UWThPh-1997-23
September 1, 1997

Existence of many-particle bound states in spite of a pair-interaction with positive scattering length

Bernhard Baumgartner
Institut für Theoretische Physik
Universität Wien
Boltzmanngasse 5, A-1090 Wien

Abstract

Examples of bound states are presented, for a system of three identical particles as well as for a system of particles on a lattice. The particles may be bosons as well as fermions. The interaction between them is given by a pair-potential, which does not allow two-particle bound states, has positive scattering length and is not too different from realistic interatomic potentials.

1 Introduction

Experiments which have produced Bose-Einstein-condensates of several different elements did spark a renewed interest in the theory of Bose-Einstein-condensation (C.N. Yang 1997, K. Huang 1996, K. Burnett 1996 and references therein). A great part of theoretical work relies on the formula

$$E/N = 2\pi(\hbar^2/m)\rho a + O(\sqrt{\rho a^3}) \tag{1}$$

for the ground-state energy of a non-relativistic Bose gas with low density ρ, where the particles interact pairwise by a potential with scattering length a. The arguments for its validity (Lieb 1965, Lieb 1963 and references therein) rest on the *assumption*, that there exists *no many-body bound state.*

A related, less discussed problem would be to find a formula for the ground state energy of a non-relativistic low density Fermi gas with pair interactions. Again it seems reasonable, that the $\rho^{5/3}$-formula for non-interacting Fermions has to be enlarged by adding low-order terms, *provided* that *no many body bound state* exists; that $E > 0$.

Concerning Bosons, a necessary condition for the positivity of the ground state energy is the non-existence of two-particle bound states, and the positivity of the scattering length a of the pair-potential v, which, throughout this work, is assumed to be a function of the particle-distance only. The message of this paper is the demonstration that this condition is *not sufficient*, neither for Bosons nor for Fermions. We present bound states for systems of three particles and for a system of particles on a lattice. The family of pair-potentials which are used are not too different from realistic interatomic potentials: They are thermodynamically stable, they have a repulsive core and an attractive well. Such examples have as far as I know never been presented before.

2 Setup: The interaction potential and statistics

The interaction potential v is a function of the interparticle distance r only. The calculations are done with $\hbar^2/m = 1$. But in the reduced two-particle system a reduced mass equal to $m/2$ has to be used and the scattering length is to be calculated by solving

$$\varphi''(r) = v(r)\varphi(r) \tag{2}$$

with

$$\varphi(0) = 0.$$

Non-existence of a two-particle bound state is equivalent to $\varphi(r)$ not changing sign. The scattering length a is

$$a := \lim_{r\to\infty}(r - \varphi/\varphi'). \tag{3}$$

Using parameters $c > 0$, $d \geq 1$ we define the potential $v(r)$ to be zero for $r > c + d$, and otherwise

$$\begin{aligned} v(r) &:= (r-c)^2 - 1 + \mu\delta(c+d-r), \\ \mu &= d + \frac{1}{c+d}. \end{aligned} \tag{4}$$

Absence of bound states and positivity of the scattering length are seen by comparison of φ with $f(r) = e^{-(r-c)^2/2}$. The Gaussian f is also a solution of (2) for $0 < r < c+d$. The Wronskian $w = \varphi' f - \varphi f'$ is constant in this interval and φ does not change sign (Sturm's oscillation theorem). The Wronskian w is strictly positive, if φ is chosen as positive. Approaching $c+d$ from the lower side one finds

$$\frac{\varphi'(c+d-0)}{\varphi(c+d)} = \frac{w}{\varphi f} + \frac{f'(c+d)}{f(c+d)} > \frac{f'(c+d)}{f(c+d)} = -d.$$

The δ-function part of the barrier makes

$$\frac{\varphi'(c+d+0)}{\varphi(c+d)} = \frac{\varphi'(c+d-0)}{\varphi(c+d)} + \mu > \frac{1}{c+d}. \tag{5}$$

Outside the barrier $\varphi(r)$ is linear, so (5) implies that it does not change sign and that a is strictly positive.

