

Absence of bound states implies non-negativity of the scattering length

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Abstract. We show that bosons interacting via pair potentials with negative scattering length form bound states for a suitable number of particles. In other words, the absence of many-particle bound states of any kind implies the non-negativity of the scattering length of the interaction potential.

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1. Introduction

While there is a huge literature on two-particle bound states in quantum mechanics, relatively little is known concerning bound states of more than two particles. Via the introduction of center-of-mass and relative coordinates, the former question reduces to a one-particle problem, i.e. the spectral analysis of an operator of the form $-\Delta + V(x)$, with Δ denoting the Laplacian and V a potential, i.e. a multiplication operator, which decays at infinity. Also for more than two particles the center-of-mass motion can be separated, but the resulting operator is more complicated, and the potential does not decay in certain directions.

In this article, we shall show that if the pair interaction potential has a negative scattering length, there always exist bound states for a suitable number of particles. At low density and low temperature such a system will thus not behave like an atomic gas, but will form molecules or even much larger bound clusters. We note that the atoms used in current experiments on Bose–Einstein condensation of ultra-cold dilute gases have scattering length of either sign; see, e.g., [3] and [2].

For $N \geq 2$, we consider the Hamiltonian

$$H_N = - \sum_{i=1}^N \Delta_i + \sum_{1 \leq i < j \leq N} v(x_i - x_j)$$

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on $L^2(\mathbb{R}^{3N})$, with Δ the usual Laplacian on \mathbb{R}^3 . We assume that $v \in L^1(\mathbb{R}^3)$ is real-valued and radial, and that $v_- \in L^{3/2}(\mathbb{R}^3)$, where v_- denotes the negative part of v , i.e. $v_-(x) = \max\{0, -v(x)\}$. Under these assumptions, the quadratic form defined by H_N is bounded from below, and hence H_N gives rise to a self-adjoint operator via the Friedrichs extension [11].

Let $E_N = \inf \text{spec } H_N$ denote the ground state energy of H_N , and let

$$\Sigma_N = \min_{1 \leq n \leq N-1} \{E_{N-n} + E_n\}$$

denote the lowest energy of two separate clusters of particles. Note that $E_N \leq \Sigma_N \leq E_{N-1}$. The HVZ Theorem [12] implies that if $E_N < \Sigma_N$, then the N -particle system has a bound state, i.e. the Hamiltonian H_N has, after removal of the center-of-mass motion, an eigenvalue at the bottom of its spectrum. We note that E_N is always attained in the sector of permutation-invariant functions [6], hence we are effectively dealing with bosons even though we defined H_N on the full space $L^2(\mathbb{R}^{3N})$ for simplicity.

The *scattering length* of the interaction potential v is defined as

$$a = \lim_{R \rightarrow \infty} a_R$$

where a_R is given by the variational principle ([8] and [7])

$$a_R = \frac{1}{8\pi} \inf \left\{ \int_{|x| \leq R} (2|\nabla f(x)|^2 + v(x)|f(x)|^2) dx : f(x) = 1 \text{ for } |x| = R \right\}. \tag{1}$$

The infimum is over all H^1 -functions on the ball $\{|x| \leq R\}$ satisfying the boundary condition $f(x) = 1$ on the boundary of the ball. Under the assumption that $H_2 \geq 0$, i.e. the absence of two-particle bound states, the existence of a minimizer for (1) was shown in [8], Appendix A. Note that since $a_{R_1} \leq a_{R_2} + (8\pi)^{-1} \int_{R_1 \leq |x| \leq R_2} v(x) dx$ for $R_2 > R_1$, the limit $\lim_{R \rightarrow \infty} a_R$ always exists for $v \in L^1(\mathbb{R}^3)$, but it could equal $-\infty$. It is easy to see that finiteness of a implies that $H_2 \geq 0$, i.e.

$$a > -\infty \implies H_2 \geq 0. \tag{2}$$

Eq. (1) is the correct definition of the scattering length only in the absence of two-particle bound states. The scattering length can be defined by other means (via the solution to the zero-energy scattering equation) even in the presence of two-particle bound states (see, e.g., [5]), but it is not given by the above variational principle in this case. Since our main concern here is the case of $H_2 \geq 0$, we find it convenient to work with the definition (1), however.

