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"Optimal" Bounds on the Ground-State Energy of N-Body Systems of Bosons and Fermions Interacting by Attractive Forces

André Martin[1]

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We present inequalities on the ground state energy of N-body systems which reduce, for bosons and fermions, to the exact solution in the limit where forces approach harmonic oscillator forces.

KEY WORDS: Quantum mechanics; many-body systems; fermions; bosons; optimal bounds.

1. PREAMBLE

It is for me a great pleasure to contribute to this festschrift in honour of my old friend Bernard Jancovici. Old is the appropriate term since we met in 1948 in "Lycée Saint Louis" and became friends while we were students at the Ecole Normale Supérieure from 1949 to 1953. We remained in close contact socially and scientifically because we were both belonging to the initial nucleus of the theoretical group of Ecole Normale founded by Maurice Lévy at the invitation of Yves Rocard (father of the French politician Michel Rocard). Initially there was very little specialization in this group. Janco was interested in nuclear physics (he dedicated to me a paper on Carbon 14 wishing me a correspondingly long life), and particle physics, and I remember vividly the excellent report he gave, after coming back from a conference at Stanford, describing the beautiful experiment of Maurice Goldhaber showing that neutrinos were left-handed. It is only

[1] Theoretical Physics Division, CERN, CH-1211 Geneva 23, Switzerland, and LAPP (URA 14-36 du CNRS, associée à L'Ecole Normale Supérieure de Lyon et à l'Université de Savoie), B.P. 110, F-74941 Annecy Le Vieux, France; e-mail: andre.martin@cern.ch.

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later that Janco turned to statistical mechanics, to some extent under the influence of Loup Verlet who initially worked on particle physics too. However, while Loup became interested in numerical simulations, Janco was more attracted by analytical aspects. I, myself, remained in the field of particle physics or more exactly at the frontier of particle physics and mathematical physics. To contribute to a festschrift which would appear in the Journal of Statistical Physics, I thought that I should at least choose a topic involving N particles, N arbitrarily large, but also arbitrarily small (as Laurent Schwartz uses to say) and I only apologize if my systems are exactly at zero temperature!

The work I want to present is not original. It started in a collaboration with Jean-Louis Basdevant and Jean-Marc Richard[1] where we found extraordinarily good lower bounds on systems of bosons of equal masses, later on extended to unequal masses with the help of Tai-Tsun Wu.[2] These bounds represented a considerable quantitative improvement on those obtained for example by Lévy–Leblond,[3] and in particular reduced smoothly to the exact solution in the case of harmonic oscillator forces. However, attempts to achieve a similar improvement for systems of fermions seemed to fail, until Jean-Louis Basdevant[4] proposed to me a rather extraordinary inequality allowing to replace a sum of two-body potentials by a sum of one particle interactions to a fixed center. I found some reasons to believe the inequality by guessing the minimizing configuration saturating it, but, in the end, a mathematician from Ecole Polytechnique, Jean-Michel Bony, told us that it was obvious, as a consequence of interpolation of inequalities connecting two ℓ^p norms.

2. BOUNDS FOR BOSONS

We consider an assembly of bosons with the following Hamiltonian:

$$H=\sum_{i=1}^{N}\frac{p_i^2}{2m}+\sum_{i>j}V(|\vec{r}_i-\vec{r}_j|) \tag{1}$$

A very simple way of getting a lower bound on the ground state of this Hamiltonian is to write it as a sum of two-body Hamiltonians:

$$\begin{aligned} H&=\sum_{i<j}h_{ij}\\ h_{ij}&=\frac{1}{N-1}\left(\frac{p_i^2}{2m}+\frac{p_j^2}{2m}\right)+V(|\vec{r}_i-\vec{r}_j|) \end{aligned} \tag{2}$$

the lower bound on H is larger or equal to the sum of the lower bounds of the h_{ij}. If we denote as $E(M, V)$ the ground state energy of a two-body system, with two masses M, and interaction potential V, we have[3]

$$h_{ij} \geqslant E((N-1)\,m, V), \tag{3}$$

hence

$$H > \frac{N(N-1)}{2}\,E((N-1)\,m, V). \tag{4}$$

This, however, as described in ref. 1, is not the best one can do. One can make use of the identity

$$\sum p_i^2 = \frac{1}{N}\left[\sum_{i>j}(p_i - p_j)^2 + \left(\sum p_i\right)^2\right] \tag{5}$$

and hence

$$H = \frac{1}{2mN}\left(\sum p_i\right)^2 + \sum_{i>j}\tilde{h}_{ij} \tag{6}$$

where

$$\tilde{h}_{ij} = \frac{1}{2mN}(p_i - p_j)^2 + V((\vec{r}_i - \vec{r}_j)) \tag{7}$$

