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Improved lower bounds for the N-fermion problem

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Abstract. Lower bound energy formulae for the N-fermion problem of the type used by Hall and by Post are considered in terms of a reduced density operator for the interparticle separation. In bounds of this type the N-body energy is bounded below by a sum of eigen-energies of states of relative motion weighted by occupations for the relative states. It is shown that the wavefunctions of relative motion are subject to constraints and in particular must be zero when the particle separation is zero. This modifies the energy spectrum of the reduced Hamiltonian of relative motion and improves the lower bound due to Hall. The improvement is demonstrated for some simple model problems. Furthermore it is shown that the bounds of this type currently known do not exhibit saturation regardless of the interaction details. This leads to some speculation on improved lower bounds.

1. Introduction

Methods for finding the ground state energy of the N-fermion problem can be divided into three classes. First there are exact upper bound energies obtained by using suitable trial wavefunctions. For example, Hartree–Fock and Hartree–Fock–Bogoliubov theories fall in this class, though the latter provides a strict upper bound only in the limit $N \to \infty$. Second is the large class of approximation methods which substitute some physical intuition for mathematical rigour. The majority of methods used in the many-body problem are of this type. The third class is that of strict lower bound energies. These can be obtained by partly relaxing the constraint that the wavefunction be totally antisymmetric, and doing this in such a way as to reduce the problem to a solvable one.

Lower bound results are important for several reasons. In the first place good lower bounds can be used to demonstrate stability properties. This is exemplified for atomic and molecular systems in an excellent review by Lieb (1976). It would be extremely useful to have comparable lower bounds for systems interacting with a wide range of forces, particularly in the limit $N \to \infty$. Such bounds might enable useful checks on nuclear matter calculations and define allowed ranges of parameters in nucleon interactions. Another important reason for pursuing exact lower bound results is that in doing so one is forced to explore the structure of general antisymmetric wavefunctions in detail. This leads to a refinement of our intuitive understanding of fermion systems which in turn can lead to better approximation methods. As an example the lower bound for atomic systems derived by Coleman (1963) in his study of reduced density matrices has led to a clearer understanding of the pair condensation phenomenon responsible for superconductivity (Coleman 1965).

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For a system of N fermions with no external forces the centre of mass degree of freedom becomes redundant. This has a significant effect on the Coleman lower bound and reduces it to a bound derived earlier by Post (1956). The quality of the Post bound is known to depend significantly on the type of interaction but in all cases becomes poor as N increases. Various other lower bounds have been derived (e.g. Carr and Post 1968, 1971, Hall 1967) with a view to improving the behaviour for large N and in general the best of these is that of Hall. The Hall bound is not as good as that of Post for very small N but usually surpasses it at some intermediate N value depending on the interaction.

In this work the various bounds of the Hall and Post type are derived in a unified way from a reduced density operator for the interparticle separation. It should be noted that the second Carr and Post bound cannot be derived in this way.

The derivation here shows that additional constraints, not previously considered, can be imposed on the wavefunctions of the relative coordinate. In particular these wavefunctions must go to zero for zero particle separation and this leads to an improvement in the Hall bound.

The improvement is demonstrated for some simple model problems in which it is shown that the modification to the Hall bound causes it to surpass the Post bound at lower N values. The behaviour of the Hall bound for large N is however not significantly changed. Furthermore, it is shown that none of these bounds exhibit saturation for interactions of the type occurring between molecules or nucleons. This leads to some discussion as to how the lower bounds must be improved to exhibit saturation.

2. Preliminary definitions

The internal energy for an interacting N-fermion system is given by the Hamiltonian

$$H = \sum_{i=1}^{N} \frac{p_i^2}{2m} + \sum_{i<j=2}^{N} v(r_i - r_j) - \frac{P^2}{2mN},$$

where the particle momenta p_i are conjugate to the coordinates r_i, v is an arbitrary (momentum-independent) interaction potential, and P is the centre of mass momentum:

$$P = \sum_{i=1}^{N} p_i.$$

For simplicity spins are not considered throughout this work although their inclusion is straightforward.

The ground state energy is the global minimum value of

$$E(\Psi) = \langle \Psi | H | \Psi \rangle$$

where $\Psi(r_1, \ldots, r_N)$ is a normalised wavefunction antisymmetric in all the coordinates r_i.

