Many-particle systems VI. *N*-fermion systems: derivation of a lower-bound shell model

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VI. N-fermion systems: derivation of a lower-bound shell model

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Abstract. The programme of reducing N-particle problems to one-particle problems is extended to include the Pauli principle. To calculate the ground-state energy of a system of N fermions interacting by pair forces, a rigorous lower-bound shell model is derived. This shell model follows a building-up principle, and tends to improve with increasing number of particles as well as with increasing strength of interaction. For twenty particles antisymmetric in ordinary space interacting by square-well interaction of strength $V_0 a^2 = 200\hbar^2/2m$ the shell model differs by less than 8% from the calculated upper bound, and hence *a fortiori* from the exact energy. In order to test the quality of the approximation for various interactions, it was necessary to calculate upper bounds.

1. Introduction

The N-particle problem has been solved exactly in quantum mechanics in the case of a few interactions (Hooke's forces‡, delta functions in one dimension§) only. The quantum-mechanical N-particle problem is, of course, simpler than the corresponding classical problem in at least two respects: we do not specify positions and momenta independently, and we have the strong symmetry restrictions arising from the non-individuality of particles.∥

The latter restriction was used in II to reduce the N-particle problem to an equivalent one-particle variational problem¶ subject to the condition that the trial functions be translation-invariant and totally symmetric (in the case of bosons) or totally antisymmetric (in the case of fermions). The requirement of translation invariance is far from trivial in its consequences. On the other hand, it is just the translation invariance requirement in conjunction with the symmetry requirement that renders the reduction of the trial function to the space of one (vector) variable difficult.

In the case of bosons we dropped the symmetry requirement to arrive at a lower bound for the ground-state energy. This lower bound turned out to be close to the exact value for a large range of interactions (III, IV, V). This was proved by comparison with an easily determined upper bound. It is still not clear why the lower bound should provide such a good estimate for bosons with short-range interactions. It is at the same time a lower bound for the energy of N fermions with the same interaction, but would hardly be expected to be close to the exact ground-state energy in that case.

In the case of fermions it can easily be proved that for $N \geqslant 3$, no single trial function in the one (vector) variable can be the projection of the totally antisymmetric wave function

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‡ For example, Post (1953); that paper and Post (1956), Post (1962), Hall and Post (1967), Hall (1967) will be referred to as I, II, III, IV and V, respectively.

§ McGuire (1964).

∥ This condition is stronger than mere indistinguishability (which is ensured by the symmetry of all operators corresponding to possible measurements). The latter would not, for instance, allow the reduction to one-particle problems used in this and preceding papers of this series.

¶ We do not consider a reduction to an irreducible two-particle problem (cf. Bopp's (1959) reduction of an N-electron atom to the helium problem) a solution of the N-body problem. Such a reduction is already implied in the limited number of double integrals involved in the case of pair interactions. We are concerned with the reduction to a one-particle problem, and are dealing with an N-particle system in translation-invariant formulation.

on to that subspace of one variable. Instead of developing a quantitative estimate of the maximum contribution of any one function, we proceed in this paper to derive a lower-bound model in the general case of N fermions. This lower-bound model is a shell model exhibiting a Pauli 'Aufbau-prinzip'.†

2. Proof

We consider a system of N identical particles with pair interaction in three dimensions. The Hamiltonian is

$$H = -\frac{\hbar^2}{2m} \sum_{i=1}^{N} \Delta_{r_i} + \sum_{i<j=1}^{N} V(|r_i - r_j|)$$

where m is the mass of any particle, and the ith particle has the position vector r_i.

Let us consider the class of normalized translation-invariant trial functions $\Psi(r_1, r_2, ..., r_N)$ for the problem, obeying the usual boundary conditions of quantum mechanics. Since we have identical particles, we further restrict this class to those functions which are symmetric with respect to the interchange of any pair of particles 1, 2, ..., N if they are bosons (or antisymmetric if they are fermions). We denote this symmetry (or antisymmetry) by writing $\Psi(\overline{r_1, r_2, ..., r_N})$ for any member of this sub-class which we label the class L. The ground-state energy E_0 for the system is given by

$$E_0 = \text{minimum of } (\Psi, H\Psi)$$

the minimization being with respect to *all functions of the class L*. We are insisting on translation invariance; therefore the variables $r_1, r_2, ..., r_N$ are not independent. Throughout this section we have only $3N$-3 *independent* variables.

We may consider E_0 to be the expectation value, minimized with respect to functions of class L, of a new Hamiltonian

$$H_1 = -\frac{\hbar^2}{2m} \Delta_{r_1} + \sum_{i=2}^{N} \left\{ -\frac{\hbar^2}{2m} \Delta_{r_i} + \tfrac{1}{2} N V(|r_i - r_1|) \right\}$$

since all Ψ are symmetric (or antisymmetric) in the particles 1, 2, ..., N. Thus

$$E_0 = \text{minimum of } (\Psi(\overline{r_1, r_2, ..., r_N}), H_1\Psi(\overline{r_1, r_2, ..., r_N})).$$

The condition of symmetry (or antisymmetry) with respect to the interchange of particle 1 with any of the particles 2, 3, ..., N is now dropped. We may now choose from a larger class of functions M when minimizing. Symmetry (or antisymmetry) in 2, 3, ..., N is a necessary condition for symmetry (or antisymmetry) in 1, 2, 3, ..., N, since L ⊂ M. With this larger choice M (retaining translation invariance and all previous conditions except for the relaxation of symmetry (antisymmetry)), it may be possible to minimize further, and in any case we can still obtain E_0 as before. Hence

$$E_0 \geqslant \text{minimum of } (\Psi_1(r_1, \overline{r_2, ..., r_N}), H_1\Psi_1(r_1, \overline{r_2, ..., r_N}))$$

where Ψ_1 denotes any member of the class M. The particular function of the class M which minimizes this will be written $\psi_1(r_1, \overline{r_2, ..., r_N})$. Thus

$$E_0 \geqslant (\psi_1, H_1\psi_1) \tag{1}$$

† This model was found by one of us several years ago. Subsequent work, also reported here, was largely devoted to the sometimes somewhat elaborate task of establishing upper bounds to arrive at an upper (pessimistic) estimate for the error involved in substituting the lower bound for the exact value of the ground-state energy. This indirect checking incidentally involved the use of computers. The object of projects like the present one is, of course, to derive a general solution, a finite expression to supersede any collection of numbers put out by computers.

where ψ_1 is symmetric (or antisymmetric) in at least particles 2, 3, ..., N.

