Reviews in Mathematical Physics
Vol. 28, No. 5 (2016) 1650010 (12 pages)

DOI: 10.1142/S0129055X16500100

Rellich's theorem and *N*-body Schrödinger operators

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Received 25 February 2016
Accepted 19 June 2016
Published 1 July 2016

We show an optimal version of Rellich's theorem for generalized N-body Schrödinger operators. It applies to singular potentials, in particular, to a model for atoms and molecules with infinite mass and finite extent nuclei. Our proof relies on a Mourre estimate [10] and a functional calculus localization technique.

Keywords: N-body Schrödinger operators; minimal non-threshold generalized eigenfunctions.

Mathematics Subject Classification 2010: 81Q10, 35A01, 35P05

1. Introduction and Results

Consider for given disjoint $R_1, \dots, R_K \in \mathbb{R}^d$ the N-body Schrödinger operator

$$H = \sum_{j=1}^{N} \left(-\frac{1}{2m_j}\Delta_{x_j} + \sum_{1\le k\le K} V_j^k(x_j - R_k) \right) + \sum_{1\le i<j\le N} V_{ij}(x_i - x_j) \qquad (1.1)$$

describing a system of N d-dimensional particles in $\Omega_1 = \mathbb{R}^d \backslash \overline{\Theta}$, where $\Theta = \bigcup_{1\le k\le K} \Theta_k$ for given open and bounded (possibly empty) subsets $\Theta_1, \dots, \Theta_K$ of $\mathbb{R}^d$. For those (possibly existing) $k = 1, \dots, K$ where $\Theta_k \neq \emptyset$, we demand that $R_k \in \Theta_k$, and for $N = 1$, the last term to the right in (1.1) is omitted. Furthermore, we assume that $d \ge 2$ and that $V_j^k(y) = q_j q^k |y|^{-1}$ and $V_{ij}(y) = q_i q_j |y|^{-1}$ (Coulomb potentials). We consider H as an operator on the Hilbert space $\mathcal{H} = L^2(\Omega)$, $\Omega = (\Omega_1)^N$, given by imposing the Dirichlet boundary condition. In [10] we proved that the set of eigenvalues and thresholds (that is eigenvalues for sub-Hamiltonians) is closed and countable and that any L^2-eigenfunction corresponding to a non-threshold eigenvalue is exponentially decaying. Under the additional condition that the exterior set Ω_1 is connected we proved that H does not have positive eigenvalues.

In this paper, we prove a version of Rellich's theorem applicable to this and other generalized N-body models. Letting $B_n = \{x \in \Omega \,|\, |x| < n\}$ we introduce the Besov space B_0^* of functions ϕ on Ω such that $1_{B_n}\phi \in \mathcal{H}$ for all $n \geq 1$ and

$$\lim_{n\to\infty} n^{-1}\|1_{B_n}\phi\|^2 = 0. \tag{1.2a}$$

Our version of Rellich's theorem for the atomic physics model (1.1) reads:

Proposition 1.1. *Suppose H is given by* (1.1) *with Coulomb potentials, and that ϕ is a generalized eigenfunction in B_0^* fulfilling the Dirichlet boundary condition on Ω and corresponding to a real non-threshold eigenvalue. Then $\phi \in \mathcal{H}$ and therefore ϕ is a genuine eigenstate (in fact $\mathrm{e}^{\epsilon|x|}\phi(x) \in L^2$ for some $\epsilon > 0$).*

We note that Isozaki in [9] showed for a class of smooth potentials in the context of usual N-body operators (i.e. N-body operators without hard-core interaction) that any non-threshold generalized eigenfunction in the weighted space $L^2_{\epsilon-1/2} = \langle x\rangle^{1/2-\epsilon}L^2$ must be in L^2 (here the weight $\langle x\rangle = (1+|x|^2)^{1/2}$ and $\epsilon > 0$). This type of problem goes back to Rellich [16]. The optimal one-body result is that any non-threshold generalized eigenfunction in B_0^* must be in L^2, cf. [12, 13, 1, 8]. The achievement of this paper is three-fold. Whence we obtain a version of Rellich's theorem for N-body operators (1) with singular pair potentials (with or without hard-core interaction), (2) stated with the optimal space, and finally (3) with a proof that appears more transparent (we think) than the one in [9].

Introducing the Besov space B^* of functions ϕ on Ω such that $1_{B_n}\phi \in \mathcal{H}$ for all $n \geq 1$ and

$$\sup_{n\geq 1} n^{-1}\|1_{B_n}\phi\|^2 < \infty, \tag{1.2b}$$

we note for comparison that $L^2_{\epsilon-1/2} \subseteq L^2_{-1/2} \subseteq B_0^* \subseteq B^* \subseteq L^2_{-1/2-\epsilon}$.