Thermodynamic stability does obviously hold only if c is not too small. We prove it for $c \geq 5$ by bounding v from below by a positive definite function. First, for any c, d under consideration,

$$v(r) \geq u_c(r) := [(r-c)^2 - 1]\theta(c+1-r),$$

bounding v from below by removing all of the barrier. For $c = 5$ it is easy to check numerically that

$$u_5(r) > g(r) := 20\, e^{-0.8\times r} - 4\, e^{-0.2\times r}.$$

This function is positive definite. Its Fourier transform as a function of $\vec{x}$ in $\mathbf{R}^3$, with $r = |\vec{x}|$, is a positive function of $\vec{k}$ with $|\vec{k}| = k$:

$$\tilde{g}(k) = \frac{2\sqrt{2/\pi}}{(0.8^2+k^2)^2(0.2^2+k^2)^2}[0.128 + 15.2k^2] > 0.$$

For $c > 5$ we make a comparison by scaling:

$$u_c(r) \geq (c/5)^2 u_5(5r/c).$$

So each $v(r)$ with $c \geq 5$ is a sum of a positive definite and a positive function, which implies thermodynamic stability (Ginibre 1968).

Concerning the statistics it will not be necessary to take special care of the Bosons. The true ground state wave function for distinguishable but equal particles is automatically symmetric under exchange. So any proof for the existence of a bound state of distinguishable particles is also a proof valid for Bosons.

The Fermions on the lattice will be satisfied with a product of one-particle wave functions which do not overlap. Such a product can be antisymmetrized without any change in energy. For three Fermions the antisymmetry is achieved by choosing the right angular momenta.

3 Existence of a three-particle bound state

The Hamiltonian

$$-\frac{1}{2}\sum_{i=1}^{3}\Delta_{x_i}+\sum_{i<j}v(|\vec{x}_i-\vec{x}_j|) \tag{6}$$

acts on $\mathcal{L}^2(\mathbf{R}^9)$.

The free movement of the center of mass with the coordinates $\vec{x}_{CM}=(\vec{x}_1+\vec{x}_2+\vec{x}_3)/3$ can be separated off. Since the transformation in $\mathbf{R}^9$ to the system of coordinates

$$\sqrt{3}\,\vec{x}_{CM}$$

$$\begin{aligned}\vec{y}_1 &= \frac{1}{\sqrt{6}}(2\vec{x}_1-\vec{x}_2-\vec{x}_3) \\ \vec{y}_2 &= \frac{1}{\sqrt{2}}(\vec{x}_2-\vec{x}_3)\end{aligned} \tag{7}$$

is orthogonal, the kinetic energy of inner rotations and oscillations is represented by

$$-\frac{1}{2}\Delta_{y_1}-\frac{1}{2}\Delta_{y_2}. \tag{8}$$

The interaction energy depends only on the $r_i=|\vec{y}_i|$ and the angle $\vartheta\in[0,\pi]$ defined by

$$\vec{y}_1\cdot\vec{y}_2=r_1r_2\cos\vartheta, \tag{9}$$

since

$$\begin{aligned}|\vec{x}_1-\vec{x}_{2(3)}| &= (3r_1^2/2+r_2^2/2-(+)\sqrt{3}\,r_1r_2\cos\vartheta)^{1/2} \\ |\vec{x}_2-\vec{x}_3| &= \sqrt{2}\,r_2.\end{aligned} \tag{10}$$

For r_1, r_2, ϑ fixed there remain the inner rotations, which may be expressed using three Euler angles.

The mathematical situation is thus analogous to the one in the treatment of the Helium atom by (Hylleraas 1928) and (Breit 1930). Restriction to s-waves of the rotation gives as the operator for the kinetic energy of oscillations:

$$-\frac{1}{2}\left[\frac{1}{r_1^2}\frac{\partial}{\partial r_1}r_1^2\frac{\partial}{\partial r_1}+\frac{1}{r_2^2}\frac{\partial}{\partial r_2}r_2^2\frac{\partial}{\partial r_2}+\left(\frac{1}{r_1^2}+\frac{1}{r_2^2}\right)\frac{1}{\sin\vartheta}\frac{\partial}{\partial\vartheta}\sin\vartheta\frac{\partial}{\partial\vartheta}\right] \tag{11}$$

acting on the Hilbert space

$$\mathcal{L}^2(\mathbf{R}_+\times\mathbf{R}_+\times[0,\pi], r_1^2r_2^2\sin\vartheta dr_1dr_2d\vartheta).$$

With a unitary transformation to the $\mathcal{L}^2$ on the same set, but with Lebesgue-measure, multiplying the wave functions by $r_1r_2\sqrt{\sin\vartheta}$, the kinetic energy operator becomes

$$-\frac{1}{2}\left[\frac{\partial^2}{\partial r_1^2}+\frac{\partial^2}{\partial r_2^2}+\left(\frac{1}{r_1^2}+\frac{1}{r_2^2}\right)\left(\frac{\partial^2}{\partial\vartheta^2}+\frac{1}{4}\left(1+\frac{1}{\sin^2\vartheta}\right)\right)\right]. \tag{12}$$

We dont have to take care of the boundary conditions, since we will finally apply this operator to functions with compact support in the interior only.

