Many-particle systems

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Abstract. A recent energy lower bound method of Carr and Post incorporates the full permutation symmetry of the N particle system, but the resulting estimates for the ground state energies appear to be inferior to those given by method I of Hall and Post for small N, and to method II of Hall for large N.

1. Introduction

An interesting new addition to the collection of energy *lower* bound methods for many-particle systems has recently been published (Carr and Post 1971). In this method (called SHIP) the lowest energy of a system of N identical fermions is shown to be bounded below by the lowest energy of a model system of N independent particles which interact with a fixed centre. Earlier methods of this kind involve the use of model systems of either one particle (eg method I, Hall and Post 1967) or of $N-1$ particles (eg method II, Hall 1967). The advantage of the SHIP method is that there is no 'loss of antisymmetry' in going from the given system to the model system. For the purpose of calculating ground state energies, however, methods I and II still appear to be the best available. This is illustrated by the following calculations for Hooke's interaction in one dimension and the inverse-square interaction in three dimensions.

2. Comparison of SHIP with methods I and II

2.1. Hooke's interaction in one dimension

For the interaction $V_{ij} = k^2(x_i - x_j)^2$ figure 1 compares the exact ground state energy $E_0 = (N^2-1)(N\hbar^2/2m)^{1/2}k$ with the lower bounds given by SHIP and methods I and II. The cases $N = 2(1)6$ are shown in table 1. We see that method I gives the highest lower bound for $N < 5$. For $N = 5$ SHIP is best and is about $2\,\%$ (of the exact energy) above method II. For all $N > 5$ method II gives the highest lower bound. In the limit of very large N, SHIP gives $71\,\%$ of the exact energy whereas method II yields $87\,\%$.

2.2. Inverse-square interaction in three dimensions

For the interaction $V_{ij} = -k/r_{ij}$ figure 2 compares SHIP with methods I and II. For $N = 2$, 3, and 4 the results are given in table 2 together with the upper bound by Levy-Leblond (1969). Of course, for $N = 2$ method I yields the *exact* energy. The energies are here measured in units of $2mk^2/\hbar^2$. By over filling the model 'shells' we get explicit

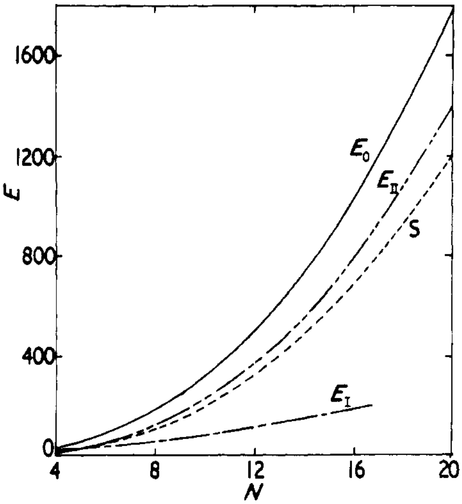

Figure 1. Hooke's interaction in one dimension. Energies in units of $(\hbar^2/2m)^{1/2}k$. Exact energy, E_0: SHIP, S; method I, E_I; method II, E_{II}.

Table 1. Ratios of lower bounds to exact energies for Hooke's interaction in one dimension

	Method I	SHIP	Method II
N	$\frac{3}{N+1}$	$\frac{N}{N+1}\frac{1}{\sqrt{2}}$	$\frac{N-1}{N+1}\frac{\sqrt{3}}{2}$
2	1·00	0·47	0·29
3	0·75	0·53	0·43
4	0·60	0·57	0·52
5	0·50	0·59	0·58
6	0·43	0·61	0·62

relations for the estimates by SHIP and method II. The formulae are as follows:

$$E_{\text{upper}} = -\frac{1}{3\pi^2 2^6} N^{1/3}(N-1)^2$$

$$E_{\text{I}} = -\tfrac{1}{128}N^2(N-1)$$

$$E_{\text{II}} = -\tfrac{1}{12}(N-1)^{1/3}N^2$$

$$E_{\text{SHIP}} = -\tfrac{1}{8}N^{4/3}(N-1).$$

We see that method I gives the highest lower bound until $N = 35$, at which point method II becomes superior. In the large-N limit method II is at least 50 % (of the exact energy) above SHIP. The upper bound by Levy-Leblond is at present the best available. It is very poor for $N = 2$ but until more computations for $N \gg 2$ are undertaken we have no way of telling which estimate, the upper bound or method II, is the nearer to the exact energy.

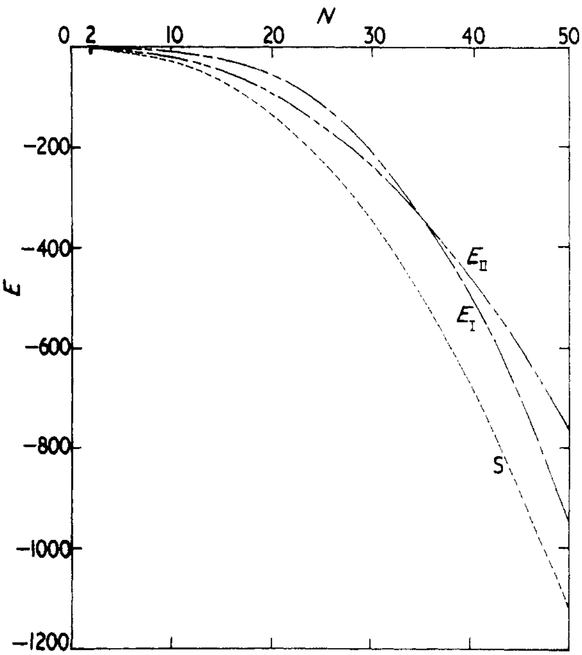

Figure 2. Inverse-square interaction in three dimensions. Energies in units of $2mk^2/\hbar^2$. SHIP, S; method I, $E_{\rm I}$; method II, $E_{\rm II}$.

Table 2. Upper and lower bounds in units of $2mk^2/\hbar^2$ for the inverse-square interaction in three dimensions

N	Method I	Method II	SHIP	Upper
2	−0·031	−0·167	−0·156	−0·00067
3	−0·141	−0·469	−0·563	−0·00305
4	−0·375	−1·000	−1·313	−0·00754

3. Conclusions

Since for large N the inclusion of the Nth particle in the SHIP model has less effect on the energy than the use of the smaller reduced mass, as in method II, we expect to get similar results to those of § 2 for all interactions. We therefore conclude that, whilst the SHIP method has the great advantage of keeping the full antisymmetry of the problem, the best available energy lower bounds appear to be those given by method I for small N, and method II for large N.

For the many-particle *excited states* it has been proved (Hall 1969) that the discrete energies of the system are rigorously bounded below (one by one) by the energies of the model system of method II (using the value $2(N-1)/N$ for the transformation parameter λ). A hopeful goal in this work is to develop general methods which, in the case of Hooke's interaction, yield the exact energies of the system. This has already been achieved for the ground states of N-boson systems (method I) and it has been shown that Hooke's interaction is the only one for which that class of lower bound methods can yield the exact energy (Hall 1972).

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