The internal energy Hamiltonian can be re-arranged as

$$H = \sum_{i<j=2}^{N} \frac{(p_j - p_i)^2}{2mN} + v(r_j - r_i)$$

and using the symmetry of the wavefunction we can write a variety of equivalent expressions for the energy, e.g.

$$E(\Psi)=\sum_{j=2}^{N}\left\langle\Psi\left|\frac{(p_j-p_1)^2}{4m}+\tfrac{1}{2}Nv(r_j-r_1)\right|\Psi\right\rangle,$$
$$E(\Psi)=(N-1)\left\langle\Psi\left|\frac{(p_2-p_1)^2}{4m}+\tfrac{1}{2}Nv(r_2-r_1)\right|\Psi\right\rangle. \tag{1}$$

Following Hall we define a set of coordinates $\rho_1, \rho_2, \ldots, \rho_N$ separating the centre of mass and at least one relative coordinate. Thus

$$\rho_i=\sum_{j=1}^{N}B_{ij}r_j \tag{2}$$

where particularly

$$\rho_1=\sum_{j=1}^{N}\frac{r_j}{N}, \qquad \rho_2=r_2-r_1,$$

and $\rho_3, \ldots, \rho_N$ are left undetermined at this stage although they are orthogonal to ρ_1. The momenta conjugate to the ρ_i are

$$\pi_i=\sum_{j=1}^{N}(B^{-1})_{ji}p_j,$$

the first of these being already determined as

$$\pi_1=P=\sum_{j=1}^{N}p_j.$$

The momentum conjugate to the interparticle separation ρ_2 will be written as

$$\pi_2=\sum_{j=1}^{N}\beta_j p_j,$$

and the coefficients β_j must satisfy

$$\sum_{j=1}^{N}\beta_j=0.$$

Relative to its rest frame Ψ is independent of ρ_1. Thus we can write

$$\Psi(r_1, \ldots, r_N)=\Phi(\rho_2, \ldots, \rho_N)$$

where Φ can be taken as normalised in the internal coordinates. The ground state energy is now given by the minimum value of

$$E(\Psi)=(N-1)\left\langle\Phi\left|\frac{(p_2-p_1)^2}{4m}+\tfrac{1}{2}Nv(\rho_2)\right|\Phi\right\rangle \tag{3}$$

Φ being restricted to a set of wavefunctions such that the corresponding Ψ is totally antisymmetric.

As shown by Hall the energy can be given entirely in terms of ρ_2 and π_2 by noting that

$$\langle\Psi|\pi_2^2|\Psi\rangle=\langle\Psi|p_1^2|\Psi\rangle\sum_{i=1}^{N}\beta_i^2+2\langle\Psi|p_1\,.\,p_2|\Psi\rangle\sum_{i<j=2}^{N}\beta_i\beta_j$$

where again use has been made of the symmetry between the particles. Defining

$$\lambda = \sum_{j=1}^{N} \beta_j^2 = -2 \sum_{i<j=2}^{N} \beta_i \beta_j$$

it follows that

$$\langle \Psi | \pi_2^2 | \Psi \rangle = \tfrac{1}{2} \lambda \langle \Psi | (p_2 - p_1)^2 | \Psi \rangle$$

and so

$$E(\Psi) = (N-1) \left\langle \Phi \left| \frac{\pi_2^2}{2m\lambda} + \tfrac{1}{2} N v(\rho_2) \right| \Phi \right\rangle. \tag{4}$$

The reduced mass factor λ depends on the transformation matrix B and has a minimum value of $\frac{1}{2}$ when $\rho_3, \ldots, \rho_N$ are all orthogonal to ρ_2. Note that as Hall uses a different normalisation for the relative coordinate his λ is twice ours.

We will write

$$K(\lambda) = \frac{\pi_2^2}{2m\lambda} + \tfrac{1}{2} N v(\rho_2)$$

and refer to this as the reduced Hamiltonian. In cases of interest it will have discrete bound eigenstates ϕ_i satisfying

$$K(\lambda) | \phi_i(\lambda) \rangle = \epsilon_i(\lambda) | \phi_i(\lambda) \rangle. \tag{5}$$

Note that each of the energy eigenvalues $\epsilon_i(\lambda)$ decreases monotonically as λ increases as π_2^2 is a positive operator.

3. The reduced density operator for the relative coordinate

In order to reduce the expression for the energy still further, it is necessary to consider resolutions of Φ of the form

$$\Phi(\rho_2, \ldots, \rho_N) = \sum_{i=0}^{\infty} c_i f_i(\rho_2) g_i(\rho_3 \ldots \rho_N) \tag{6}$$

where f_i and g_i are separately normalised. A theorem due to Schmidt (see Coleman 1963) shows that the most rapidly convergent such series expansion is obtained by taking the f_i as eigenstates of the integral operator with kernel

$$D(\rho_2, \rho_2') = (N-1) \int \mathrm{d}\rho_3 \ldots \mathrm{d}\rho_N \Phi(\rho_2 \rho_3 \ldots \rho_N) \Phi^*(\rho_2' \rho_3 \ldots \rho_N).$$

This operator, denoted simply by D, will be called the reduced density operator for the relative coordinate ρ_2. It can be shown to be a Hermitian, positive, bounded operator and therefore has eigenstates f_i satisfying

$$D | f_i \rangle = \gamma_i | f_i \rangle,$$

all the γ_i being real and positive. We have chosen D to be normalised so that

$$\mathrm{Tr}(D) = \sum_{i=0}^{\infty} \gamma_i = N - 1$$

for convenience below.