The s-waves of Euler angles are not allowed for Fermions. They require higher angular momentum introducing a centrifugal force. More details of the necessary modifications for their treatment follow at the end of this section.

We restrict our attention to "small" oscillations near the minimum of the potential, assuming the parameters c and d to be large. The final change of coordinates is therefore

$$\begin{aligned} u &:= \frac{1}{\sqrt{2}}\,(r_1 + r_2) - c \\ v &:= \frac{1}{\sqrt{2}}\,(r_1 - r_2) \\ w &:= \frac{1}{2}\,c\left(\vartheta - \frac{\pi}{2}\right). \end{aligned} \tag{13}$$

These coordinates are chosen according to symmetries: u is the coordinate for a "breathing mode", where ϑ and $r_1/r_2 = 1$ remain fixed. Because of the symmetry under particle exchange, the other oscillations should be degenerate, with equal frequencies.

Expanding the potential in powers of u, v and $\vartheta - \pi/2$ about its minimum at $r_1 = r_2 = c/\sqrt{2}$, $\vartheta = \pi/2$ gives an expansion in powers of $1/c$. This expansion of the interaction energies involves

$$\begin{aligned} (|\vec{x}_1 - \vec{x}_{2(3)}| - c)^2 &= \left(u + \frac{v}{2} - (+)\,\frac{\sqrt{3}}{2} w\right)^2 + O\left(\frac{1}{c}\right) \\ (|\vec{x}_2 - \vec{x}_3| - c)^2 &= (u - v)^2. \end{aligned} \tag{14}$$

Summing up gives the potential energy

$$V = -3 + 3u^2 + \frac{3}{2}\,v^2 + \frac{3}{2}\,w^2 + O\left(\frac{1}{c}\right). \tag{15}$$

The operator for the kinetic energy is now

$$-\frac{1}{2}\Delta_{u,v,w} + \frac{1}{2}\left[1 - \frac{c^2}{4}\left(\frac{1}{r_1^2} + \frac{1}{r_2^2}\right)\right]\frac{\partial^2}{\partial w^2} - \frac{1}{8}\left(1 + \frac{1}{\sin^2\vartheta}\right)\left(\frac{1}{r_1^2} + \frac{1}{r_2^2}\right), \tag{16}$$

$$\Delta_{u,v,w} := \frac{\partial^2}{\partial u^2} + \frac{\partial^2}{\partial v^2} + \frac{\partial^2}{\partial w^2}.$$

The harmonic-oscillator Hamiltonian made from the leading terms,

$$-\frac{1}{2}\,\Delta_{u,v,w} + 3u^2 + \frac{3}{2}v^2 + \frac{3}{2}w^2 - 3 \tag{17}$$

has the negative ground state energy

$$\frac{1}{2}\,\sqrt{6} + \sqrt{3} - 3 = -0.043... \tag{18}$$

It remains to discuss the corrections from the anharmonic terms in (15) and (16), and also from the restriction to a compact support. All these corrections can be bounded and the bounds can be controlled in the limit of large c, since they fall off at least as $1/c$, as is shown in the appendix. Hence it is proven, that there exists a bound state, a molecule of three Bosonic atoms arranged in an equilateral triangle.

When treating the model with Fermions, we introduce the antisymmetrizing factor

$$\frac{(\vec{y}_1 \times \vec{y}_2) \cdot \vec{a}}{|\vec{y}_1 \times \vec{y}_2|}$$

where $\vec{a}$ is a constant vector. This is a function of the Euler angles, determining the rotational state of the molecule. It is completely antisymmetric under particle exchange. Its contribution to the kinetic energy gives the angular momentum barrier

$$\left(\frac{1}{r_1^2} + \frac{1}{r_2^2}\right) \frac{1}{\sin^2 \vartheta},$$

which has to be added to the Hamiltonian of the oscillations, in formulas (11), (12) and (16).

The trial wave functions for oscillations have to be completely symmetric under particle exchange. We may use the same functions as in the case of the Bosons. Once their support is sufficiently restricted, the symmetrization has no effect on kinetic or potential energy.

And the contribution from the angular momentum is of the order of $1/c^2$.