Let the mass of particle 1 be denoted by m_1. The Hamiltonian H_1 becomes

$$H_2 \equiv -\frac{\hbar^2}{2m_1}\Delta_{r_1} + \sum_{i=2}^{N}\left\{-\frac{\hbar^2}{2m}\Delta_{r_i} + \tfrac{1}{2}NV(|r_i - r_1|)\right\} = H_1 \qquad (2)$$

when $m_1 = m$. If the mass m_1 is increased, the expectation value

$$(\psi_1(r_1, \overline{r_2, ..., r_N}), H_2\psi_1(r_1, \overline{r_2, ..., r_N}))$$

if we keep the same function ψ_1 defined as above, decreases algebraically, i.e.

$$(\psi_1, H_2\psi_1)_{m_1 \geqslant m} \leqslant (\psi_1, H_2\psi_1)_{m_1 = m}. \qquad (3)$$

This follows immediately from noting that

$$-(\psi_1, \Delta_{r_i}\psi_1) = (\nabla_{r_i}\psi_1, \nabla_{r_i}\psi_1) \geqslant 0$$

and hence that $-(\hbar^2/2m)(\psi_1, \Delta_{r_i}\psi_1)$ is a decreasing function of m. Thus from (1), (2) and (3), for any $m_1 \geqslant m$,

$$E_0 \geqslant (\psi_1, H_1\psi_1) \geqslant (\psi_1, H_2\psi_1). \qquad (4)$$

We introduce new coordinates ρ_i by means of the transformation

$$\begin{pmatrix} M^{1/2}\rho_1 \\ m^{1/2}\rho_2 \\ m^{1/2}\rho_3 \\ \vdots \\ m^{1/2}\rho_N \end{pmatrix} = \begin{pmatrix} \left(\frac{m_1}{M}\right)^{1/2} & \left(\frac{m}{M}\right)^{1/2} & \left(\frac{m}{M}\right)^{1/2} & \cdots & \left(\frac{m}{M}\right)^{1/2} \\ -\left(\frac{m}{m+m_1}\right)^{1/2} & \left(\frac{m_1}{m+m_1}\right)^{1/2} & 0 & & 0 \\ -\left(\frac{m}{m+m_1}\right)^{1/2} & 0 & \left(\frac{m_1}{m+m_1}\right)^{1/2} & & 0 \\ & & & \text{etc.} \\ \vdots & & & \\ -\left(\frac{m}{m+m_1}\right)^{1/2} & 0 & 0 & & \left(\frac{m_1}{m+m_1}\right)^{1/2} \end{pmatrix} \begin{pmatrix} m_1^{1/2}r_1 \\ m^{1/2}r_2 \\ m^{1/2}r_3 \\ \vdots \\ m^{1/2}r_N \end{pmatrix}. \qquad (5)$$

M is the total mass of the system, i.e. $M = m_1 + (N-1)m$. Thus from (4)

$$E_0 \geqslant (\psi_1, H_2\psi_1) \equiv (\psi_1, H_3\psi_1) \qquad (6)$$

where

$$H_3 = -\frac{\hbar^2}{2M}\Delta_{\rho_1} - \frac{\hbar^2}{2m}\sum_{i=2}^{N}\Delta_{\rho_i} - \frac{\hbar^2}{m+m_1}\sum_{i<j=1}^{N}\nabla_{\rho_i}\cdot\nabla_{\rho_j} + \tfrac{1}{2}N\sum_{i=2}^{N}V\left\{\left(\frac{m+m_1}{m_1}\right)^{1/2}\rho_i\right\}.$$

The expectation values $(\psi_1, H_2\psi_1)$ and $(\psi_1, H_3\psi_1)$ denote the same *physical* quantity. The transformation (5) merely changes the coordinates. It should be noted that ρ_1 is the centre-of mass coordinate and is orthogonal to $\rho_2, \rho_3, ..., \rho_N$. Initially we took ψ_1 to be translation-invariant. Thus, if we denote by ψ_2 the function obtained by expressing ψ_1 in terms of $\rho_1, \rho_2, ..., \rho_N$ then

$$\psi_1(r_1, \overline{r_2, ..., r_N}) \equiv \psi_2(\rho_2, ..., \rho_N).$$

(ψ_2 is symmetric (or antisymmetric) in at least particles 2, 3, ..., N.) Hence from (6)

$$E_0 \geqslant (\psi_1, H_3\psi_1) \equiv (\psi_2, H_3\psi_2). \qquad (7)$$

The only term in H_3 which contains ρ_1 is the kinetic energy term for the centre of mass.

Thus from (7), for any $m_1 \geqslant m$,

$$E_0 \geqslant (\psi_2, H_3\psi_2) \equiv (\psi_2(\boldsymbol{\rho}_2, ..., \boldsymbol{\rho}_N), H_4\psi_2(\boldsymbol{\rho}_2, ..., \boldsymbol{\rho}_N))$$

$$H_4 = -\frac{\hbar^2}{2m} \sum_{i=2}^{N} \Delta_{\rho_i} - \frac{\hbar^2}{m+m_1} \sum_{i<j=2}^{N} \nabla_{\rho_i} \cdot \nabla_{\rho_j} + \tfrac{1}{2}N \sum_{i=2}^{N} V\left\{\left(\frac{m+m_1}{m_1}\right)^{1/2} \rho_i\right\}. \quad (8)$$

From (6), (7) and (8) we have $(\psi_1, H_2\psi_1) \equiv (\psi_2, H_4\psi_2)$; thus the inequality (3) becomes

$$(\psi_2, H_4\psi_2)_{m_1 \geqslant m} \leqslant (\psi_2, H_4\psi_2)_{m_1=m}. \quad (9)$$

Now, let $m_1 \to \infty$ while retaining the trial function ψ_2. All the elements of the square matrix in (5) tend to zero except the diagonal elements, which tend to unity. The coordinates $\boldsymbol{\rho}_2, ..., \boldsymbol{\rho}_N$ become orthogonal and identical with $\boldsymbol{r}_2, ..., \boldsymbol{r}_N$, respectively. In the limit (9) becomes

$$\lim_{m_1 \to \infty} (\psi_2, H_4\psi_2) \leqslant (\psi_2, H_4\psi_2)_{m_1=m}. \quad (10)$$

