Energy lower bound of a many-fermion system

E B Balbutsev and I N Mikhailov

Joint Institute for Nuclear Research, Dubna 141980, USSR

Abstract. A more detailed consideration of a trial wavefunction antisymmetry makes it possible to raise an energy lower bound of a many-fermion system. The method is particularly effective for a small number of particles.

1. Introduction

A translation invariant system of N identical fermions with binary interaction $v(r_i - r_j)$ is considered. An improvement is proposed to the method by Carr and Post (1968, 1977) of calculating a lower bound $\mathscr{E}$ for the ground-state energy E_0. In the quoted paper E_0 was defined as a minimum of the functional $\langle \psi | H | \psi \rangle$, where

$$H = \sum_{i=2}^{N} \left(-\frac{\hbar^2}{2\mu} \frac{\partial^2}{\partial \boldsymbol{\rho}_i^2} + \frac{N}{2} v(\boldsymbol{\rho}_i) \right) = \sum_{i=2}^{N} h_i$$

is the model operator with eigenfunctions ϕ_α and eigenvalues ϵ_α:

$$H\phi_\alpha = \epsilon_\alpha \phi_\alpha, \qquad \phi_\alpha = \det \varphi_n(\boldsymbol{\rho}_i), \qquad h_i \varphi_n(\boldsymbol{\rho}_i) = e_n \varphi_n(\boldsymbol{\rho}_i), \qquad \mu = m(N-1)/N,$$

m is the mass of a particle, $\boldsymbol{\rho}_i = r_i - r_1$, and $\psi(\boldsymbol{\rho}_2, \boldsymbol{\rho}_3, \ldots, \boldsymbol{\rho}_N)$ is the trial function which must be antisymmetric in particles $1, 2, \ldots, N$.

Carr and Post (1968, 1977) symmetrise ψ in particles $2, 3, \ldots, N$ only, thus enlarging the class of trial functions, and obtain in this way the lower bound for E_0.

2. Improvement on the Carr and Post method

Any antisymmetric function is equal to zero when the coordinates of two particles coincide. Hence, the function $\psi(\boldsymbol{\rho}_2, \boldsymbol{\rho}_3, \ldots, \boldsymbol{\rho}_N)$ should vanish when any of the relative coordinates $\boldsymbol{\rho}_i = r_i - r_1$ is zero and the spin coordinates of particles i and 1 are the same. We use this property to improve the lower estimate for E_0: antisymmetrising ψ in particles $2, 3, \ldots, N$ only, we also require it to vanish at $\boldsymbol{\rho}_i = 0$.

For simplicity we consider the case of spinless fermions. Now, the variational problem is

$$\mathscr{E} = \min\langle \psi | H | \psi \rangle, \qquad \langle \psi | \psi \rangle = 1,$$

$$\psi(\boldsymbol{\rho}_2, \ldots, \boldsymbol{\rho}_{i-1}, \boldsymbol{\rho}_i = 0, \boldsymbol{\rho}_{i+1}, \ldots, \boldsymbol{\rho}_N) = 0.$$

Expanding ψ over eigenfunctions of H,

$$\psi = \sum_{n=1}^{\infty} c_{\alpha_n} \phi_{\alpha_n}(\boldsymbol{\rho}_2, \ldots, \boldsymbol{\rho}_N),$$

we arrive at the system of equations for coefficients c_α

$$\mathcal{E} = \min \sum_{n=1}^{\infty} |c_{\alpha_n}|^2 \epsilon_{\alpha_n},$$

$$\sum_{n=1}^{\infty} |c_{\alpha_n}|^2 = 1, \tag{1}$$

$$\sum_{n=1}^{\infty} c_{\alpha_n} \phi_{\alpha_n}(\boldsymbol{\rho}_2, \ldots, \boldsymbol{\rho}_i = 0, \ldots, \boldsymbol{\rho}_N) = 0. \tag{2}$$

As an illustration, we shall consider the problem for a four-particle system in one dimension with the oscillator interaction. A possible method of generalisation will become apparent during the procedure.

Consider the first term in (2), putting $i = 2$:

$$\phi_{012}(x_2 = 0, x_3, x_4) = \begin{vmatrix} \varphi_0(0) & \varphi_1(0) & \varphi_2(0) \\ \varphi_0(x_3) & \varphi_1(x_3) & \varphi_2(x_3) \\ \varphi_0(x_4) & \varphi_1(x_4) & \varphi_2(x_4) \end{vmatrix}$$

$$= \varphi_0(0) \begin{vmatrix} \varphi_1(x_3) & \varphi_2(x_3) \\ \varphi_1(x_4) & \varphi_2(x_4) \end{vmatrix} + \varphi_2(0) \begin{vmatrix} \varphi_0(x_3) & \varphi_1(x_3) \\ \varphi_0(x_4) & \varphi_1(x_4) \end{vmatrix}.$$