The space B^* is a natural space for generalized eigenfunctions. In fact, the generalized eigenfunctions in the range of the delta function

$$\delta(H-E) = \lim_{\epsilon\to 0} \frac{1}{\pi}\mathrm{Im}\,(H-E-\mathrm{i}\epsilon)^{-1},$$

defined on yet another Besov space $B \subseteq \mathcal{H}$ for any non-threshold and non-eigenvalue E, are in B^* and they span the continuous subspace of H. We shall not here elaborate on the precise meaning of the above limit. For usual N-body operators, an optimal form of the limiting absorption principle was given in [11]. For a version of LAP that applies to more singular Hamiltonians (in particular hard-core Hamiltonians), we refer to [10, Appendix B]. We claim, although here being unjustified, that the sharp form of LAP is valid for the Hamiltonians considered in [10] as well, in particular for the one of Proposition 1.1. Whence for any non-threshold and non-eigenvalue E Proposition 1.1 provides the following dichotomy for the mapping $\delta(H-E) : B \to B^*$. For $f \in B$ either $\phi = \delta(H-E)f \in B^*\backslash B_0^*$ or $\phi = 0$.

This is a general feature for N-body Hamiltonians due to the present paper. However, this being said, the generalized eigenfunctions in B^* are poorly understood, see [18] for some results. In particular it is not known if $\mathrm{Ran}(\delta(H-E))$ contains all generalized eigenfunctions in B^* (fulfilling the Dirichlet boundary condition for hard-core Hamiltonians). It is believed to be true and it is believed that all scattering information is encoded in this space (confirmed for the one-body problem).

1.1. *Generalized N-body models*

We will work in a generalized framework. This is given by a real finite dimensional vector space $\mathbf{X}$ with an inner product and a finite family of subspaces $\{\mathbf{X}_a \,|\, a \in \mathcal{A}\}$ closed with respect to intersection. We refer to the elements of $\mathcal{A}$ as *cluster decompositions* although this terminology is not motivated here. The orthogonal complement of $\mathbf{X}_a$ in $\mathbf{X}$ is denoted $\mathbf{X}^a$, and correspondingly we decompose $x = x^a \oplus x_a \in \mathbf{X}^a \oplus \mathbf{X}_a$. We order $\mathcal{A}$ by writing $a_1 \subset a_2$ if $\mathbf{X}^{a_1} \subset \mathbf{X}^{a_2}$. It is assumed that there exist $a_{\min}, a_{\max} \in \mathcal{A}$ such that $\mathbf{X}^{a_{\min}} = \{0\}$ and $\mathbf{X}^{a_{\max}} = \mathbf{X}$. Let $\mathcal{B} = \mathcal{A} \backslash \{a_{\min}\}$. The length of a chain of cluster decompositions $a_1 \subsetneq \cdots \subsetneq a_k$ is the number k. Such a chain is said to connect $a = a_1$ and $b = a_k$. The maximal length of all chains connecting a given $a \in \mathcal{A}\backslash\{a_{\max}\}$ and $a_{\max}$ is denoted by $\#a$. We define $\#a_{\max} = 1$ and denoting $\#a_{\min} = N+1$ we say the family $\{\mathbf{X}^a \,|\, a \in \mathcal{A}\}$ is of *N-body type.*

To define the generalized hard-core model more structure is needed: For each $a \in \mathcal{B}$ there is given an open subset $\Omega_a \subset \mathbf{X}^a$ with $\mathbf{X}^a \backslash \Omega_a$ compact, possibly $\Omega_a = \mathbf{X}^a$. Let for $a_{\min} \neq b \subset a$

$$\Omega^a_b = (\Omega_b + \mathbf{X}_b) \cap \mathbf{X}^a = \Omega_b + \mathbf{X}_b \cap \mathbf{X}^a,$$

and for $a \neq a_{\min}$

$$\Omega^a = \bigcap_{a_{\min} \neq b \subset a} \Omega^a_b.$$

We define $\Omega^{a_{\min}} = \{0\}$ and $\Omega = \Omega^{a_{\max}}$.

Our "soft potentials" fulfill:

Condition 1.2. There exists $\varepsilon > 0$ such that for all $b \in \mathcal{B}$ there is a splitting into (real-valued) terms $V_b = V_b^{(1)} + V_b^{(2)}$, where

(1) $V_b^{(1)}$ is smooth on the closure of Ω_b and

$$\partial_y^\alpha V_b^{(1)}(y) = O(|y|^{-\varepsilon-|\alpha|}). \tag{1.3a}$$

(2) $V_b^{(2)}$ vanishes outside a bounded set in Ω_b, and

$$V_b^{(2)} : H_0^1(\Omega_b) \to H_0^1(\Omega_b)^* \text{ is compact.} \tag{1.3b}$$

We consider for $a \in \mathcal{B}$ the Hamiltonian

$$H^a = -\frac{1}{2}\Delta_{x^a} + V^a, \quad V^a(x^a) = \sum_{b \subset a} V_b(x^b),$$

on the Hilbert space $L^2(\Omega^a)$ with the Dirichlet boundary condition on $\partial\Omega^a$, in particular,

$$H = H^{a_{\max}} = \frac{1}{2}\Delta + V = H_0 + V \quad \text{on } \mathcal{H} := L^2(\Omega)$$

with the Dirichlet boundary condition on $\partial\Omega$. More precisely the Hamiltonian H^a, henceforth referred to as a hard-core Hamiltonian, is given by its quadratic form. The form domain is the standard Sobolev space $H_0^1(\Omega^a)$, and the corresponding action is the (naturally defined) Dirichlet form. Due to the continuous embedding $H_0^1(\Omega^a) \subset H_0^1(\Omega^a_b)$ for $a_{\min} \neq b \subset a$ we conclude that indeed H^a is self-adjoint, cf. [15, Theorem X.17]. We define $H^{a_{\min}} = 0$ on $\mathbb{C}$. The thresholds of H are the eigenvalues of sub-Hamiltonians, that is more precisely, the set of thresholds is given by

$$\mathcal{T} = \bigcup_{a \in \mathcal{A}, \# a \geq 2} \sigma_{\mathrm{pp}}(H^a). \tag{1.4}$$