The optimally convergent series (6) is now obtained by taking the states f_i in order of decreasing γ_i. For each f_i the corresponding co-factor g_i and coefficient c_i is determined by

$$c_i g_i(\rho_3, \ldots, \rho_N) = \int \mathrm{d}\rho_2 f_i^*(\rho_2)\Phi(\rho_2, \rho_3, \ldots, \rho_N),$$

and it should be noted that these co-factors are themselves orthogonal. The coefficients c_i are simply related to the γ_i by

$$\gamma_i = (N-1)|c_i|^2.$$

and the γ_i can be regarded as occupation probabilities of the various relative states f_i.

It must be made quite clear at this stage that the operator D as defined above depends on the definition of the internal coordinates $\rho_3, \ldots, \rho_N$. For two distinct B matrices defining different sets of internal coordinates (2) there appears in general to be no simple relation between the corresponding reduced density operators. On the other hand, if the two sets are such that one can be obtained from the other simply by a transformation of the form

$$\tilde{\rho}_i = \sum_{j=3}^{N} R_{ij}\rho_j; \qquad i = 3, \ldots, N$$

which does not involve ρ_2 then it can be shown that the D operators are in fact the same (the Jacobian $|R|$ cancels as we require Φ to be normalised in both cases). This result can be expressed more succinctly by saying that D only depends on the coefficients β_i which define π_2.

The energy (4) can now be written in terms of D as

$$E(\Psi) = \mathrm{Tr}(DK(\lambda)) = \sum_{i=0}^{\infty} \gamma_i \langle f_i|K(\lambda)|f_i\rangle. \tag{7}$$

The problem of finding the ground state energy is therefore equivalent to minimising the right-hand side of (7) subject to the constraint of antisymmetry in the original wavefunction. This identifies a 'representability problem' similar to that studied by Coleman and others for the reduced density operators for particle coordinates r_i. Explicitly, we would like to know a necessary and sufficient set of conditions on the γ_i and f_i which would ensure that they can arise from a totally antisymmetric N-fermion wavefunction Ψ.

In the absence of a sufficient set of constraints for the γ_i and f_i, a lower bound energy can still be obtained by minimising (7) subject to any known necessary constraints. For a complex system of constraints such a minimisation could pose an insoluble problem in itself. However, the result is straightforward for constraints of the following type

$$\gamma_i \leqslant q \qquad f_i \in M$$

where q is an upper bound for any relative state occupation and M is a linear subspace of allowed relative states f_i. Both q and M might depend on N.

The lower bound energy is obtained under these conditions by identifying the eigenstates f_i of D with those of the reduced Hamiltonian restricted to the subspace M. If P is the projection operator onto this subspace we have

$$PK(\lambda)P|\chi_i\rangle = \xi_i(\lambda)|\chi_i\rangle. \tag{8}$$

Numbering the states so that the ξ_i are non-decreasing the lower bound energy is

$$E_L = \sum_{i=0}^{p-1} q\xi_i + \alpha\xi_p \tag{9}$$

where the first p states have the maximum occupation q and p is determined as the largest integer satisfying

$$pq \leqslant N-1.$$

The overflow into the last occupied state is

$$\alpha = N-1-pq.$$

It has been assumed here that there are at least $(p+1)$ bound states. If this is not the case, the lower bound is obtained by giving the maximal occupation to all the bound states. The total occupation is made up to $(N-1)$ by filling states f_i in the continuum which can be chosen to contribute negligibly to the energy. Thus p in (9) becomes the number of bound states and α becomes zero. Although the density operator D associated with such a lower bound describes an unbound N-body state (the probability of large particle separation does not go to zero) it cannot be assumed that the exact ground state solution has this character.