We have from (8) and (10)

$$E_0 \geqslant \lim_{m_1 \to \infty} (\psi_2, H_4\psi_2) = (\psi_2(\overline{\boldsymbol{r}_2, ..., \boldsymbol{r}_N}), \mathscr{H}\psi_2(\overline{\boldsymbol{r}_2, ..., \boldsymbol{r}_N})) \quad (11)$$

where

$$\mathscr{H} = \sum_{i=2}^{N} \left\{-\frac{\hbar^2}{2m} \Delta_{r_i} + \tfrac{1}{2}NV(r_i)\right\}.$$

The expectation value of $\mathscr{H}$ is now minimized with respect to the functions of class M, thus maintaining or strengthening the inequality (11). The minimizing function is the lowest eigenfunction of $\mathscr{H}$, which we denote by $\Phi(\overline{\boldsymbol{r}_2, \boldsymbol{r}_3, ..., \boldsymbol{r}_N})$. Let

$$h_i = -\frac{\hbar^2}{2m}\Delta + \tfrac{1}{2}NV(r_i)$$

with

$$h_i\varphi_n(\boldsymbol{r}_i) = \epsilon_n\varphi_n(\boldsymbol{r}_i);$$

we take φ_n to be normalized to unity. Then

$$\mathscr{H} = \sum_{i=2}^{N} h_i.$$

We have a shell system of $N-1$ independent particles interacting with a fixed centre of force, a model whose ground-state energy is a lower bound to the true energy of the original problem.

To construct the lower bound, we simply fill the lowest $N-1$ levels of the shell model. For a boson system all particles may occupy the same state. The function Φ is simply the product $\varphi_0(\boldsymbol{r}_2) \varphi_0(\boldsymbol{r}_3) ... \varphi_0(\boldsymbol{r}_N)$, where φ_0 is the ground state of h_i, giving a lower bound which we shall denote by $\mathscr{E}$, such that $E_0 \geqslant \mathscr{E} = (N-1)\epsilon_0$, where ϵ_0 is the lowest eigenvalue of h_i.

For fermions each shell-model particle must occupy a different state. The lowest eigenfunction of $\mathscr{H}$ will be the Slater determinant formed from the first $N-1$ eigenfunctions of h_i, namely

$$\frac{1}{\{(N-1)!\}^{1/2}} \begin{vmatrix} \varphi_0(\boldsymbol{r}_2) & \varphi_1(\boldsymbol{r}_2) & \cdots & \varphi_{N-2}(\boldsymbol{r}_2) \\ \varphi_0(\boldsymbol{r}_3) & \varphi_1(\boldsymbol{r}_3) & & \\ \vdots & & & \\ \varphi_0(\boldsymbol{r}_N) & & & \varphi_{N-2}(\boldsymbol{r}_N) \end{vmatrix}$$

giving a lower bound $\mathscr{E} = \epsilon_0 + \epsilon_1 + ... + \epsilon_{N-2}$. If we introduce spin the degeneracies of the shell-model levels are correspondingly increased.

3. Hooke's interaction

The method described above will be applied to some fermion systems with central force interactions. The lower bound will be compared with upper bounds obtained using the Rayleigh–Ritz variational principle. First, however, we discuss a system for which the true energy is known. The problem of N fermions interacting by Hooke's law forces has been solved exactly. We shall use the solution given by Post (1953). The ground-state energy in the one-dimensional problem is given by $E_0 = (N^2-1)\sqrt{N}k'$, for an interaction $V_{ij} = k^2(x_i - x_j)^2$ between the ith and jth particles $(k' = (\hbar^2/2m)^{1/2}k)$. For the same problem the lower bound is given by $\mathscr{E} = (N-1)^2(\tfrac{1}{2}N)^{1/2}k'$.

As a criterion of quality we take the ratio of exact (or upper-bound) to lower-bound energies when these are measured in the usual manner from the bottom of the continuous spectrum. This ratio will be less than unity and must increase to show improvement. For bound states the energies will be negative, the corresponding magnitudes being the 'binding energies'. In the case of the 'harmonic oscillator' interaction, however, the energies are positive and the concept of 'binding energy' is not strictly applicable. The zero of energy in the case of 'harmonic oscillator' interaction is taken for all particles coincident, with no kinetic energy. From above $E_0/\mathscr{E} = \sqrt{2}(N+1)/(N-1)$, which is greater than unity and decreases monotonically with N. In this sense the lower bound improves in this case as the number of particles is increased.

For an interaction $V_{ij} = k^2(\mathbf{r}_i - \mathbf{r}_j)^2$ in three dimensions we do not have an explicit energy expression for any and all N. The energy of the ground state is given by $E_0 = (3+5+5+5+ \ldots)\sqrt{N}k' - 3\sqrt{N}k'$ to N terms in the bracket. We have 'shells' of $\tfrac{1}{2}(m+1)(m+2)$ levels, each level of energy $(2m+3)\sqrt{N}k'$; $m = 0, 1, 2, \ldots$. For the corresponding lower bound $\mathscr{E} = (3+5+5+5+ \ldots)(\tfrac{1}{2}N)^{1/2}k'$ to $N-1$ terms in the bracket. Again each shell has $\tfrac{1}{2}(m+1)(m+2)$ levels, but of energy $(2m+3)(\tfrac{1}{2}N)^{1/2}k'$; $m = 0, 1, 2, \ldots$. We see that $(E_0/\mathscr{E})_N > (E_0/\mathscr{E})_{N+1}$ except when N gives a closed 'shell' for the exact problem.

Let us consider those values of N which give $q+1$ closed 'shells' for the exact problem, i.e.

$$N = \sum_{m=0}^{q} \tfrac{1}{2}(m+1)(m+2) = \tfrac{1}{6}(q+1)(q+2)(q+3).$$

For these cases we can write

$$E_0 = \sum_{m=0}^{q} \tfrac{1}{2}(m+1)(m+2)(2m+3)\sqrt{N}k' - 3\sqrt{N}k'$$

$$= \tfrac{1}{4}(q+1)(q+2)^2(q+3)\sqrt{N}k' - 3\sqrt{N}k'$$

and

$$\mathscr{E} = \sum_{m=0}^{q} \tfrac{1}{2}(m+1)(m+2)(2m+3)(\tfrac{1}{2}N)^{1/2}k' - (2q+3)(\tfrac{1}{2}N)^{1/2}k'$$

$$= \tfrac{1}{4}(q+1)(q+2)^2(q+3)(\tfrac{1}{2}N)^{1/2}k' - (2q+3)(\tfrac{1}{2}N)^{1/2}k'.$$

Comparing successive closed 'shells', we see that $(E_0/\mathscr{E})_q > (E_0/\mathscr{E})_{q+1}$. We have the same overall trend of improvement as N increases.

