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Many-particle systems VII. Angular momenta and an improved lower bound: an approach towards shell theory

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Abstract. The shell model previously developed by Carr and Post consisting of strictly independent particles is shown to provide lower bounds to the energies of any N-fermion system for states of each angular momentum separately. An improved lower-bound shell model retaining antisymmetry in all N particles is derived, and applied to Hooke's law, inverse square, rectangular well, and exponential interactions. Upper bounds to the deviations of our model energy values from the exact values are given. An approach to shell theory is sketched.

1. Introduction

In this paper we prove that the method introduced in paper VI (Carr and Post 1968)† may be used to establish a lower energy bound for states of any given angular momentum separately. This is a further step towards shell theory, whose main success lies in the prediction of (or at least the exclusion of certain values from a set of values for) the angular momenta of ground states for successive numbers of nucleons, rather than in the prediction of energies (see Lovell 1959).

On the basis of paper VI we may assert that the binding energy of the ground state of an N-nucleon system (assuming any given pair interaction) is not greater than the value for our corresponding shell model (which is easily calculated, our shell model being a *strict* independent particle model). The ground state of our model will, of course, have a definite angular momentum, or degenerate set of angular momenta. We have not proved that these values are the values for the ground state of the actual system. To do this, we have to establish (i) a lower bound for the energy of states of other angular momentum and (ii) an upper bound for the ground state. If (ii) is lower than (i), the other angular momentum is excluded from the ground state.

(i) is established by the proof in § 2. The calculation of upper bounds is a straightforward, though sometimes tedious, procedure. In many cases we have found upper bounds for the ground state reasonably close to our (HIP model) lower bound. The possible 'error' in our model value, thus calculated, may be reduced further by improving our lower bound model as in § 3. In so far as we may ignore the 'error' in our model (to be precise: in so far as the difference in 'errors' is smaller than the spacing between model levels of different angular momenta) our model provides the basis for a shell theory of angular momenta.

† Post (1953), Post (1956), Post (1962), Hall and Post (1967), and Hall (1967b) will be referred to as papers I, II, III, IV and V, respectively. We call the lower-bound model introduced in paper II the OP (one particle) model and that of paper VI the HIP (heavy independent particle) model.

2. Angular momentum

We continue the study commenced in paper VI, of a translation invariant system of N fermions in three dimensions. The Hamiltonian is

$$H = -\frac{\hbar^2}{2m}\sum_{i=1}^{N}\Delta_{r_i} + \sum_{i<j=1}^{N}\sum V_{ij} \tag{1}$$

where m is the mass of any particle, and the ith particle has the position vector $\boldsymbol{r}_i$.

Suppose the exact energy eigenvalues are E_i, $i = 1, 2, 3, \ldots$, with corresponding eigenstates Ψ_i, such that $H\Psi_i = E_i\Psi_i$. Some of the E_i may be equal. The lower bound shell model of paper VI has the Hamiltonian

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

Let the eigenvalues for this system be $\mathscr{E}_j$ with eigenstates Φ_j, such that $\mathscr{H}\Phi_j = \mathscr{E}_j\Phi_j$; $j = 1, 2, 3, \ldots$. Again some of the $\mathscr{E}_j$ may be degenerate.

We examine the internal angular momentum, for the exact problem and the lower bound shell model. For the exact problem the total angular momentum may be expressed by

$$\sum_{i=1}^{N}\boldsymbol{r}_i \times \boldsymbol{p}_i.$$

The internal angular momentum is translation invariant and depends on $2N-2$ vector variables; we denote it by $\boldsymbol{L}$. If

$$\boldsymbol{L} \equiv (L_1, L_2, L_3)$$

then

$$L^2\Psi_i = l(l+1)\hbar^2\Psi_i \qquad l = 0, 1, 2, \ldots$$
$$L_3\Psi_i = m_l\hbar\Psi_i \qquad m_l = 0, \pm 1, \pm 2, \ldots, \pm l.$$

The angular momentum for the lower bound shell model $\mathscr{L}$ depends on the same number of vector variables. If $\mathscr{L} \equiv (\mathscr{L}_1, \mathscr{L}_2, \mathscr{L}_3)$, then

$$\mathscr{L}^2\Phi_j = l(l+1)\hbar^2\Phi_j \qquad l = 0, 1, 2, \ldots$$
$$\mathscr{L}_3\Phi_j = m_l\hbar\Phi_j \qquad m_l = 0, \pm 1, \pm 2, \ldots, \pm l.$$

For all cartesian coordinate systems the position and momentum coordinates $\boldsymbol{p}_i$, $\boldsymbol{q}_i$ are related by the correspondence $\boldsymbol{p}_i = -i\hbar\nabla_{q_i}$, that is, $\boldsymbol{p}_i$ and $\boldsymbol{q}_i$ are mutually covariant. In paper VI the mass of particle 1 enters only implicitly via the momentum. The quantities $\boldsymbol{p}_i \times \boldsymbol{q}_i$ are therefore formally independent of the particular choice of coordinates when we change the mass of particle 1 and thus the internal angular momentum in the exact problem is formally identical with the total angular momentum for the lower bound shell model. Since moreover the commutation rules in the two problems are the same we have complete identity†.