4. Specific lower bound formulae

If the coordinates $\rho_3, \ldots, \rho_N$ are all chosen to be symmetric in r_1 and r_2 it is clear that the relative states $f_i(\rho_2)$ must carry the antisymmetry between r_1 and r_2. This implies that P becomes the projection operator onto the space of odd functions. Furthermore, the momentum conjugate to ρ_2 is just

$$\pi_2 = \tfrac{1}{2}(p_2 - p_1)$$

and so

$$\lambda = \tfrac{1}{2}.$$

This value of λ maximises the eigenvalues $\xi_i(\lambda)$ and only those corresponding to odd states can occur in the lower bound (9). Unfortunately, the best upper bound q for the occupations currently known in this case is the trivial one

$$\gamma_i \leqslant N-1.$$

The lower bound energy that results is

$$E_{L1} = (N-1)\xi_0(\tfrac{1}{2}) \tag{10}$$

$\xi_0(\frac{1}{2})$ here being the lowest eigenvalue of $K(\frac{1}{2})$ corresponding to an odd state. This lower bound result is due originally to Post (1956) and, as has already been pointed out, the Coleman (1963) bound reduces to this in the absence of external forces.

Another choice for the coordinates $\rho_3, \ldots, \rho_N$ is

$$\rho_i = r_i - r_1, \qquad i = 3, \ldots, N,$$

for which we can derive

$$\lambda = \frac{N-1}{N}.$$

With this set of coordinates $\Phi(\rho_2, \ldots, \rho_N)$ must be antisymmetric in the ρ_i because of the antisymmetry of Ψ in $r_2, \ldots, r_N$. Therefore, Φ has the characteristics of an $(N-1)$-fermion state and in particular

$$\gamma_i \leqslant 1. \tag{11}$$

Ignoring any constraints on the relative states f_i, we have immediately a second lower bound

$$E_{L2} = \sum_{i=0}^{N-2} \epsilon_i\left(\frac{N-1}{N}\right), \tag{12}$$

being the sum over the $N-1$ lowest eigenvalues of $K((N-1)/N)$. Because the $\epsilon_i(\lambda)$ decrease as λ increases, it is apparent that

$$E_{L3} = \sum_{i=0}^{N-2} \epsilon_i(1) \tag{13}$$

is also a lower bound energy and this is in fact the first Carr and Post (1968) bound.

Hall (1967) showed that the value of λ can be decreased to $\frac{2}{3}$ by suitable choice of the coordinates ρ_i while still retaining the occupation upper bound (11). Specifically the occupation upper bound (11) can be derived provided

$$\rho_3 = r_3 - r_1$$

and $\rho_4, \ldots, \rho_N$ are all symmetric in r_1, r_2 and r_3. Under these conditions the minimum value of λ turns out to be $\frac{2}{3}$ and thus we have the Hall lower bound

$$E_{L4} = \sum_{i=0}^{N-2} \epsilon_i(\tfrac{2}{3}). \tag{14}$$

Obviously, Hall's bound (14) is equivalent to (12) for $N = 3$ and is superior for $N > 3$. It is superior to the Carr and Post bound (13) for all N.

These last three bounds have all ignored the possibility that the f_i states might be constrained to some subspace. In fact there is one such constraint that can be applied in all three cases. Because $\Phi(\rho_2, \ldots, \rho_N)$ must vanish whenever $\rho_2 = 0$ $(r_1 = r_2)$ it follows that

$$c_i f_i(\rho_2) = \int \mathrm{d}\rho_3 \ldots \mathrm{d}\rho_N g_i(\rho_3, \ldots, \rho_N)^* \Phi(\rho_2, \rho_3, \ldots, \rho_N)$$

must also vanish. Consequently, all the occupied f_i must satisfy:

$$f_i(0) = 0.$$

The odd eigenstates of (5) already satisfy this constraint, but provided the interaction is non-singular at the origin there will be S-state solutions in three dimensions and even state solutions in one dimension which violate it. By solving the projected problem (9), we find an upward shift in the eigenvalues ϵ_i for these solutions and a consequent improvement in the lower bound. This effect is considered in detail in the next section.

5. Solutions of the constrained eigenproblem

In order to solve the constrained problem (8), it is convenient to regard the constraint introduced in the last section as an orthogonality condition. In fact the allowed wavefunctions must be orthogonal to the δ function as

$$\langle \delta | f \rangle = \int \mathrm{d}\rho \, \delta(\rho) f(\rho) = f(0) = 0.$$

The projection operator P in (8) projects onto the subspace orthogonal to $|\delta\rangle$. Now if f is an eigenstate of the projected reduced Hamiltonian it must satisfy

$$P(K-\xi)|f\rangle = 0$$

or equivalently

$$(K-\xi)|f\rangle = \mu|\delta\rangle \tag{15}$$

for some μ. The solutions f to (15) fall into two classes. If $\mu = 0$, we have

$$(K-\xi)|f\rangle = 0$$

and by definition f satisfies the constraint

$$\langle \delta | f \rangle = 0.$$

Such solutions are just those solutions of the unconstrained problem which satisfy the constraint coincidentally. If $\mu \neq 0$ we can extract the equation

$$\langle \delta | (K-\xi)^{-1} | \delta \rangle = 0 \tag{16}$$

for ξ. For each ξ_i satisfying this equation, the solution f_i is given by

$$|f_i\rangle = \mu_i (K-\xi_i)^{-1} |\delta\rangle$$

where μ_i is now seen to be a normalisation factor. From what has been said the f_i obtained this way must all be orthogonal to one another and orthogonal to the $\mu = 0$ solutions. This result could also be derived directly.