Our main result is the following.

Theorem 1. *If $H_N \geq 0$ for all $N \geq 2$, then $a \geq 0$.*

As discussed above, finiteness of a implies that $E_2 = 0$. If $a < 0$, Theorem 1 implies the existence of an $N \geq 3$ with $\Sigma_N = 0$ but $E_N < 0$. In other words, negativity of the scattering length of v implies the existence of bound states of some kind. We note that the converse of Theorem 1 does not hold. There exist interaction potentials v with positive scattering length such that $H_2 \geq 0$ but H_3 has negative spectrum, i.e. with three-particle bound states but no two-particle bound states [1].

For large, negative a , the existence of three-particle bound states is well known; see [4], [14], [9], [13], and [10]. Our Theorem 1 implies that a does not actually have to be large for bound states to exist. As long as it is negative, bound states exist, but they might require more than three particles.

We note that if $\int_{\mathbb{R}^3} v(x)dx < 0$, then $a < 0$. In this case, it is not difficult to see that there exist bound states for an infinite sequence of particle numbers. This follows from the fact that $E_N \sim -\text{const } N^2$ for large N , while obviously $E_N \sim \text{const } N$ if bound states exist only for finitely many particle numbers. It remains an open problem to decide whether bound states exist for an infinite sequence of particle numbers for all interaction potentials with $a < 0$.

Theorem 1 can be extended to dimensions larger than three. It does not extend to one and two dimensions, however. The corresponding expression (1) in one or two dimensions is always positive in the absence of two-particle bound states; see [8] and [7]. Another important difference concerns the fact that arbitrarily shallow negative potentials lead to the existence of two-particle bound states in one and two dimensions, which is not the case in three and more dimensions.

2. Proof of Theorem 1

We shall assume that $a < 0$, and show that for large enough N we can find a $\Psi \in L^2(\mathbb{R}^{3N})$ with $\langle \Psi | H_N \Psi \rangle < 0$. Since $a < 0$ and $v \in L^1(\mathbb{R}^3)$, we can find an $R > 0$ such that $a_R + (8\pi)^{-1} \int_{|x|>R} v(x)dx < 0$. As a consequence, there exists a non-negative function $\varphi : \mathbb{R}_+ \rightarrow \mathbb{R}_+$ with $\varphi(t) = 1$ for $t \geq R$ such that

$$b = \int_{\mathbb{R}^3} (2\varphi'(|x|)^2 + v(x)\varphi(|x|)^2)dx < 0. \tag{3}$$

For instance, one can choose φ to be the minimizer of (1) for $|x| \leq R$. By an approximation argument, we can assume φ to be bounded without loss of generality. That is, for some $c \geq 0$, we have

$$\varphi(t)^2 \leq 1 + c \theta(R - t)$$

for all $t \geq 0$, with θ denoting the Heaviside step function

$$\theta(t) = \begin{cases} 1 & \text{for } t \geq 0, \\ 0 & \text{for } t < 0. \end{cases}$$

For $g \in C_0^\infty(\mathbb{R}^3)$ real-valued and with $\int_{\mathbb{R}^3} g(x)^2 dx = 1$, we shall consider the function

$$\Psi(x_1, \dots, x_N) = \varphi(t) \prod_{k=1}^N g(x_k),$$

where

$$t = t(x_1, \dots, x_N) = \min_{1 \leq i < j \leq N} |x_i - x_j|.$$

Note that t is Lipschitz continuous and differentiable almost everywhere. A simple calculation yields

$$\sum_{k=1}^N |\nabla_k \varphi(t)|^2 = 2\varphi'(t)^2.$$

An integration by parts shows that

$$\begin{aligned} & \sum_{k=1}^N \int_{\mathbb{R}^{3N}} |\nabla_k \Psi|^2 dx_1 \cdots dx_N \\ &= 2 \int_{\mathbb{R}^{3N}} \varphi'(t)^2 \prod_{j=1}^N g(x_j)^2 dx_j - N \int_{\mathbb{R}^{3N}} g(x_1) \Delta g(x_1) \varphi(t)^2 dx_1 \prod_{j=2}^N g(x_j)^2 dx_j. \end{aligned} \tag{4}$$

