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Absence of Negative Energy Spectrum for *N*-Particle Hamiltonians

Michael O'Carroll[1]

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We consider the spectrum of the quantum Hamiltonian H for a system of N one-dimensional particles. H is given by $H=\sum_{i=1}^{N}-\frac{1}{2m_i}\frac{\partial^2}{\partial x_i^2}+\sum_{1\leqslant i<j\leqslant N}V_{ij}(x_i-x_j)$ acting in $L^2(R^N)$. We assume that each pair potential is a sum of a hard core for $|x|\leqslant a$, $a>0$, and a function $V_{ij}(x)$, $|x|>a$, with $\int_a^\infty |x-a|\,|V_{ij}(x)|\,dx<\infty$. We give conditions on $V_{ij}^-(x)$, the negative part of $V_{ij}(x)$, which imply that H has no negative energy spectrum for all N. For example, this is the case if $V_{ij}^-(x)$ has finite range 2a and

$$2m_i\int_a^{2a}|x-a|\,|V_{ij}^-(x)|\,dx<1.$$

If V_{ij}^- is not necessarily small we also obtain a thermodynamic stability bound $\inf\sigma(H)\geqslant -cN$, where $0<c<\infty$, is an N-independent constant.

KEY WORDS: N-particle Hamiltonian spectrum; quantum thermodynamic stability bound; N-particle Schrödinger operator spectrum.

Let us consider the spectrum of the N-particle Hamiltonian, with $\vec{x}_k\in R^d$,

$$H=\sum_{i=1}^{N}-\frac{1}{2m_i}\Delta_i+\sum_{1\leqslant i<j\leqslant N}V_{ij}(\vec{x}_i-\vec{x}_j)\equiv T+V$$

acting in $L^2(R^{dN})$. In particular, we are interested in lower bounds for the spectrum of H and conditions on the pair potentials V_{ij} which imply that H has no negative energy spectrum. Conditions on V_{ij} which imply self-adjointness and lower boundedness of H are well-known (see refs. 1 and 2). However, the form of the lower bound cannot be used to exclude negative

[1] Departamento de Física, ICEx, Universidade Federal de Minas Gerais, C.P. 702, cep 30123-970, Belo Horizonte, Minas Gerais, Brasil; e-mail: ocarroll@fisica.ufmg.br

energy spectrum. Another form of a lower bound has recently been given in ref. 3, namely, denoting $\sigma(A)$ for the spectrum of A,

$$\inf \sigma(H) \geqslant \sum_{i<j} \inf \sigma(h'_{ij})$$

where $h'_{ij} = \frac{-1}{(N-1)\, 2\mu_{ij}} \Delta^{\times}_{\vec{x}} + V_{ij}(\vec{x}^{\times})$, $\mu_{ij} = m_i m_j/(m_i + m_j)$, is a one-particle Hamiltonian acting in $L^2(R^d)$. For $d = 3$ it is known that if V^-_{ij}, the negative part of V_{ij}, satisfies

$$(N-1)(2\mu_{ij})\left(\frac{1}{4\pi}\right)\left[\int |V^-_{ij}(x)|\, |x-y|^{-2}\, |V^-_{ij}(y)|\, dx\, dy\right]^{\frac{1}{2}} < 1$$

then $\inf \sigma(h'_{ij}) \geqslant 0$. Thus $\inf \sigma(H) \geqslant 0$. This condition holds if each $V_{ij} \in L^{\frac{3}{2}}(R^3)$ and small which is an improvement over the result of Theorem X.111.27 of ref. 4 which requires $V_{ij} \in L^{\frac{3}{2}+\varepsilon} \cap L^{\frac{3}{2}-\varepsilon}$ for some $\varepsilon > 0$. The drawback of this bound is that the potentials are smaller as N increases.

Thus the following question arises: can any region of negative potential in the pair potential be permitted so that H has no negative energy spectrum for all N. We are unaware of any result of this nature. Another question concerning the negative part of the pair potential is how rough and singular it can be and still insure the thermodynamic stability bound (see refs. 5 and 6 for sufficient conditions). For low density systems in three dimensions a bound of the form $H > cN$, $c > 0$ has been obtained in ref. 7 and as the density goes to zero an exact lower bound is obtained. These results are obtained assuming that the pair potential is *positive*. It is conjectured that the same bound holds if the two-body scattering length is positive and there are no N-body bound states. Of course in treating neutral atoms or molecules as point particles there is always the van der Waals long range *negative* potential.

Let us now consider one-dimensional systems with hard core two-body potentials which are rough (but locally integrable). If the negative part falls off sufficiently rapidly at infinity in a integrable sense and if it is small (see the theorem below for the precise condition) we show that there is no negative energy spectrum for all N. Without the smallness condition a thermodynamic stability bound is also obtained. Our proof of these results is suprisingly simple. The analogous questions in two or three dimensions are important and open.