4. Square-well interaction

The problem of interaction by 'square-well' forces will be considered next. First, we take the one-dimensional case:

$$V_{ij} = -V_0 f\left(\frac{x_{ij}}{a}\right), \qquad f(x) = \begin{cases} 1, & x < 1 \\ 0, & x > 1. \end{cases}$$

The reduced Hamiltonian

$$h_i = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x_i^2} - \tfrac{1}{2}NV_0 f\left(\frac{|x_i|}{a}\right).$$

We introduce the dimensionless quantities E' and V', defined as

$$E' = \frac{2mEa^2}{\hbar^2}, \qquad V' = \frac{2mV_0a^2}{\hbar^2}.$$

Eigenvalues of h_i are found by solving the equations

$$\begin{aligned} \alpha \tan \alpha &= \beta \qquad \text{(even solutions)} \\ \alpha \cot \alpha &= -\beta \qquad \text{(odd solutions)} \end{aligned} \tag{12}$$

where

$$\alpha = (\tfrac{1}{2}NV' + E')^{1/2}, \qquad \beta = (-E')^{1/2}.$$

We do not have explicit solutions for the equations (12), but if α_m satisfies one of them we may write

$$\tfrac{1}{2}m\pi \leqslant \alpha_m \leqslant \tfrac{1}{2}(m+1)\pi; \qquad m = 0, 1, 2, \ldots .$$

These inequalities lead to bounds on the shell-model energy $\mathscr{E}'$:

$$\tfrac{1}{4}\pi^2 \sum_{m=0}^{N-2} m^2 - \tfrac{1}{2}N(N-1)V' \leqslant \mathscr{E}' \leqslant \tfrac{1}{4}\pi^2 \sum_{m=0}^{N-2} (m+1)^2 - \tfrac{1}{2}N(N-1)V'$$

i.e.

$$\frac{\pi^2}{24}(N-1)(N-2)(2N-3) - \tfrac{1}{2}N(N-1)V' \leqslant \mathscr{E}' \leqslant \frac{\pi^2}{24}N(N-1)(2N-6) - \tfrac{1}{2}N(N-1)V'.$$

The relations are valid only for $V' > (N-1)^2\pi^2/2N$, in order that all filled shell-model levels are bound.

The single-particle 'infinitely deep square-well' problem with potential function

$$V(x) = \begin{cases} 0, & 0 < x < 1 \\ \infty, & x < 0, x > 1 \end{cases}$$

has solutions

$$\phi_n(x) = \begin{cases} \sqrt{2}\sin n\pi x, & 0 < x < 1 \\ 0, & x < 0, x > 1. \end{cases}$$

We construct from these solutions a trial function Φ to give an upper bound E' to the exact energy:

$$\Phi = \frac{1}{\sqrt{N!}} \begin{vmatrix} \phi_1(x_1) & \phi_1(x_2) & \cdots & \phi_1(x_N) \\ \phi_2(x_1) & \phi_2(x_2) & & \phi_2(x_N) \\ \vdots & & & \\ \phi_N(x_1) & \phi_N(x_2) & \cdots & \phi_N(x_N) \end{vmatrix}.$$

This is not translation-invariant, and the resulting upper bound will contain some centre-of-mass energy. But this is positive (kinetic energy) and will only lead to the upper bound being weaker. The effect of using Φ as a trial function is to confine all the particles to the region $0 < x < 1$. We have a 'collapsed state', in which each particle lies within range of every other. The expectation value with respect to Φ of the true Hamiltonian is easily evaluated, giving

$$E' = \sum_{n=1}^{N} (n\pi)^2 - \tfrac{1}{2}N(N-1)V' = \tfrac{1}{6}N(N+1)(2N+1)\pi^2 - \tfrac{1}{2}N(N-1)V'.$$

The 'collapsed-state' upper bound does not give any useful information as to the increase of $E/\mathscr{E}$ with N. In fact, for any given V' the upper bound always becomes positive for sufficiently large N. The kinetic energy is proportional to N^3, while the potential energy is proportional to N^2 when N is large. However, the binding energy of the lower-bound shell model increases with N. Here the number of bound single-particle states

is for large N proportional to $(NV')^{1/2}$. As N increases, there will be an insufficient number of bound states to accommodate all the shell-model particles. In filling the shell-model levels, when all the bound states have been assigned the remaining particles can only be given states in the continuous spectrum with $\epsilon_i = 0$. Thus not all shell-model particles contribute to the overall binding energy, but the number of available bound states increases with N. The condition that the 'collapsed-state' energy E' is negative ensures at least $N-1$ bound states in the lower-bound shell model. For $V' \rightarrow \infty$ we see that $E/\mathscr{E} \rightarrow 1$ for all N.

We now examine the two- and three-particle cases more closely. Table 1 gives the lower bound for two particles and the corresponding exact solution. $E_0/\mathscr{E}$ increases with V' and $E_0/\mathscr{E} \rightarrow 1$ for $V' \rightarrow \infty$. $E_0' = 0$ for $V' = \frac{1}{2}\pi^2$.

Table 1. Two particles in one dimension with square-well interaction

V'	E_0'	$\mathscr{E}'$	$E_0/\mathscr{E}$
10	$-1 \cdot 863$	$-8 \cdot 593$	$0 \cdot 217$
20	$-9 \cdot 248$	$-18 \cdot 361$	$0 \cdot 504$
30	$-17 \cdot 946$	$-28 \cdot 241$	$0 \cdot 636$
40	$-27 \cdot 116$	$-38 \cdot 164$	$0 \cdot 711$
50	$-36 \cdot 524$	$-48 \cdot 109$	$0 \cdot 759$
60	$-46 \cdot 073$	$-58 \cdot 067$	$0 \cdot 793$
70	$-55 \cdot 712$	$-68 \cdot 033$	$0 \cdot 819$
80	$-65 \cdot 415$	$-78 \cdot 006$	$0 \cdot 839$
90	$-75 \cdot 165$	$-87 \cdot 982$	$0 \cdot 854$
100	$-84 \cdot 950$	$-97 \cdot 962$	$0 \cdot 867$
110	$-94 \cdot 762$	$-107 \cdot 945$	$0 \cdot 878$
120	$-104 \cdot 600$	$-117 \cdot 929$	$0 \cdot 887$

