ABSENCE OF POSITIVE EIGENVALUES FOR HARD-CORE N-BODY SYSTEMS

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We give an account of a recent work on absence of positive eigenvalues for generalized 2-body hard-core Schrödinger operators [12]. We show absence of such eigenvalues under the condition of bounded strictly convex obstacles. A scheme for showing absence of positive eigenvalues for generalized N-body hard-core Schrödinger operators, $N \geq 2$, is presented. This scheme involves high energy resolvent estimates, and for $N = 2$ it is implemented by a Mourre commutator type method. A particular example is the Helium atom with the assumption of infinite mass and finite extent nucleus.

Keywords: Schrödinger operator with obstacle, Mourre estimate, high-energy resolvent estimate.

1. Introduction and result for Helium type atom

Consider the N-body Schrödinger operator

$$H = \sum_{j=1}^{N} \Big(-\frac{1}{2m_j}\Delta_{x_j} + V_j^{\mathrm{ncl}}(x_j)\Big) + \sum_{1\leq i<j\leq N} V_{ij}^{\mathrm{elec}}(x_i - x_j) \tag{1}$$

for a system of N d-dimensional particles in the exterior of a bounded strictly convex obstacle $\Theta_1 \subset \mathbb{R}^d$ (for $N = 1$ the last term is omitted). Whence H is an operator on the Hilbert space $L^2(\Omega)$; $\Omega = (\Omega_1)^N$, $\Omega_1 = \mathbb{R}^d \setminus \overline{\Theta}_1$. It is defined more precisely by imposing the Dirichlet boundary condition. This operator models a system of N d-dimensional charged particles interacting with a fixed charged nucleus of finite extent, for example a ball (or possibly a somewhat deformed ball). In particular (assuming $0 \in \Theta_1$) we could have Coulomb interactions $V_j^{\mathrm{ncl}}(y) = q_j q^{\mathrm{ncl}}|y|^{-1}$ and $V_{ij}^{\mathrm{elec}}(y) = q_i q_j |y|^{-1}$ in dimension $d \geq 2$. We address the problem of proving absence of positive eigenvalues. While this property is well-known for the N-body problem with "soft potentials" [5] and for one-body potential or obstacle problems [6, 11, 15], the N-body obstacle problem is open for $N \geq 2$. We introduce for problems of this type a general procedure involving high energy resolvent estimates for effective sub-Hamiltonians. We show that this scheme can be implemented for the case $N = 2$. In this case essentially such an effective sub-Hamiltonian is a one-body Hamiltonian for an exterior region. The result is shown in the so-called generalized 2-body hard-core framework.

Specializing to the model (1) with Coulomb interactions we have:

Theorem 1.1. *For $N = 2$ charged particles confined to the exterior of a bounded strictly convex obstacle $\Theta_1 \subset \mathbb{R}^d$ containing 0, $d \geq 2$, the corresponding Hamiltonian H given by* (1) *with Coulomb interactions $V_j^{\mathrm{ncl}}(y) = q_j q^{\mathrm{ncl}} |y|^{-1}$ and $V_{ij}^{\mathrm{elec}}(y) = q_i q_j |y|^{-1}$ does not have positive eigenvalues.*

As it is indicated above we have a partial result for $N \geq 3$ only. Another open problem would be to relax the assumption of strict convexity of the obstacle. Yet another related open problem would be to treat unbounded obstacles.[a]

2. Generalized N-body hard-core systems

We work in a generalized framework. The outset is the same as for model without obstacles, i.e. the model defined by "soft potentials". This is given by real finite dimensional vector space $\mathbf{X}$ with an inner product q, i.e. $(\mathbf{X}, q)$ is Euclidean space, and a finite family of subspaces $\{X_a |\ a \in \mathcal{A}\}$ closed with respect to intersection. We refer to the elements of $\mathcal{A}$ as *cluster decompositions* (not to be motivated here). The orthogonal complement of $\mathbf{X}_a$ in $\mathbf{X}$ is denoted $\mathbf{X}^a$, and correspondingly we decompose $x = x^a \oplus x_a = \pi^a x \oplus \pi_a x \in \mathbf{X}^a \oplus \mathbf{X}_a$. 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 $X^{a_{\max}} = \mathbf{X}$. Let $\mathcal{B} = \mathcal{A} \setminus \{a_{\min}\}$. 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 $a \in \mathcal{A} \setminus \{a_{\max}\}$ 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. Whence the generalized 2-body framework is characterized by the condition $X_a \cap X_b = \{0\}$ for $a, b \neq a_{\min}$, $a \neq b$.

