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THE METHOD OF ESTIMATE OF LOWER  
BOUND FOR ENERGY OF A MANY-BODY  
QUANTUM SYSTEM

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## 1. INTRODUCTION

Post and Hall <sup>/1/</sup> have shown, that the symmetry or antisymmetry of the many-body wave function could be used for the simple estimates of the energy lower bound. The method based on this idea is proposed in this paper. Its derivation can be found in Section 2. The advantages of our method over the well-known Carr and Post <sup>/2/</sup> method are demonstrated by the example of a harmonic oscillator in Section 3. Here we pointed out also that the improvement suggested by Carr and Post <sup>/3/</sup> is erroneous. In Section 4 we compare the exact energy with its lower bound for a system of many bosons, interacting with the oscillator and  $\delta$ -type forces.

## 2. The Derivation of the Method

An internal motion of the  $N$ -body system is described by the Hamiltonian:

$$H_{in} = \sum_{i,j=1}^N \left\{ \frac{(p_i - p_j)^2}{2mN} + v(r_i - r_j) \right\}.$$

The ground state energy of the system is the average:

$$E_0 = \langle \Psi_0 | H_{in} | \Psi_0 \rangle,$$

where  $\Psi_0$  is the eigenfunction of  $H_{in}$  corresponding to the lowest eigenvalue.  $\Psi_0$  is antisymmetric or symmetric (for fermions or bosons respectively), so the next equality is valid:

$$E_0 = \frac{N(N-1)}{2} \langle \Psi_0 | \frac{(p_i - p_j)^2}{2mN} + v(r_i - r_j) | \Psi_0 \rangle,$$

where  $i$  and  $j$  are any indices from 1 to  $N$ ;  $i \neq j$ . Let us take the new coordinates

$$r_{ij} = r_i - r_j, \quad R_{ij} = r_i + r_j.$$

With them  $p_i - p_j = -2i\hbar \frac{\partial}{\partial r_{ij}}$  and

$$E_0 = \frac{N(N-1)}{2} \langle \Psi_0 | -4 \frac{\hbar^2}{2mN} \frac{\partial^2}{\partial r_{ij}^2} + v(r_{ij}) | \Psi_0 \rangle.$$

Take  $j=1$  and denote  $r_{i1} = \rho_i$ ,  $\mu = m/2$ . Then

$$E_0 = (N-1) \langle \Psi_0 | -\frac{\hbar^2}{2\mu} \frac{\partial^2}{\partial \rho_i^2} + \frac{N}{2} v(\rho_i) | \Psi_0 \rangle = \langle \Psi_0 | \sum_{i=2}^N \left\{ -\frac{\hbar^2}{2\mu} \frac{\partial^2}{\partial \rho_i^2} + \frac{N}{2} v(\rho_i) \right\} | \Psi_0 \rangle = \langle \Psi_0 | \mathcal{H} | \Psi_0 \rangle.$$

$\mathcal{H}$  is the single particle operator with its eigenfunctions and eigenvalues:

$$\mathcal{H}\phi^a = \varepsilon^a \phi^a.$$

Writing  $\Psi_0$  in the form  $\Psi_0 = \sum_a c_a \phi^a$  we get:

$$E_0 = \sum_a |c_a|^2 \varepsilon^a$$

Replacing here all the  $\varepsilon^a$  by the lowest eigenvalue  $\varepsilon_0$  we come to the inequality

$$E_0 \geq \varepsilon_0.$$

So the lowest eigenvalue of the more simple Hamiltonian  $\mathcal{H}$  can serve as the lower bound for  $E_0$ .