4 A manybody bound state in the form of a lattice

The setup is the same as above, only at the end some variations on defining the interaction potential will be discussed. The number of particles is very large or infinity. We will calculate the energy of one particle in the interior. As the state of the many particle system we choose a product of independent one-particle states. Each one-particle state is defined by the Gaussian wave function

$$\psi(\vec{x}) = (\lambda/\pi)^{3/4}\, e^{-\lambda\, \vec{x}^2/2} \tag{19}$$

translated to be centered at a lattice point of a fcc or hcp lattice (close packing with 12 nearest neighbours). The distance of neighbours is chosen as c, the parameter which defines the distance of two particles at the minimum of interaction potential. (This choice is not optimal in minimizing the energy, but it simplifies the calculations.)

The kinetic energy per particle is

$$E_{\text{kin}} = 3\lambda/4. \tag{20}$$

The potential energy of a pair of particles, belonging to a pair of lattice points in the distance $b = |\vec{b}|$, is

$$\begin{aligned} E_{\text{pair},b} &= \iint v(|\vec{z}-\vec{y}|)\psi^2(\vec{z})\psi^2(\vec{y}-\vec{b})d^3z d^3y = \\ &= \int v(|\vec{x}|)\left(\int \psi^2(\vec{x}+\vec{y})\psi^2(\vec{y}-\vec{b})d^3y\right) d^3x. \end{aligned} \tag{21}$$

Straightforward this can be reduced to

$$E_{\text{pair},b} = \left(\frac{\lambda}{2\pi}\right)^{1/2} \frac{1}{b}\int_0^\infty v(r)\left[e^{-\lambda(r-b)^2/2} - e^{-\lambda(r+b)^2/2}\right] r dr. \tag{22}$$

In order to get a low energy, we have to place the cut-off distance $c+d$ of the interaction potential between the distances to nearest and next nearest neighbours. For example at half way:

$$d = \frac{\sqrt{2}-1}{2}\, c.$$

Then the contributions of the next nearest and all the other far away located particles to the energy are small, according to the fall-off of the Gaussians. The nearest neighbours are located at distance $b = c$, where the bottom of $v(r)$ lies. The harmonic part of $v(r)$ near its bottom gives thus the main contribution to the integral (22). The negative Gaussian and the boundaries to the harmonic part at $r = 0$ and $r = c + d$ have little influence, again according to the fall-off of the Gaussians. The approximate main contribution to the potential energy per particle, half of the pair interactions with 12 nearest neighbours, can thus be calculated analytically as

$$6\left(\frac{\lambda}{2\pi}\right)^{1/2} \frac{1}{c}\int_{-\infty}^{+\infty} [(r-c)^2 - 1] e^{-\lambda(r-c)^2/2} r dr = 6\left(\frac{1}{\lambda} - 1\right). \tag{23}$$

The energy per particle, the sum of (20) and (23)

$$\frac{3\lambda}{4} + \frac{6}{\lambda} - 6 \tag{24}$$

is minimized with $\lambda = 2\sqrt{2}$:

$$E = 3\sqrt{2} - 6 \approx -1.757. \tag{25}$$

This model can also be used for Fermions: One may proceed by restricting the one-particle wave functions to a compact support, so that they do not overlap. This procedure will decrease the potential energy and increase the kinetic energy. The correction is always to be measured by the fall-off of the Gaussian. (See the Appendix.) Antisymmetrization has then no effect on the energy.

5 Discussion

Having established the existence of many body bound states we would like to identify the reason why the "repulsive effect" of the positive scattering length breaks down: It is essentially the dominance of many-particle-correlations, when they cannot be decomposed into pair-correlations. For three particles this correlation has to be fine tuned, determining the wave functions of relative motion, and it leads to weak binding. For many particles much cruder correlations, determining only the relative mean positions, give stronger binding. (One may then consider pair potentials which are more realistic, with reduced repulsive barrier outside the attractive well.)

Dropping the requirement for thermodynamic stability, there are much simpler arguments against the sufficiency of the positive scattering length as a condition for the absence of bound states: Consider a pair potential which is negative for small r in a neighbourhood of the origin ($v(r) = (r^2 - 3)\theta(d - r) + d\delta(r - d)$ for example). Then, N particles in a cluster with such a small diameter will have a negative potential energy, proportional to N^2. But kinetic energies need not increase faster than N in the case of Bosons, $N^{5/3}$ in the case of Fermions. (Considering Bosons, already three of them can have a bound state with the given example potential.)

In a low-density gas the occurrence of special structures has low probability, so one might philosophize, that a gaseous state without bounds persists some time as a metastable state. Such considerations have already been stated in connection with the existence of a Bose-condensed gas in spite of a negative scattering length (R.J. Dodd 1996, B.D. Esry 1996).

