_\delta^e \geq (1 - \epsilon_0) \mathbb{1}_{\mathcal{H}^e} - C f_{E,\kappa}^\perp (H_v^e)^2 \langle H_v^e \rangle - K_0 \quad (5.29)$$

for all  $E \in J$  and  $v \in \mathcal{B}_\gamma(v_0)$ , as a form on  $\mathcal{D}((M_\delta^e)^{1/2}) \cap \mathcal{D}(H_v^e)$ .

**Remark.** As in Corollary 5.11, the constant  $\gamma$  can be chosen to only depend on  $\epsilon_0, J, v_0$  and  $\delta$ , and as in the associated remark one can in fact choose it uniformly in  $0 < \delta \leq \delta_0$ .

*Proof.* We fix  $v_0, J$  and  $\epsilon_0$  as in the statement of the theorem.

We begin by taking  $\delta'_0$  to be the  $\delta_0$  coming from Corollary 5.11. Secondly we fix  $C'_B$  and  $c'_0$  to be the two constants from Lemma 5.10 (3).

We can now choose  $0 < \delta_0 \leq \delta'_0$  such that

$$d(\delta_0) \geq \max\{C'_B + 2, \max_{E \in J} 2C'_B(E + c'_0)\}. \quad (5.30)$$

Here we used that  $\lim_{t \rightarrow 0^+} d(t) = +\infty$ . Fix now a  $0 < \delta \leq \delta_0$  and denote by  $\gamma$  the radius coming from Corollary 5.11.

The above choices anticipates the proof below, but we make them here to make it evident that we pick the constants in the right order.

We begin the verification of the commutator estimate for  $v \in B_\gamma(v_0)$  by computing as a form on  $\mathcal{D}((M_\delta^e)^{1/2}) \cap \mathcal{D}(H^e)$

$$\mathcal{U}^{-1} [M_\delta^e + R_\delta^e] \mathcal{U} = [M_\delta + R_\delta] \otimes P_\Omega + [M_\delta \otimes \mathbb{1} + \mathbb{1} \otimes \widehat{M}_\delta + R_\delta \otimes \mathbb{1}] \mathbb{1} \otimes \bar{P}_\Omega. \quad (5.31)$$

We apply Corollary 5.11 to the first term in the r.h.s. of (5.31), with the given  $\delta$  (apart from  $v_0, J$  and  $\epsilon_0$ ). This yields a  $C'_4$ , a  $\kappa' > 0$ , and a compact operator  $K'_0$  (apart from  $\gamma$ ) such that the following bound holds

$$[M_\delta + R_\delta] \otimes P_\Omega \geq [(1 - \epsilon_0) \mathbb{1} - C'_4 f_{E,\kappa'}^\perp (H_v^{\text{PF}})^2 \langle H_v^{\text{PF}} \rangle - K'_0] \otimes P_\Omega. \quad (5.32)$$

Observe that the bound above also holds with  $\kappa'$  replaced by any  $0 < \kappa \leq \kappa'$ .

To bound from below the second term on the r.h.s. of (5.31), we use Lemma 5.10. Together with (5.28) and (5.30), this implies

$$\begin{aligned} & \left[ \mathbb{1} \otimes \widehat{M}_\delta + R_\delta \otimes \mathbb{1} \right] \mathbb{1} \otimes \bar{P}_\Omega \\ & \geq \left[ \mathbb{1} \otimes d(\delta) \left( d\Gamma(\hat{h}) + \frac{1}{2} \right) - C'_B (H_v^{\text{PF}} \otimes \mathbb{1} + c'_0) \otimes \mathbb{1} \right] \mathbb{1} \otimes \bar{P}_\Omega \\ & \geq \left[ (d(\delta) - C'_B) \mathbb{1} \otimes d\Gamma(\hat{h}) - C'_B (\widehat{H}_v^e - E) + \frac{d(\delta)}{2} - C'_B (E + c'_0) \right] \mathbb{1} \otimes \bar{P}_\Omega \\ & \geq \left[ 2 - C'_B (\widehat{H}_v^e - E) \right] \mathbb{1} \otimes \bar{P}_\Omega, \end{aligned} \quad (5.33)$$

Here we also made use of (5.10) and that  $\hat{h} \geq 0$ . We now pick a  $0 < \kappa \leq \kappa'$  such that  $3\kappa C'_B \leq 1$ . Inserting  $1 = f_{E,\kappa}^2 + 2f_{E,\kappa} f_{E,\kappa}^\perp + (f_{E,\kappa}^\perp)^2$  into (5.33) yields the bound

$$\left[ \mathbb{1} \otimes \widehat{M}_\delta + R_\delta \otimes \mathbb{1} \right] \mathbb{1} \otimes \bar{P}_\Omega \geq \left[ 1 - C'_B(1 + E') f_{E,\kappa}^\perp (\widehat{H}_v^e)^2 \langle \widehat{H}_v^e \rangle \right] \mathbb{1} \otimes \bar{P}_\Omega,$$

where  $E' = \max_{E \in J} |E|$ . This estimate together with (5.31) and (5.32) lead to the statement of the theorem with  $C_4 = \min\{C'_4, C'_B(1 + E')\}$  and  $K_0 = \mathcal{U}[K'_0 \otimes P_\Omega] \mathcal{U}^{-1}$ .  $\square$

## 5.5 Checking the Abstract Assumptions

The purpose of this subsection is to complete the proof of Theorem 5.5. We do this by running through the abstract assumptions in Section 2 pertaining to Theorems 2.5 and 2.10, from which Theorem 5.5 then follows. In accordance with Remark 2.11 4), we ensure that all constants can be chosen locally uniformly in energy  $E$  and form factor  $v$ . This ensures local uniformity in Theorem 5.5.

We fix  $v_0 \in \mathcal{I}_{\text{PF}}(d)$  and  $E_0 \in \sigma(H_{v_0}^{\text{PF}})$ . Observe that there exists  $e_0$  such that  $e_0 < \inf \sigma(H_v^{\text{PF}})$  for all  $v \in \mathcal{B}_{\gamma_0}(v_0)$ , where  $\gamma_0$  comes from Lemma 5.10. Put  $J = [e_0, E_0]$ . Let  $\gamma$  and  $\delta'_0$  be fixed by Theorem 5.12 and choose a  $\delta < \delta'_0$ , which from now on is fixed.

We begin by postulating the objects for which the abstract assumptions in Conditions 2.1 should hold. We take

$$\begin{aligned} \mathcal{H} &= \mathcal{H}^e \\ H &= H_v^e \\ A &= A_\delta^e \\ N &= K^\rho \otimes \mathbb{1}_{\Gamma(\mathfrak{h}^e)} + \mathbb{1}_{\mathcal{K}} \otimes d\Gamma(h') + \mathbb{1}_{\mathcal{H}^e}, \quad \max\{2\tau, \tfrac{1}{2}\} < \rho < 1 \\ H' &= [M_\delta^e + R_\delta^e]_{|\mathcal{D}(N)}. \end{aligned} \tag{5.34}$$

The constant  $\tau$  appearing above is the one from **(II)**. Observe that  $R_\delta^e$  and  $M_\delta^e$  are  $N$ -bounded. See Lemma 5.13 just below.

We make use of the following dense subspace of  $\mathcal{H}$

$$\mathcal{S} = \mathcal{D}(K) \otimes \Gamma_{\text{fin}}(C_0^\infty(\mathbb{R}) \otimes L^2(\mathcal{S}^{d-1})) \subseteq \mathcal{H}^e.$$

The tensor product is algebraic. Observe that  $\mathcal{S}$  is a core for  $H$ ,  $N$ , and  $A$ . We recall that we can construct the group  $e^{itA}$  explicitly. Let  $\psi_t$  denote the (global) flow for the 1-dimensional ODE  $\dot{\psi}_t(\omega) = m_\delta^e(\psi_t(\omega))$ . Then, for continuous compactly supported  $f$ ,

$$(e^{ita_\delta^e} f)(\omega) = e^{\frac{1}{2} \int_0^t (m_\delta^e)'(\psi_s(\omega)) ds} f(\psi_t(\omega)).$$

This in particular implies that

$$e^{itA_\delta^e} = \Gamma(e^{ita_\delta^e}) : \mathcal{S} \rightarrow \mathcal{S}. \tag{5.35}$$

We begin with the following lemma which implies that  $R_\delta^e$  is  $N$ -bounded.

**Lemma 5.13.** *Let  $v \in \mathcal{O}_\tau$  and  $\kappa = 1/4 - \tau/(2\rho)$ . Then  $\mathcal{D}(N^{1-2\kappa}) \subseteq \mathcal{D}(\phi(v))$ , and for  $f \in \mathcal{D}(N)$  we have*

$$\|\phi(v^e) f\| \leq C \|v\|_\tau \|N^{1-2\kappa} f\|,$$

where  $C$  does not depend on  $v$  nor on  $f$ .