Recall that odd Hermite polynomials become zero at $x = 0$. The next term in (2) is

$$\phi_{013}(0, x_3, x_4) = \varphi_0(0) \begin{vmatrix} \varphi_1(x_3) & \varphi_3(x_3) \\ \varphi_1(x_4) & \varphi_3(x_4) \end{vmatrix},$$

and so on. The sum in (2) consists of all possible determinants of second rank. As these are all linearly independent and the equality (2) holds for any x_3, x_4, the coefficients at each determinant should be equal to zero. Thus, the condition (2) yields an infinite system of linear homogeneous equations for c_α which splits into independent subsystems. Here are the first few subsystems (φ_i means $\varphi_i(0)$):

$$\begin{cases} c_{012}\varphi_2 + c_{014}\varphi_4 + c_{016}\varphi_6 + \ldots \equiv f_{01} = 0 \\ c_{012}\varphi_0 + c_{412}\varphi_4 + c_{612}\varphi_6 + \ldots \equiv f_{21} = 0 \\ c_{014}\varphi_0 + c_{412}\varphi_2 + c_{416}\varphi_6 + \ldots \equiv f_{41} = 0 \\ \qquad\qquad \cdot \quad \cdot \quad \cdot \quad \cdot \end{cases}$$

$$\{ c_{013}\varphi_0 + c_{213}\varphi_2 + c_{413}\varphi_4 + \ldots \equiv f_{13} = 0 \tag{3}$$

$$\begin{cases} c_{032}\varphi_2 + c_{034}\varphi_4 + c_{036}\varphi_6 + \ldots \equiv f_{03} = 0 \\ c_{032}\varphi_0 + c_{432}\varphi_4 + c_{632}\varphi_6 + \ldots \equiv f_{23} = 0 \\ c_{034}\varphi_0 + c_{432}\varphi_2 + c_{436}\varphi_6 + \ldots \equiv f_{43} = 0 \\ \qquad\qquad \cdot \quad \cdot \quad \cdot \quad \cdot \\ \qquad\qquad \cdot \quad \cdot \quad \cdot \quad \cdot \end{cases}$$

Now, the subsidiary conditions (1) and (3) are taken into account by introducing Lagrange multipliers into the variation of $\mathscr{E}$:

$$\delta\left(\mathscr{E} - \lambda \sum_{n=1}^{\infty} |c_{\alpha_n}|^2 - \mu_{01}f_{01} - \mu_{21}f_{21} - \ldots - \mu_{13}f_{13} - \mu_{03}f_{03} - \ldots\right) = 0.$$

That gives

$$c_{012} = \frac{\mu_{01}\varphi_2 + \mu_{21}\varphi_0}{2(\epsilon_{012} - \lambda)}, \qquad c_{014} = \frac{\mu_{01}\varphi_4 + \mu_{41}\varphi_0}{2(\epsilon_{014} - \lambda)}, \qquad c_{016} = \frac{\mu_{01}\varphi_6 + \mu_{61}\varphi_0}{2(\epsilon_{016} - \lambda)}, \ldots$$

$$c_{412} = \frac{\mu_{21}\varphi_4 + \mu_{41}\varphi_2}{2(\epsilon_{412} - \lambda)}, \qquad c_{612} = \frac{\mu_{21}\varphi_6 + \mu_{61}\varphi_2}{2(\epsilon_{612} - \lambda)}, \ldots$$

. . . .

$$c_{013} = \frac{\mu_{13}\varphi_0}{2(\epsilon_{013} - \lambda)}, \qquad c_{213} = \frac{\mu_{13}\varphi_2}{2(\epsilon_{213} - \lambda)}, \qquad c_{413} = \frac{\mu_{13}\varphi_4}{2(\epsilon_{413} - \lambda)}, \ldots$$

. . . .

Substituting c_α into (3) we obtain a system of linear homogeneous equations for μ:

$$\begin{cases} \dfrac{\mu_{01}\varphi_2^2 + \mu_{21}\varphi_0\varphi_2}{\epsilon_{012} - \lambda} + \dfrac{\mu_{01}\varphi_4^2 + \mu_{41}\varphi_0\varphi_4}{\epsilon_{014} - \lambda} + \dfrac{\mu_{01}\varphi_6^2 + \mu_{61}\varphi_0\varphi_6}{\epsilon_{016} - \lambda} + \ldots = 0 \\[3mm] \dfrac{\mu_{01}\varphi_2\varphi_0 + \mu_{21}\varphi_0^2}{\epsilon_{012} - \lambda} + \dfrac{\mu_{21}\varphi_4^2 + \mu_{41}\varphi_2\varphi_4}{\epsilon_{412} - \lambda} + \dfrac{\mu_{21}\varphi_6^2 + \mu_{61}\varphi_2\varphi_6}{\epsilon_{612} - \lambda} + \ldots = 0 \end{cases}$$

. . . . .

$$\begin{cases} \dfrac{\mu_{13}\varphi_0^2}{\epsilon_{013} - \lambda} + \dfrac{\mu_{13}\varphi_2^2}{\epsilon_{213} - \lambda} + \dfrac{\mu_{13}\varphi_4^2}{\epsilon_{413} - \lambda} + \ldots = 0 \end{cases} \tag{4}$$

. . . .