Before stating our result we make some comments on the intuition for forming or excluding bound states for large N. If the pair potential is an attractive square well a simple variational calculation shows that $\inf \sigma(H) < -cN^2$, $c > 0$, as each pair potential makes an order 1 contribution and the kinetic energy contributes order N. This can be avoided with a repulsive core. In the extreme case of an infinite hard core of radius R_0 and an attractive well of radius roughly $2R_0$ then the potential energy term should only make an order N contribution (2 nearest neighbors for dim. 1; 6 (12) nearest neighbors for dimension 2(3); 2d for a Z^d lattice Hamiltonian). For a bound state the particles are partially localized so the kinetic energy should be of order N. Thus for a sufficiently shallow well the energy is positive. For the one-dimensional case a region of positive potential is needed even for two particles as an arbitrarily small negative potential gives rise to a bound state.

For our one-dimensional result in the theorem below we impose an infinite hard core condition on the pair potentials. R^N is replaced by $R_c^N = \{x = (x_1, ..., x_N) \in R^N \mid |x_i - x_j| > a;\ a > 0, \text{ for all } i \neq j\}$ and Dirichlet conditions are taken on the boundary. We assume that each $V_{ij}(u) \in R$, $u \in R$, $|u| > a$, is even and $\int_a^\infty (u-a)\,|V_{ij}(u)|\,du < \infty$. Then H is defined as the self-adjoint operator associated with the form closure of the form sum on $C_0^\infty(R_c^N) \times C_0^\infty(R_c^N) \subset L^2(R_c^N) \times L^2(R_c^N)$.

To state our result, we introduce a potential $W_i^-(x)$ which is, roughly speaking, the most negative potential felt by particle i at x due to particles $1, 2, ..., i-1, i+1, ..., N$ at fixed positions. The rather complicated definition below becomes clear in the course of the proof of the theorem.

Let B_{li}, $l = 1, 2, ..., N-1$, $i = 1, 2, ..., N$, be the set of l element subsets of $(1, 2, ..., i-1, i+1, ..., N)$. Let π_l be a permutation of $(b_1, ..., b_l) \in B_{li}$. Further let $u^l \equiv (u_1, ..., u_l)$, u_k an integer, with $u_1 = 0$, $u_{s+1} + a < u_s$. We define a potential $W_i^-(x_i)$, $x_i \in (a, \infty)$, by

$$W_i^-(x_i) \equiv \inf_{l,\, u^l,\, B_{li},\, \pi_l} \sum_{m=1}^{l} V_{i\pi_e(b_m)}^-(x_i - u_m). \tag{1}$$

We have the

Theorem.

(a) If

$$c_i = 2m_i \int_a^\infty |u-a|\, |W_i^-(u)|\, du < 1 \tag{2}$$

for all i, then H has no negative energy spectrum for all N.

(b) If $c = \max c_i < \infty$ then we have the bound $\inf \sigma(H) \geqslant -c'N$ for some N-independent $c' < \infty$.

We remark that if $V_{ij}^-(x)$ has finite range then there are only a finite number of terms (independent of N) that contribute to the sum on the right side of $W_i^-(x)$ of (1). Also if the pair potential is bounded above by $-c(1+|x|)^{-\alpha}$, $c>0$, it is known that there are an infinite number of negative energy bound states for $\alpha>2$. The above integral in (2) is finite for $\alpha>3$ which is an indication of the influence of distant particles to enhance binding.

We prove the theorem for an εZ^N lattice approximation to H then the theorem follows by norm resolvent convergence (see refs. 8 and 9) of the lattice approximation to the continuum. In this way, we keep the proof elementary, avoiding direct integral decompositions and singular subsets of R^N.

We define the quadratic form

$$(f, H^\varepsilon f) = \sum_i \left(f, -\frac{\Delta_i^\varepsilon}{2m_i} f \right) + \sum_{\substack{1 \leqslant i < j \leqslant N \\ x}} \varepsilon f(x)\, V_{ij}^\varepsilon(x_i - x_j)\, f(x)$$

where the inner product $(\cdot,\cdot)$ is in $l_2(\varepsilon Z_c^N)$, $Z_c^N = \{x=(x_1, x_2,..., x_N) \in \varepsilon Z^N\ |x_i - x_j| > a,\ a \in \varepsilon Z$ for all $i \neq j\}$, $f \in l_2(\varepsilon Z_c^N)$ has finite support and $(f, -\Delta_i^\varepsilon f) = \sum_x \varepsilon^{-1} |f(..., x_i+\varepsilon,...) - f(..., x_i,...)|^2$ where the sum is over $x \in \varepsilon Z^N$. $V_{ij}^\varepsilon(u)$ is a smooth approximation which cuts off $|V_{ij}(u)|$ at ε^{-1}. From now on, for simplicity, we suppress ε from the notation. We also use the following facts. Let $A_1, A_2,...$ be self-adjoint;