*Proof.* Adopting notation from [GGM2] we put  $C_0(v) = \|v(K+1)^{-\tau}\|^2$  and  $C_2(v) = \|[(K+1)^{-\tau} \otimes \mathbb{1}_{\mathfrak{h}}]v\|^2$ . We estimate for  $f \in \mathcal{S}$ , repeating the argument for [GGM2, (3.14) and (3.16)], and get

$$\|a^*(v^e)f\|^2 \leq C_0(v)\|(K+1)^\tau \otimes \mathbb{1}_{\Gamma(\mathfrak{h}^e)}f\|^2 + C_0(v)\langle f, (K+1)^{2\tau} \otimes \mathcal{N}^e f \rangle$$

and

$$\|a(v^e)f\|^2 \leq C_2(v)\langle f, (K+1)^{2\tau} \otimes \mathcal{N}^e f \rangle.$$

Observing the bound, with  $2\kappa = 1/2 - \tau/\rho$  and some  $C' > 0$ ,

$$\begin{aligned} (K+1)^{2\tau} \otimes \mathcal{N}^e &\leq \frac{\tau}{\rho(1-2\kappa)}(K+1)^{2\rho(1-2\kappa)} \otimes \mathbb{1}_{\Gamma(\mathfrak{h}^e)} \\ &+ \frac{1}{2(1-2\kappa)}(\mathcal{N}^e)^{2(1-2\kappa)} \leq C'N^{2(1-2\kappa)}, \end{aligned}$$

yields

$$\|\Phi(v^e)f\| \leq C\|v\|_\tau\|N^{1-2\kappa}f\| \quad (5.36)$$

a priori as a bound for elements of  $\mathcal{S}$ . The lemma now follows since  $\mathcal{S}$  is a core for  $N$ .  $\square$

*Condition 2.1 (1):* We make use of the fact (given the invariance of  $\mathcal{S}$  mentioned in (5.35)) that our Condition 2.1 (1) is equivalent to Mourre's conditions,  $e^{itA}\mathcal{D}(N) \subseteq \mathcal{D}(N)$  (i.e.  $\mathcal{D}(N)$  is invariant) and that  $i[N, A]$  extends from a form on  $\mathcal{S}$  to an element of  $\mathcal{B}(N^{-1}\mathcal{H}; \mathcal{H})$ . See [Mo, Proposition II.1].

From the computation

$$i[h', a_\delta^e] = m_\delta^e h''$$

it follows that the following identity holds in the sense of forms on  $\mathcal{S}$

$$N' = i[N, A_\delta^e] = \mathbb{1}_{\mathcal{K}} \otimes d\Gamma(m_\delta^e h''). \quad (5.37)$$

Since  $m_\delta^e$  is bounded and  $\sup_{\omega \in \mathbb{R}} |h''(\omega)|/h'(\omega) < \infty$ , we find that  $N'$  extends from  $\mathcal{S}$  to a bounded operator on  $\mathcal{D}(N)$ , and the extension is in fact an element of  $\mathcal{B}(N^{-1}\mathcal{H}; \mathcal{H})$  as required.

It remains to check that  $\mathcal{D}(N)$  is invariant under  $e^{itA_\delta^e}$ . For this we compute strongly on  $\mathcal{S}$

$$Ne^{itA_\delta^e} = e^{itA_\delta^e}(K^\rho \otimes \mathbb{1}_{\Gamma(\mathfrak{h}^e)} + \mathbb{1}_{\mathcal{K}} \otimes d\Gamma(h' \circ \psi_{-t})).$$

Since  $t \rightarrow \psi_t(\omega)$  is increasing and  $\omega \rightarrow h'(\omega)$  is decreasing (and positive) we find for  $t \leq 0$

$$0 \leq h' \circ \psi_{-t} \leq h'.$$

For positive  $t$  we estimate  $\omega - Ct \leq \psi_{-t}(\omega) \leq \omega$ , for some  $C > 0$ , where we used that  $m_\delta^e$  was a bounded function. This gives for  $t > 0$

$$0 \leq h' \circ \psi_{-t}(\omega) = \max\{1, e^{-\psi_{-t}(\omega)} + \psi_{-t}(\omega)\} \leq \max\{1, e^{-\omega+Ct} + \omega - Ct\}.$$

Using that  $e^{-\omega+\alpha} + \omega \leq C_\alpha(e^{-\omega} + \omega)$ , we get for any  $t$  a  $C' = C'(t)$  such that  $(h' \circ \psi_{-t})^2 \leq C'(h')^2$  and hence by [GGM2, Proposition 3.4] we arrive at

$$d\Gamma(h' \circ \psi_{-t})^2 \leq C'd\Gamma(h')^2.$$

Since  $\mathcal{S}$  was a core for  $N$  we now conclude that  $e^{itA_\delta^e}\mathcal{D}(N) \subseteq \mathcal{D}(N)$ . This completes the verification of Condition 2.1 (1).

*Condition 2.1 (2):* We begin by observing that  $N$  and  $H_0^e$  commute. In particular we can compute as a form on  $\mathcal{S}$

$$i[N^{-1}, H_v^e] = iN^{-1}\phi(v^e) - i\phi(v^e)N^{-1}.$$

This computation in conjunction with Lemma 5.13 implies that  $i[N^{-1}, H_v^e]$  extends from a form on  $\mathcal{D}(H_v^e)$  to a bounded operator and hence  $N$  is of class  $C^1(H)$ .

Since the commutator form  $i[N, H]$  extends from  $\mathcal{D}(N) \cap \mathcal{D}(H)$  to a bounded form on  $\mathcal{D}(N)$  it suffices to compute it on a core for  $N$ . Here we take again  $\mathcal{S}$  and compute

$$\begin{aligned} i[N, H] &= [K^\rho \otimes \mathbb{1}_{\Gamma(\mathfrak{h}^e)}, \phi(v^e)] + \phi(ih'v^e) \\ &= \phi([K^\rho \otimes \mathbb{1}_{\mathfrak{h}^e}]v^e - v^e K^\rho) + \phi(iv^e). \end{aligned} \quad (5.38)$$

That the second term extends by continuity to a bounded form on  $\mathcal{D}(N^{\frac{1}{2}-\kappa})$  follows from Lemma 5.13 (applied with  $iv^e$  instead of  $v^e$ ) and interpolation.

In order to deal with the first term in (5.38) we write

$$\phi([K^\rho \otimes \mathbb{1}_{\mathfrak{h}^e}]v^e - v^e K^\rho) = \mathcal{U} \left( \phi([K^\rho \otimes \mathbb{1}_{\mathfrak{h}}]\tilde{v} - \tilde{v}K^\rho) \otimes \mathbb{1}_{\Gamma(\mathfrak{h})} \right) \mathcal{U}^{-1}.$$

Here we need the new assumption **(I4)**. We will immediately verify that the above expression extends to a bounded form on  $\mathcal{D}(N^{1/2-\kappa})$  for some  $\kappa > 0$ . This implies the required property for  $i[H, N]^0$ .

We employ the representation formula (3.5) with  $K$  instead of  $N$ . Compute as a form on  $\mathcal{D}(K \otimes \mathbb{1}_{\mathfrak{h}}) \times \mathcal{D}(K)$

$$\begin{aligned} (K^\rho \otimes \mathbb{1}_{\mathfrak{h}})\tilde{v} - \tilde{v}K^\rho &= -c_\rho \int_0^\infty t^\rho [((K+t)^{-1} \otimes \mathbb{1}_{\mathfrak{h}})\tilde{v} - \tilde{v}(K+t)^{-1}] dt \\ &= B - c_\rho \int_1^\infty t^\rho ((K+t)^{-1} \otimes \mathbb{1}_{\mathfrak{h}}) [\tilde{v}K - (K \otimes \mathbb{1}_{\mathfrak{h}})\tilde{v}] (K+t)^{-1} dt, \end{aligned}$$

where  $B$  is the contribution from the integral between 0 and 1, which due to **(I1)** is a bounded operator.

By **(I4)** we have

$$\begin{aligned} c_1 &:= \left\| (\tilde{v}K - (K \otimes \mathbb{1}_{\mathfrak{h}})\tilde{v})(K+1)^{-\frac{1}{2}} \right\| < \infty, \\ c_2 &:= \left\| (K+1)^{-\frac{1}{2}} \otimes \mathbb{1}_{\mathfrak{h}} (\tilde{v}K - (K \otimes \mathbb{1}_{\mathfrak{h}})\tilde{v}) \right\| < \infty. \end{aligned}$$

Let  $\tau' < 1/2$  be chosen such that  $\rho/2 > \tau' > \rho - 1/2$ . This is possible due to the choice of  $\rho$ . We estimate for  $\psi \in \mathcal{D}(K \otimes \mathbb{1}_{\mathfrak{h}})$  and  $\varphi \in \mathcal{D}(K)$

$$\langle \psi, ((K^\rho \otimes \mathbb{1}_{\mathfrak{h}})\tilde{v} - \tilde{v}K^\rho)\varphi \rangle \leq \|B\| \|\psi\| \|\varphi\| + \frac{c_1 c_\rho}{\frac{1}{2} + \tau' - \rho} \|\psi\| \|(K+1)^{\tau'} \varphi\|.$$

Similarly we get

$$\langle \psi, ((K^\rho \otimes \mathbb{1}_{\mathfrak{h}})\tilde{v} - \tilde{v}K^\rho)\varphi \rangle \leq \|B\| \|\psi\| \|\varphi\| + \frac{c_2 c_\rho}{\frac{1}{2} + \tau' - \rho} \|(K \otimes \mathbb{1}_{\mathfrak{h}} + 1)^{\tau'} \psi\| \|\varphi\|.$$

We have thus established that the first term in (5.38) is the (expanded) field operator associated to an operator in  $\mathcal{O}_{\tau'}$ . We can thus employ Lemma 5.13 again, this time with  $v^e$  replaced by  $[K^\rho \otimes \mathbb{1}_{\mathfrak{h}^e}]v^e - v^e K^\rho$  and  $\kappa$  replaced by  $0 < \kappa' = 1/4 - \tau'/(2\rho) < 1/4$ .

Together with an interpolation argument this ensures that  $\phi((K^\rho \otimes \mathbb{1}_{\mathfrak{h}^e})v^e - v^e K^\rho)$  extends by continuity to a bounded form on  $\mathcal{D}(N^{1/2-\kappa'})$ .