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

$$\Omega_b^a = \{\Omega_b + \mathbf{X}_b\} \cap \mathbf{X}^a = \Omega_b + \mathbf{X}_b \cap \mathbf{X}^a,$$

[a]Note added in proof: We recently solved two of these problems. More precisely we have generalized the above result to arbitrary $N \geq 2$ without assuming strict convexity of Θ_1, although keeping the condition this set be bounded. As a substitute for the strict convexity assumption we need only $\Omega_1 = \mathbb{R}^d \setminus \overline{\Theta}_1$ to be connected. See "Absence of positive eigenvalues for hard-core N-body systems", Institut Mittag-Leffler Preprint Series, fall 2012 no. 31

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

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

We define $\Omega^{a_{\min}} = \{0\}$ and $\Omega = \Omega^{a_{\max}}$. The generalized N-body hard-core Hamiltonian is the following operator H on the Hilbert space $\mathcal{H} = L^2(\Omega)$ with form domain $Q(H) = H^1_0(\Omega)$,

$$H = -\tfrac{1}{2}\Delta + V, \quad V = \sum_{b \in \mathcal{B}} V_b(x^b), \tag{2a}$$

where we impose:

Condition 2.1. There exists $\varepsilon > 0$ such that for all $b \in \mathcal{B}$ there is a splitting $V_b = V_b^{(1)} + V_b^{(2)}$, where

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

$$\partial_y^\alpha V_b^{(1)}(y) = O\big(|y|^{-\varepsilon-|\alpha|}\big). \tag{2b}$$

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

$$V_b^{(2)} \in \mathcal{C}\big(H^1_0(\Omega_b), H^1_0(\Omega_b)^*\big). \tag{2c}$$

Here and henceforth, given Banach spaces X_1 and X_2, the notation $\mathcal{C}\big(X_1, X_2\big)$ and $\mathcal{B}\big(X_1, X_2\big)$ refer to the set of compact and the set of bounded operators $T : X_1 \to X_2$, respectively.

3. Basic properties of generalized N-body hard-core Hamiltonians

As for N-body Hamiltonians with soft potentials we have the notions of sub-Hamiltonians and thresholds, and in fact there is a Mourre estimate. This is under the conditions of the previous section.

Let $-\Delta^a = (p^a)^2$ and $-\Delta_a = p_a^2$ denote (minus) the Laplacians on $L^2(\Omega^a)$ and $L^2(\mathbf{X}_a)$, respectively. Here $p^a = \pi^a p$ and $p_a = \pi_a p$ denote the internal (i.e. within "clusters") and the external (i.e. "inter-cluster") components of the momentum operator $p = -\mathrm{i}\nabla$, respectively. For $a \in \mathcal{B}$, denote

$$V^a(x^a) = \sum_{b \subset a} V_b(x^b), \quad I_a(x) = \sum_{b \not\subset a} V_b(x^b),$$

$$H^a = -\tfrac{1}{2}\Delta^a + V^a(x^a), \quad H_a = H^a - \tfrac{1}{2}\Delta_a.$$

Note that the operators H^a and $H_a = H^a \otimes I + I \otimes \frac{1}{2}p_a^2$ are defined on $L^2(\Omega^a)$ and $L^2(\Omega^a) \otimes L^2(\mathbf{X}_a)$, respectively. We define $H^{a_{\min}} = 0$ on $L^2(\mathbf{X}^{a_{\min}}) := \mathbb{C}$. The generalized many-body Hamiltonian H^a is the sub-Hamiltonian associated with the cluster decomposition a and I_a is the sum of all inter-cluster interactions. The detailed expression of H^a depends on the choice of coordinates on $\mathbf{X}^a$.

The set of thresholds of the generalized N-body Hamiltonian $H = H^{a_{\max}}$ is the set

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

The bottom of the essential spectrum of H is given by the well-known HVZ theorem, that is by the formulas

$$\inf \sigma_{\rm ess}(H) = \min_{a\in\mathcal{A}\setminus\{a_{\max}\}} \inf \sigma(H^a) = \min_{a\in\mathcal{A},\#a=2} \inf \sigma(H^a) = \min \mathcal{T},$$

in fact $\sigma_{\rm ess}(H) = [\min \mathcal{T}, \infty)$.

