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INTERPARTICLE DISTANCE IN N BOSON SYSTEMS

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ABSTRACT

We find the order of magnitude of the interparticle distance in a system of N bosons interacting via a power-like two-body attractive interaction, including in particular a gravitational interaction. This can be generalized to monotonous attractive potentials, but our procedure fails for potentials of positive type.

1. - INTRODUCTION

It is with great pleasure that I have accepted to write a paper to celebrate Gérard Wanders' 60th birthday. I have always had a great admiration for Gérard, for his immense culture, his sense of rigor, his desire to be in contact with physical reality. All these qualities were in action when we were both working, in parallel, on the rigorous aspects of pion-

pion scattering and where he was the first to see that rigorous inequalities would severely restrict acceptable models for pion-pion phase shifts. This is just an example, which will be developed by others in this volume. So I had to speak of something else, if possible rigorous. A question by Philippe Choquard, asked during a joint colloquium between the EPFL and the University of Lausanne gives me the opportunity to do this, even though the answer is not as complete as one would like it to be. The problem is to estimate the mean distance between pairs of particles in an assembly of bosons interacting by two-body forces.

Recently, J.L. Basdevant, J.M. Richard and I [1,2] have obtained rather remarkably accurate lower bounds on ground state energies of N boson systems, interacting by two-body attractive potentials (attractive means $\frac{dV}{dr} > 0$). The fact that they are accurate is demonstrated by comparison with upper bounds coming from various variational approaches, including hyperspherical expansions for the three-body case. For gravitational forces, the upper bound differs from the lower by at most 16 %. For harmonic oscillator forces our lower bound coincides with the exact ground state energy.

Denoting $E_N(M, V)$, a function of N and M, a functional of V, as the binding energy of N bosons of mass M interacting by two-body potentials $V(r_{ij})$ the inequality we use is

$$E_N(M,V) \ge \frac{N(N-1)}{2} E_2(\frac{NM}{2},V).$$
 (1)

In fact we have learnt recently that this inequality can be found in a paper by Hall and Post [3] dating from 1967!

To prove this, we split the N particle hamiltonian, into two-body subhamiltonians, after removing the centre-of-mass motion:

$$H = \sum_{i} \frac{p_i^2}{2M} + \sum_{i \ge i} V(r_{ij}) = \frac{1}{2NM} (\Sigma p_i)^2 + \sum_{i \ge i} h_{ij}$$
 (2)

with

$$h_{ij} = \frac{4\pi_{ij}^2}{2MN} + V(r_{ij}) \tag{3}$$

where π_{ij} is the moment conjugate to r_{ij} . The lower bound on H is just the sum of the lower bounds of the h_{ij} 's, i.e., $\frac{N(N-1)}{2}$ times the ground state energy of h_{12} . The success of the very simple approach in which pairs of particles are treated independently led Philippe

Choquard, during a colloquium in Lausanne, to ask the question if the interparticle distance is effectively given by looking at the interparticle distance in the lower eigenstate of the subhamiltonian h_{ij} given by Eq. (3). The answer to this question for attractive power-like interactions, i.e., $V(r_{ij}) = \epsilon(\beta)r_{ij}^{\rho}$, is affirmative. It is also probably affirmative for attractive monotonous potentials, but unfortunately we cannot give any answer for the case of potentials of positive type (i.e., with positive three-dimensional Fourier transform) for which one has classical stability [4].

2. - THE GRAVITATIONAL CASE

Here

$$V(r_{ij}) = -\frac{\kappa}{r_{ij}},$$

$$\kappa = G M^{2}$$
(4)

G being Newton's constant. We can get an upper bound of the N body Hamiltonian by taking a wave function

$$\Psi = \pi \psi(r_i) \tag{5}$$

In Ref. [1] we used

$$\psi = \exp{-\lambda\sqrt{\mu r^2 + 1}}\tag{6}$$

but for our needs, the wave function used previously by Lévy-Leblond [5], is good enough:

$$\psi = \exp{-\lambda r} \tag{7}$$

and will be used systematically later. If one uses (7), and optimizes in λ , one gets [5]

$$E < -\frac{1}{8} \left(\frac{5}{8}\right)^2 N(N-1)^2 \kappa^2 M \tag{8}$$

with $\frac{1}{8} (\frac{5}{8})^2 = 0.0488$, while with (6) one gets [1]

$$E < -0.0542 \ N(N-1)^2 \kappa^2 M \tag{9}$$

and, solving the integral equation giving the best possible ψ [6]

$$E < -0.05426 \ N(N-1)^2 \kappa^2 M. \tag{10}$$

Now, since we are dealing with bosons, the expectation value of h_{ij} in the true ground

state is independent of i and j, so

$$\langle h_{ij} \rangle < -\frac{0.0542 \ N(N-1)^2 \kappa^2 M}{N(N-1)/2} = -0.1084(N-1)\kappa^2 M$$
 (11)