Equation (16) for ξ can be written as

$$\sum_{i=0}^{\infty} \frac{|\phi_i(0)|^2}{\epsilon_i - \xi} = 0 \tag{17}$$

from which it can be seen that the solutions ξ are sandwiched between the poles of the left-hand side. These poles are just the eigenvalues corresponding to unconstrained solutions of (5) which violate the constraint.

For the model problems to be considered below the $\phi_i(0)$ are all known and (17) can be used to evaluate the energies ξ_j. However, for a general interaction v this approach is not possible and (15) must be solved directly.

6. The improved bounds for some model problems

The first model problem we consider is that of N fermions in one dimension interacting with harmonic forces. This problem has been discussed by Post and Hall for the

earlier bounds and the exact solution is known (Post 1953). The interaction is

$$v(x_i - x_j) = k^2(x_i - x_j)^2$$

and the unconstrained reduced Hamiltonian problem is

$$\left(-\frac{\hbar^2}{2m\lambda}\frac{\mathrm{d}^2}{\mathrm{d}x^2} + \frac{Nk^2}{2}x^2 - \epsilon_i\right)\phi_i(x) = 0.$$

The solutions of this are well known as

$$\epsilon_i = (2i+1)e(\lambda)$$

where

$$e(\lambda) = \left(\frac{Nk^2\hbar^2}{4m\lambda}\right)^{1/2}. \tag{18}$$

The odd states (i odd) satisfy the constraint

$$\phi_i(0) = 0$$

whereas the even ones do not and their eigen-energies become shifted. The constrained energies can be obtained using

$$\phi_{2i}(0) = (-1)^i \pi^{-1/4} \frac{\sqrt{(2i)!}}{2^i i!}.$$

Introducing the dimensionless energy variable

$$\nu = \xi / e(\lambda),$$

the equation for ν is

$$S(\nu) \equiv \sum_{i=0}^{\infty} \frac{1 \cdot 3 \ldots (2i-1)}{2 \cdot 4 \ldots (2i)} \frac{1}{4i+1-\nu} = 0.$$

The ratio of successive terms in this series, for large i becomes

$$\frac{t_{i+1}}{t_i} = 1 - \frac{3}{2i} + \mathrm{O}\left(\frac{1}{i^2}\right),$$

and so by Raabes test (Ferrar 1938) the series converges even though it does so very slowly. Fortunately the series can be expressed in terms of the Γ function after noting that

$$\int_0^1 \mathrm{d}x\, x^{-\mu}(1-x)^{-1/2}$$

$$= \sum_{i=0}^{\infty} \frac{1 \cdot 3 \ldots (2i-1)}{2 \cdot 4 \ldots (2i)} \frac{1}{i+1-\mu}$$

$$= \Gamma(\tfrac{1}{2})\Gamma(1-\mu)/\Gamma(\tfrac{3}{2}-\mu).$$

For $\mu > 1$ this relation still holds using the standard analytic continuation of the Γ function (Copson 1935). It follows that

$$S(\nu) = \frac{\frac{1}{4}\Gamma(\frac{1}{2})\Gamma(\frac{1}{4}(1-\nu))}{\Gamma(\frac{1}{4}(3-\nu))}.$$

The zeros of $S(\nu)$ are given by the poles of the denominator on the right-hand side and we have immediately:

$$\xi_i = (4i+3)e(\lambda).$$

The constraint therefore shifts each even state energy by $2e$ to become degenerate with the next odd state.

Figure 1 shows the resulting modified Hall bound as a function of N and compares it with the other lower bounds and the exact result.