Our Mourre estimate is given in terms of the conjugate operator

$$A = A_R = \omega_R(x)\cdot p + p\cdot \omega_R(x);\ R > 1. \tag{3}$$

Here $\omega_R(x) := R\omega(\frac{x}{R})$ is the rescaled Graf vector field, see the comment after Lemma 3.2 stated below. We also introduce a function $d:\mathbb{R}\to\mathbb{R}$ by

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

These devices enter into the following Mourre estimate (there exists a different Mourre estimate [2]). We remark that all inputs needed for a proof [10, 17] are stated in Lemma 3.2.

Lemma 3.1. *For all $E\in\mathbb{R}$ and $\epsilon > 0$ there exists $R_0 > 1$ such that for all $R \geq R_0$ there is a neighbourhood $\mathcal{V}$ of E and a compact operator K on $L^2(\Omega)$ such that*

$$f(H)^*{\rm i}[H, A_R]f(H) \geq f(H)^*\{4d(E) - \epsilon - K\}f(H) \text{ for all } f \in C_{\rm c}^\infty(\mathcal{V}).$$

We use below the notation $\mathbb{N}_0 = \mathbb{N}\cup\{0\}$.

Lemma 3.2. *There exist [4, 9] a smooth positive and convex function on $\mathbf{X}$, denoted by r, and a partition of unity $\{\tilde q_a\}_{a\in\mathcal{A}}$ consisting of smooth functions, $0 \leq \tilde q_a \leq 1$, such that for some positive constants r_1 and r_2 and with the vector field $\omega := \frac{1}{2}\nabla r^2$ (with derivative denoted by ω_*):*

(1) $\omega_*(x) \geq \sum_a \pi_a \tilde q_a$.
(2) $\omega^a(x) = 0$ *if* $|x^a| < r_1$.
(3) $|x^b| > r_1$ *on* $\operatorname{supp}(\tilde q_a)$ *if* $b \not\subset a$.
(4) $|x^a| < r_2$ *on* $\operatorname{supp}(\tilde q_a)$.
(5) For all $\alpha \in \mathbb{N}_0^{\dim X}$ *and* $k\in\mathbb{N}_0$ *there exist* $C\in\mathbb{R}$:

$$|\partial_x^\alpha \tilde q_a| + |\partial_x^\alpha (x\cdot\nabla)^k\{r^2 - x^2\}| \leq C.$$

The rescaled Graf vector field entering in (3) corresponds to the rescaled potential function $r_R(x) = Rr(x/R)$. We choose R so big that (intuitively) ω_R acts tangentially at the boundary of Ω, cf. Lemma 3.2 (2). Dropping henceforth the subscript R we have the more precise statement that the restriction of the vector field ω to Ω is *complete*. A consequence of this property is that ${\rm e}^{{\rm i}tA}$ preserves the form domain $Q(H)$ and that

$$\sup_{|t|<1} \|{\rm e}^{{\rm i}tA}\|_{\mathcal{B}(Q(H))} < \infty.$$

In fact H is $C^1(A_{Q(H)}, A_{Q(H)^*})$ [8]. In particular the following formal computation of the commutator has a precise (and useful) interpretation as a "derivative" [8]:

$$\mathrm{i}[H, A] = 2p\omega_*(x)p - \tfrac{1}{4}\left(\Delta^2 r^2\right)(x) - 2\omega \cdot \nabla V. \tag{4a}$$

This formula can be viewed as a first step of a proof of Lemma 3.1. Notice that Lemma 3.2 (1) guarentees that indeed the first term to the right is non-negative. However the Hessian is degenerate and this is the main source of complication, not only for the Mourre estimate, but in fact in a more profound way for our procedure of showing absence of positive eigenvalues (to be briefly outlined in the next section). The content of positivity is most conveniently expressed in terms of "quadratic" partition functions, say $q_a = q_{a,R}$, so we deduce from (4a) that

$$\mathrm{i}[H, A] \geq 2\sum_b q_b\, p_b^2\, q_b + O\left(R^{-\min\{2,\varepsilon\}}\right). \tag{4b}$$

We note some standard applications of the Mourre estimate: The set of thresholds $\mathcal{T}$ is closed and countable, and the eigenvalues can at most accumulate at $\mathcal{T}$. Another consequence [5, 10] is that non-threshold eigenstates decay exponentially with rates determined by the distance to the lowest threshold above the eigenvalue. In particular absence of positive eigenvalues would follow by an inductive procedure as for soft potentials [5] provided one could exclude the existence of super-exponentially decaying eigenstates. Whence the latter problem is the incomplete part of a scheme for showing absence of positive eigenvalues. The problem is solved for $N = 1$ [11]. Our procedure for attacking it for $N \geq 2$ is based on a virial type argument using (4b).