This definition of thresholds conforms with the notion of thresholds for usual N-body operators, and we recall that the so-called HVZ theorem asserts that the essential spectrum of H is given by the formula

$$\sigma_{\mathrm{ess}}(H) = [\min \mathcal{T}, \infty),$$

cf. [15, Theorem XIII.17]. We proved in [10] that $\mathcal{T}$ is closed and countable. It is also known that under rather general conditions H does not have positive eigenvalues and the negative non-threshold eigenvalues can at most accumulate at the thresholds and only from below, cf. [4, 10, 14].

In [10] we proved a version of the Mourre estimate using constructions of [2, 6]. This is more precisely given in terms of the (rescaled) Graf vector field $\tilde{\omega}_R(x) = R\tilde{\omega}(\frac{x}{R})$ and the corresponding operator

$$A = A_R = \frac{1}{2}(\tilde{\omega}_R(x) \cdot p + p \cdot \tilde{\omega}_R(x)); \quad R > 1, p = -\mathrm{i}\nabla. \tag{1.5}$$

We introduce a function $d : \mathbb{R} \to \mathbb{R}$ by

$$d(E) = \begin{cases} \inf_{\tau \in \mathcal{T}(E)}(E - \tau), & \mathcal{T}(E) := \mathcal{T} \cap]-\infty, E] \neq \emptyset, \\ 1, & \mathcal{T}(E) = \emptyset, \end{cases} \tag{1.6}$$

where $\mathcal{T}$ is given by (1.4).

Lemma 1.3. *For all $\kappa > 0$ and compact $I \subset \mathbb{R}$ with $I \cap \mathcal{T} = \emptyset$ there exists $R_0 > 1$ such that for all $R \geq R_0$ and all $E \in I$: There exists a neighborhood $\mathcal{U}$ of E and a compact operator K on $\mathcal{H}$ such that*

$$f(H)^* \mathrm{i}[H, A_R] f(H) \geq f(H)^* \{2d(E) - \kappa - K\} f(H) \quad \textit{for all real } f \in C_c^\infty(\mathcal{U}). \tag{1.7a}$$

The rescaled Graf vector field $\tilde{\omega}_R$ is complete on Ω. The Graf vector field is a gradient vector field, $\tilde{\omega} = \nabla r^2/2$ for some positive function r. We also note that by definition the "commutator" $\mathrm{i}[H, A_R]$ is given by its formal expression

$$\mathrm{i}[H, A_R] = p\tilde{\omega}_*(x/R)p - (2R^2)^{-1}(\Delta^2 r^2)(x/R) - \tilde{\omega}_R \cdot \nabla V. \tag{1.7b}$$

1.2. *Rellich's theorem in the generalized framework*

We need to be precise about the meaning of generalized eigenfunctions in B_0^* fulfilling the Dirichlet boundary condition: We say $\phi \in B_0^*$ (meaning that (1.2a) is fulfilled for the function $\phi : \Omega \to \mathbb{C}$) is a *generalized Dirichlet eigenfunction* with eigenvalue E if for all $n \geq 1$ the function $\chi_n(|x|)\phi \in H_0^1$ and in the distributional sense $(H - E)\phi = 0$. Here $\chi \in C^\infty(\mathbb{R})$ is real-valued,

$$\chi(t) = \begin{cases} 1 & \text{for } t \leq 1, \\ 0 & \text{for } t \geq 2, \end{cases} \tag{1.8}$$

and $\chi_n(t) = \chi(t/n)$. The main result of this paper reads.

Theorem 1.4. *Suppose Condition* 1.2. *Any generalized Dirichlet eigenfunction in* B_0^* *with a real non-threshold eigenvalue is in* $\mathcal{H} = L^2(\Omega)$.

We refer the reader to the proof of [10, Corollary 1.8] to see how Proposition 1.1 follows from Theorem 1.4. Note that it follows from [10, Appendix C] that non-threshold L^2-eigenfunctions have exponential decay. This is a consequence of Lemma 1.3. Our proof of Theorem 1.4 is also based on Lemma 1.3, however we shall proceed very differently. Whence exponential decay of non-threshold B_0^*-eigenfunctions is obtained by a combination of methods. A uniform approach seems out of reach.

2. Proof of Theorem 1.4

We introduce and discuss various preliminaries needed in the proof. It is easy to see that operators of the form $f(H)$, $f \in C_c^\infty(\mathbb{R})$, preserve any of the weighted L^2-spaces and Besov spaces introduced in Sec. 1, cf. Lemma A.1 stated below and [8, Theorem 14.1.4]. In particular $f(H)$ is a well-defined operator on B_0^*. It is also easy to see that for any generalized Dirichlet eigenfunction $\phi \in B_0^*$ with eigenvalue E we have $f(H)\phi = f(E)\phi$. Whence if $f(E) = 1$ we have the representation $\phi = f(H)\phi$.