Here we have also used the permutation-symmetry of Ψ in the last term, in order to replace the sum over k by just one summand, multiplied by N . We can bound

$$\varphi'(t)^2 \leq \sum_{i < j} \varphi'(|x_i - x_j|)^2$$

and hence the first term on the right side of (4) is bounded above by

$$N(N - 1) \int_{\mathbb{R}^6} g(x)^2 \varphi'(|x - y|)^2 g(y)^2 dx dy.$$

To bound the second term, we simply use $\varphi(t)^2 \leq 1 + c$. We shall also drop the positive part of $g(x) \Delta g(x)$, and arrive at the upper bound

$$\begin{aligned} & \sum_{k=1}^N \int_{\mathbb{R}^{3N}} |\nabla_k \Psi|^2 dx_1 \cdots dx_N \\ & \leq N(N - 1) \int_{\mathbb{R}^6} g(x)^2 \varphi'(|x - y|)^2 g(y)^2 dx dy + (1 + c)N \|[g \Delta g]_-\|_1, \end{aligned} \tag{5}$$

where $[s]_- = \max\{0, -s\}$ denotes the negative part.

Next we shall investigate the expectation value of the interaction potential. Because of the permutation-symmetry of Ψ , it suffices to consider $\langle \Psi | v(x_1 - x_2) \Psi \rangle$, multiplied by $N(N - 1)/2$, the number of pairs of particles. To bound this term, we shall use the fact that

$$\begin{aligned}
 & |\varphi(t)^2 - \varphi(|x_1 - x_2|)^2| \\
 & \leq (1 + c) \left(\sum_{j=3}^N \theta(R - |x_1 - x_j|) + \sum_{k=2}^N \sum_{j=k+1}^N \theta(R - |x_k - x_j|) \right). \tag{6}
 \end{aligned}$$

To see the validity of this bound, note that the left side is at most $1 + c$. The right side is at least $1 + c$, unless all the pairs (x_k, x_j) with $\{k, j\} \neq \{1, 2\}$ are separated a distance larger than R , in which case it equals zero. Also the left side is then zero, however; either $|x_1 - x_2| \geq R$, in which case it is zero since also $t \geq R$ and $\varphi(s) = 1$ for $s \geq R$, or $|x_1 - x_2| < R$, in which case $t = |x_1 - x_2|$. In any case, (6) holds.

Using (6), we have

$$\begin{aligned}
 & \langle \Psi | v(x_1 - x_2) \Psi \rangle \\
 & \leq \int_{\mathbb{R}^6} g(x)^2 v(x - y) \varphi(|x - y|)^2 g(y)^2 dx dy \\
 & \quad + (1 + c) \frac{(N - 2)(N - 3)}{2} \left(\int_{\mathbb{R}^6} g(x)^2 |v(x - y)| g(y)^2 dx dy \right) \\
 & \quad \quad \quad \times \left(\int_{\mathbb{R}^6} g(x)^2 \theta(R - |x - y|) g(y)^2 dx dy \right) \\
 & \quad + 2(1 + c)(N - 2) \int_{\mathbb{R}^9} g(x)^2 |v(x - y)| g(y)^2 \theta(R - |y - z|) g(z)^2 dx dy dz. \tag{7}
 \end{aligned}$$

The terms on the second line on the right side can be bounded with the aid of a Schwarz inequality as

$$\int_{\mathbb{R}^6} g(x)^2 |v(x - y)| g(y)^2 dx dy \leq \|v\|_1 \|g\|_4^4$$

and

$$\int_{\mathbb{R}^6} g(x)^2 \theta(R - |x - y|) g(y)^2 dx dy \leq \frac{4\pi}{3} R^3 \|g\|_4^4.$$