4. Results for generalized models

In addition to Condition 2.1 we impose henceforth

Condition 4.1. Suppose $N \geq 2$. For all $b \in \mathcal{B} \setminus \{a_{\max}\}$ with $\Omega_b \subsetneq \mathbf{X}^b$ the set $\Theta_b := \mathbf{X}^b \setminus \overline{\Omega_b} \neq \emptyset$ has smooth boundary $\partial\Theta_b = \partial\Omega_b$ and is strictly convex.

Our main result reads:

Theorem 4.1. *Suppose $N = 2$ and Conditions 2.1 and 4.1. Suppose that for all $b \in \mathcal{B} \setminus \{a_{\max}\}$ with $\Omega_b \subsetneq \mathbf{X}^b$ the term $V_b^{(2)} = 0$ while for all $b \in \mathcal{B} \setminus \{a_{\max}\}$ with $\Omega_b = \mathbf{X}^b$*

$$x^b \cdot \nabla V_b^{(2)}(x^b),\ (x^b \cdot \nabla)^2 V_b^{(2)}(x^b) \in \mathcal{C}\big(H^1(\mathbf{X}^b), H^1(\mathbf{X}^b)^*\big).$$

Suppose that any eigenstate of H vanishing at infinity must be zero (the unique continuation property). Then H does not have positive eigenvalues.

The unique continuation property is a well-studied subject [7, 14, 15]. It is valid for a large class of potential singularities given connectivity of Ω. The latter connectivity is indeed valid for the application stated above as Theorem 1.1, and the unique continuation property is valid too [15].

To state a partial result for $N \geq 3$ we first introduce a non-negative $\chi \in C^\infty(\mathbb{R})$ with $0 \leq \chi \leq 1$ and

$$\chi(t) = \begin{cases} 0 & \text{for } t \leq 5/4, \\ 1 & \text{for } t \geq 7/4. \end{cases}$$

We shall use the rescaled function

$$\chi_\nu(t) = \chi(t/\nu), \quad \nu > 1,$$

and the notation $\chi_\nu^+ = \chi_\nu$ and $\chi_\nu^- = 1 - \chi_\nu$. Introduce then the following function on Ω,

$$s(x) = \chi_{\nu/2}^+(r)(|\mathrm{d}r| - 1)/\sqrt{2} + 1/\sqrt{2}; \quad \nu > 1.$$

From Lemma 3.2 (5) we deduce that

$$\forall \alpha \in \mathbb{N}_0^{\dim \mathbf{X}} : |\partial_x^\alpha \big(s(x) - 1/\sqrt{2}\big)| \leq C_\alpha \nu^{-2}.$$

So in the regime $\nu >> 1$ we have $s(x) \approx 1/\sqrt{2}$.

Next we introduce for large $\sigma, \nu > 1$ the operators

$$\widetilde{H}_b = \widetilde{H}^b + \tilde{p}_b^2 \chi^-_{\sigma^2/2}\left(\tilde{p}_b^2\right);$$
$$\widetilde{H}^b = s(x)^{-1} H^b s(x)^{-1}, \quad \tilde{p}_b^2 = \tfrac{1}{2} s(x)^{-1} p_b^2 s(x)^{-1}.$$

The operator $\widetilde{H}_b - \sigma^2$ should be thought of as an effective approximation to

$$2|\mathrm{d}r|^{-1}\left(H_b - \tfrac{\sigma^2}{2}|\mathrm{d}r|^2\right)|\mathrm{d}r|^{-1} \approx 2H_b - \sigma^2 = 2H^b + p_b^2 - \sigma^2$$

in the large r regime and in the low energy regime of p_b^2 (the latter regime is the "bad one" destroying positivity in (4b)). In turn (in an equally imprecise sense), if $(H - E)\phi = 0$ with $\phi_\sigma := \mathrm{e}^{\sigma r}\phi \in \mathcal{H}$ for all $\sigma > 1$, then