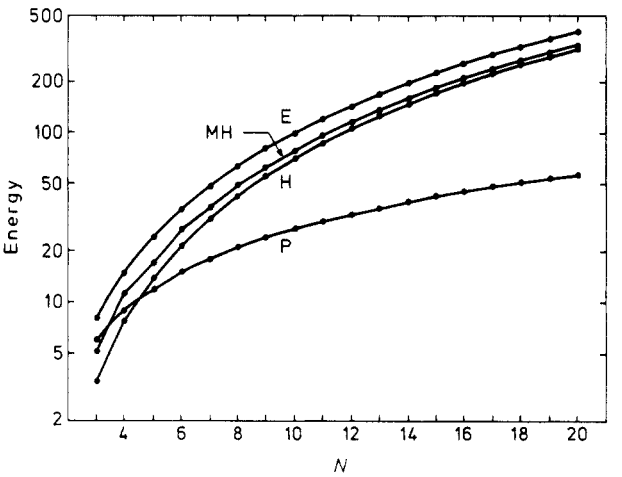

Figure 1. The Post (P), Hall (H) and modified Hall (MH) lower bound energies, for the one-dimensional harmonic force problem, compared with the exact energy (E) as a function of N, the number of fermions. The energy is given in units of $e(\frac{1}{2})$ defined by equation (18).

The second model problem we consider is that of N fermions in three dimensions interacting with harmonic forces. The interaction is

$$v(r_i - r_j) = k^2(r_i - r_j)^2$$

and the treatment of this closely parallels that of the one-dimensional case above.

The unconstrained eigenvalues for the reduced Hamiltonian are

$$\epsilon_{nlm} = (4n+2l+3)e(\lambda)$$

where

$$e(\lambda) = \left(\frac{Nk^2\hbar^2}{4m\lambda}\right)^{1/2}. \tag{19}$$

Only the S-states ($l=0$) violate the constraint and the corresponding constrained energies ξ must satisfy

$$\nu = \xi/e(\lambda),$$

$$S(\nu) = \sum_{n=0}^{\infty} \frac{3.5\ldots(2n+1)}{2.4\ldots(2n)} \frac{1}{4n+3-\nu} = 0.$$

The infinite series can be treated similarly to that in the one-dimensional case and the equation for ν becomes

$$S(\nu)=\frac{\frac{1}{4}\Gamma(-\frac{1}{2})\Gamma(\frac{1}{4}(7-\nu))}{\Gamma(\frac{1}{4}(5-\nu))}=0.$$

Immediately then the shifted energies are at

$$\xi_n=(4n+5)e(\lambda),$$

the shift being just $2e$ for each S-state.

Figure 2 shows the resulting modified Hall bound in this case and compares it with the other lower bounds and the exact result.

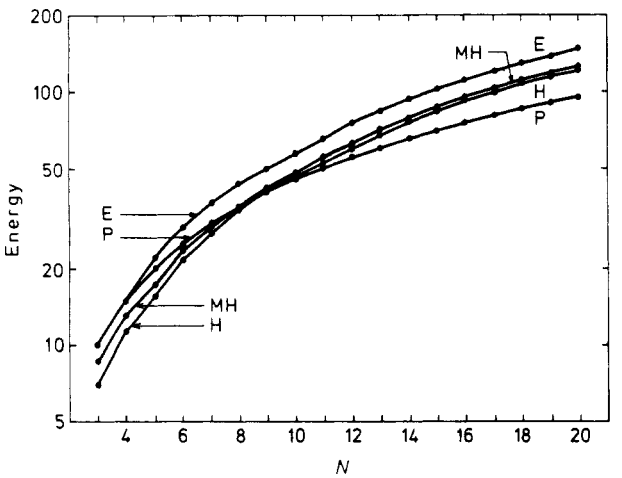

Figure 2. The Post (P), Hall (H) and modified Hall (MH) lower bound energies, for the three-dimensional harmonic force problem, compared with the exact energy (E) as a function of N, the number of fermions. The energy is given in units of $e(\frac{1}{2})$ defined by equation (19).

The third model problem we shall consider is the rather more realistic one of an attractive 'gravitational' force in three dimensions. In this case the exact result is not known but a comparison of the various lower bounds is still of interest.

The interaction potential is

$$v(r_i-r_j)=-\frac{k}{|r_i-r_j|}$$

and the unconstrained reduced Hamiltonian is equivalent to that of the hydrogen atom.