We notice that $\frac{1}{2}(\vec{p}_i - \vec{p}_j)$ is conjugate to $(\vec{r}_i - \vec{r}_j)$. Hence, the "reduced mass" in (7) is $mN/4$, equivalent to two equal masses $Nm/2$. Since $(\sum p_i)^2$ is positive, and, in fact vanishes in the centre-of-mass, we can replace (4) by

$$H > \frac{N(N-1)}{2}\,E\left(\frac{Nm}{2}, V\right) \tag{8}$$

and, since the binding energy of any system is a *decreasing* function of the mass, we see that (8) represents an improvement of (4) for any $N \geqslant 3$. In fact, the bigger is N, the bigger is the improvement.

For instance if we take

$$V(r) = -\frac{\kappa}{r}, \tag{9}$$

we know that by scaling the N-body energy is proportional to the mass and we get an improvement by a factor 2 for very large N. By comparison with variational trial functions one finds that for any N the ratio of the lower bound (8) to the variational upper bound is less than 1.172.

Furthermore, it is easy to see that the lower bound (8) coincides with the exact ground state energy for $V = gr^2$. Numerical experiments, based on calculations using the hyperspherical harmonics for the special case of three bodies show that the error is very small for $V = r^q$, $-1 \leqslant q \leqslant +3$. For instance, for $V = r$ we have

$$\frac{E_{exact}}{E_{lowerbound}} < 1.00077$$

In general, we believe that for attractive potentials, such that $dV/dr > 0$, the lower bound (8) gives always excellent results. It is clear, however, that this will not be the case for interactions such that one has saturation, i.e., that the binding energy grows, in absolute value, like N (this is the case, for instance, if a V has a positive Fourier transform). Indeed we see that since the two-body binding energy decreases with the mass, (8) decreases necessarily at least as fast as $-N^2$ for $N \to \infty$, if the potential has a negative part in r space. We shall not describe here the intricacies of the case of unequal masses which has been clarified only for $N = 3$.[2]

3. THE CASE OF FERMIONS

For a long time, we thought that the Fermion case was untractable, because splitting the Hamiltonian as a sum of $\tilde{h}_{ij}$, as is done in (6) destroys the antisymmetry of the wave function. In the original paper of Lévy-Leblond[3] devoted to gravitational interactions, but which can be generalized to arbitrary two-body potentials the Hamiltonian (1) is written as a sum of one-body Hamiltonians.

$$\begin{aligned} H &= \frac{1}{N-1} \sum_i h_i \\ h_i &= \sum_{j \neq i} \frac{p_j^2}{2m} + \frac{1}{2} V(|r_i - r_j|). \end{aligned} \tag{10}$$

For simplicity we take "spinless fermions," i.e., the space wave function is completely antisymmetric. To get the energy we have to take the expectation value of H with a completely antisymmetric wave function ψ. Hence if we take the expectation value of h_i we must take it with a wave function antisymmetric in all r_j's, $j \neq i$. Hence if $e_1, e_2, \ldots, e_n$ are the eigenvalues of h_i

we have $\langle\psi| h_i |\psi\rangle \geqslant e_1 + e_2 + \cdots e_{N-1}$. By using this technique, Lévy-Leblond succeeded to prove, for instance, that if you have N fermions in gravitational interaction, their binding energy is lower-bounded by $-CN^{7/3}$, while in the boson case you get $-CN^3$.

However, there is one thing which is not satisfactory which is that when you apply this trick to the case of $V=r^2$, you do not get the exact answer, which is known, but you are off by a factor $\sqrt{2}$. This is not a catastrophy, but when one compares with the boson case, for which one gets then the exact answer by using the decomposition (6), it is irritating.

What I want to describe here is the content of ref. 4, in which we succeed in finding a bound which reduces smoothly to the exact answer for harmonic oscillator forces. Unfortunately, if we restrict ourselves to power potentials, $V=\varepsilon(q)\, r^q$, the improvement works only for $1<q<\infty$, which means that we do not get any improvement in the "realistic" case of $V=-\kappa/r$, which is the case of neutron stars in the non-relativistic limit.