For three particles in one dimension we obtain an improved upper bound by a new method. It is necessary that our upper-bound trial functions be antisymmetric and square-integrable. Furthermore, the upper bound is improved be insisting on translation invariance. Let the coordinates of the problem be x_1, x_2, x_3. Any function ψ antisymmetric in these coordinates may be written $\psi = D\phi$, where

$$D = \prod_{i<j=1}^{3} (x_i - x_j) = \begin{vmatrix} 1 & 1 & 1 \\ x_1 & x_2 & x_3 \\ x_1^2 & x_2^2 & x_3^2 \end{vmatrix}$$

and ϕ is a function symmetric in x_1, x_2, x_3 (Weyl 1946, p. 34). We introduce coordinates ξ_1, ξ_2, ξ_3 and separate off the centre of mass by the orthogonal transformation

$$\begin{pmatrix} \xi_1 \\ \xi_2 \\ \xi_3 \end{pmatrix} = \begin{pmatrix} \dfrac{1}{\sqrt{3}} & \dfrac{1}{\sqrt{3}} & \dfrac{1}{\sqrt{3}} \\ \dfrac{1}{\sqrt{2}} & -\dfrac{1}{\sqrt{2}} & 0 \\ \dfrac{1}{\sqrt{6}} & \dfrac{1}{\sqrt{6}} & -\dfrac{2}{\sqrt{6}} \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix}.$$

ξ_1 is the centre-of-mass coordinate. The reduced configuration space is two-dimensional. The planes $x_i = x_j$ become the lines $\xi_2 = 0$, $\xi_2 = \pm\sqrt{3}\xi_3$. We shall denote points in the (ξ_2, ξ_3) plane by polar coordinates (R, ϕ) such that $\xi_2 = R\sin\phi$, $\xi_3 = R\cos\phi$; $R \geqslant 0, 0 \leqslant \phi < 2\pi$. Written in reduced coordinates

$$D = \frac{1}{\sqrt{2}}(3\xi_2\xi_3^2 - \xi_2^3) = \frac{R^3}{\sqrt{2}}\sin 3\phi.$$

$R = (\xi_2{}^2 + \xi_3{}^2)^{1/2}$ is invariant under the interchange of any pair of particles; hence we may multiply D by any suitable normalizing function of R and take $F(R) \sin 3\phi$ as trial function. The $\sin 3\phi$ term provides three nodes coincident with the lines $\xi_2 = 0$, $\xi_2 = \pm\sqrt{3}\xi_3$.

The choice of the function $F(R)$ is based on the ground state of the corresponding two-particle problem. A trial function with range p is taken:

$$F(R) = \begin{cases} AR^{a_3} \cos a_1 R, & R < p \\ BR^{a_3} \exp(-\tfrac{1}{2}a_2 R), & R > p \end{cases} \tag{13}$$

where a_1, a_2, a_3 are variable parameters and A, B are normalization constants. The resulting expression for the upper bound energy E' is given in the appendix. This energy was minimized numerically with respect to a_1, a_2, a_3 by the method of Rosenbrock (1960). Table 2 gives the minimizing values of a_1, a_2, a_3 and corresponding E' for given V' and

Table 2. Three particles in one dimension with square-well interaction

V'	a_1	a_2	a_3	p	E'	$\mathscr{E}'$	$E/\mathscr{E}$
10	6·528	8·3	4·2	0·087	−4·310	−22·426	0·192
20	1·765	9·5	2·9	0·689	−22·557	−51·277	0·440
30	1·820	11·5	2·6	0·694	−45·766	−80·717	0·567
40	1·873	13·4	2·5	0·693	−71·364	−110·365	0·647
50	1·912	15·1	2·5	0·692	−98·269	−140·117	0·701
60	1·940	16·7	2·5	0·692	−125·955	−169·929	0·741
70	1·961	18·2	2·4	0·693	−154·142	−199·780	0·772
80	1·977	19·6	2·4	0·694	−182·670	−229·658	0·795
90	1·990	20·8	2·4	0·694	−211·445	−259·556	0·815
100	2·002	21·6	2·4	0·693	−240·405	−289·468	0·831
110	2·011	22·9	2·3	0·695	−269·503	−319·392	0·844
120	2·020	23·8	2·3	0·694	−298·714	−349·325	0·855

the shell-model lower bound $\mathscr{E}'$ is compared with this upper bound. As in the two-particle case, $E/\mathscr{E}$ improves with increasing V'. The lower bound $\mathscr{E}'$ passes through the origin. To find the point at which the energy E' becomes positive a numerical minimization of V', keeping $E' = 0$, was performed. It was found that E' becomes positive for $V' = 6\cdot0698$, i.e. for V' greater than this figure there is certainly an antisymmetric bound state. Comparing the two- and three-particle cases (table 1 with table 2), we see that for every value of V' taken $(E_0/\mathscr{E})_2 > (E/\mathscr{E})_3$. We have failed to demonstrate improvement with increasing N in this, the one-dimensional case. Experience with other trial functions leads us to believe that the upper bound is close to the exact ground state and that we have a counter example to the conjecture of improvement with increasing N.

We now turn to the three-dimensional case. As in the one-dimensional case, we shall not attempt to evaluate the energy levels of the lower-bound shell model for N particles exactly but will give convenient bounds. Let us consider the infinitely deep spherical-well problem. The kinetic energies of the levels are found by solving the equation

$$J_{l+\frac{1}{2}}(\sqrt{\tau'}) = 0$$

where $J_{l+\frac{1}{2}}(x)$ is a Bessel function of the first kind of order $l+\frac{1}{2}$ and $\tau' = (2ma^2/\hbar^2)$. (kinetic energy). Margenau (1934) showed that in going from an infinitely deep to a finite-depth spherical well all the energy levels are depressed, and that in this displacement the level corresponding to $j_{l+\frac{1}{2},n}$ for infinite depth never falls below the original energy value corresponding to $j_{l-\frac{1}{2},n}$. Thus for the finite-depth spherical-well problem we may write

$$j_{l-\frac{1}{2},n}^2 \leqslant \tau' \leqslant j_{l+\frac{1}{2},n}^2.$$

The resulting bounds on the shell-model energy $\mathscr{E}'$ are

$$\mathscr{L}' = \sum j_{l-\frac{1}{2},n}^2 - \tfrac{1}{2}N(N-1)V' \leqslant \mathscr{E}' \leqslant \sum j_{l+\frac{1}{2},n}^2 - \tfrac{1}{2}N(N-1)V'.$$

The summation is over the lowest $N-1$ states of the shell model, note being taken of the $2l+1$ degeneracy of each level. As in the one-dimensional case for the corresponding bounds, the above relations are only true when V' is large enough to ensure that all occupied shell-model states considered are bound.