The unconstrained energies are therefore

$$\epsilon_{nlm}=-\frac{e(\lambda)}{(n+l+1)^2},$$

where the energy scale is now

$$e(\lambda)=\frac{\lambda mN^2k^2}{8\hbar^2}. \tag{20}$$

Once again the constraint that the wavefunction go to zero at zero particle separation affects only the S-states. To evaluate the shifted energies for these states we use (17) and

$$\phi_{n00}(0) = \pi^{-1/2}\left(\frac{Nkm\lambda}{\hbar^2(n+1)}\right)^{3/2}.$$

It is convenient now to introduce the dimensionless variable μ so

$$\xi = -e(\lambda)/\mu^2$$

and the equation for μ becomes

$$S(\mu) = \sum_{n=0}^{\infty} \frac{1}{(n+1)^3 - \mu^2(n+1)} = 0.$$

The author has been unable to find any useful expression for this series comparable to the two previous cases. However, this series is rapidly convergent and it is quite easy to solve the last equation numerically. It should be noted that neglected terms in the series can be bracketed by the inequalities

$$\int_{m+1}^{\infty} \frac{dx}{x^3 - \mu^2 x} < \sum_{n=m}^{\infty} \frac{1}{(n+1)^3 - \mu^2(n+1)} < \int_{m}^{\infty} \frac{dx}{x^3 - \mu^2 x}$$

where

$$\int_{m}^{\infty} \frac{dx}{x^3 - \mu^2 x} = \frac{1}{\mu^2} \ln\left(\frac{m}{(m^2 - \mu^2)^{1/2}}\right).$$

Using this result the maximum error in the numerical solution can be carefully controlled. We have obtained the following values for the first four roots:

$$\mu = 1{\cdot}691,\ 2{\cdot}751,\ 3{\cdot}780,\ 4{\cdot}799$$

or

$$\xi = 0{\cdot}350e(\lambda),\ 0{\cdot}132e(\lambda),\ 0{\cdot}070e(\lambda),\ 0{\cdot}043e(\lambda).$$

Figure 3 shows the resulting modification to the Hall bound and gives the Post bound for comparison.

7. Behaviour of the lower bounds as $N \to \infty$

In the case of the harmonic interaction problems for one or three dimensions discussed above, the lower bound energy behaves asymptotically as N^2. The exact energy which is known in this case also behaves asymptotically as N^2. For the gravitational problem the lower bound energy collapses as $N^{7/3}$ and in this case an upper bound has been derived (Levy-Leblond 1969) which also collapses as $N^{7/3}$. Thus it is heartening to observe that the lower bound gives the correct power law behaviour for these non-saturating cases. However, the lower bound formulae developed so far unfortunately do not give the correct asymptotic behaviour for saturating potentials (for which the exact energy goes as N).

To demonstrate this point we consider a potential with a finite negative part, the minimum (negative) value being $V_{\min}$. Given a suitable repulsive core we can expect the N-fermion ground state energy to be proportional to N for large N. The

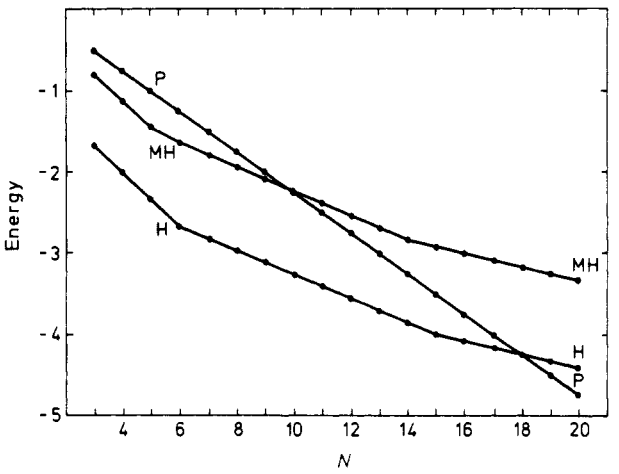

Figure 3. The Post (P), Hall (H) and modified Hall (MH) lower bound energies, for the attractive gravitational force, as a function of N, the number of fermions. The energy is given in units of $e(\frac{1}{2})$ defined by equation (20).

eigenvalues of (5) will now be written as $\epsilon_i(N)$ to emphasise their dependence on N. It is obvious that the $\epsilon_i(N)$ decrease monotonically as N increases, but the rate of decrease is bounded below by

$$\tfrac{1}{2}NV_{\min} < \epsilon_i(N).$$

Furthermore, it follows from the work of Martin (1972) that for any

$$e > V_{\min}$$

the number of eigenvalues less than $\frac{1}{2}Ne$, i.e., satisfying

$$\tfrac{1}{2}NV_{\min} < \epsilon_i(N) \leqslant \tfrac{1}{2}Ne$$

increases asymptotically as $N^{3/2}$. As a corollary of this the Nth eigenvalue must satisfy

$$\epsilon_N(N) \leqslant \tfrac{1}{2}Ne$$

for N sufficiently large. Thus, in the large-N limit the lower bound

$$E_L(N) = \sum_{i=0}^{N-1} \epsilon_i(N)$$

consists of N terms all approaching $\frac{1}{2}NV_{\min}$ whence

$$E_L \sim \tfrac{1}{2}N^2 V_{\min}.$$

The author believes that this result also holds for (8) when the relative wavefunctions are subject to some general constraint. It certainly holds for the specific constraint

$$\phi_i(0) = 0$$

which was considered in detail above.