We have thus verified Condition 2.1 (2) with the smallest of the two kappa's. In addition we observe that the  $\mathcal{B}(N^{-1/2+\kappa}\mathcal{H}; N^{1/2-\kappa}\mathcal{H})$ -norm of  $i[N, H]^0$  is bounded by a constant times  $\|v\|_{\text{PF}}$ , cf. Remark 2.11 4).

**Remark 5.14.** We observe from the discussion above that we could relax **(I4)** and require instead that  $[K^\rho \otimes \mathbb{1}_{\tilde{\mathfrak{h}}}] \tilde{v} - \tilde{v} K^\rho$  extends to an element of  $\mathcal{B}(\mathcal{D}(K^\eta); \mathcal{K} \otimes \tilde{\mathfrak{h}}) \cap \mathcal{B}(\mathcal{K}; \mathcal{D}(K^\eta)^* \otimes \tilde{\mathfrak{h}})$ , for some  $1/2 \leq \eta < 1 - \tau$ , where  $\tau$  is coming from **(I1)**. This would still leave room to choose  $\rho$  and  $\tau'$  (in the argument above) such that  $1 > \rho > 2\tau$  and  $\rho/2 > \tau' > \rho + \eta - 1$ .

While we do not know the domain of  $H$ , it turns out that we can indeed compute the intersection domain  $\mathcal{D}(H) \cap \mathcal{D}(N)$ . This is done in the following lemma.

**Lemma 5.15.** *We have the identity*

$$\mathcal{D}(H) \cap \mathcal{D}(N) = \mathcal{D}(K \otimes \mathbb{1}_{\Gamma(\mathfrak{h}^e)}) \cap \mathcal{D}(\mathbb{1}_{\mathcal{K}} \otimes d\Gamma(\max\{h', \omega\})) \quad (5.39)$$

and  $\mathcal{S}$  is dense in  $\mathcal{D}(H) \cap \mathcal{D}(N)$  with respect to the intersection topology.

*Proof.* Let for the purpose of this proof  $H_0 = H_0^e$ , the unperturbed expanded Hamiltonian, and denote by  $\mathcal{D}$  the right-hand side of (5.39). Since  $N$  controls the unphysical part of  $d\Gamma(h)$ , due to the choice of extension of  $\omega$  by an exponential, we observe that the identity (5.39) holds if  $H$  is replaced by  $H_0$ . Since  $H_0$  and  $N$  commute we find that  $T_0 = N + iH_0$  is a closed operator on  $\mathcal{D}$  and it clearly generates a contraction semigroup.

We now construct the formal operator sum  $N + iH$  in two different ways. By Lemma 5.13  $\mathcal{D}(\phi(v^e)) \subset \mathcal{D}(N^{1-2\kappa})$  and hence for  $u \in \mathcal{D}$

$$\|\phi(v^e)u\| \leq c\|N^{1-2\kappa}u\| + c'\|u\| \leq \frac{1}{4}\|Nu\| + c''\|u\| \leq \frac{1}{4}\|T_0u\| + c''\|u\|.$$

From this estimate we deduce that  $T_1 = T_0 + i\phi(v) =: N + iG$  is a closed operator on  $\mathcal{D}$  and it generates a contraction semigroup. See [RS, Lemma preceding Theorem X.50]. Here  $G$  is implicitly defined as the operator sum  $G = H_0 + \phi(v^e)$  with domain  $\mathcal{D}$ .

On the other hand, since we have just established Condition 2.1 (2), we conclude from [GGM1, Theorem 2.25] that  $T_{2,\pm} = N \pm iH$  are closed operators on  $\mathcal{D}(H) \cap \mathcal{D}(N)$ . In addition we have  $T_{2,\pm}^* = T_{2,\mp}$  and since  $T_{2,\pm}$  are both accretive we conclude that  $T_{2,+}$  generates a contraction semigroup. See [RS, Corollary to Theorem X.48].

We proceed to argue that  $T_2 = T_{2,+}$  is an extension of  $T_1$ , i.e.  $T_1 \subset T_2$ . Since  $\mathcal{S} \subseteq \mathcal{D}$ ,  $G$  is a symmetric extension of  $H|_{\mathcal{S}}$  and  $\mathcal{S}$  is a core for  $H$  we deduce that  $H$  is an extension of  $G$ . Hence indeed  $T_1 \subset T_2$ .

We now argue that in fact  $T_1 = T_2$ , or more poignantly that their domains coincide. This will follow if the intersection of the resolvent sets is non-empty. Indeed, let  $\zeta \in \rho(T_1) \cap \rho(T_2)$ . Then

$$(T_2 - \zeta)(T_1 - \zeta)^{-1} = (T_1 - \zeta)(T_1 - \zeta)^{-1} = \mathbb{1},$$

and hence  $(T_2 - \zeta)^{-1} = (T_1 - \zeta)^{-1}$  and the domains must coincide. But by the Hille-Yosida theorem [RS, Theorem X.47a] we have  $(-\infty, 0) \subset \rho(T_1) \cap \rho(T_2)$ . Here we used that both  $T_1$  and  $T_2$  generate contraction semigroups.

It remains to ascertain that  $\mathcal{S}$  is dense in  $\mathcal{D}$  with respect to the intersection topology of  $\mathcal{D}(H) \cap \mathcal{D}(N)$ . We begin by verifying that  $\mathcal{S}$  is dense in  $\mathcal{D}$  with respect to the graph norm of  $T_0$ , which induces the intersection topology of  $\mathcal{D}(H_0) \cap \mathcal{D}(N) = \mathcal{D}$ .

Let  $\psi \in \mathcal{D}$ . Observe first that  $\lim_{n \rightarrow \infty} \mathbb{1}_{\mathcal{N}^e \leq n} \psi \rightarrow \psi$  in the graph norm of  $T_0$ , since  $\mathcal{N}^e$  and  $T_0$  commute. Similarly we find that  $\mathbb{1}_{\mathcal{K}} \otimes \Gamma(\mathbb{1}_{|\omega| \leq \ell}) \psi \rightarrow \psi$  in the graph norm of  $T_0$ . Hence it suffices to approximate  $\psi \in \mathcal{D}$  with  $\Gamma(\mathbb{1}_{|\omega| \leq \ell}) \mathbb{1}_{\mathcal{N}^e \leq n} \psi = \psi$ , for some  $\ell$  and  $n$ , by elements from  $\mathcal{S}$  in the graph norm of  $T_0$ . Fix now such a  $\psi$ ,  $n$  and  $\ell$ .

Since  $\mathcal{S}$  is a core for  $K \otimes \mathbb{1}_{\Gamma(\mathfrak{h}^e)}$  we can find a sequence  $\{\psi_j\} \subset \mathcal{S}$  with  $\psi_j \rightarrow \psi$  in  $\mathcal{D}(K \otimes \mathbb{1}_{\Gamma(\mathfrak{h}^e)})$ . Put  $\tilde{\psi}_j = \mathbb{1}_{\mathcal{N}^e \leq n} [\mathbb{1}_{\mathcal{K}} \otimes \Gamma(f)] \psi_j \in \mathcal{S}$ , where  $f \in C_0^\infty(\mathbb{R})$ , with  $0 \leq f \leq 1$  and  $f = 1$  on  $[-\ell, \ell]$ . Then  $\tilde{\psi}_j \rightarrow \psi$  in  $\mathcal{D}(K \otimes \mathbb{1}_{\Gamma(\mathfrak{h}^e)})$  as well. We now observe that  $T_0 \tilde{\psi}_j = (iK \otimes \mathbb{1}_{\Gamma(\mathfrak{h}^e)} + B_{n,\ell}) \tilde{\psi}_j$ , for some bounded operator  $B_{n,\ell}$ . This implies density of  $\mathcal{S}$  in  $\mathcal{D}$  in the graph norm of  $T_0$ .

By the closed graph theorem  $H(T_0 - \zeta)^{-1}$  and  $N(T_0 - \zeta)^{-1}$  are bounded, and hence  $\mathcal{S}$  is also dense in  $\mathcal{D}(H) \cap \mathcal{D}(N) = \mathcal{D}$  with respect to the indicated intersection topology.  $\square$

*Condition 2.1 (3):* Let  $\sigma$  be such that  $R(\eta)$  preserves  $\mathcal{D}(N)$  for  $\eta$  with  $|\operatorname{Im} \eta| \geq \sigma$ . It suffices to establish the identity

$$R(\eta)H - HR(\eta) = -iR(\eta)H'R(\eta),$$

for  $\eta$  with  $|\operatorname{Im} \eta| \geq \sigma$ , as a form on  $\mathcal{D}(H) \cap \mathcal{D}(N)$ , since this set is dense in  $\mathcal{D}(H) \cap \mathcal{D}(N^{1/2})$  by Remark 3.5.

By Lemma 5.15, we can on the set  $\mathcal{D}(H) \cap \mathcal{D}(N)$  express  $H$  and  $H'$  as sums of operators  $H = H_0^e + \phi(v^e)$  and  $H' = d\Gamma(h') - \phi(ia_\delta^e v^e)$ .