(1) If $A = \sum_n A_n$ then $\inf \sigma(A) \geqslant \sum_n \inf \sigma(A_n)$

(2) If $A = \sum_n \oplus A_n$ then $\inf \sigma(A) = \inf_n (\inf \sigma(A_n))$.

We partition H as

$$H = \sum_i \left\{ \left[\frac{-1}{2m_i} \Delta_i + \frac{1}{2} \sum_{j \neq i} V_{ij}(x_i - x_j) \right] \equiv H_i \right\}.$$

Thus $\inf \sigma(H) \geqslant \sum_i \inf \sigma(H_i)$. But $H_i = \sum_r \oplus H_{ir}$, $r \equiv (r_1, r_2, ..., \hat{r}_i, ..., r_N)$, $|r_k - r_l| > a$, $k \neq l$, where $\hat{r}_i$ means omit r_i, and

$$H_{ir} = \frac{-1}{2m_i} \Delta_i + \frac{1}{2} \sum_{j \neq i} V_{ij}(x_i - r_j), \tag{3}$$

i.e., a one particle Hamiltonian for particle i moving in a potential with the jth particle fixed at r_j. We refer to r_j as the center of the potential. The set r, considered as a subset of Z, decomposes Z into disjoint internal intervals I_r. Furthermore, H_{ir} of (3) decomposes into a direct sum over these intervals, i.e., H_{ir} can be written

$$H_{ir} = \sum_{Ir} \oplus H_{il_r}$$

where H_{il_r} acts in $l_2(I_r)$. Thus $\inf \sigma(H_{ir}) = \inf_{Ir} \sigma(H_{il_r})$ and

$$\inf \sigma(H) \geqslant \sum_i \inf_{r, I_r} \sigma(H_{il_r}).$$

Thus the problem is reduced to obtaining a lower bound for the spectrum of H_{il_r}.

Consider the case $i = 1$ and $r_2 < r_3 < \cdots < r_N$. The other cases are treated similarly. For the interval (r_k, r_{k+1}), $2 \leqslant k \leqslant N-1$, the Hamiltonian under consideration is

$$H_{1k} = \frac{-\Delta_1}{2m_1} + \frac{1}{2} \sum_{j=2}^{N} V_{1j}(x_1 - r_j) \tag{4}$$

where $x_1 \in (r_k + a, r_{k+1} - a)$ and Δ_1 has Dirichlet boundary conditions (b.c.) at $r_k + a$ and $r_{k+1} - a$. We further partition the Hamiltonian of (4) writing

$$H_{1k} = \left[\frac{1}{2}\frac{-\Delta_1}{2m_1} + \frac{1}{2}\sum_{j \leqslant k} V_{1j}(x_1 - r_j)\right] + \left[\frac{1}{2}\frac{-\Delta_1}{2m_1} + \frac{1}{2}\sum_{j > k} V_{1j}(x_1 - r_j)\right] \equiv H_{k+} + H_{k-}.$$

H_{k+} (H_{k-}) takes into account the effect of the particles to the left (right) of particle one. We now obtain lower bounds for $\inf \sigma(H_{k\pm})$. We note that $\inf \sigma(H_{k+})$ is bounded below by $\inf \sigma(H'_{k+})$ where H'_{k+} is H_{k+} extended to the semi-infinite interval $(r_k + a, \infty)$ replacing the Dirichlet Laplacian with Dirichlet b.c. only at $r_k + a$ and replacing each V_{ij} with its negative part. Similarly $\inf \sigma(H_{k-})$ is bounded below by $\inf \sigma(H'_{k-})$ where H'_{k-} is H_{k-} extended to the semi-infinite interval $(-\infty, r_{k+1} - a)$.