The proof of Theorem 1.4 will rely on Lemma 1.3. We abbreviate $A = A_R$ in Lemma 1.3 using the result at a given non-threshold E leading to the following form of the estimate

$$f(H)\mathrm{i}[H, A]f(H) \geq f(H)(\sigma - K)f(H), \tag{2.1}$$

where $\sigma > 0$, $f \in C_c^\infty(\mathbb{R})$ is real-valued with $f(E) = 1$ and K is compact. Below the positivity of σ will be crucial, but its size will not have importance.

Another ingredient of our proof is the operator

$$B = \frac{1}{2}(\omega(x) \cdot p + p \cdot \omega(x)),$$

where $\omega = \omega_R = \tilde{\omega}_R / r_R$, $r_R(x) = Rr(\frac{x}{R})$. Recall for comparison that

$$2A = \tilde{\omega}_R(x) \cdot p + p \cdot \tilde{\omega}_R(x) = r_R \omega_R \cdot p + p \cdot r_R \omega_R.$$

We shall suppress the dependence of the parameter R (which is considered as a fixed large number). In particular we shall slightly abuse the notation writing for example r rather than the rescaled version r_R. Using the notation $\mathbf{D}$ for the Heisenberg derivative $\mathrm{i}[H, \cdot]$ we note the formal computations $B = \mathbf{D}r$, $A = r^{1/2} B r^{1/2}$ and

$$\mathbf{D}B = r^{-1/2}(\mathbf{D}A - B^2) r^{-1/2} + O(r^{-3}). \tag{2.2}$$

Here the function

$$O(r^{-3}) = \frac{1}{4} \omega \cdot (\nabla^2 r) \omega / r^2 = r^{-3} v(x),$$

where v belongs to the algebra $\mathcal{V}$ of smooth functions on Ω obeying

$$\forall \, \alpha \in \mathbb{N}_0^{\dim \mathbf{X}} \quad \text{and} \quad k \in \mathbb{N}_0 : |\partial_x^\alpha (x \cdot \nabla)^k v(x)| \leq C_{\alpha,k}.$$

This is due to the fact that the function $r^2 - x^2 \in \mathcal{V}$, cf. [10, (2.1b)]. We note that the expression (1.7b) for $\mathbf{D}A$ takes the form

$$\mathbf{D}A = \sum_{|\alpha| \leq 2} v_\alpha p^\alpha; \quad v_\alpha \in \mathcal{V},$$

which makes sense as a bounded form on $\mathcal{H}^1 = Q(H) = H_0^1$. For computations we will need the following rigorous version of (2.2), cf. [10, Lemma A.8]: In the sense of strong limit in the space of bounded operators $\mathcal{B}(\mathcal{H}^1, \mathcal{H}^{-1})$

$$\mathbf{D}B := \operatorname*{s-lim}_{t \to 0} t^{-1} (H \mathrm{e}^{\mathrm{i}tB} - \mathrm{e}^{\mathrm{i}tB} H) = r^{-1/2} (\mathbf{D}A - B^2) r^{-1/2} + r^{-2} v, \tag{2.3}$$

where $v \in \mathcal{V}$. Here we use that $\mathrm{e}^{\mathrm{i}tB} \in \mathcal{B}(\mathcal{H}^1) \cap \mathcal{B}(\mathcal{H}^{-1})$, cf. [10, Lemma A.6]. With a similar interpretation it follows that $\mathrm{ad}_B(\mathbf{D}B) = [\mathbf{D}B, B] \in \mathcal{B}(\mathcal{H}^1, \mathcal{H}^{-1})$. Although this will not be needed; in fact, all higher order repeated commutators $\mathrm{ad}_B^k(\mathbf{D}B)$ exist in this sense.

The above computations were used in [5], in fact our proof of Theorem 1.4 will to a large extent rely on ideas from [5] similarly to [9]. On the more technical level a certain part of Isozaki's proof also relies on ideas of [4], whereas the analogous difficulty at the threshold zero for a one-body problem was treated in [17] using a propagation of singularity result. We will present a new approach based on a conveniently chosen partition of unity.

As in [5] phase-space localization in terms of functional calculus of the operators B and H will be important. If $f \in C_c^\infty(\mathbb{R})$ (or for example $f = \chi$) the operator $f(B)$ preserves the spaces mentioned at the beginning of this section (like $f(H)$ does), and more generally $f(B)$ and $f(H)$ enjoy good properties regarding commutation with functions of r. These properties are studied in [5, Sec. 2] and will be used frequently below, however our presentation will be self-contained. It is based on an abstract result in Appendix A.