Appendix: Bounds to the effects of localization of the wave functions and of anharmonic terms

We use a continuous cut-off approximation to the ground state wave function $\varphi(x)$ of a harmonic oscillator (1-dimensional, centered at $x = 0$):

$$\psi(x) = \gamma \left(\frac{\omega^2}{\pi}\right)^{1/4} \left[e^{-x^2\omega^2/2} - e^{-\ell^2\omega^2/2}\right] \theta(\ell - |x|).$$

The normalization factor γ is greater than 1. It can be bounded by

$$\gamma < \left(1 - \frac{2}{\sqrt{\pi}\,\omega\ell}\, e^{-\ell^2\omega^2} - 4e^{-\ell^2\omega^2/2}\right)^{-1/2}.$$

(Derived by finding lower bounds to the integrals which determine $\|\psi\|$.)

The expectation value of any increasing positive $V(|x|)$ (the interaction with a partner at the right distance) gets smaller by this cut-off. The line of reasoning is:

$\gamma > 1 \Rightarrow \psi'(x) < \varphi'(x)$ for $x \in (0,\ell) \Rightarrow \psi - \varphi$ is decreasing on $(0,\ell) \Rightarrow \psi^2 - \varphi^2$ is decreasing $\Rightarrow$ (by Chebyshev's inequality)

$$\int_0^\infty V(x)\psi^2(x)dx = \int_0^\ell V\psi^2 < \int_0^\ell V\varphi^2 < \int_0^\infty V\varphi^2.$$

The kinetic energy increases in the procedure of cutting-off. This increase is bounded:

$$\int_{-\infty}^{+\infty} |\psi'(x)|^2 dx = \gamma^2 \int_{-\ell}^{+\ell} |\varphi'|^2 < \gamma^2 \int_{-\infty}^{+\infty} |\varphi'|^2.$$

For the three particle model, $\ell < c/2$ will guarantee that ψ is in the Hilbert space. Also $\ell < d/2$ is useful, in order not to involve the δ-barrier as contributing to the energy. (Otherwise, the fall-off of the Gaussian would make good bounds to these contributions.) Finally, ℓ/c shall be small.

The trial function $\psi_1(u)\psi_2(v)\psi_3(w)$ (with the appropriate ω_i) is used to estimate the ground state energy of the Hamiltonian (16) + (15). For the harmonic-oscillator part we get (18) plus the changes discussed above. In the anharmonic part,

$$f(r_1,r_2)\frac{\partial^2}{\partial w^2} + g(r_1,r_2,\vartheta) + V_{\mathrm{anh}}(u,v,w),$$

g is of no concern for Bosons, since it is negative, see (16). For Fermions it is positive (the angular momentum barrier), of the order of $1/c^2$. The anharmonic part of the potential can be studied by expanding the interactions as Taylor series in u, v, w, see (14). That the corrections to the harmonic quadratic terms are of the order $1/c$ can be understood as a geometric effect.

The operator $f\dfrac{\partial^2}{\partial w^2}$ contributes the kinetic energy of $\psi_3(w)$, multiplied by the expectation of $f = \dfrac{c^2}{4}\left(\dfrac{1}{r_1^2} + \dfrac{1}{r_2^2}\right) - 1$. On the support of $\psi_1\psi_2$ this function is bounded by $\dfrac{\ell}{c} + \dfrac{2\ell^2}{(c-2\ell)^2}$.

References

G. Breit 1930: Phys. Rev. **35**, 569–78

K. Burnett, M. Edwards and C.W. Clark (Editors) 1996: Special Issue: Bose Einstein Condensation. J. Res. Natl. Inst. Stand. Technol. **101** (4)

R.J. Dodd et al. 1996: Phys. Rev. **A54**, 661–4

B.D. Esry et al. 1996: J. Phys. **B29**, L51-7

J. Ginibre 1968: Commun. Math. Phys. **8**, 26–51

K. Huang and P. Tommasini 1996: J. Res. Natl. Inst. Stand. Technol. **101**, 435–42

E.A. Hylleraas 1928: Z. Phys. **48**, 469–94

E.H. Lieb 1963: Phys. Rev. **130**, 2518–28

E.H. Lieb 1965: The Bose Fluid. In: W.E. Brittin (Ed.): Lectures in Theoretical Physics VII C, The University of Coloredo Press, Boulder

C.N. Yang 1997: Int. J. Mod. Phys. **B11**, 683–4