Now we can use the operator inequality

$$\pi_{ij}^2 > \frac{1}{4r_{ij}^2} \tag{12}$$

and get the operator inequality

$$h_{ij} > \frac{1}{2MN} \frac{1}{r_{ij}^2} - \frac{\kappa}{r_{ij}}$$
 (13)

and hence, using (11),

$$\left\langle \frac{1}{2MN} \frac{1}{r_{ij}^2} - \frac{\kappa}{r_{ij}} \right\rangle < -0.05 N \kappa^2 M, \qquad N \ge 2$$
 (14)

We can divide both sides by $N\kappa^2M$, and, introducing

$$X = \frac{1}{MN\kappa} \frac{1}{r_{ii}} \tag{15}$$

we get

$$\left\langle \frac{1}{2} X^2 - X \right\rangle = < -0.05$$

and using Schwarz inequality we get

$$\frac{1}{2}\left\langle X^{2}\right\rangle -\sqrt{\left\langle X^{2}\right\rangle }+0.05<0$$

and hence

$$1 - \sqrt{0.9} < \sqrt{\langle X^2 \rangle} < 1 + \sqrt{0.9}$$

OL

$$0.05MN\kappa < \left\langle \frac{1}{r_{ij}^2} \right\rangle^{1/2} < 2 MN\kappa \tag{16}$$

which means, crudely speaking, that the interparticle distance is of the order of $(MN\kappa)^{-1}$.

From (16), it also follows that

$$(\langle r_{ij}^2 \rangle)^{1/2} > \frac{1}{2MN\kappa} \tag{17}$$

but, strictly speaking, this method does not allow us to find an upper bound on $\left\langle r_{ij}^2 \right\rangle^{1/2}$.

3. - THE CASE OF POWER POTENTIALS

The case where

$$V(r_{ij}) = g\epsilon(\beta)r_{ij}^{\beta}$$

$$g > 0, \beta > -2, \beta \neq 0, \epsilon(\beta) = \text{sign of } \beta$$
(18)

will be a carbon copy of the Coulomb case, except for the fact that Hölder inequalities will be used instead of Schwarz inequalities.

Again we try to get an upper bound on the ground-state energy of the system by using the trial function

$$\Psi = \pi \exp{-\lambda r_{ij}}$$

In this way we get

$$E < \frac{N}{2M}\lambda^2 + \frac{N(N-1)}{2}g \ \epsilon(\beta)\lambda^{-\beta} \ K(\beta)$$
 (19)

with

$$K(\beta) = \frac{\int e^{-2|x|} |x - x'|^{\beta} e^{-2|x'|} d^3x d^3x'}{(\int e^{-2|x|} d^3x)^2}$$
(20)

Minimizing (19) with respect to λ we get

$$\lambda_{min} = [(N-1)M \ g \ K(\beta)|\beta|]^{\frac{1}{\beta+2}}$$
 (21)

and

$$E < N(N-1)^{\frac{2}{\beta+2}} M^{-\frac{\beta}{\beta+2}} \frac{\beta+2}{2\beta} [|\beta| g K(\beta)]^{\frac{2}{\beta+2}}$$
 (22)

then from

$$\langle h_{ij} \rangle = \frac{2E}{N(N-1)}$$

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$$\left\langle \frac{1}{2MN\ r_{ij}^2} + g\epsilon(\beta)r_{ij}^\beta \right\rangle$$

$$< [(N-1)M]^{-\frac{\beta}{\beta+2}} \left(\frac{\beta+2}{\beta}\right) [g|\beta|K(\beta)]^{\frac{2}{\beta+2}} \tag{23}$$