Let

$$H(m_1) = -\frac{h^2}{2m_1}\Delta_{r_1} - \sum_{i=2}^{N}\frac{h^2}{2m}\Delta_{r_i} + \sum_{i<j=1}^{N}\sum V(|\boldsymbol{r}_i - \boldsymbol{r}_j|)$$

† The change of coordinates given by (3) is a point transformation and is therefore canonical.

such that for $m_1 = m$, $H(m_1)$ is the same Hamiltonian as that given by (1). In paper VI it was shown that increasing the mass m_1 in the expectation value $(\Psi_i, H(m_1)\Psi_i)$, while retaining the same function Ψ_i, lowers the expectation value algebraically, that is

$$E_i = (\Psi_i, H(m_1)\Psi_i)_{m_1=m} \geqslant (\Psi_i, H(m_1)\Psi_i)_{m_1>m}. \tag{2}$$

We introduce the relative coordinates $\boldsymbol{\rho}_i$, $i = 1, 2, \ldots, N$ of paper VI (see (5)).

$$\boldsymbol{\rho}_1 = \frac{m_1\boldsymbol{r}_1 + \sum_{i=2}^{N} m\boldsymbol{r}_i}{M}$$

centre of mass coordinate

$$\boldsymbol{\rho}_i = \left(\frac{m_1}{m+m_1}\right)^{1/2}(\boldsymbol{r}_i - \boldsymbol{r}_1) \tag{3}$$

where M is the total mass

$$M = m_1 + (N-1)m.$$

Let $\Psi_i\,\overline{(\boldsymbol{r}_1, \boldsymbol{r}_2, \ldots, \boldsymbol{r}_N)} \equiv \Psi_i'(\boldsymbol{\rho}_2, \ldots, \boldsymbol{\rho}_N)$; $\boldsymbol{\rho}_1$ does not enter since we have translation invariance. Ψ_i' is an eigenfunction of $\boldsymbol{L}^2$ and L_3 with eigenvalues $l(l+1)\hbar^2$ and $m_l\hbar$ respectively. The inequality (2) becomes

$$E_i \geqslant (\Psi_i'(\boldsymbol{\rho}_2, \ldots, \boldsymbol{\rho}_N), H'(m_1)_{m_1>m}\Psi_i'(\boldsymbol{\rho}_2, \ldots, \boldsymbol{\rho}_N))$$

where

$$H'(m_1) = -\frac{\hbar^2}{2m}\sum_{i=2}^{N}\Delta_{\boldsymbol{\rho}_i} - \frac{\hbar^2}{m+m_1}\sum_{i<j=2}^{N}\sum \nabla_{\boldsymbol{\rho}_i}\cdot\nabla_{\boldsymbol{\rho}_j} + \tfrac{1}{2}N\sum_{i=2}^{N} V\left(\left(\frac{m+m_1}{m_1}\right)^{1/2}\rho_i\right).$$

For $m_1 \to \infty$, $H'(m_1) \to \mathscr{H}$. This gives

$$E_i \geqslant (\Psi_i', \mathscr{H}\Psi_i'). \tag{4}$$

Since $\boldsymbol{L}$ and $\mathscr{L}$ are identical, Ψ_i' is an eigenfunction of $\mathscr{L}^2$ and $\mathscr{L}_3$ with eigenvalues $l(l+1)\hbar^2$ and $m_l\hbar$. However Ψ_i' is not (in general) an eigenstate of $\mathscr{H}$. This implies by the variational principle the existence of a lower bound shell model state Φ_j which is simultaneously an eigenstate of $\mathscr{L}^2$, $\mathscr{L}_3$ and $\mathscr{H}$, such that

$$(\Psi_i', \mathscr{H}\Psi_i') \geqslant (\Phi_j, \mathscr{H}\Phi_j)$$

where

$$\mathscr{H}\Phi_j = \mathscr{E}_j\Phi_j \qquad \mathscr{L}^2\Phi_j = l(l+1)\hbar^2\Phi_j$$

and

$$\mathscr{L}_3\Phi_j = m_l\hbar\Phi_j.$$

Thus from (4) we have $E_i \geqslant \mathscr{E}_j$. The angular momentum spectrum will usually be degenerate; for a given eigenvalue of $\mathscr{L}^2$ and $\mathscr{L}_3$ choosing the eigenstate which gives lowest energy with respect to $\mathscr{H}$ will ensure the truth of the above inequality. Hence for a state Ψ_i of the exact problem with energy E_i and angular momentum quantum numbers l, m_l the energy of the lowest state in the lower bound shell model having the same quantum numbers l, m_l will give a lower bound to E_i.