We are thus reduced to verifying the following two form identities on  $\mathcal{D}(H) \cap \mathcal{D}(N)$

$$R(\eta)H_0^e - H_0^e R(\eta) = -iR(\eta)\mathbb{1}_{\mathcal{K}} \otimes d\Gamma(m_\delta^e h')R(\eta) \quad (5.40)$$

$$R(\eta)\phi(v^e) - \phi(v^e)R(\eta) = iR(\eta)\phi(ia_\delta^e v^e)R(\eta). \quad (5.41)$$

Since all operators appearing in (5.40) commute with  $\mathcal{N}^e$  it suffices to verify this identity on each fixed expanded particle sector with  $\mathcal{N}^e = n$ . Introduce for  $\ell$  a positive integer the semibounded dispersion  $h_\ell(\omega) = \max\{-\ell, h(\omega)\}$  and a cutoff expanded free Hamiltonian  $H_{0,\ell} = K \otimes \mathbb{1}_{\Gamma(\mathfrak{h}^e)} + \mathbb{1}_{\mathcal{K}} \otimes d\Gamma(h_\ell)$ . Then on a particle sector  $H_{0,\ell}$  is of class  $C_{\text{Mo}}^1(A)$  such that we can compute for  $|\operatorname{Im} \eta| \geq \sigma_{n,\ell}$

$$R(\eta)H_{0,\ell} - H_{0,\ell}R(\eta) = -iR(\eta)\mathbb{1}_{\mathcal{K}} \otimes d\Gamma(m_\delta^e h'_\ell)R(\eta).$$

as a form on  $\mathbb{1}_{[\mathcal{N}^e = n]} \mathcal{D}$ . Here  $\sigma_{n,\ell}$  is some positive constant. Since both sides are analytic in  $\eta$  for  $|\operatorname{Im} \eta| \geq \sigma$  we conclude the above identity for all such  $\eta$ . Appealing to the explicit form of the domain  $\mathcal{D}$  we find that we can remove the cutoff  $\ell \rightarrow \infty$  by the dominated convergence theorem. This yields (5.40) for  $|\operatorname{Im} \eta| \geq \sigma$ .

As for (5.41) we recall that we have already established that  $N$  is of class  $C_{\text{Mo}}^1(A)$ . It is a consequence of the proof of [Mo, Proposition II.1], that  $i[\phi(v^e), A]$  read as a form on  $\mathcal{D}(N) \cap \mathcal{D}(A)$  can be represented by an extension from the form computed on  $\mathcal{S}$ . Here we used (5.35). As a form on  $\mathcal{S}$  we clearly have  $i[\phi(v^e), A] = -\phi(ia_\delta^e v^e)$ , which extends to an  $N$ -bounded operator by Lemma 5.13. The computation  $R(\eta)\phi(v^e) - \phi(v^e)R(\eta) = R(\eta)[\phi(v^e), A]R(\eta)$  as forms on  $\mathcal{D}(N)$  now concludes the verification of (5.41), and hence of Condition 2.1 (3).

*Condition 2.1 (4):* We compute first as a form on  $\mathcal{S}$

$$i[H', A] = H'' = \mathbb{1}_{\mathcal{K}} \otimes d\Gamma\left(m_\delta^e \frac{dm_\delta^e}{d\omega} h' + (m_\delta^e)^2 h''\right) - \phi((a_\delta^e)^2 v^e)$$

and observe that the right-hand side extends by continuity to an  $N$ -bounded operator, cf. Lemma 5.13. Again, by the proof of [Mo, Proposition II.1], cf. (5.35), we conclude that the operator on the right-hand side of the formula also represents the commutator form  $i[H', A]$  on  $\mathcal{D}(N) \cap \mathcal{D}(A)$ .

*Condition 2.2:* By Lemma 5.15 and Remark 3.5, it suffices to check the form bound in the virial condition on  $\mathcal{S}$ . In addition, since  $K^\rho \leq \mathbb{1} + K$ , it suffices to check the estimate with  $\rho = 1$ .

Recalling (5.11) and (5.15) we observe that  $\hat{h} \leq \hat{h}'$ , and hence  $h + h' \geq 0$ . Making use of this observation we find that

$$\begin{aligned} K \otimes \mathbb{1}_{\Gamma(\mathfrak{h}^e)} + \mathbb{1}_{\mathcal{K}} \otimes d\Gamma(h') &\leq K \otimes \mathbb{1}_{\Gamma(\mathfrak{h}^e)} + \mathbb{1}_{\mathcal{K}} \otimes (d\Gamma(h) + 2d\Gamma(h')) \\ &\leq K \otimes \mathbb{1}_{\Gamma(\mathfrak{h}^e)} + \mathbb{1}_{\mathcal{K}} \otimes d\Gamma(h) + 2M_\delta^e. \end{aligned}$$

We now add and subtract  $\Phi(v^e) + 2R_\delta^e$  to obtain

$$K \otimes \mathbb{1}_{\Gamma(\mathfrak{h}^e)} + \mathbb{1}_{\mathcal{K}} \otimes d\Gamma(h') \leq H_v^e + 2H' - \Phi(v^e) - 2R_\delta^e.$$

We now make use of the fact that

$$C = \|(\Phi(v^e) + 2R_\delta^e)(K \otimes \mathbb{1}_{\Gamma(\mathfrak{h}^e)} + \mathbb{1}_{\mathcal{K}} \otimes d\Gamma(h') + 1)^{-\frac{1}{2}}\| < \infty$$

to conclude the form estimate

$$K \otimes \mathbb{1}_{\Gamma(\mathfrak{h}^e)} + \mathbb{1}_{\mathcal{K}} \otimes d\Gamma(h') \leq H_v^e + 2H' + \frac{1}{2}(K \otimes \mathbb{1}_{\Gamma(\mathfrak{h}^e)} + \mathbb{1}_{\mathcal{K}} \otimes d\Gamma(h') + 1) + \frac{1}{2}C^2.$$

This completes the verification of the virial bound. We again observe that the constants involved can be chosen independent of  $E$  in a bounded set and  $v \in \mathcal{B}_\gamma(v_0)$ .

*Condition 2.3:* This condition has already been essentially verified in the form of Theorem 5.12. We only need to observe that the form bound extends by continuity from  $\mathcal{D}(H) \cap \mathcal{D}(N)$  to  $\mathcal{D}(H) \cap \mathcal{D}(N^{1/2})$ , cf. Remark 3.5.

*The condition (2.7):* Let  $\psi^e$  be a bound state for  $H = H_v^e$ . That is  $\psi^e \in \mathcal{D}(H_v^e)$  and  $H_v^e \psi^e = E \psi^e$ , for some  $E \in \mathbb{R}$ . Recall that  $\psi^e = \mathcal{U}(\psi \otimes \Omega)$ , where  $\psi \in \mathcal{D}(\tilde{H}_v^{\text{PF}})$  and  $\tilde{H}_v^{\text{PF}} \psi = E \psi$ . From [GGM2, Proposition 6.5] we conclude that  $\psi \in \mathcal{D}(\mathcal{N}^{1/2})$ . Hence we conclude that  $\psi^e \in \mathcal{D}(d\Gamma(h')^{1/2}) \cap \mathcal{UD}(\tilde{H}_v^{\text{PF}} \otimes \mathbb{1}_{\Gamma(\tilde{\mathfrak{h}})})$ . In particular we find that  $\psi^e \in \mathcal{D}(H) \cap \mathcal{D}(N^{1/2})$  and the result follows from the virial estimate in Condition 2.2. Observe again that  $\|N^{1/2}\psi\|$  can be bounded uniformly in  $v \in \mathcal{B}_{\gamma_0}(v_0)$  and  $E \in [e_0, E_0]$ .

*Condition 2.8  $k_0 = 1$ :* This merely amounts to checking the statement in (2.11) with  $\ell = 0$ . But this is trivially satisfied since  $[N, N'] = 0$ . See (5.37).

This completes the verification of the conditions needed to conclude Theorem 5.5 from Theorems 2.5 and 2.10.

## 6 AC-Stark type models

### 6.1 The Model and the Result

We will work in the framework of generalized  $N$ -body systems, which we review briefly. Let  $\mathcal{A}$  be a finite index set and  $X$  a finite dimensional real vector-space with inner product.

There is an injective map from  $\mathcal{A}$  into the subspaces of  $X$ ,  $\mathcal{A} \ni a \rightarrow X^a \subseteq X$ , and we write  $X_a = (X^a)^\perp$ . We introduce a partial ordering on  $\mathcal{A}$ :

$$a \subset b \Leftrightarrow X^a \subseteq X^b$$

and assume the following

1. There exist  $a_{\min}, a_{\max} \in \mathcal{A}$  with  $X^{a_{\min}} = \{0\}$  and  $X^{a_{\max}} = X$ .
2. For each  $a, b \in \mathcal{A}$  there exists  $c = a \cup b \in \mathcal{A}$  with  $X_a \cap X_b = X_c$ .

We will write  $x^a$  and  $x_a$  for the orthogonal projection of a vector  $x$  onto the subspaces  $X^a$  and  $X_a$  respectively.

We will work with a generalized potential

$$V = V(t, x) = \sum_{a \in \mathcal{A} \setminus \{a_{\min}\}} V_a(t, x^a),$$

where  $V_a$  is a real-valued function on  $\mathbb{R} \times X^a$ . In the conditions below  $\alpha$  denotes multi-indices.

**Conditions 6.1.** Let  $k_0 \in \mathbb{N}$  be given. For each  $a \neq a_{\min}$  the following holds. The pair-potential  $\mathbb{R} \times X^a \ni (t, y) \rightarrow V_a(t, y) \in \mathbb{R}$  is a continuous function satisfying

- (1) Periodicity:  $V_a(t+1, y) = V_a(t, y)$ ,  $t \in \mathbb{R}$  and  $y \in X^a$ .
- (2) Differentiability in  $y$ : For all  $\alpha$  with  $|\alpha| \leq k_0 + 1$  there exist  $\partial_y^\alpha V_a \in C(\mathbb{R} \times X^a)$ .
- (3) Global bounds: For all  $\alpha$  and  $k \in \mathbb{N} \cup \{0\}$  with  $|\alpha| + k \leq k_0 + 1$  there are global bounds  $|\partial_y^\alpha (y \cdot \nabla_y)^k V_a(t, y)| \leq C$ .
- (4) Decay at infinity:  $|V_a(t, y)| + |y \cdot \nabla_y V_a(t, y)| = o(1)$  uniformly in  $t$ .
- (5) Regularity in  $t$ : There exists  $\partial_t V_a \in C(\mathbb{R} \times X^a)$  and there is a global bound  $|\partial_t V_a(t, y)| \leq C$ .