In the three-dimensional case we take as trial function for the upper bound the Slater determinant formed from the lowest N states of the infinitely deep spherical-well problem. Expressed in the usual spherical polar coordinates these states are

$$\phi_{n,l,m}(\boldsymbol{r}) = \begin{cases} Ar^{-1/2}\mathrm{J}_{l+\frac{1}{2}}(\sqrt{\tau'}r)\,Y_{l,m}(\theta,\phi), & r < \tfrac{1}{2} \\ 0, & r > \tfrac{1}{2}. \end{cases}$$

$Y_{l,m}(\theta,\phi)$ is a spherical harmonic and A a normalization constant. It is now necessary for the state function to vanish whenever $r > \frac{1}{2}$, in order to confine all particles within a collapsed state. The upper bound we obtain is

$$E' = \sum 4j^2_{l+\frac{1}{2},n} - \tfrac{1}{2}N(N-1)V'.$$

The summation covers the lowest N states, the $2l+1$ degeneracy being included as before.

To discuss the increase of $E/\mathscr{E}$ with N, we are obliged to take a numerical example as our upper and lower bounds are not explicit. The potential well chosen must be deep enough for the two-particle upper bound to be negative. We take $V' = 200$ as convenient and consider up to twenty particles. Table 3 compares the lower bound to the shell-model

Table 3. N particles in three dimensions with square-well interaction

$V' = 200$

N	E'	$\mathscr{L}'$	$E/\mathscr{L}$
2	−79·76	−197·53	0·404
3	−399·00	−587·66	0·679
4	−918·23	−1177·8	0·780
5	−1585·4	−1967·9	0·806
6	−2452·5	−2947·7	0·832
7	−3519·6	−4127·5	0·853
8	−4786·8	−5507·4	0·869
9	−6253·9	−7087·2	0·882
10	−7896·0	−8867·0	0·891
11	−9700·6	−10845	0·895
12	−11705	−13012	0·900
13	−13910	−15378	0·905
14	−16315	−17945	0·909
15	−18919	−20712	0·914
16	−21724	−23679	0·918
17	−24729	−26846	0·921
18	−27890	−30212	0·923
19	−31251	−33773	0·925
20	−34813	−37533	0·928

energy $\mathscr{L}'$ with the 'collapsed-state' upper bound E' for this choice. We note that $E/\mathscr{L}$ increases monotonically with N, indicating that the lower bound $\mathscr{E}'$ improves with N. The kinetic energy of both E' and $\mathscr{L}'$ is independent of V'. Thus, for $V' \to \infty$, $E/\mathscr{E} \to 1$ for all N.

To see how far the 'collapsed-state' upper bound lies above the exact energy and how far below the shell-model energy the lower bound lies we examine table 4. The upper bound E' is poor, but the lower bound $\mathscr{L}'$ gives values quite close to the true shell-model energy $\mathscr{E}'$. Thus it may be concluded from table 4 that the quality of the shell-model lower bound is indeed better than table 3 suggests. Ideally we require $\lim\limits_{N\to\infty}(E/\mathscr{L})$, but no suitable analytic solution of the two-body problem is available. Our purpose is to

investigate the quality of the lower bound; the lack of definite conclusions throughout the paper does not reflect on the lower-bound method itself.

The lower bound for two particles is compared with the exact solution in table 5.

Table 4. Three-dimensional square-well interaction

$V' = 200$		$N = 2$	$N = 3$
Collapsed-state upper bound	E'	$-79\cdot759$	$-398\cdot996$
Exact ground state	E_0'	$-166\cdot789$	—
Shell-model energy	$\mathscr{E}'$	$-191\cdot399$	$-573\cdot155$
Lower bound	$\mathscr{L}'$	$-197\cdot533$	$-587\cdot663$

Table 5. Two particles in three dimensions with square-well interaction

V'	E_0'	$\mathscr{E}'$	$E_0/\mathscr{E}$
10	—	$-4\cdot624$	—
20	$-0\cdot099$	$-13\cdot558$	$0\cdot007$
30	$-6\cdot381$	$-23\cdot036$	$0\cdot277$
40	$-14\cdot328$	$-32\cdot708$	$0\cdot438$
50	$-22\cdot934$	$-42\cdot475$	$0\cdot540$
60	$-31\cdot898$	$-52\cdot298$	$0\cdot610$
70	$-41\cdot087$	$-62\cdot158$	$0\cdot661$
80	$-50\cdot427$	$-72\cdot043$	$0\cdot700$
90	$-59\cdot876$	$-81\cdot947$	$0\cdot731$
100	$-69\cdot407$	$-91\cdot864$	$0\cdot756$
110	$-78\cdot999$	$-101\cdot792$	$0\cdot776$
120	$-88\cdot642$	$-111\cdot729$	$0\cdot793$

$E_0/\mathscr{E}$ increases with V' and, as we expect from previous considerations, $E_0/\mathscr{E} \to 1$ for $V' \to \infty$. E_0' becomes zero for $V' = 2\pi^2$ and $\mathscr{E}' = 0$ for $V' = \frac{1}{4}\pi^2$.

5. Exponential interaction

For N particles interacting by exponential forces in one dimension

$$V_{ij} = -V_0 \exp\left(-\frac{|x_{ij}|}{a}\right)$$

the reduced Hamiltonian h_i is

$$-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x_i^2} - \tfrac{1}{2}NV_0 \exp\left(-\frac{|x_i|}{a}\right).$$

Its eigenvalues are found by solving the equations

$$\mathrm{J}_k(y_0) = 0, \qquad \text{for odd solutions}$$

and

$$\mathrm{J}_k'(y_0) = 0, \qquad \text{for even solutions}$$

where

$$k^2 = -4E', \qquad y_0^2 = 2NV'.$$

Here

$$E' = \frac{2mEa^2}{\hbar^2}, \qquad V' = \frac{2mV_0 a^2}{\hbar^2}$$

as in §4; $J_k(y)$ is a Bessel function of the first kind of order k (Bates 1961, p. 113). Table 6 compares the lower bound for two particles with the corresponding exact solution. It should be noted that $E_0/\mathscr{E}$ increases with V'. For $V' \to \infty$, $E_0/\mathscr{E} \to 1$. E_0' becomes zero for $V' = 2\cdot892$.