We need a cut-off function $\eta_\epsilon \in C^\infty(\mathbb{R})$ with special properties: The parameter $\epsilon > 0$ is considered small, and we define $\eta_\epsilon(x) = \frac{1}{\epsilon}\eta(\frac{x}{\epsilon})$, where $\eta'(x) > 0$ for $|x| < 1$, $\eta(x) = 0$ for $x \leq -1$ and $\eta(x) = 1$ for $x \geq 1$. We can construct η such that η' is even, $\sqrt{\eta'} \in C^\infty(\mathbb{R})$ and for some $c > 0$

$$\eta'(x) \geq c\,\eta(x) \quad \text{for } x \in (-1, 1/2]. \tag{2.4}$$

The optimal choice of such c (a necessary condition is $c \leq 2\ln 2$) is not important for us since we will only need (2.4) in the following disguised form: For any $\tilde{c} > 0$ and all ϵ small enough ($\epsilon^2 \leq \frac{2}{3}c\tilde{c}$ suffices)

$$\left(\frac{\epsilon}{2} - b\right)\eta_\epsilon(b) \leq \tilde{c}\,\eta_\epsilon'(b) \quad \text{for all } b \in \mathbb{R}. \tag{2.5}$$

Note also that since η_ϵ' is even $\epsilon^{-1} = \eta_\epsilon(b) + \eta_\epsilon(-b)$. We shall use the function $\zeta_\epsilon(b) = \eta_\epsilon(b) - \eta_\epsilon(-b)$.

Let $h_\kappa(r) = \frac{r}{1+\kappa r}$ for $\kappa \geq 0$, and let X_κ and Y_κ be the operators of multiplication by h_κ and $\frac{1}{1+\kappa r}$, respectively. Writing $X = X_0$ we note that $X_\kappa = XY_\kappa$. Note also that $\nabla h_\kappa(r) = (1+\kappa r)^{-2}\omega$, whence for example $\mathbf{D}X_\kappa = Y_\kappa B Y_\kappa$.

With these preliminaries we now embark on proving Theorem 1.4. Let $\phi \in B_0^*$ be a given generalized Dirichlet eigenfunction with a non-threshold eigenvalue E. We shall first show that $\phi \in L^2_{-1/4}$ and then use this property to show by a similar procedure that $\phi \in L^2$. Write $\phi = f(H)\phi$ where $f \in C_c^\infty(\mathbb{R})$, $f(E) = 1$ and (2.1) holds.

Step I. We outline the ideas of the proof of the property $\phi \in L^2_{-1/4}$. We shall consider the "propagation observable"

$$P = P_\kappa = f(H)X_\kappa^{1/4}\zeta_\epsilon(B)X_\kappa^{1/4}f(H), \quad \kappa > 0.$$

The parameter $\epsilon > 0$ will be fixed shortly small enough. Note that X_κ and P_κ are bounded due to the appearance of the factor $\frac{1}{1+\kappa r}$. Eventually this factor will be removed by letting $\kappa \to 0$. More precisely we shall demonstrate some "essential positivity" of $\mathbf{D}P$ persisting in the $\kappa \to 0$ limit. For any n the function $\phi_n = \chi_n(r)\phi \in H_0^1$, $(H-E)\phi_n = -\mathrm{i}(\mathbf{D}\chi_n)\phi$ and whence the expectation

$$\langle \mathbf{D}P\rangle_{\phi_n} = -2\mathrm{Re}\,\langle(\mathbf{D}\chi_n)P\chi_n\rangle_\phi. \tag{2.6a}$$

Since $\phi \in B_0^*$ the term to the right vanishes as $n \to \infty$, so it remains to study the term to the left in this limit. We compute

$$4\mathbf{D}X_\kappa^{1/4} = Y_\kappa^2 X_\kappa^{-3/4}B + \frac{3}{8}\mathrm{i}\omega^2 X_\kappa^{-7/4}Y_\kappa^4 + \mathrm{i}\kappa\omega^2 X_\kappa^{-3/4}Y_\kappa^3.$$

With commutation errors this should give

$$\begin{aligned} &2\mathrm{Re}((\mathbf{D}X_\kappa^{1/4})\zeta_\epsilon(B)X_\kappa^{1/4}) \\ &\quad = \frac{1}{2}Y_\kappa X_\kappa^{-1/4}B\zeta_\epsilon(B)X_\kappa^{-1/4}Y_\kappa + X^{-3/4}O(\kappa^0)X^{-3/4}. \end{aligned} \tag{2.6b}$$

Similarly, letting $\theta_\epsilon = \sqrt{\eta'_\epsilon}$,

$$X_\kappa^{1/4}(\mathbf{D}\zeta_\epsilon(B))X_\kappa^{1/4} \approx X_\kappa^{1/4}(\theta_\epsilon(B)(\mathbf{D}B)\theta_\epsilon(B) + \theta_\epsilon(-B)(\mathbf{D}B)\theta_\epsilon(-B))X_\kappa^{1/4}. \tag{2.6c}$$

Now we insert (2.2) into this expression and then estimate by (2.1) (here ignoring factors of $f(H)$). Ignoring the contribution from the compact operator K in (2.1) (which should be controllable in the state ϕ_n) we should end up with the effective lower bounds

$$\begin{aligned} X_\kappa^{1/4}(\mathbf{D}\zeta_\epsilon(B))X_\kappa^{1/4} &\geq (\sigma - \epsilon^2)X_\kappa^{1/4}X^{-1/2}(\eta'_\epsilon(B) + \eta'_\epsilon(-B))X^{-1/2}X_\kappa^{1/4} + X^{-3/4}O(\kappa^0)X^{-3/4} \\ &\geq (\sigma - \epsilon^2)Y_\kappa X_\kappa^{-1/4}(\eta'_\epsilon(B) + \eta'_\epsilon(-B))X_\kappa^{-1/4}Y_\kappa + X^{-3/4}O(\kappa^0)X^{-3/4}. \end{aligned} \tag{2.6d}$$