We consider under Condition 6.1 the Hamiltonian  $h = h(t) = p^2 + V$ ,  $p = -i\nabla$ , on the Hilbert space  $L^2(X)$ . The corresponding propagator  $U$  satisfies: It is two-parameter strongly continuous family of unitary operators which solves the time-dependent Schrödinger equation

$$i \frac{d}{dt} U(t, s) \phi = h(t) U(t, s) \phi \quad \text{for } \phi \in \mathcal{D}(p^2).$$

The family satisfies the Chapman Kolmogorov equations

$$U(s, r) U(r, t) = U(s, t), \quad r, s, t \in \mathbb{R},$$

the initial condition  $U(s, s) = \mathbb{1}$  for any  $s \in \mathbb{R}$  and the periodicity equation

$$U(t+1, s+1) = U(t, s), \quad s, t \in \mathbb{R}.$$

The operator  $U(1, 0)$  is called the *monodromy operator*. For each  $a \neq a_{\max}$  the sub-Hamiltonian monodromy operator is  $U^a(1, 0)$ ; it is defined as the monodromy operator on  $\mathcal{H}^a = L^2(X^a)$  constructed for  $a \neq a_{\min}$  from  $h^a = (p^a)^2 + V^a$ ,  $V^a = \sum_{a_{\min} \neq b \subset a} V_b(t, x^b)$ . If  $a = a_{\min}$  we define  $U^a(1, 0) = \mathbb{1}$  (implying  $\sigma_{\text{pp}}(U^{a_{\min}}(1, 0)) = \{1\}$ ). The set of *thresholds* is then

$$\mathcal{F}(U(1, 0)) = \bigcup_{a \neq a_{\max}} \sigma_{\text{pp}}(U^a(1, 0)), \quad (6.1)$$

We recall from [MS] that the set of thresholds is closed and countable, and non-threshold eigenvalues, i.e. points in  $\sigma_{\text{pp}}(U(1,0)) \setminus \mathcal{F}(U(1,0))$ , have finite multiplicity and can only accumulate at the set of thresholds. Moreover any corresponding bound state is exponentially decaying, the singular continuous spectrum  $\sigma_{\text{sc}}(U(1,0)) = \emptyset$  and there are integral propagation estimates for states localized away from the set of eigenvalues and away from  $\mathcal{F}(U(1,0))$ . It should be remarked that the weakest condition, Condition 6.1 with  $k_0 = 1$ , corresponds to [MS, Condition 1.1] (more precisely Condition 6.1 with  $k_0 = 1$  is slightly weaker than [MS, Condition 1.1], and we also remark that [MS] goes through with this modification). All of the above properties are proven in [MS] either under [MS, Condition 1.1] or under weaker conditions allowing local singularities. In particular local singularities up to the Coulomb singularity are covered in [MS]. See Subsection 6.3 for a new result for Coulomb systems.

In the following subsection we establish the theorem below, which implies Theorem 1.6 (2).

**Theorem 6.2.** *Suppose Conditions 6.1, for some  $k_0 \in \mathbb{N}$ . Let  $\phi$  be an bound state for  $U(1,0)$  pertaining to an eigenvalue  $e^{-i\lambda} \notin \mathcal{F}(U(1,0))$ . Then  $\phi \in \mathcal{D}(|p|^{k_0+1})$ .*

## 6.2 Regularity of Non-threshold Bound States

The principal tool in the proof of Theorem 6.2 will be Floquet theory (in common with [MS] and other papers) which we briefly review. The Floquet Hamiltonian associated with  $h(t)$  is

$$H = \tau + h(t) = H_0 + V, \quad \text{on } \mathcal{H} = L^2([0,1]; L^2(X)). \quad (6.2)$$

Here  $\tau$  is the self-adjoint realization of  $-i\frac{d}{dt}$ , with periodic boundary conditions. The spectral properties of the monodromy operator and the Floquet Hamiltonian are equivalent. We have the following relations

$$\sigma_{\text{pp}}(U(1,0)) = e^{-i\sigma_{\text{pp}}(H)}, \quad \sigma_{\text{ac}}(U(1,0)) = e^{-i\sigma_{\text{ac}}(H)}, \quad \sigma_{\text{sc}}(U(1,0)) = e^{-i\sigma_{\text{sc}}(H)},$$

and the multiplicity of an eigenvalue  $z = e^{-i\lambda}$  of  $U(1,0)$  is equal to the multiplicity of  $\lambda$  as an eigenvalue of  $H$  (regardless of the choice of  $\lambda$ ). We also recall that the Floquet Hamiltonian is the self-adjoint generator of the strongly continuous unitary one-parameter group on  $\mathcal{H}$  given by

$$(e^{-isH}\psi)(t) = U(t, t-s)\psi(t-s - [t-s]), \quad (6.3)$$

where  $[r]$  is the integer part of  $r$ . In particular any bound state of the monodromy operator,  $U(1,0)\phi = e^{-i\lambda}\phi$ , gives rise to a bound state of the Floquet Hamiltonian,  $H\psi = \lambda\psi$ , by the formula

$$\psi(t) = e^{it\lambda}U(t,0)\phi. \quad (6.4)$$

**Proposition 6.3.** *Suppose Conditions 6.1 for some  $k_0 \in \mathbb{N}$  and suppose  $H\psi = \lambda\psi$  for  $e^{-i\lambda} \notin \mathcal{F}(U(1,0))$ . Then  $\psi \in \mathcal{D}(|p|^{k_0+1})$ .*

*Proof.* We shall use Corollary 4.13 with  $H$  being the Floquet Hamiltonian and  $N = p^2 + 1$ . This amounts to checking the assumptions given in terms of Conditions 2.1–2.3, Condition 2.6, Condition 2.8 and (for  $k_0 \geq 2$  only) Condition 4.11 (same  $k_0$ ). We take  $A = \frac{1}{2}(x \cdot p + p \cdot x)$  and compute with direct reference to Conditions 2.1, Condition 2.6

and Condition 2.8

$$H' = 2p^2 - x \cdot \nabla V, \quad (6.5a)$$

$$i[N, H]^0 = p \cdot \nabla V + \nabla V \cdot p = \sum_{j=1}^{\dim X} ((p_j \partial_j V + (\partial_j V) p_j), \quad (6.5b)$$

$$N' = 2p^2, \quad (6.5c)$$

$$i^\ell \text{ad}_A^\ell(N') = 2^{\ell+1} p^2, \quad i \text{ad}_N(i^\ell \text{ad}_A^\ell(N')) = 0; \quad \ell \leq k_0 - 1, \quad (6.5d)$$

$$i^l \text{ad}_A^l(H') = 2^{l+1} p^2 + (-1)^{l+1} (x \cdot \nabla)^{l+1} V; \quad l \leq k_0. \quad (6.5e)$$

A comment on (6.5a) is due. We need to show Condition 2.1 (3) using the expression (6.5a): First we remark that the operators  $\tau$ ,  $p^2$  and  $H_0$  are simultaneously diagonalizable. Therefore  $\mathcal{D}(H) \cap \mathcal{D}(N) = \mathcal{D}(\tau) \cap \mathcal{D}(N)$  is dense in  $\mathcal{D}(H) \cap \mathcal{D}(N^{1/2})$ . (See also Remark 3.5.) Moreover  $p^2$ ,  $V$  and  $R(\eta)$  are obviously fibered (i.e. they act on the fiber space  $L^2(X)$ ) and  $R(\eta)$  preserves  $\mathcal{D}(p^2)$  and  $\mathcal{D}(|p|)$  for  $|\eta|$  large enough. Whence as a form on  $\mathcal{D}(\tau) \cap \mathcal{D}(N)$

$$i[H, R(\eta)] = i[p^2 + V, R(\eta)] = -R(\eta) i[p^2 + V, A] R(\eta) = -R(\eta) H' R(\eta).$$

The last identity for fiber operators is well-known in standard Mourre theory for Schrödinger operators. Finally we extend the shown version of (2.2) by continuity to a form identity on  $\mathcal{D}(H) \cap \mathcal{D}(N^{1/2})$  yielding Condition 2.1 (3).

Clearly (2.4) holds with  $C_1 = 0$ ,  $C_2 = 1/2$  and  $C_3 = 1 + \sup x \cdot \nabla V(t, x)/2$ . As for (2.5) a stronger version follows from [MS, Theorem 4.2]

$$H' \geq c_0 \mathbb{1} - C_4 f_\lambda^\perp(H)^2 - K_0. \quad (6.6)$$

Finally it follows from [MS, Proposition 4.1] that indeed the condition of Corollary 4.13,  $\psi \in \mathcal{D}(N^{1/2}) = \mathcal{D}(|p|)$ , is fulfilled. This shows the proposition in the case  $k_0 = 1$ .

For  $k_0 \geq 2$  it remains to verify Condition 4.11. For this purpose it is helpful to notice that

$$i \text{ad}_A(p_j) = p_j, \quad (6.7a)$$

$$i \text{ad}_A((N + t_j)^{-1}) = -2(N + t_j)^{-1} (N - 1) (N + t_j)^{-1}. \quad (6.7b)$$

Moreover all computations are in terms of fiber operators (in particular  $M_1$ ,  $M_2$  and  $M_3$  are all fibered operators), and recalling [Mo, Proposition II.1] and using the fact that  $N^{1/2} \in C_{\text{Mo}}^1(A)$  it suffices to do the computations in terms of forms on the Schwartz space  $\mathcal{S}(X)$ .