### 3. FERMIONS WITH OSCILLATOR FORCES

An accuracy of such estimates is tested usually by the exactly soluble problem of the one-dimensional harmonic oscillator:

$$\sum_{i,j=1}^N \left\{ \frac{(p_i - p_j)^2}{2mN} + \gamma(x_i - x_j)^2 \right\} \Psi_0 = E_0 \Psi_0.$$

For fermions  $E_0 = (N^2-1)(\frac{1}{2}\hbar^2\gamma N/m)^{1/2}$  and  $\varepsilon_0 = (N-1)^2(\frac{1}{2}\hbar^2\gamma N/m)^{1/2}$ . The ratio of these two quantities

$$\varepsilon_0/E_0 = \frac{N-1}{N+1}$$

goes to unity as  $N \rightarrow \infty$ . The known result of Carr and Post /2/

$$\varepsilon_0/E_0 = \frac{1}{\sqrt{2}} \frac{N-1}{N+1}$$

gives  $1/\sqrt{2}$  when  $N \rightarrow \infty$ . It is not difficult to understand an origin of the factor  $1/\sqrt{2}$  by comparing the ways of deriving of these formulas. Carr and Post consider the motion of the  $N-1$  independent particles relative to the first particle. They suppose for simplicity its mass  $m_1 = \infty$ , i.e., fix it in a space. We also consider the motion of all the rest particles relative to the first one, but now it may move. The first particle movement is taken into account as usual by reduced mass

$$\mu = \frac{m_1 m}{m_1 + m} = \frac{m}{2}, \quad m_1 = m.$$

The very factor  $1/2$  gives us at the end the possibility of getting rid of the factor  $1/\sqrt{2}$ .

In the paper by Carr and Post /3/ their method had been "improved" and as a result

$$\varepsilon_0/E_0 = \frac{1}{\sqrt{2}} \frac{N}{N+1}$$

was obtained. We have attempted to improve our method

by this way in order to get  $\varepsilon_0/E_0 = \frac{N}{N+1}$ . But more careful

consideration shows that such an "improvement" is impossible. The reason is that Carr and Post made an error in their previous paper /2/. They had changed va-

riables there  $\rho_j = (r_i - r_j) \sqrt{m_1/(m_1+m)}$  and decided that  $\rho_i \rightarrow r_i$ , when  $m_1 \rightarrow \infty$ . It is clear however that  $\rho_i \rightarrow r_i - r_1$ . This error had not influenced the results of the paper /2/. But the "improvement" proposed in /3/ is based only on it.

4. *BOSONS WITH THE OSCILLATOR AND  $\delta$ -TYPE FORCES*

Let us consider a many-boson system. Here the lower bound estimate on the ground state energy of the one-dimensional harmonic oscillator gives us the exact eigenvalue:

$$\xi_0 = (N-1) \left( \frac{1}{2} \hbar^2 \gamma N/m \right)^{1/2} = E_0.$$

The one-dimensional N-bosons problem can be solved in the case of the attractive  $\delta$ -type forces as well:

$$\sum_{i=1}^N \left\{ \frac{(p_i - p_j)^2}{2mN} - g\delta(x_i - x_j) \right\} \Psi_0 = E_0 \Psi_0.$$

The single bound state has the energy /4/

$$E_0 = - \frac{1}{48} g^2 N(N^2 - 1) \frac{2m}{\hbar^2}.$$

The solution of the problem with the more simple Hamiltonian

$$H = \sum_{i=1}^N \left\{ - \frac{\hbar^2}{2\mu} \frac{\partial^2}{\partial p_i^2} - \frac{N}{2} g\delta(p_i) \right\}$$

gives /5/

$$\xi_0 = - \frac{1}{8} \left( \frac{N}{2} g \right)^2 (N-1) \frac{2m}{\hbar^2} = - \frac{1}{32} g^2 N^2 (N-1) \frac{2m}{\hbar^2}.$$

Hence

$$\xi_0/E_0 = \frac{3}{2} \frac{N}{N+1}.$$

This ratio is equal to unity for  $N=2$  and goes to  $3/2$  when  $N \rightarrow \infty$ .

*REFERENCES*

1. H.R.Post. *Proc. Phys. Soc.*, 69, 936 /1956/.
- R.L.Hall, H.R.Post. *Proc. Phys. Soc.*, 90, 381 /1967/.
2. R.J.M.Carr, H.R.Post. *J.Phys.*, A1, 596 /1968/.
3. R.J.M.Carr, H.R.Post. *J.Phys.*, A4, 665 /1971/.

4. J.B.McGuire. *J.Math.Phys.*, 5, 622 /1964/.
5. P.M.Morse, H.Feshbach. *Methods of Theoretical Physics, part II, New-York, 1953.*

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