This suggests we should have ϵ so small that $2\epsilon^2 < \sigma$ since then $\sigma - \epsilon^2 \geq \sigma/2$. In total, we are led to consider

$$\frac{1}{2}Y_\kappa X_\kappa^{-1/4}(B\eta_\epsilon(B) - B\eta_\epsilon(-B) + \sigma\eta'_\epsilon(B) + \sigma\eta'_\epsilon(-B))X_\kappa^{-1/4}Y_\kappa.$$

Using (2.5) with $\tilde{c} = \sigma$ and any possibly smaller ϵ, whenceforth considered fixed, we arrive at the lower bound

$$\frac{\epsilon}{4}Y_\kappa X_\kappa^{-1/4}(\eta_\epsilon(B) + \eta_\epsilon(-B))X_\kappa{}^{-1/4}Y_\kappa = \frac{1}{4}X_\kappa^{-1/2}Y_\kappa^2.$$

Whence, given that error terms can be controlled, we obtain from these arguments the uniform bound

$$\|X_\kappa^{-1/4}Y_\kappa\phi\|^2 = \lim_{n\to\infty}\|X_\kappa^{-1/4}Y_\kappa\phi_n\|^2 \leq C_\phi. \tag{2.7}$$

By letting $\kappa \to 0$ in (2.7), it follows that $\phi \in L^2_{-1/4}$. The constant C_ϕ arises from bounding errors in (2.6b)–(2.6d) as well as from bounding the contribution from the operator K in (2.1) to supplement (2.6d). As we will see, in agreement with (2.6b) and (2.6d) it can be taken of the form $C_\phi = C\|X^{-3/4}\phi\|^2$.

Step II. To implement the scheme of Step I we provide details on estimating errors from various commutation and the outlined application of (2.1).

Right-hand side of (2.6a): We have

$$\mathbf{D}\chi_n = \chi'_n B - \frac{\mathrm{i}}{2}\omega^2\chi''_n,$$

and therefore using that BP is bounded and that $\phi \in B_0^*$ indeed

$$\lim_{n\to\infty}\mathrm{Re}\langle(\mathbf{D}\chi_n)P\chi_n\rangle_\phi = 0.$$

Left-hand side of (2.6a): We calculate

$$\mathbf{D}P = \mathrm{i}f(H)\big[\tilde{H}, X_\kappa^{1/4}\zeta_\epsilon(B)X_\kappa^{1/4}\big]f(H),$$

where $\tilde{H} = g(H)$ with $g(\lambda) = \lambda\tilde{f}(\lambda)$ and real-valued $\tilde{f} \in C_c^\infty(\mathbb{R})$ chosen such that $\tilde{f}(\lambda) = 1$ in a neighborhood of the support of f. Whence denoting $\tilde{\mathbf{D}}$ the Heisenberg derivative $\mathrm{i}[\tilde{H}, \cdot]$ we need to examine (2.6b) and (2.6c) with $\mathbf{D}$ replaced by $\tilde{\mathbf{D}}$.

<u>(2.6b) *with* $\tilde{\mathbf{D}}$</u>: Based on the representation (A.1b) (applied to $B = H$) we compute

$$4\tilde{\mathbf{D}}X_\kappa{}^{1/4} = g'(H)Y_\kappa^2 X_\kappa^{-3/4}B + X^{-3/4}O(\kappa^0)X^{-1},$$

and therefore

$$4f(H)(\tilde{\mathbf{D}}X_\kappa{}^{1/4}) = f(H)Y_\kappa^2 X_\kappa^{-3/4}B + X^{-3/4}O(\kappa^0)X^{-1}.$$

Using again Lemma A.1, we then obtain

$$\begin{aligned} &2f(H)\mathrm{Re}((\tilde{\mathbf{D}}X_\kappa^{1/4})\zeta_\epsilon(B)X_\kappa^{1/4})f(H) \\ &\quad = \frac{1}{2}f(H)Y_\kappa X_\kappa{}^{-1/4}B\zeta_\epsilon(B)X_\kappa{}^{-1/4}Y_\kappa f(H) + X^{-3/4}O(\kappa^0)X^{-3/4}. \end{aligned}$$

<u>(2.6c) *and* (2.6d) *modified*</u>: Using (2.3) and Lemma A.1 we can write

$$\begin{aligned} X_\kappa^{1/4}(\tilde{\mathbf{D}}\zeta_\epsilon(B))X_\kappa^{1/4} &= X_\kappa^{1/4}(\theta_\epsilon(B)(\tilde{\mathbf{D}}B)\theta_\epsilon(B) + \theta_\epsilon(-B)(\tilde{\mathbf{D}}B)\theta_\epsilon(-B))X_\kappa^{1/4} \\ &\quad + X^{-3/4}O(\kappa^0)X^{-3/4}. \end{aligned} \tag{2.8}$$