What remains of the ideas of Lévy-Leblond is that one should replace H by an independent particle Hamiltonian. What one has to do is to try to generalize the method used to treat the case of harmonic oscillator forces. Then one uses identity (5) in r space, i.e.,

$$N\sum r_i^2 - \left(\sum \vec{r}_i\right)^2 = \sum (\vec{r}_i - \vec{r}_j)^2. \tag{11}$$

In the case where the potential is $V=\varepsilon(q)\, r^q$, $1<q<\infty$, we replace (11) by two inequalities which have been guessed by Jean-Louis Basdevant and proved with the help of Jean-Michel Bony. They are

$$4\sum\sum_{1\leqslant i<j\leqslant N}\left|\frac{\vec{r}_i-\vec{r}_j}{2}\right|^q + N^2\left|\frac{\sum_{i=1}^N \vec{r}_i}{N}\right|^q \gtrless N\sum_{i=1}^N |r_i|^q \tag{12}$$

$$\sum\sum_{1\leqslant i<j\leqslant N} |\vec{r}_i-\vec{r}_j|^q + \left|\sum_{i=1}^N \vec{r}_i\right|^q \lessgtr N\sum_{i=1}^N |r_i|^q \tag{13}$$

where the upper inequality holds for $1\leqslant q\leqslant 2$, and the lower one for $2\leqslant q\leqslant\infty$; $|r|$ is the Euclidean norm of $r\in R^3$.

The proof of these inequalities is based on the Riesz–Thorin theorem of interpolation of inequalities between ℓ^p norms. We shall not give any detail here. The reader may consult for instance Reed and Simon.[5] The fact is that all conditions are fullfilled to guarantee the validity of the inequalities provided they hold for $q=1$, $q=2$, and $q=\infty$.

If we take, for instance (12), it is true for $q=2$, since then it coincides with identity (11). It is also very easy to see that it holds for $q=1$, because

$$x_i = \frac{1}{N}\left(\sum_j (x_i - x_j) + \sum_j x_j\right) \tag{14}$$

$$|x_i| \leqslant \frac{1}{N}\left(\sum_j |x_i - x_j| + \left|\sum_j x_j\right|\right) \tag{15}$$

and, summing over i, we get (12) in the special case $q = 1$.

It is clear that since (12) and (13) connect smoothly with (11) for $q \to 2$, the upper and lower bounds obtained by using these inequalities will approach the exact answer for $q \to 2$.

Now the procedure is the following: we add $\sum p_i^2$ to both sides of, for instance, (12) (from now on, we shall take $2m = 1$). On the left-hand side we have a Hamiltonian with a two-body interaction $|r_i - r_j|^q$, plus a potential acting only on the centre-of-mass. On the right-hand side we have an independent particle Hamiltonian, whose ground state energy, for fermions, is the sum of the first N energy levels.

If we denote ε_1 as the ground state energy in the potential $V = r^q$, and f_N the sum of the first N energy levels in the potential $V = r^q$ we get, for $1 < q < 2$,

$$2^{(2(q-2)/(q+2)}[N^{2/(q+2)} f_N - N^{(4-q)/(q+2)} \varepsilon_1] \leqslant E_F^N \leqslant N^{2/(q+2)} f_N - N^{q/(q+2)} \varepsilon_1 \tag{16}$$

For N large, f_N can be estimated by using semi-classical estimates, or even exact bounds:

$$f_N \sim N^{(5q+6)/(3q+6)} \tag{17}$$

and one sees that in (16) it dominates over the terms containing ε_1, which come from the centre-of-mass motion effect. So, asymptotically, the ratio between the right-hand side and left-hand side of (16), for $1 < q < 2$ becomes

$$2^{2(2-q)/(2+q)} \tag{18}$$

for $q = 3/2$, for instance, it is about 1.22, which is not too bad!

The conclusion is that we should be satisfied, since we have been able to find upper and lower bounds valid for any finite N which approach the exact solution for fermions in the case of harmonic oscillator forces. However, we have not been able to improve the lower bounds for the case of $V = \varepsilon(q)\, r^q$, $-2 < q < +1$, and in particular in the case of gravitational forces. In that case, there are asymptotic theorems showing that in the large N limit, and provided the strength of the interaction decreases in an appropriate way with N, the Thomas–Fermi limit is approached.[6]

However, this is not exactly equivalent to strict bounds, since the gravitational interaction is extremely small but not zero.

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