Table 6. Two-particles in one dimension with exponential interaction

V'	Exact solution E_0'	Lower bound $\mathscr{E}'$	$E_0/\mathscr{E}$
10	$-1\cdot1006$	$-6\cdot0432$	$0\cdot182$
20	$-4\cdot3648$	$-13\cdot476$	$0\cdot324$
30	$-8\cdot5374$	$-21\cdot294$	$0\cdot401$
40	$-13\cdot248$	$-29\cdot332$	$0\cdot452$
50	$-18\cdot333$	$-37\cdot520$	$0\cdot489$
60	$-23\cdot700$	$-45\cdot819$	$0\cdot517$
70	$-29\cdot291$	$-54\cdot207$	$0\cdot540$
80	$-35\cdot067$	$-62\cdot666$	$0\cdot560$
90	$-40\cdot999$	$-71\cdot185$	$0\cdot576$
100	$-47\cdot064$	$-79\cdot757$	$0\cdot590$
110	$-53\cdot248$	$-88\cdot373$	$0\cdot603$
120	$-59\cdot535$	$-97\cdot029$	$0\cdot614$

Table 7. Three particles in one dimension with exponential interaction

V'	a_1	a_2	Upper bound E'	Lower bound $\mathscr{E}'$	$E/\mathscr{E}$
10	$0\cdot8$	$2\cdot0$	$-3\cdot00$	$-13\cdot96$	$0\cdot215$
20	$1\cdot9$	$2\cdot2$	$-12\cdot31$	$-33\cdot14$	$0\cdot372$
30	$2\cdot9$	$2\cdot2$	$-24\cdot34$	$-53\cdot91$	$0\cdot452$
40	$3\cdot9$	$2\cdot3$	$-38\cdot10$	$-75\cdot59$	$0\cdot503$
50	$4\cdot5$	$2\cdot3$	$-52\cdot88$	$-97\cdot89$	$0\cdot540$
60	$5\cdot7$	$2\cdot3$	$-68\cdot47$	$-120\cdot7$	$0\cdot568$
70	$6\cdot6$	$2\cdot3$	$-84\cdot80$	$-143\cdot8$	$0\cdot590$
80	$7\cdot3$	$2\cdot3$	$-101\cdot7$	$-167\cdot2$	$0\cdot608$
90	$8\cdot3$	$2\cdot4$	$-119\cdot1$	$-190\cdot9$	$0\cdot624$
100	$9\cdot0$	$2\cdot4$	$-136\cdot9$	$-214\cdot8$	$0\cdot637$
110	$9\cdot8$	$2\cdot4$	$-155\cdot1$	$-238\cdot9$	$0\cdot649$
120	11	$2\cdot6$	$-174\cdot3$	$-263\cdot2$	$0\cdot662$

An upper bound for the three-particle problem was obtained using a trial function of the form $F(R) \sin 3\phi$ (see §4). We made the choice $F(R) = AR^{a_2} \exp(-\tfrac{1}{2}a_1R^2)$, bearing in mind the ground state of the corresponding two-particle problem which is roughly 'Gaussian' in shape. The normalization constant is given by

$$A = \left\{ \frac{2a_1^{1+a_2}}{\pi\Gamma(1+a_2)} \right\}^{1/2}.$$

Taking the expectation value of the exact Hamiltonian with respect to this trial function, we may express the upper-bound energy E' by

$$E' = a_1\left(1 + \frac{9}{a_2}\right) - \frac{24V'a_1^{1+a_2}I_1}{\pi\Gamma(1+a_2)}$$

where

$$I_1 = \int_0^\infty \int_0^{\pi/2} R^{1+2a_2} \exp\{-(a_1R^2 + \sqrt{2}R\sin\phi)\} \sin^2 3\phi \, d\phi \, dR.$$

This E' (essentially Ea^2) was minimized numerically with respect to the parameters a_1, a_2 in a manner similar to that for the 'square-well' interaction. Table 7 gives the minimizing values of these parameters with resulting E' for given V' and the shell-model lower bound $\mathscr{E}'$ is compared with this upper bound. The ratio $E/\mathscr{E}$ improves with increasing V' as for two particles. The upper bound E' becomes positive for $V' = 3\cdot696$. (This value was obtained by minimizing V' numerically, keeping $E' = 0$.) Comparing table 6 with table 7, we see that for the points considered the lower bound $\mathscr{E}'$ is always better for three particles, i.e. we have improvement as N increases in this case.

6. Conclusion

A simple method has been devised to give a rigorous lower bound to the energy of N fermions interacting by pair forces. This lower bound improves monotonically as we deepen the potential well. For the non-saturating interactions studied the ratio of upper and lower estimates, and hence *a fortiori* of exact to lower-bound values, tends to unity as the potential depth increases. We may understand this when we consider that in deriving our lower bound we effectively retained all $\frac{1}{2}N(N-1)$ pair interactions by scaling up the shell-model central force by a factor of $\frac{1}{2}N$. This gives a good potential energy approximation, and thus in deep wells where the potential energy dominates over the kinetic energy we obtain a good result for systems which do not saturate.

With one exception, all our examples give better lower bounds for greater numbers of particles. It was at first conjectured that this improvement with increasing N held generally. However, for 'square-well' interaction in one dimension the collapsed-state upper bound failed to demonstrate this. An improved upper bound minimized simultaneously with respect to three parameters still fails to show a monotonic increase in the ratio of upper and lower bounds with increasing N. Thus we may have a counter example to the conjecture of monotonic improvement of the lower bound with increasing N.

To derive the shell-model lower bound we proceeded in two steps. Firstly, we relaxed the antisymmetry condition with respect to the interchange of particle 1 with any of the particles 2, 3, ..., N. Secondly, we let the mass of particle 1 become very large, associating the centre of mass of the system with this particle. Since the first step interferes with one particle in N, we expect the overall binding energy to be little affected when 1 is small compared with N. (cf. the smallness of the symmetry-restriction effect in IV.) Thus for large numbers of particles it is the second step, which we shall call the mass effect, that contributes most to the difference between the exact energy and the shell-model lower bound. This 'mass effect' depends on the interaction (cf. the 'reduced mass effect' of IV).

It may be noted from §§ 4 and 5 for one-dimensional problems that the lower bound $\mathscr{E}'$ always passes through the origin. This is true generally, for the lower bound admits even parity states, the lowest two-particle state in one dimension being bound for all V'. The three-particle upper bounds are believed to be close to the exact energy, and since considerable effort is required to obtain such bounds for spatial antisymmetry they should serve as a useful standard for future work. The lower-bound method will be most interesting for large numbers of particles, but in this case obtaining corresponding upper bounds for comparison is tedious. For square-well interaction in three dimensions the upper and lower bounds differ by less than 8% for twenty particles and a strength of interaction $V' = 200$. However, we are less interested in the closeness of upper and lower bounds than in the existence of a lower bound following a building-up principle.