Now we distinguish

(i)
$$-2 < \beta < 0$$

Then we have

$$\left\langle \left(\frac{1}{r_{ij}}\right)^{|\beta|} \right\rangle < \left\langle \frac{1}{r_{ij}^2} \right\rangle^{\frac{|\beta|}{2}}$$

and hence

$$\frac{1}{2MN} \left\langle \frac{1}{r_{ij}^2} \right\rangle - g \left\langle \frac{1}{r_{ij}^2} \right\rangle^{\frac{|\beta|}{2}} < \left[\frac{NM}{2} \right]^{-\frac{\beta}{\beta+2}} \frac{\beta+2}{\beta} \left[g|\beta|K(\beta) \right]^{\frac{2}{\beta+2}} \tag{24}$$

(here we use $N-1>\frac{N}{2}$ for $N\geq 2$). Then defining

$$X = \frac{1}{r_{ij}^2} (MNg)^{\frac{2}{\beta+2}} \tag{25}$$

we get

$$\frac{1}{2}\langle X \rangle - \langle X \rangle^{\frac{|\beta|}{2}} < -K'(\beta) \tag{26}$$

where K' is positive.

Inequality (26) is easy to study by looking at the function

$$y = \frac{x}{2} - x^{\frac{|\beta|}{2}}$$

This function for $|\beta| < 2$ has a single minimum, is negative for small x, positive for large x. The equation $y = -K'(\beta)$ has either zero or two positive solutions, x_1^2 and x_2^2 . It is necessarily the second half of the alternative which is correct. Therefore we have

$$x_1(MNg)^{\frac{1}{\beta+2}} < \left\langle \frac{1}{r_{ij}^2} \right\rangle^{1/2} < x_2(MNg)^{\frac{1}{\beta+2}}$$
 (27)

Therefore the interparticle distance is of the order of $(MNg)^{-\frac{1}{\beta+2}}$.

(ii)
$$\beta > 0$$

Here we use

$$\left\langle r_{ij}^{\beta} \right\rangle > \left\langle r_{ij}^{-2} \right\rangle^{rac{eta}{2}}$$

and get back again to inequality (27). However, in that case, one can also get directly a double inequality on $\left\langle r_{ij}^2 \right\rangle$ if $\beta > 2$ indeed. Then, one has $\left\langle r_{ij}^2 \right\rangle^{\frac{\beta}{2}} < \left\langle r_{ij}^{\beta} \right\rangle$ and $\left\langle r_{ij}^2 \right\rangle^{-1} < \left\langle r_{ij}^{-2} \right\rangle$.

4. - SOME CONSIDERATIONS ON GENERAL POTENTIALS

In general the expectation value of the two-body Hamiltonian defined by (3) in the ground state of the full N-body system is given by

$$\langle h_{12} \rangle = \frac{2}{N(N-1)} E_N(M,V) \tag{28}$$

and therefore if one has a variational upper bound E_N^{var}

$$\langle h_{12} \rangle \le \frac{2}{N(N-1)} E_N^{var} \tag{29}$$

Now if we write the wave function of the N-body system as

$$\Psi(r_1, r_2, \dots r_N) = \Phi(r_1 - r_2, r_1 + r_2, r_3 \dots r_N)$$
(30)

we can expand Φ in eigenstates of h_{12} :

$$\Phi(r_1 - r_2, r_1 + r_2, r_3 \dots r_N) = \sum \psi_K(r_1 - r_2) \chi_K(r_1 + r_2, r_3, \dots r_N)$$
(31)

then if the $e'_K s$ are the ordered eigenvalues of h_{12} we have

$$\langle h_{12} \rangle = \sum e_K C_K < \frac{2}{N(N-1)} E_N^{var}$$
 (32)

where

$$C_K = \int |\chi_K|^2 \tag{33}$$

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Assume

$$e_M > \frac{2}{N(N-1)} E_N^{var}$$

Then, since

$$\sum C_K = 1 \tag{34}$$

from normalization, we have

$$\left[e_{M} - \frac{2}{N(N-1)} E_{N}^{var}\right] \left(1 - \sum_{K=1}^{M-1} C_{K}\right) < \sum_{K=1}^{M-1} C_{K} \left(\frac{2}{N(N-1)} E_{N}^{var} - e_{K}\right)$$
(35)

which means that the first M-1 components in (31) dominate and that the spatial extension of the pair 12 is given dominantly by the spatial extension of the two-body wave functions

$$\psi_1 \ \psi_2 \dots \psi_{M-1}$$

We can illustrate this by taking again the case of attractive two-body potentials $-\frac{\kappa}{r_{ij}}$. In that case the energy levels of h_{12} are given by