**Re  $M_1$ :** We shall apply (6.7a) in combination with (6.5b) to verify the part of Condition 4.11 that involves  $M_1$ . Let us first look at the particular choice in (4.21) for  $M_1$  given by taking all the  $T$ 's equal  $N^{1/2}$ . That is we will demonstrate that for  $m = 1, \dots, k_0 - 1$

$$i^m \text{ad}_{N^{1/2}}^m(M_1) \text{ is } |p| \text{-bounded.} \quad (6.8)$$

We compute

$$\begin{aligned} i^m \text{ad}_{N^{1/2}}^m(M_1) &= -(i c_{\frac{1}{2}})^{m+1} \int_0^\infty dt_{m+1} t_{m+1}^{\frac{1}{2}} \cdots \int_0^\infty dt_2 t_2^{\frac{1}{2}} \int_0^\infty t_1^{\frac{1}{2}} \\ &(N + t_1)^{-1} \cdots (N + t_{m+1})^{-1} \text{ad}_{p^2}^{m+1}(V) (N + t_{m+1})^{-1} \cdots (N + t_1)^{-1} dt_1, \end{aligned}$$

and in turn,

$$\begin{aligned} \text{ad}_{p^2}^{m+1}(V) &= \sum_{|\alpha+\beta|=m+1} c_{\alpha,\beta} p^\alpha (\partial^{\alpha+\beta} V) p^\beta = T_1 + T_2 + T_3; \\ T_1 &= \sum_{|\alpha+\beta|=m+1, |\beta|\geq 1} c_{\alpha,\beta} p^\alpha (\partial^{\alpha+\beta} V) p^\beta, \\ T_2 &= \sum_{|\alpha+\beta|=m+1, |\beta|=1} -i c_{\alpha+\beta,0} p^\alpha (\partial^{\alpha+2\beta} V), \\ T_3 &= \sum_{|\alpha+\beta|=m+1, |\beta|=1} c_{\alpha+\beta,0} p^\alpha (\partial^{\alpha+\beta} V) p^\beta. \end{aligned}$$

Now in front of the bounded derivative of any of the terms of the expressions  $T_1$ ,  $T_2$  and  $T_3$  we move the factor  $p^\alpha$  to the left in the integral representation and use the bound

$$\|N^s(N+t)^{-1}\| \leq C_s(1+t)^{s-1}; \quad s \in [0, 1]. \quad (6.9)$$

We obtain

$$\|p^\alpha(N+t_{m+1})^{-1} \cdots (N+t_1)^{-1}\| \leq C_s^{m+1} \prod_{j=1}^{m+1} (1+t_j)^{s-1}; \quad s = \frac{|\alpha|}{2(m+1)}.$$

Using (6.9) for the factors of  $p^\beta$  to the right (in case of  $T_1$  and  $T_3$ ) combined with the resolvents to the right and an additional factor  $N^{-1/2}$  we obtain

$$\|p^\beta(N+t_{m+1})^{-1} \cdots (N+t_1)^{-1} N^{-\frac{1}{2}}\| \leq C_\sigma^{m+1} \prod_{j=1}^{m+1} (1+t_j)^{\sigma-1}; \quad \sigma = \frac{|\beta|-1}{2(m+1)}.$$

To treat  $T_2$  we notice that

$$\|(N+t_{m+1})^{-1} \cdots (N+t_1)^{-1}\| \leq \prod_{j=1}^{m+1} (1+t_j)^{-1}. \quad (6.10)$$

Now the integrand with an additional factor  $N^{-1/2}$  to the right is a sum of terms either bounded (up to a constant) by

$$\prod_{j=1}^{m+1} t_j^{\frac{1}{2}} (1+t_j)^{\frac{|\alpha|}{2(m+1)}-1} (1+t_j)^{\frac{|\beta|-1}{2(m+1)}-1} = \prod_{j=1}^{m+1} t_j^{\frac{1}{2}} (1+t_j)^{-\frac{3}{2}-\frac{1}{2(m+1)}}$$

(these terms come from  $T_1$  and  $T_3$ ), or (for any term of  $T_2$ ) by

$$\prod_{j=1}^{m+1} t_j^{\frac{1}{2}} (1+t_j)^{\frac{|\alpha|}{2(m+1)}-1} (1+t_j)^{-1} = \prod_{j=1}^{m+1} t_j^{\frac{1}{2}} (1+t_j)^{\frac{m}{2(m+1)}-2}.$$

Whence in all cases the integral with an additional factor  $N^{-1/2}$  to the right is convergent in norm, which finishes the proof of the special case where all of the  $T$ 's are equal to  $N^{1/2}$ . The general case follows the same scheme. Some of the commutators with  $A$  "hit" the potential part introducing a change  $W(t, x) \rightarrow -x \cdot \nabla W(t, x)$ . Other commutators with  $A$  hit a factor  $p_j$  in which case we apply (6.7a). Finally yet other commutators with  $A$  hit a factor  $(N+t_j)^{-1}$  in which case we apply (6.7b) and (6.10).

**Re  $M_2$  and  $M_3$ :** The contributions to (4.21) from the first term of (6.5a), i.e. contributions from the expression  $2p^2N^{-1/2}$ , vanish except for the case where all of the  $T$ 's are equal to  $A$ . In this case we compute

$$i^m \text{ad}_A^m (2p^2N^{-\frac{1}{2}}) = (2t \frac{d}{dt})^m f(t) \Big|_{t=p^2}; \quad f(t) = 2t(t+1)^{-\frac{1}{2}}. \quad (6.11)$$

Obviously the right hand side of (6.11) is  $N^{1/2}$ -bounded.

The contributions to (4.21) from the expressions  $-x \cdot \nabla V N^{-1/2}$  and  $-N^{-1/2} x \cdot \nabla V$  are treated like the term  $M_1$  in fact slightly simpler. The iterated commutators are all bounded in this case. We leave out the details.  $\square$

**Remark.** Since  $H$  is not elliptic (more precisely  $|p|(H_0 - i)^{-1}$  is unbounded) we do not see an ‘‘easy way’’ to get the conclusion of Proposition 6.3. For instance we need to use the assumption that  $e^{-i\lambda}$  is non-threshold. See [KY] for a related result for the one-body AC-Stark problem.

*Proof of Theorem 6.2:* We mimic the proof of [MS, Theorem 1.8]. Recall the notation  $I_{in}(N) = n(N+n)^{-1}$  and  $N_{in} = NI_{in}(N)$ . Due to Proposition 6.3 and the representation (6.4) there exists  $t_0 \in [0, 1[$  such that

$$U(t_0, 0)\phi \in \mathcal{D}(N^{(k_0+1)/2}). \quad (6.12)$$

In particular  $\psi(t) = e^{it\lambda}U(t, 0)\phi \in \mathcal{D}(p^2)$  for all  $t$ . Next we compute

$$\frac{d}{dt} \langle \psi(t), N_{in}^{k_0+1} \psi(t) \rangle = \langle \psi(t), i[V, N_{in}^{k_0+1}] \psi(t) \rangle, \quad (6.13a)$$

$$i[V, N_{in}^{k_0+1}] = \sum_{0 \leq p \leq k_0} N_{in}^p i[V, N_{in}] N_{in}^{k_0-p}, \quad (6.13b)$$

$$i[V, N_{in}] = -I_{in}(N) \sum_{j=1}^{\dim X} ((p_j \partial_j V + (\partial_j V) p_j) I_{in}(N)). \quad (6.13c)$$

We plug (6.13c) into (6.13b) and then in turn (6.13b) into the right hand side of (6.13a). We expand the sum and redistribute for each term at most  $k_0$  derivatives by pulling through the factor  $\partial_j V$  obtaining terms on a more symmetric form, more precisely on the form

$$\langle N^{\frac{k_0+1}{2}} \psi(t), B_n N^{\frac{k_0+1}{2}} \psi(t) \rangle \text{ where } \sup_n \|B_n\| < \infty. \quad (6.14)$$

Notice that for all terms the operator  $B_n$  involves at most  $k_0 + 1$  derivatives of  $V$ . Thanks to the Cauchy-Schwarz inequality and Proposition 6.3 any expression like (6.14) can be integrated on  $[t_0, 1]$  and the integral is bounded uniformly in  $n$ . In combination with (6.12) we conclude that

$$\sup_n \langle \psi(1), N_{in}^{k_0+1} \psi(1) \rangle < \infty,$$

whence  $\phi = \psi(1) \in \mathcal{D}(N^{(k_0+1)/2})$ .  $\square$

### 6.3 Regularity of Non-threshold Atomic Type Bound States

The generator of the evolution of the a system of  $N$  particles in a time-periodic Stark-field with zero mean (AC-Stark field) is of the form

$$h_{\text{phy}}(t) = p^2 - \mathcal{E}(t) \cdot x + V_{\text{phy}}$$

on  $L^2(X)$ . Assuming that the field is 1-periodic the condition  $\int_0^1 \mathcal{E}(t) dt = 0$  leads to the existence of unique 1-periodic functions  $b$  and  $c$  such that

$$\frac{d}{dt}b(t) = \mathcal{E}(t), \quad \frac{d}{dt}c(t) = 2b(t) \quad \text{and} \quad \int_0^1 c(t) dt = 0;$$

see [MS] for details. For simplicity let us here assume that  $\mathcal{E} \in C([0, 1]; X)$ , see Remark 6.4 for an extension. The potential  $V_{\text{phy}}$  is a sum of time-independent real-valued ‘‘pair-potentials’’

$$V_{\text{phy}} = V_{\text{phy}}(x) = \sum_{a \in \mathcal{A} \setminus \{a_{\min}\}} V_a(x^a).$$