It is interesting that the lower-bound model obtained is a strict shell model. We might hope to derive a similar shell model for the upper bound, and perhaps the existence of an exact solution of this type between these bounds.

The pragmatic situation is this: whilst no exact general solution of the N-body problem has been found, nature provides us with solutions exhibiting some aspects of a shell model, mainly in the form of some limited evidence in nuclear physics relating to the sequence of angular momenta with increasing N (Haxel *et al.* 1950). This evidence relates to fermion systems which also exhibit saturation. A further task in our programme would be to introduce saturating interactions.

Acknowledgments

Appendix

We consider the upper-bound energy expression E' for three particles in one dimension interacting by 'square-well' forces. This was obtained for a trial function of the form $F(R) \sin 3\phi$, where $F(R)$ is given by (13) of § 4.

The condition that $F(R)$ and its first derivative be continuous at $R = p$ gives the relations

$$A \cos a_1 p = B \exp(-\tfrac{1}{2}a_2 p)$$

and

$$a_1 \tan a_1 p = \tfrac{1}{2}a_2.$$

Normalization requires that $\pi(A^2 I_1 + B^2 I_2) = 1$ where

$$I_1 = \int_0^p R^{1 + 2a_3} \cos^2 a_1 R \, \mathrm{d}R$$

and

$$I_2 = \int_p^\infty R^{1 + 2a_3} \exp(-a_2 R) \, \mathrm{d}R.$$

The kinetic energy is easily expressed in terms of integrals involving R only as $\pi(A^2 I_3 + B^2 I_4)$:

$$I_3 = \int_0^p F_3(R) \, \mathrm{d}R \qquad\qquad I_4 = \int_p^\infty F_4(R) \, \mathrm{d}R$$

$$F_3(R) = \{(9 - a_3{}^2)R^{2a_3 - 1} + a_1{}^2 R^{2a_3 + 1}\} \cos^2 a_1 R + a_1(a_3 + \tfrac{1}{2})R^{2a_3} \sin 2a_1 R$$

$$F_4(R) = \{(9 - a_3{}^2)R^{2a_3 - 1} + a_2(a_3 + \tfrac{1}{2})R^{2a_3} - \tfrac{1}{4}a_1{}^2 R^{2a_3 + 1}\} \exp(-a_2 R).$$

For the potential energy the expectation value of $-3V'f(\sqrt{2}R|\sin \phi|)$ is required. Since $f(\sqrt{2}R|\sin \phi|)\sin^2 3\phi$ is symmetric about both the ξ_2 and ξ_3 axes it is not necessary to integrate over the whole of reduced configuration space. The obligatory area of integration is reduced to the shaded strip in the first quadrant (figure 1). This gives rise to

$$\int_0^{\sin^{-1}(1/\sqrt{2}R)} \sin^2 3\phi \, \mathrm{d}\phi$$

which we denote $\phi(R)$. This may be expressed in closed form as

$$\frac{1}{2}\left\{ \sin^{-1}\left(\frac{1}{\sqrt{2}R} \right) - \frac{(2R^2 - 1)^{1/2}}{2R^2} g\left(\frac{1}{R^2} \right) \right\}$$

where

$$g(x) = 1 - \tfrac{8}{3}x + \tfrac{4}{3}x^2.$$

In terms of the above function $\phi(R)$ the potential energy may now be written involving integration with respect to R only. For $p < 1/\sqrt{2}$ we have

$$-12V'\{\tfrac{1}{4}\pi(A^2 I_5 + B^2 I_6) + B^2 I_7\}$$

where

$$I_5 = \int_0^p R^{1 + 2a_3} \cos^2 a_1 R \, \mathrm{d}R, \qquad\qquad I_6 = \int_p^{1/\sqrt{2}} R^{1 + 2a_3} \exp(-a_2 R) \, \mathrm{d}R$$

and

$$I_7 = \int_{1/\sqrt{2}}^{\infty} R^{1+2a_3} \exp(-a_2 R)\, \phi(R)\, \mathrm{d}R.$$

When $p > 1/\sqrt{2}$ the potential energy takes the somewhat different form

$$-12V'\{A^2(\tfrac{1}{4}\pi I_5 + I_6) + B^2 I_7\}$$

the integrals being

$$I_5 = \int_0^{1/\sqrt{2}} R^{1+2a_3} \cos^2 a_1 R\, \mathrm{d}R, \qquad I_6 = \int_{1/\sqrt{2}}^{p} R^{1+2a_3} \cos^2 a_1 R\, \phi(R)\, \mathrm{d}R$$

and

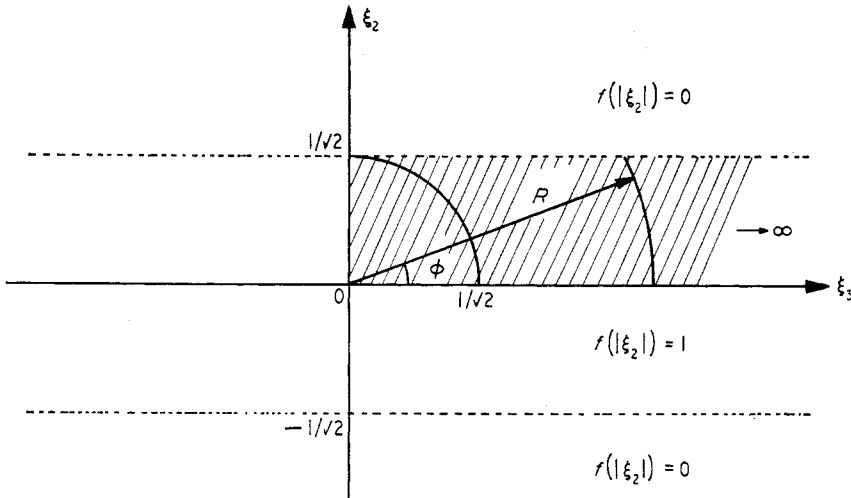$$I_7 = \int_p^{\infty} R^{1+2a_3} \exp(-a_2 R)\, \phi(R)\, \mathrm{d}R.$$

Figure 1. Reduced configuration space for three particles in one dimension interacting by 'square-well' forces. For $-1/\sqrt{2} < \xi_2 < 1/\sqrt{2}, f(|\xi_2|) = 1$; elsewhere $f(|\xi_2|) = 0$.

The total energy E' depends on the six variables a_1, a_2, a_3, p, A, B. Three of these are redundant owing to the conditions of normalization and continuity. For the purpose of minimization a_1, a_2, a_3 were chosen for variation.

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