Indeed by (A.1b) (with interchanged roles of B and H) and (2.3)

$$\tilde{\mathbf{D}}B = \int_{\mathbb{C}} (H-z)^{-1}(\mathbf{D}B)(H-z)^{-1}\mathrm{d}\mu(z) \in \mathcal{B}(\mathcal{H}),$$

and therefore in turn similarly

$$\begin{aligned} [\tilde{\mathbf{D}}B, B] &= \operatorname*{s-lim}_{t\to 0} \frac{1}{\mathrm{i}t}((\tilde{\mathbf{D}}B)\mathrm{e}^{\mathrm{i}tB} - \mathrm{e}^{\mathrm{i}tB}(\tilde{\mathbf{D}}B)) \\ &= \int_{\mathbb{C}} (H-z)^{-1}[\mathbf{D}B, B](H-z)^{-1}\mathrm{d}\mu(z) \\ &\quad + 2\mathrm{i}\int_{\mathbb{C}} (H-z)^{-1}(\mathbf{D}B)(H-z)^{-1}(\mathbf{D}B)(H-z)^{-1}\mathrm{d}\mu(z) \in \mathcal{B}(\mathcal{H}). \end{aligned}$$

In fact it follows from this representation that

$$X^s[\tilde{\mathbf{D}}B, B]X^{2-s} \in \mathcal{B}(\mathcal{H}) \quad \text{for all } s \in \mathbb{R}.$$

Now we use this property with $s = 1$ and (A.1g) with $D_r = 0$ although we could take D_r to be the contribution to $\tilde{\mathbf{D}}B$ from the last term in (2.3). In any case (2.8) follows.

We multiply by $f(H)$ from the left and from the right and commute these factors next to the factor $\tilde{\mathbf{D}}B$ in the middle. We note

$$[f(H), X_\kappa^{1/4}] = X^{-3/4}O(\kappa^0),$$

and therefore we can bound the commutation errors obtaining

$$\begin{aligned} &f(H)X_\kappa^{1/4}(\tilde{\mathbf{D}}\zeta_\epsilon(B))X_\kappa^{1/4}f(H) \\ &\quad = X_\kappa^{1/4}(\theta_\epsilon(B)f(H)(\tilde{\mathbf{D}}B)f(H)\theta_\epsilon(B) + \theta_\epsilon(-B)f(H)(\tilde{\mathbf{D}}B)f(H)\theta_\epsilon(-B))X_\kappa^{1/4} \\ &\qquad + X^{-3/4}O(\kappa^0)X^{-3/4}. \end{aligned}$$

Now we can replace $\tilde{\mathbf{D}}$ by $\mathbf{D}$, use (2.3) and implement (2.1) after commutation of factors of $r^{-1/2}$ (recall that f was chosen with small support so that (2.1) applies) and then move the factors of $f(H)$ back where they came from. As in (2.6d), we then obtain a lower bound of the form

$$(\sigma-\epsilon^2)f(H)X_\kappa^{1/4}X^{-1/2}(\eta'_\epsilon(B)+\eta'_\epsilon(-B))X^{-1/2}X_\kappa^{1/4}f(H)+X^{-3/4}O(\kappa^0)X^{-3/4}$$

plus the contribution from K that was ignored in the heuristic bound (2.6d). This contribution is treated by first fixing a big $m\in\mathbb{N}$ such that (with ϵ given as before)

$$\sigma-\epsilon^2-\|K-\chi_m K\chi_m\|\geq\sigma/2,$$

and then noting that the contribution from the operator $\chi_m K\chi_m$ is bounded by $C\|X^{-3/4}\phi\|^2$.

In total, we have proved

$$\|X_\kappa^{-1/4}Y_\kappa\phi\|^2=\lim_{n\to\infty}\|X_\kappa^{-1/4}Y_\kappa f(H)\phi_n\|^2\leq C\|X^{-3/4}\phi\|^2,$$

leading to the desired conclusion, $\phi\in L^2_{-1/4}$, by letting $\kappa\to 0$.

Step III. We complete the proof of the assertion $\phi\in L^2$. This part is very similar to the previous part and therefore we leave out the details of the proof. We consider the observable

$$P=P_\kappa=f(H)X_\kappa^{1/2}\zeta_\epsilon(B)X_\kappa^{1/2}f(H),\quad \kappa>0,$$

where $\epsilon>0$ is chosen with $2\epsilon^2<\sigma$ and such that (2.5) applies with $\tilde{c}=\sigma/2$ (rather than $\tilde{c}=\sigma$ as before). Redoing the commutator arguments with slight modifications and by using that $\phi\in L^2_{-1/4}\subseteq L^2_{-1/2}$ with the proven bound

$$\|X^{-1/4}\phi\|^2\leq C\|X^{-3/4}\phi\|^2,$$

we obtain the bound

$$\|Y_\kappa\phi\|^2=\lim_{n\to\infty}\|Y_\kappa f(H)\phi_n\|^2\leq C\|X^{-3/4}\phi\|^2. \tag{2.9}$$

By letting $\kappa\to 0$ we deduce that $\phi\in L^2$.