In terms of these quantities we introduce Hamiltonians

$$\begin{aligned} h_{\text{aux}}(t) &= p^2 + 2b(t) \cdot p + V_{\text{phy}}, \\ h(t) &= p^2 + V_{\text{phy}}(\cdot + c(t)). \end{aligned}$$

The propagators  $U_{\text{phy}}$ ,  $U_{\text{aux}}$  and  $U$  of  $h_{\text{phy}}$ ,  $h_{\text{aux}}$  and  $h$ , respectively, are linked by Galileo type transformations. Define

$$S_1(t) = e^{ic(t) \cdot p} \quad \text{and} \quad S_2(t) = e^{i(b(t) \cdot x - \alpha(t))}; \quad \alpha(t) = \int_0^t |b(s)|^2 ds.$$

Then

$$U_{\text{phy}}(t, 0) = S_2(t) U_{\text{aux}}(t, 0) S_2(0)^{-1}, \quad (6.15a)$$

$$U(t, 0) = S_1(t) U_{\text{aux}}(t, 0) S_1(0)^{-1}, \quad (6.15b)$$

$$U_{\text{phy}}(t, 0) = S_2(t) S_1(t)^{-1} U(t, 0) S_1(0) S_2(0)^{-1}. \quad (6.15c)$$

The bulk of [MS] is a study of the Floquet Hamiltonian of  $h$ . Spectral information is consequently deduced for the monodromy operator  $U(1, 0)$ . Finally the formula (6.15c) then gives spectral information for the physical monodromy operator  $U_{\text{phy}}(1, 0)$ . The part of [MS] concerning potentials with local singularities contains an incorrect reference in that it is referred to [Ya] for the existence of the propagator  $U$  (see [MS, Remark 1.4]). However although the issue of Yajima’s paper is the existence of an appropriate dynamics for singular time-dependent potentials the paper as well as the method of proof is for the one-body problem only. This point is easily fixed as follows, see Remark 6.4 for a more complicated procedure for  $\mathcal{E} \in L^1([0, 1]; X) \setminus C([0, 1]; X)$ : We use Yosida’s theorem which is in fact also alluded to in [MS, Remark 1.4] (see [Si, Theorem II.21] for a statement of the theorem). If  $V_{\text{phy}}$  is  $\epsilon$ -bounded relatively to  $p^2$  (which is the case under the conditions considered in [MS]) then indeed the propagator  $U_{\text{aux}}$  exists and we can use (6.15a) and (6.15b) to define  $U_{\text{phy}}$  and  $U$ . In particular we can use (6.15c) and obtain not only the existence of  $U_{\text{phy}}$  but various spectral information of the corresponding monodromy operator  $U_{\text{phy}}(1, 0)$  (see the introduction of [MS] for details). We remark that the construction of the Floquet Hamiltonian of  $h$  is done independently of  $U$  although of course (6.3) may be taken as a definition.

Let us for completeness note the following by-product of Yosida’s theorem (intimately related to its proof): Pick  $\lambda_0 \in \mathbb{R}$  such that  $h_{\text{aux}}(t) \geq \lambda_0 + 1$  for all  $t$ . The crucial assumption in the theorem is the boundedness of the function

$$t \rightarrow \|(h_{\text{aux}}(t) - \lambda_0)^{-1} \frac{d}{dt}(h_{\text{aux}}(t) - \lambda_0)^{-1}\|. \quad (6.16)$$

Since, by assumption  $\mathcal{E} \in C([0, 1]; X)$ , clearly the following constant is a bound of (6.16),

$$C := 2 \sup_t |\mathcal{E}(t)| \sup_t \| |p|(h_{\text{aux}}(t) - \lambda_0)^{-1} \|.$$

We have the explicit bound of the dynamics restricted to  $\mathcal{D}(p^2)$ .

$$\|(h_{\text{aux}}(t) - \lambda_0)U_{\text{aux}}(t, 0)\phi\|^2 \leq e^{2C|t|} \|(h_{\text{aux}}(0) - \lambda_0)\phi\|^2 \text{ for } \phi \in \mathcal{D}(p^2).$$

Let us also note the following property of the dynamics restricted to  $\mathcal{D}(|p|)$ , cf. [Si, Theorems II.23 and II.27],

$$\begin{aligned} & \|(h_{\text{aux}}(t) - \lambda_0)^{1/2}U_{\text{aux}}(t, 0)\phi\|^2 \\ & \leq e^{\tilde{C}|t|} \|(h_{\text{aux}}(0) - \lambda_0)^{1/2}\phi\|^2 \text{ for } \phi \in \mathcal{D}(|p|); \end{aligned} \quad (6.17)$$

here

$$\tilde{C} := 2 \sup_t |\mathcal{E}(t)| \sup_t \| |p|^{1/2}(h_{\text{aux}}(t) - \lambda_0)^{-1/2} \|^2.$$

**Remark 6.4.** If  $\mathcal{E} \in L^1([0, 1]; X)$  but possibly  $\mathcal{E} \notin C([0, 1]; X)$  we can still show that there exists an appropriate dynamics  $U$  under the conditions considered in [MS], although possibly not one that preserves  $\mathcal{D}(p^2)$ . We can use [Si, Theorem II.27] directly on  $h$ . For the borderline case, the Coulomb singularity, Hardy's inequality [MS, (6.2)] is needed to verify the assumptions of this theorem; the details are not discussed here. This yields a dynamics  $U$  preserving  $\mathcal{D}(|p|)$  which is good enough for getting the conclusions of [MS] related to the condition  $\mathcal{E} \in L^1([0, 1]; X)$ . The results presented below can similarly be extended to  $\mathcal{E} \in L^1([0, 1]; X)$ .

The following condition is an extension of [MS, Condition 1.3] (which corresponds to  $k_0 = 1$  below). The Coulomb potential commonly used to describe atomic and molecular systems (here with moving nuclei) is included.

**Conditions 6.5.** Let  $k_0 \in \mathbb{N}$  be given. For each  $a \neq a_{\min}$  the following holds. The pair-potential  $X^a \ni y \rightarrow V_a(y) \in \mathbb{R}$  splits into a sum  $V_a = V_a^1 + V_a^2$  where

- (1) Differentiability:  $V_a^1 \in C^{k_0+1}(X^a)$  and  $V_a^2 \in C^{k_0+1}(X^a \setminus \{0\})$ .
- (2) Global bounds: For all  $\alpha$  with  $|\alpha| \leq k_0 + 1$  there are bounds  $|y|^{|\alpha|} |\partial_y^\alpha V_a^1(y)| \leq C$ .
- (3) Decay at infinity:  $|V_a^1(y)| + |y \cdot \nabla_y V_a^1(y)| = o(1)$ .
- (4) Dimensionality:  $V_a^2 = 0$  if  $\dim X^a < 3$ .
- (5) Local singularity:  $V_a^2$  is compactly supported and for all  $\alpha$  with  $|\alpha| \leq k_0 + 1$  there are bounds  $|y|^{|\alpha|+1} |\partial_y^\alpha V_a^2(y)| \leq C$ ;  $y \neq 0$ .

We note that the part of time-dependent potential  $V_{\text{phy}}(\cdot + c(t))$  coming from the first term  $V_a^1$  of the splitting of  $V_a$  in Condition 6.5 conforms with Condition 6.1. The part from  $V_a^2$  does not, and we do not in general expect there to be an analogue of Theorem 6.2 in this case for  $k_0 > 1$ . It is an open problem to determine whether there is an analogue statement of Theorem 6.2 for  $k_0 = 1$ . Notice that the lowest degree of regularity,  $\phi \in \mathcal{D}(|p|)$ , holds even without the non-threshold condition, cf. [MS, Theorem 1.8]. On the other hand since the singularity is located at  $x = -c(t)$  we would expect and we will indeed prove regularity with respect to the observable

$$A = A(t) = \frac{1}{2}((x + c(t)) \cdot p + p \cdot (x + c(t))) = S_1(t) \frac{1}{2}(x \cdot p + p \cdot x) S_1(t)^{-1}. \quad (6.18)$$

This regularity is the content of Theorem 6.6 stated below; see [MS, Proposition 8.7 (ii)] for a related result in the case  $k_0 = 1$  at the level of Floquet theory, cf. Proposition 6.7 stated below. The  $A$ -regularity statement of the theorem for  $k_0 > 1$  is new. The set of thresholds is defined as before, see (6.1).

**Theorem 6.6.** *Suppose Conditions 6.5 for some  $k_0 \in \mathbb{N}$ . Let  $\phi$  be a bound state for  $U(1, 0)$  pertaining to an eigenvalue  $e^{-i\lambda} \notin \mathcal{F}(U(1, 0))$ . Then  $\phi \in \mathcal{D}(A(1)^{k_0})$  where  $A(1)$  is given by taking  $t = 1$  in (6.18).*

The above theorem implies Theorem 1.6 (1). We shall prove Theorem 6.6 along the same lines as that of the proof of Theorem 6.2. Whence we introduce the Floquet Hamiltonian by the expression (6.2) (with  $V = V_{\text{phy}}(\cdot + c(t))$ ). By [MS, Theorem 6.2]  $V$  is  $\epsilon$ -bounded relatively to  $H_0$  whence  $H$  is self-adjoint.