$$e_n = -\frac{\kappa^2}{8} NM \frac{1}{n^2}$$

with a degeneracy n^2 . The variational upper bound gives

$$\frac{2E_N^{var}}{N(N-1)} < -0.1084(N-1) \kappa^2 M$$

Hence

$$e_2 > \frac{2E_N^{var}}{N(N-1)}$$

and we get (taking the limit case $N \to \infty$)

$$\frac{C_1}{1 - C_1} > 4.64\tag{36}$$

Therefore the interparticle distance is most of the time given by the groundstate wave function of h_{12} .

Similarly if one takes a two-body potential

$$\begin{pmatrix} V(0) & = -V_0 \text{ at } r = 0 \\ V'(0) & = 0 \\ V''(0) & > 0 \text{ and } V'' \text{ continuous} \\ V(\infty) & = 0 \end{pmatrix}$$

$$(37)$$

one can take a trial function $\pi(\exp{-\lambda r_i^2})$ to get an upper bound of the total energy, and choose for large N, $\lambda \simeq C\sqrt{N}$. Then only the short-range part of the potential is used and V can be replaced by a harmonic oscillator

$$\bar{V} = -V_0 + q r^2$$

Then, in this approximation, it is not a surprise to find that the variational energy

$$E_N^{var} = 3N \sqrt{N-1} \sqrt{\frac{g}{2M}} - \frac{N(N-1)}{2} V_0$$

corresponding, as expected, to $\lambda = \sqrt{\frac{g(N-1)M}{2}}$, gives, when divided by $\frac{N(N-1)}{2}$, a number which coincides with the ground state energy of h_{12} (except for the placement of $N^{-1/2}$ by $(N-1)^{-1/2}$) which means $C_1 = 1 - O(\frac{1}{N})$.

One can try to estimate the error committed by expanding V further:

$$V = -V_0 + g r^2 + k r^4 + \dots$$

keeping

$$\lambda = \sqrt{\frac{g(N-1)M}{2}}$$

one gets an extra contribution to E_N^{var} which is

$$\frac{15}{4} \frac{kN}{gM}$$

on the other hand, the anharmonic correction to e_1 , the ground-state energy of h_{12} , is

$$\frac{15}{4} \; \frac{k}{gNM}$$

So we get

$$\left(\frac{E_N^{var}}{\frac{N(N-1)}{2}} - e_1\right) \sim \frac{15}{4} \frac{k}{gNM}$$

while the first excitation e2 has an energy

$$\frac{7}{2}\sqrt{\frac{8g}{MN}}$$

Therefore $1 - C_1$ is of the order of $N^{-1/2}$, i.e., negligible for large N, and the interparticle spacing is given by looking at the two-body subsystem.

However, a case where this method fails - and this is normal - is that of a two-body potential of positive type (more exactly non-negative type). "Positive type" means that the three-dimensional Fourier transform of the potential is positive. If we take a product trial function $\pi\psi(r_i)$ to get an upper bound on E_N , the potential energy contribution is:

$$\frac{N(N-1)}{2} \int |\psi(r_i)|^2 |V(r_i-r_j)|\psi(r_j)|^2 d^3r_i d^3r_j$$

If $\xi(p)$ is the Fourier transform of $|\psi(r)|^2$, this becomes, except for 4π factors:

$$\frac{N(N-1)}{2}\int \tilde{V}(p)|\xi(p)|^2d^3p$$

which is manifestly positive. It is therefore impossible to get a negative upper bound for E_N in the Hartree approximation. However, $\tilde{V}(p)$ may be positive everywhere without V(r) being positive everywhere. For instance

$$V(r) = \frac{16e^{-4r}}{r} - \frac{e^{-r}}{r}$$

is negative for r large enough but has a positive Fourier transform

$$\tilde{V}(p) = \frac{16}{16 + p^2} - \frac{1}{1 + p^2}$$

Then our approach fails completely because E_N^{var} is unavoidably positive while e_1 , lowest eigenvalue of h_{12} approaches the negative minimum of V(r) for $N \to \infty$.

This is not a surprise. It is known that potentials of positive type give rise to 'stability", i.e., in particular that, as N increases, the total energy does not decrease faster than -N [4]. If there is any anomaly in the particle-particle correlation, our method cannot detect it.

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