Acknowledgments

K.I. is supported by JSPS KAKENHI grant number 25800073. E.S. is supported by DFF grant number 4181-00042.

Appendix A. Functional Calculus

The following abstract result is a particular time-independent version of [7, Lemma 3.5] adapted to the proof of Theorem 1.4, although the notation for operators does not conform with that of the proof of Theorem 1.4. There are many similar results in the literature, see for example [5, Sec. 2] or [3, Appendix C]. The function η referred to in (C) below is the function introduced at (2.4).

Lemma A.1. *Suppose B is a self-adjoint operator on a complex Hilbert space $\mathcal{H}$, and that H is a symmetric operator on $\mathcal{H}$ with domain $\mathcal{D}=\mathcal{D}(H)=\mathcal{D}(B)$. Suppose* *that the commutator form* $i[H, B]$ *defined on* $\mathcal{D}$ *is a symmetric operator with the same domain* $\mathcal{D}$. *Let* $\mathbf{D} = \mathrm{i}[H, \cdot]$ *Then*:

(A) *For any given* $F \in C_c^\infty(\mathbb{R})$ *we let* $\tilde{F} \in C_c^\infty(\mathbb{C})$ *denote an almost analytic extension. In particular*

$$F(B) = \frac{1}{\pi}\int_{\mathbb{C}} (\bar{\partial}\tilde{F})(z)(B-z)^{-1} dudv, \quad z = u + \mathrm{i}v, \tag{A.1a}$$

and

$$\mathbf{D}F(B) = -\frac{1}{\pi}\int_{\mathbb{C}} (\bar{\partial}\tilde{F})(z)(B-z)^{-1}(\mathbf{D}B)(B-z)^{-1} dudv. \tag{A.1b}$$

In particular if $\mathbf{D}B$ *is bounded then for any* $\epsilon > 0$ (*with* $\langle z\rangle = (1+|z|^2)^{\frac{1}{2}}$)

$$\|\mathbf{D}F(B)\| \le C_\epsilon \sup_{z\in\mathbb{C}} (\langle z\rangle^{\epsilon+2} |\mathrm{Im}\, z|^{-2} |(\bar{\partial}\tilde{F})(z)|)\|\mathbf{D}B\|. \tag{A.1c}$$

(B) *Suppose in addition that we can split* $\mathbf{D}B = D + D_r$, *where* D *and* D_r *are symmetric operators on* $\mathcal{D}$, *and that similarly for* $k = 1$ *the form* $\mathrm{i}^k \mathrm{ad}_B^k(D) = \mathrm{i}[\mathrm{i}^{k-1}\mathrm{ad}_B^{k-1}(D), B]$ *defined on* $\mathcal{D}$ *is a symmetric operator on* $\mathcal{D}$. *Here by definition* $\mathrm{ad}_B^0(D) = D$, *and we note that the form* $\mathrm{ad}_B^2(D)$ *appearing below makes sense without further assumptions. Then the contribution from* D *to* (A.1b) *can be written as*

$$\begin{aligned} -\frac{1}{\pi}\int_{\mathbb{C}} &(\bar{\partial}\tilde{F})(z)(B-z)^{-1} D (B-z)^{-1} dudv \\ &= \frac{1}{2}(F'(B)D + DF'(B)) + R_1(t); \end{aligned} \tag{A.1d}$$

$$R_1 = \frac{1}{2\pi}\int_{\mathbb{C}} (\bar{\partial}\tilde{F})(z)(B-z)^{-2}\mathrm{ad}_B^2(D)(B-z)^{-2} dudv.$$

For all $f \in C_c^\infty(\mathbb{R})$,

$$\frac{1}{2}(f^2(B)D + Df^2(B)) = f(B)Df(B) + R_2; \tag{A.1e}$$

$$\begin{aligned} R_2(t) = \frac{1}{2\pi^2}\int_{\mathbb{C}}\int_{\mathbb{C}} &(\bar{\partial}\tilde{f})(z_2)(\bar{\partial}\tilde{f})(z_1)(B-z_2)^{-1}(B-z_1)^{-1} \\ &\mathrm{ad}_B^2(D)(B-z_1)^{-1}(B-z_2)^{-1} du_1 dv_1 du_2 dv_2. \end{aligned}$$

(C) *Suppose in addition to the previous assumptions that the operator* D_r *extends to a bounded self-adjoint operator. Let* $F = \eta$ *where* η *is the function from above. Then there exists an almost analytic extension with*

$$|(\bar{\partial}\tilde{F})(z)| \le C_k \langle z\rangle^{-1-k} |\mathrm{Im}\, z|^k; \quad k \in \mathbb{N}, \tag{A.1f}$$

yielding the representation

$$\mathbf{D}F(B) = F'^{\frac{1}{2}}(B) D F'^{\frac{1}{2}}(B) + R_1 + R_2 + R_3, \tag{A.1g}$$

where R_1 *is given by* (A.1d), R_2 *by* (A.1e) *with* $f = \sqrt{F'}$ *and* R_3 *is the contribution from* D_r *to* (A.1b) (*the latter possibly estimated as in* (A.1c) *with* $\epsilon = 1$).

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