**Proposition 6.7.** *Suppose Conditions 6.5 for some  $k_0 \in \mathbb{N}$  and suppose  $H\psi = \lambda\psi$  for  $e^{-i\lambda} \notin \mathcal{F}(U(1, 0))$ . Then for any  $k, \ell \geq 0$ , with  $k + \ell \leq k_0$ , we have  $\psi \in \mathcal{D}(A^k \langle p \rangle A^\ell)$  where  $A$  is given by (6.18).*

*Proof.* It is tempting to try to apply Corollary 2.9 with  $H$  being the Floquet Hamiltonian,  $A$  being as stated and  $N = p^2 + 1$ . In fact all of the conditions of Corollary 2.9 can be verified except for Condition 2.1 (2) (notice that the formal analogue of (6.5b) might be too singular). This deficiency will be discussed at the end of the proof. All other conditions can be verified with

$$H' = 2p^2 - (x + c) \cdot \nabla V + 2b \cdot p, \quad (6.19a)$$

$$N' = 2p^2, \quad (6.19b)$$

$$i^\ell \text{ad}_A^\ell(N') = 2^{\ell+1} p^2, \quad i \text{ad}_N(i^\ell \text{ad}_A^\ell(N')) = 0; \quad \ell \leq k_0 - 1, \quad (6.19c)$$

$$i^\ell \text{ad}_A^\ell(H') = 2^{\ell+1} p^2 + (-1)^{\ell+1} ((x + c) \cdot \nabla)^{\ell+1} V + 2b \cdot p; \quad \ell \leq k_0. \quad (6.19d)$$

Comments are due. First, the second and the third terms of (6.19a) are bounded relatively to  $|p|$  uniformly in  $t$ , cf. the Hardy inequality [MS, (6.2)], and whence indeed (6.19a) is  $N$ -bounded. We need to verify Condition 2.1 (3) using the expression (6.19a): The operators  $p^2$ ,  $V$  and  $R(\eta)$  are fibered and  $R(\eta)$  preserves  $\mathcal{D}(p^2)$  and  $\mathcal{D}(|p|)$  for  $|\eta|$  large enough (uniformly in  $t$ ). Whence as a form on  $\mathcal{D}(\tau) \cap \mathcal{D}(N)$

$$i[h, R(\eta)] = -R(\eta)i[p^2 + V, A]R(\eta) = -R(\eta)(2p^2 - (x + c) \cdot \nabla V)R(\eta),$$

$$i[\tau, R(\eta)] = -R(\eta)2b \cdot pR(\eta),$$

and therefore

$$i[H, R(\eta)] = -R(\eta)H'R(\eta).$$

Using again that  $\mathcal{D}(H) \cap \mathcal{D}(N) = \mathcal{D}(\tau) \cap \mathcal{D}(N)$  is dense in  $\mathcal{D}(H) \cap \mathcal{D}(N^{1/2})$ , cf. Remark 3.5, the latter form identity can be extended by continuity to a form identity on  $\mathcal{D}(H) \cap \mathcal{D}(N^{1/2})$  yielding Condition 2.1 (3).

As for (6.19b), (6.19c), (6.19d), Conditions 2.1 (1) and (4), Condition 2.6 and Condition 2.8 the verification is straightforward (omitted here).

To show (2.4) we first introduce the natural notation  $V = V^1 + V^2$  reflecting the splitting of Conditions 6.5. Then we introduce

$$C = \||p|^{-\frac{1}{2}}((x + c) \cdot \nabla V^2 - 2b \cdot p)|p|^{-\frac{1}{2}}\| \quad \text{and} \quad \tilde{C} = \|(x + c) \cdot \nabla V^1\|;$$

the norm is the operator norm on  $\mathcal{H}$ . Then we note that

$$N \leq \frac{1}{2}H' + \frac{1}{2}C|p| + 1 + \frac{1}{2}\tilde{C},$$

yielding (2.4) with  $C_1 = 0$ ,  $C_2 = 1$  and  $C_3 = 1 + C^2/4 + \tilde{C}$  understood as a form on  $\mathcal{D}(N^{1/2})$ . We have verified Condition 2.2.

As for (2.5) a stronger version follows from [MS, Proposition 6.4]

$$H' \geq c_0\mathbb{1} - C_4 f_\lambda^\perp(H)^2 - K_0. \quad (6.20)$$

Here we use the condition that  $e^{-i\lambda} \notin \mathcal{F}(U(1,0))$ . The estimate (6.20) is valid as a form on  $\mathcal{D}(N^{1/2})$ . Finally it follows from [MS, Theorem 6.3] that indeed the condition of Corollary 2.9,  $\psi \in \mathcal{D}(N^{1/2}) = \mathcal{D}(|p|)$ , is fulfilled.

Now to the deficiency given by the lack of Condition 2.1 (2). Checking the proof of Corollary 2.9 it is realized that Condition 2.1 (2) is used only to assure boundedness of  $N^{1/2}BN^{-1/2}$ , where under the assumption (2.5) we have  $B = C_4 f_\lambda^\perp(H)^2 \langle H \rangle (H - \lambda)^{-1}$ . In our case we have a slightly stronger version of the Mourre estimate, (6.20), so what we really need is

$$N^{\frac{1}{2}}BN^{-\frac{1}{2}} \in \mathcal{B}(\mathcal{H}) \text{ where } B = g(H); g(E) = f_\lambda^\perp(E)^2(E - \lambda)^{-1}. \quad (6.21)$$

So let us show (6.21) without invoking a condition like Condition 2.1 (2). Clearly it suffices to show that the commutator

$$[N^{\frac{1}{2}}, g(H)] \in \mathcal{B}(\mathcal{H}). \quad (6.22)$$

But

$$\begin{aligned} [N^{\frac{1}{2}}, g(H)] &= c_{\frac{1}{2}} \int_0^\infty t^{\frac{1}{2}}(N+t)^{-1} [N, g(H)](N+t)^{-1} dt, \\ [N, g(H)] &= [H - V + I - \tau, g(H)] = -[\tau, g(H)] + T, \\ -[\tau, g(H)] &= \frac{1}{\pi} \int_{\mathbb{C}} (\bar{\partial}\tilde{g})(\eta)(H - \eta)^{-1} [\tau, V](H - \eta)^{-1} du dv, \\ -[\tau, V] &= i2b \cdot \nabla V. \end{aligned}$$

Here the term  $T$  is bounded since  $V$  is bounded relatively to  $H$ ; whence indeed  $T$  gives a bounded contribution to the commutator in (6.22). As for the contribution from the term  $-[\tau, g(H)]$  only the part from  $V^2$  is non-trivial. For that part we use [MS, (6.6)] to obtain

$$\|(H - \eta)^{-1} 2b \cdot \nabla V^2 (H - \eta)^{-1}\| \leq C \max(|\operatorname{Im} \eta|^{-2}, |\operatorname{Im} \eta|^{-\frac{1}{2}}).$$

Whence we can bound the integral

$$\begin{aligned} &\left\| \int_{\mathbb{C}} (\bar{\partial}\tilde{g})(\eta)(H - \eta)^{-1} 2b \cdot \nabla V^2 (H - \eta)^{-1} du dv \right\| \\ &\leq C \int_{\mathbb{C}} |(\bar{\partial}\tilde{g})(\eta)| \max(|\operatorname{Im} \eta|^{-2}, |\operatorname{Im} \eta|^{-\frac{1}{2}}) du dv < \infty. \end{aligned}$$

This means that also the first term  $-[\tau, g(H)]$  is bounded and whence in turn its contribution to the commutator in (6.22) agrees with the statement of (6.22). We have proven (6.22).  $\square$

*Proof of Theorem 6.6:* We mimic the proof of Theorem 6.2. Recall the notation  $I_n(A) = -in(A - in)^{-1}$  and  $A_n = AI_n(A)$ . Due to Proposition 6.7 and the representation (6.4) there exists  $t_0 \in [0, 1[$  such that

$$U(t_0, 0)\phi \in \mathcal{D}(|p|) \cap \mathcal{D}(A(t_0)^{k_0}). \quad (6.23)$$

In particular  $\psi(t) = e^{it\lambda}U(t, 0)\phi \in \mathcal{D}(|p|)$  for all  $t$ , cf. (6.15b) and (6.17). Moreover  $\psi(\cdot)$  is differentiable as a  $\mathcal{D}(|p|)^*$ -valued function, and in this sense

$$i\frac{d}{dt}\psi(t) = (h(t) - \lambda)\psi(t).$$

Whence we can compute

$$\frac{d}{dt}\|A_n^{k_0}\psi(t)\|^2 = 2\operatorname{Re}\langle A_n^{k_0}\psi(t), (i[h(t), A_n^{k_0}] + \frac{d}{dt}A_n^{k_0})\psi(t)\rangle, \quad (6.24a)$$

$$i[h(t), A_n^{k_0}] + \frac{d}{dt}A_n^{k_0} = \sum_{0 \leq p \leq k_0 - 1} A_n^p (i[h(t), A_n] + \frac{d}{dt}A_n) A_n^{k_0 - p - 1}, \quad (6.24b)$$

$$i[h(t), A_n] + \frac{d}{dt}A_n = I_n(A)(2p^2 + 2b \cdot p - (x + c) \cdot \nabla V)I_n(A). \quad (6.24c)$$

We plug (6.24c) into (6.24b) and then in turn (6.24b) into the right hand side of (6.24a). We expand the sum and redistribute for each term at most  $k_0 - 1$  factors of  $A$  obtaining terms on a more symmetric form, more precisely on the form

$$\operatorname{Re}\langle \langle p \rangle A^{k_0}\psi(t), B \langle p \rangle A^k \psi(t) \rangle \text{ where } k \leq k_0 - 1 \text{ and } \sup_{n,t} \|B\| < \infty. \quad (6.25)$$

Thanks to the Cauchy-Schwarz inequality and Proposition 6.7 any expression like (6.25) can be integrated on  $[t_0, 1]$  and the integral is bounded uniformly in  $n$ . In combination with (6.23) we conclude that

$$\sup_n \|A(1)_n^{k_0}\psi(1)\|^2 < \infty,$$

whence  $\phi = \psi(1) \in \mathcal{D}(A(1)^{k_0})$ . □

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