A nontrivial solution exists if the determinant of the system is zero. This yields an equation for λ. Since the system (4) as well as (3) consists of independent subsystems, its determinant has a block-diagonal form and is equal to the product of determinants of individual subsystems. Hence, a solution can be found by equating to zero each of those determinants independently. For instance we obtain from the first subsystem

$$\begin{vmatrix} \left(\dfrac{\varphi_2^2}{\epsilon_{012} - \lambda} + \dfrac{\varphi_4^2}{\epsilon_{014} - \lambda} + \dfrac{\varphi_6^2}{\epsilon_{016} - \lambda} + \ldots\right) & \dfrac{\varphi_2\varphi_0}{\epsilon_{210} - \lambda} & \cdots \\[4mm] \dfrac{\varphi_0\varphi_2}{\epsilon_{012} - \lambda} & \left(\dfrac{\varphi_0^2}{\epsilon_{210} - \lambda} + \dfrac{\varphi_4^2}{\epsilon_{214} - \lambda} + \dfrac{\varphi_6^2}{\epsilon_{216} - \lambda} + \ldots\right) \cdots \\ \vdots & \vdots \end{vmatrix} = 0 \tag{5}$$

from the second

$$\frac{\varphi_0^2}{\epsilon_{013} - \lambda} + \frac{\varphi_2^2}{\epsilon_{213} - \lambda} + \frac{\varphi_4^2}{\epsilon_{413} - \lambda} + \ldots = 0, \tag{6}$$

and so on. Most of the determinants turn out to be of infinite rank. Their matrix

elements decrease quite rapidly with increasing number of the row and column. Therefore, λ can be obtained within the desired accuracy by cutting off the determinants.

The lower bound of energy we are looking for equals the minimal value of λ. It is not known *a priori* whether either equations (5) or (6) or some other, have as a solution the minimal $\lambda = \lambda_0$. We know, however, that solutions to equation (5) are above ϵ_{012}, to equation (6) above ϵ_{013}, and for subsequent equations above ϵ_{023}, etc. Therefore, if λ_0 found from (5) is smaller than ϵ_{013}, the problem is solved. If it is larger than ϵ_{013}, it should be compared with the solution to equation (6). If both the solutions are larger than ϵ_{023}, a subsequent equation is to be solved, and so on. Obviously, this procedure is not infinite as we should not go above the exact energy value.

It can be seen that the method proposed for solving the variational problem is extended, without change, to systems with $N > 4$.

For $N \leqslant 10$ we have calculated the ratios of the lower bound $\mathscr{E}$ to the exact value E_0. These are listed in table 1 where the ratios which can be obtained from Carr and Post (1968, 1977) are also given for comparison;

$$\mathscr{E}/E_0 = \frac{1}{\sqrt{2}} \frac{N-1}{N+1} \left(\frac{N}{N-1}\right)^{1/2}.$$

Table 1 also contains the results by Post (1956) and the ratios

$$\mathscr{E}/E_0 = \frac{\sqrt{3}}{2} \frac{N-1}{N+1}$$

from Hall (1967) obtained by another method. The comparison shows that our version of the Carr and Post method provides better results for $N \leqslant 9$ while for $N \geqslant 10$ the method of Hall works better.

The above concerns the one-dimensional harmonic oscillator. The generalisation to the three-dimensional system of particles with spin interacting through arbitrary forces is straightforward. The only note should be made that all equations, (5), (6), etc. include the wavefunctions which are not equal to zero at zero point. The same will be true in the general case, i.e. equations will contain only the s-state wavefunctions.

Table 1. Ratios of lower bounds to exact energies for the one-dimensional system of N spinless fermions with the oscillator interaction.

	N	2	3	4	5	6	7	8	9	10
	This paper	1	0·70	0·71	0·69	0·71	0·70	0·71	0·70	0·70
$\mathscr{E}/E_0$	Carr and Post	0·33	0·43	0·49	0·53	0·55	0·57	0·59	0·60	0·61
	Hall	0·29	0·43	0·52	0·58	0·62	0·65	0·67	0·69	0·71
	Post	1	0·75	0·60	0·50	0·43	0·37	0·33	0·30	0·27

References

Carr R J M and Post H R 1968 *J. Phys. A: Gen. Phys.* **1** 596–609
—— 1977 *J. Phys. A: Math. Gen.* **10** L59–61
Hall R L 1967 *Proc. Phys. Soc.* **91** 16–22
Post H R 1956 *Proc. Phys. Soc.* **69** 936–8