$$\left(s^{-1} H s^{-1} - \sigma^2\right)(s\phi_\sigma) \approx s^{-1}\big(H - \tfrac{\sigma^2}{2}|\mathrm{d}r|^2\big)\phi_\sigma \approx 0,$$

leading to the following approximation on the support of the partition function q_b entering in (4b),

$$(\widetilde{H}_b - \sigma^2)(s\phi_\sigma) \approx 0. \tag{5}$$

The form domain of $\widetilde{H}_b$ is

$$Q(\widetilde{H}_b) = L^2(\mathbf{X}_b, H_0^1(\Omega^b); \mathrm{d}x_b) \subset \mathcal{H}_b := L^2(\Omega^b) \otimes L^2(\mathbf{X}_b).$$

We introduce a high energy type condition.

Condition 4.2. For all $b \neq a_{\max}$ the following bound holds uniformly in all large $\sigma, \nu > 1$, $\epsilon \in (0, 1]$ and reals λ near 1:

$$\|\delta_\epsilon(\widetilde{H}_b/\sigma^2 - \lambda)\|_{\mathcal{B}(B(|x^b|), B(|x^b|)^*)} \leq C\sigma. \tag{6}$$

Here, by definition, for any self-adjoint operator T

$$\delta_\epsilon(T) = \pi^{-1}\Im(T - \mathrm{i}\epsilon)^{-1}.$$

The space $B(\cdot)$ is the Besov space, here used for the operator of multiplication by $|x^b|$. Note that (6) is trivially fulfilled for $b = a_{\min}$ (by the spectral theorem). We derive the bounds for $N = 2$ under the conditions of Theorem 4.1 by a modification of the Mourre commutator method. Note that for $N = 2$ and $b \notin \{a_{\min}, a_{\max}\}$ only $b' = b$ obeys $a_{\min} \neq b' \subset b$, and hence for such b we have $\Omega^b = \Omega_b$ and (6) is an effective high energy bound for a bounded obstacle (hence one-body type). More generally we prove (6) for b with $\#b = N$ under the additional regularity conditions for Ω_b and V_b. High energy resolvent bounds are studied previously in the literature [1, 13, 16, 18, 19]. Although slightly weaker bounds than (6) will suffice (Besov spaces can be replaced by weighted spaces for example) we need the linear dependence of σ on the right-hand side. Whence the slightly weaker dependence $\sigma \ln \sigma$ found in recent works on one-body obstacle problems [3] would not suffice, cf. the bounds below.

In our virial type argument we apply (5), (6) and Lemma 3.2 (4) in combination with the following bound valid for all $\chi, g \in C_{\mathrm{c}}(\mathbb{R})$ and $\kappa > 0$, provided $\sigma > 1$ is large enough,

$$\begin{aligned} &\|\chi(|x^b|)g\big(\sigma(\widetilde{H}_b/\sigma^2 - 1)\big)\chi(|x^b|)\| \\ &\le \sigma^{-1}\|g\|_{L^1} \sup_{\epsilon\in(0,1],\, |\lambda-1|\le\kappa} \|\chi(|x^b|)\delta_\epsilon(\widetilde{H}_b/\sigma^2 - \lambda)\chi(|x^b|)\| \\ &\le C\|g\|_{L^1} \text{ for } \sigma \ge \sigma_0 = \sigma_0(\operatorname{supp} g, \kappa) \text{ and with } C = C(\chi, \kappa). \end{aligned}$$

Note that we used (6) to obtain a bound independent of σ.

We have the following partial result for arbitrary $N \ge 2$.

Proposition 4.1. *Suppose $N \ge 2$ and Conditions 2.1 and 4.2. Suppose H does not have positive thresholds. Suppose that any eigenstate of H vanishing at infinity must be zero (the unique continuation property). Then H does not have positive eigenvalues.*

By imposing the analogous version of Condition 4.2 for sub-Hamiltonians as well as the unique continuation property for these operators and for H (in addition to Condition 2.1) we obtain that H does not have positive thresholds nor positive eigenvalues, cf. the inductive scheme discussed in the previous section. However since we are only able to verify Condition 4.2 for $N = 2$ using Condition 4.1 we need these restrictions in Theorem 4.1. Nevertheless, since verifying Condition 4.2 for higher N under Condition 2.1 possibly as well as under Condition 4.1 could be a purely technical difficulty, we consider Proposition 4.1 as a result of independent interest.

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