The picture now emerges for obtaining a potential and Hamiltonian such that the inf of its spectrum is a lower bound for the spectrum of each component Hamiltonian of a partition. We see that each Hamiltonian of a partition is bounded below by a Hamiltonian with a Dirichlet Laplacian on a semi-infinite interval and a potential which is a sum of a subset of the pair potentials $\{V_{1j}: j > 1\}$ with the centers placed outside the semi-infinite interval. By translation invariance of the pair potentials we can take the semi-infinite interval to be (a, ∞) and the centers of the potentials to lie in $(\infty, 0]$ with one of the centers at zero. These same considerations apply for $i > 1$. Minimizing the potential over the number in a subset and locations of the centers of the pair potentials gives us the minimum potential

$W_i^-(x_i)$, $x_i \in (a, \infty)$, which is defined in (1) before the theorem. Thus we arrive at

$$\inf \sigma(H) \geqslant \sum_i 2 \inf \sigma\left(\frac{-\Delta_i^D}{4m_i} + \frac{1}{2} W_i^-\right) = \sum_i \inf \sigma\left(\frac{-\Delta_i^D}{2m_i} + W_i^-\right). \tag{5}$$

The operator on the righthand side of (5) is a discrete version of the zero angular momentum radial Schrödinger operator. Passing to the continuum there is no negative energy spectrum if

$$2m_i \int_a^\infty |u-a|\, |W_i^-(u)|\, du < 1$$

by Thm. XIII.9 of ref. 4. Similar considerations hold for the ε approximate by treating V_{ij}^- as a perturbation of $-\frac{1}{2m_i} \Delta_i^D$ in the resolvent equation and using the explicit form for the $(-\frac{1}{2m_i} \Delta_i^D - z)^{-1}$ for $z \notin [0, \infty)$.

We make these remarks more explicit. On the half-line $x \in [0, \infty]$, the resolvent of $-d^2/dx^2$ with Dirichlet boundary conditions at zero, is, for $z \notin [0, \infty)$, $x, y \geqslant 0$,

$$(H_D - z)^{-1}(x, y) = \frac{1}{2\sqrt{-z}} [e^{-\sqrt{-z}\,|x-y|} - e^{-\sqrt{-z}\,|x|} e^{-\sqrt{-z}\,|y|}].$$

The resolvent for $H = H_D \pm W$ exists for $z = -\kappa^2$ if the Hilbert–Schmidt norm of $W^{\frac{1}{2}}(H_D + \kappa^2)^{-1} W^{\frac{1}{2}}$, with W positive, is less than one as the Neumann series for

$$(H-z)^{-1} = (H_D - z)^{-\frac{1}{2}} [1 + (H_D - z)^{-\frac{1}{2}} W^{\frac{1}{2}} W^{\frac{1}{2}} (H_D - z)^{-\frac{1}{2}}]^{-1} (H_D - z)^{-\frac{1}{2}}$$

converges. Here we use $|A^+A| \leqslant |A^+A|_{H-S} = |AA^+|_{H-S}$ with $A = W^{\frac{1}{2}}(H_D - z)^{-\frac{1}{2}}$. We write $M_{\gtrless}(x, y) = \chi(x_{\gtrless}\, y)\, W^{\frac{1}{2}}(x)(H_D - z)^{-1}(x, y)\, W^{\frac{1}{2}}(y)$ and for $z = -\kappa^2$

$$\begin{aligned}
|M_>|_{H-S}^2 &= \frac{1}{\kappa^2} \int_0^\infty W(x)\, e^{-2\kappa x} \int_0^x \sinh^2 \kappa y W(y)\, dy\, dx \\
&\leqslant \int_0^\infty W(x)\, x e^{-2\kappa x} \frac{\sinh \kappa x}{\kappa x} \left[\int_0^x \frac{\sinh \kappa y}{\kappa y} W(y)\, y\, dy\right] dx \\
&\leqslant \left[\sup_{x > y \geqslant 0,\, \kappa > 0} \left(e^{-2\kappa x} \frac{\sinh \kappa x}{\kappa x} \frac{\sinh \kappa y}{\kappa y}\right)\right] \\
&\quad \times \int_0^\infty W(x)\, x \left[\int_0^x W(y)\, y\, dy\right] dx.
\end{aligned}$$

Since $\frac{\sinh u}{u} = \int_0^1 \cosh \alpha u \, d\alpha$ is monotone increasing and $\leqslant \cosh u$ the first factor in $[\cdot]$ is bounded by 1 and the iterated integral is $\frac{1}{2} (\int_0^\infty W(u) \, u \, du)^2$. The same bound holds for $M_<$ so that, for $\kappa > 0$,

$$|M|_{H-S} \leqslant \int_0^\infty W(u) \, u \, du$$

which leads to our smallness condition on the pair potential in part (a) of the theorem.

Furthermore by the Lebesgue dominated convergence theorem $|M|_{H-S} \xrightarrow{\kappa \to \infty} 0$ which proves our assertion for the thermodynamic stability bound of part (b) of the theorem. By strengthening the conditions on W we can obtain a more explicit lower bound for $\sigma(H)$.

In this way, we obtain the integral condition on the pair potentials of the theorem and the proof is complete.

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