Similarly, we can bound the integral in the last line of (7) as

$$\int_{\mathbb{R}^9} g(x)^2 |v(x - y)| g(y)^2 \theta(R - |y - z|) g(z)^2 dx dy dz \leq \frac{4\pi}{3} R^3 \|v\|_1 \|g\|_\infty^2 \|g\|_4^4.$$

As a result, we have thus shown that

$$\begin{aligned} & \langle \Psi | v(x_1 - x_2) \Psi \rangle \\ & \leq \int_{\mathbb{R}^6} g(x)^2 v(x-y) \varphi(|x-y|)^2 g(y)^2 dx dy \\ & \quad + (1+c) \frac{2\pi}{3} (N-2) R^3 \|v\|_1 ((N-3) \|g\|_4^8 + 4 \|g\|_\infty^2 \|g\|_4^4). \end{aligned} \quad (8)$$

By combining the bounds (5) and (8), we obtain

$$\begin{aligned} & \langle \Psi | H_N \Psi \rangle \\ & \leq \frac{N(N-1)}{2} \int_{\mathbb{R}^6} g(x)^2 h(x-y) g(y)^2 dx dy \\ & \quad + (1+c) N \left(\| [g\Delta g]_- \|_1 + \frac{\pi}{3} N^2 R^3 \|v\|_1 \|g\|_4^4 (N \|g\|_4^4 + 4 \|g\|_\infty^2) \right) \end{aligned}$$

where h denotes the function

$$h(x) = 2\varphi'(|x|)^2 + v(x)\varphi(|x|)^2.$$

Note that $\int_{\mathbb{R}^3} h(x) dx = b < 0$ by (3).

Let $g_0 \in C_0^\infty(\mathbb{R}^3)$ be real-valued and L^2 -normalized. For $L > 0$, we shall choose

$$g(x) = L^{-3/2} g_0(x/L).$$

Then g is also L^2 -normalized, and satisfies

$$\|g\|_4 = L^{-3/4} \|g_0\|_4, \quad \|g\|_\infty = L^{-3/2} \|g_0\|_\infty, \quad \| [g\Delta g]_- \|_1 = L^{-2} \| [g_0\Delta g_0]_- \|_1.$$

Denoting the various constants collectively by C , we thus have

$$\begin{aligned} & \langle \Psi | H_N \Psi \rangle \\ & \leq \frac{N(N-1)}{2} \int_{\mathbb{R}^6} g(x)^2 h(x-y) g(y)^2 dx dy + C \frac{N}{L^2} \left(1 + \|v\|_1 \frac{N^3 R^3}{L^4} \right). \end{aligned} \quad (9)$$

The first term on the right side equals

$$\frac{N(N-1)}{2L^6} \int_{\mathbb{R}^6} g_0(x/L)^2 h(x-y) g_0(y/L)^2 dx dy.$$

Since h is an L^1 -function, we can use dominated convergence in Fourier space to

conclude that

$$\begin{aligned} & \lim_{L \rightarrow \infty} L^{-3} \int_{\mathbb{R}^6} g_0(x/L)^2 h(x-y) g_0(y/L)^2 dx dy \\ &= \int_{\mathbb{R}^3} h(x) dx \|g_0\|_4^4 \\ &= b \|g_0\|_4^4 < 0. \end{aligned}$$

For all L large enough, we can thus bound

$$\frac{N(N-1)}{2L^6} \int_{\mathbb{R}^6} g_0(x/L)^2 h(x-y) g_0(y/L)^2 dx dy \leq \frac{b}{4} \frac{N(N-1)}{L^3} \|g_0\|_4^4$$

(where the 4 in the denominator could be replaced by any number larger than 2). If we choose $L \ll N \ll L^{3/2}$, the last term in (9) is much smaller than N^2/L^3 for large L . For this choice of N , we thus have $\langle \Psi | H_N \Psi \rangle < 0$ for large enough L . This concludes the proof.

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