This analysis shows that the lower bounds for fermion systems do not exhibit saturation even though the interaction may have an infinite hard core and require saturation classically on simple geometrical grounds. Clearly the constraints that have been imposed on the reduced density operator D so far are still seriously deficient for large N.

The nature of this deficiency can be seen in more detail by considering the behaviour of the correlation function for the lower bound system. For any choice (2) of coordinates the correlation function is proportional to the diagonal part

$$D(\rho_2, \rho_2)$$

of the reduced density operator. The constant of proportionality depends on the normalisation chosen for the correlation function and need not concern us. For the lower bound system

$$D(\rho_2, \rho_2) = q \sum_{i=0}^{p-1} |\phi_i(\rho_2)|^2 + \alpha |\phi_p(\rho_2)|^2$$

and from the analysis above the wavefunctions ϕ_i are confined around the minimum of the potential $V(\rho_2)$ as $N \to \infty$. The resulting correlation function is small except in the neighbourhood of this minimum. The picture emerges then of one particle at the centre of a sphere on which the remaining $N-1$ particles are held by the interaction with the first. Antisymmetry has been imposed on the $N-1$ particles, but does not extend to the particle at the centre. Removing this antisymmetrisation constraint, which was necessary to obtain a soluble problem, has removed the effect of the interaction between the $N-1$ particles and thus allowed the collapse.

Having identified the nature of the problem in this way the question arises as to how the reduced density operator D can be further constrained to prevent the collapse. In terms of the occupations γ_i of the relative states, it is clear that the number of occupied states must increase at least as fast as $N^{3/2}$. This question of additional constraints on D will be taken up in a subsequent paper.

8. Conclusion

It has been shown that currently known lower bound energies for many-fermion systems can be viewed in a unified way using the reduced density operator D for the interparticle separation. Furthermore, there is a range of possibilities for D associated with the freedom of choice in the internal coordinates.

Lower bound energies are obtained simply from partial solutions of the representability problem for D. In fact the quality of the lower bound result can be taken as a useful measure of how close we are to the full solution of the representability problem.

The freedom of choice in the internal coordinates also affects the reduced Hamiltonian K and the constraints on D which make up a partial solution of the representability problem. It has been seen that no single choice for D gives the best lower bound for all N. Here we have finally used two choices, corresponding to the Post and modified Hall bounds, after discarding others which gave inferior bounds. Whereas Hall (1967) has discussed an 'optimum' choice for the internal coordinates it must now be realised that this was done in the context of a particular partial solution to the representability problem. With the simple improvement to the solution of the

representability problem introduced above Hall's internal coordinates are still optimal. However, there is no guarantee that they will remain so for subsequent improvements. Indeed this is already demonstrated by the Post bound which exploits an alternative partial solution of the representability problem and produces a better lower bound for small N.

Apart from the small-N limit the modified Hall bound presented here is the best such lower bound for general fermion interactions. It should be noted here that we are not comparing with bounds of the type described by Balbutsev *et al* (1976) which depend on a knowledge of solutions for the few (>2)-body problem. Despite the fact that this is the best known lower bound it is not able to exhibit saturation for the type of interactions occurring between molecules or nucleons. To obtain saturating lower bounds further understanding must be gained of the constraints on the relative coordinate reduced density operator which must hold for many-particle systems.

References

Balbutsev E B, Irgasiev B F, Majling L, Mikhailov I N and Řizek J 1976 *J. Phys. G: Nucl. Phys.* **2** 681–8
Carr R J M and Post H R 1968 *J. Phys. A: Gen. Phys.* **1** 596–609
—— 1971 *J. Phys. A: Gen. Phys.* **4** 665–78
Coleman A J 1963 *Rev. Mod. Phys.* **35** 668–89
—— 1965 *J. Math. Phys.* **6** 1425–31
Copson E T 1935 *An Introduction to the Theory of Functions of a Complex Variable* (London: Oxford University Press) p 212
Ferrar W L 1938 *A Text-Book of Convergence* (London: Oxford University Press) p 30
Hall R L 1967 *Proc. Phys. Soc.* A **91** 16–22
Levy-Leblond J-M 1969 *J. Math. Phys.* **10** 806–12
Lieb E H 1976 *Rev. Mod. Phys.* **48** 553–69
Martin A 1972 *Helv. Phys. Acta* **45** 140
Post H R 1953 *Proc. Phys. Soc.* **66** 649–52
—— 1956 *Proc. Phys. Soc.* **69** 936–8