3. An improved lower-bound antisymmetric in all N particles

In our usual notation, let the ground state of the exact problem be $\psi_0(\boldsymbol{r}_1, \boldsymbol{r}_2, \ldots, \boldsymbol{r}_N)$. This will be a function of class L in the nomenclature of paper VI. The ground state energy is given by $E_0 = (\psi_0, H\psi_0)$.

We express this as the expectation value of a sum of N new Hamiltonians H_i; thus

$$E_0 = \frac{1}{N}\left(\psi_0, \left[\sum_{i=1}^{N} H_i\right]\psi_0\right) = \frac{1}{N}\sum_{i=1}^{N}(\psi_0, H_i\,\psi_0) \tag{5}$$

where

$$H_i = -\frac{\hbar^2}{2m}\Delta_{r_i} + \sum_{\substack{j=1\\ j\neq i}}^{N}\left\{-\frac{\hbar^2}{2m}\Delta_{r_j} + \frac{N}{2}V(|\boldsymbol{r}_j - \boldsymbol{r}_1|)\right\}.$$

That is we 'pick out' each of the particles 1, 2, 3, ..., N in turn.

Consider a typical term $(\psi_0, H_i\psi_0)$ in the expression (5). It was shown previously that

$$(\psi_0, H_i\psi_0)_{m_i=m} \geqslant (\psi_0, H_i\psi_0)_{m_i>m}.$$

We express $(\psi_0, H_i\psi_0)$ in terms of the relative coordinates $\boldsymbol{\rho}_i$ using (3), and let $m_i \to \infty$ on the right hand side of the inequality. In the limit, $\boldsymbol{\rho}_i \to \boldsymbol{r}_i$, $i = 1, 2, 3, \ldots, N$ and we have

$$(\psi_0, H_i\psi_0)_{m_i=m} \geqslant (\psi_0, \mathscr{H}_i'\psi_0) \tag{6}$$

where

$$\mathscr{H}_i' = \sum_{\substack{j=1\\ j\neq i}}^{N}\left\{-\frac{\hbar^2}{2m}\Delta_{r_j} + \frac{N}{2}V(r_j)\right\}$$

$$= \sum_{\substack{j=1\\ j\neq i}}^{N} h_j.$$

$$h_j = -\frac{\hbar^2}{2m}\Delta_{r_j} + \frac{N}{2}V(r_j).$$

(A neater proof of the paper VI lower bound result (HIP model) is obtained by noting that

$$E_0 = (\psi_0, H_1\psi_0)_{m_1=m} \geqslant (\psi_0, \mathscr{H}_1'\psi_0)$$

and minimizing the expectation value of $\mathscr{H}_1'$ with respect to functions of class M.)

Applying (6) to each term in (5), we replace $(\psi_0, H_i\psi_0)$ by $(\psi_0, \mathscr{H}_i'\psi_0)$; $i = 1, 2, 3, \ldots, N$, which gives

$$E_0 \geqslant \frac{1}{N}\sum_{i=1}^{N}(\psi_0, \mathscr{H}_i'\psi_0) \tag{7}$$

$$= \frac{1}{N}\left(\psi_0, \left[\sum_{i\neq 1} h_i + \sum_{i\neq 2} h_i + \ldots + \sum_{i\neq N} h_i\right]\psi_0\right)$$

$$= \frac{N-1}{N}\left(\psi_0, \sum_{i=1}^{N} h_i\psi_0\right) = \frac{N-1}{N}(\psi_0, H_s\psi_0)$$

where

$$H_s = \sum_{i=1}^{N} h_i.$$

ψ_0 will not (in general) be an eigenstate of H_s. We minimize with respect to normalized functions obeying the usual boundary conditions of quantum mechanics and antisymmetric with respect to the interchange of any pair of particles 1, 2, 3, ..., N. The inequality (7) is maintained or strengthened, giving

$$E_0 \geqslant \frac{N-1}{N}(\Phi_s, H_s\Phi_s) \tag{8}$$

where Φ_s is the lowest eigenstate of H_s subject to the above constraints, a Slater determinant formed from the first N eigenstates of h_i. In the notation of paper VI $h_i\varphi_n(\boldsymbol{r}_i) = \epsilon_n\varphi_n(\boldsymbol{r}_i)$, the φ_n are normalized to unity.

The inequality (8) becomes

$$E_0 \geqslant \frac{N-1}{N}\sum_{i=1}^{N}\epsilon_i = S.$$

We have an N-particle shell model retaining antisymmetry in all N particles, which we call the SHIP (symmetrized heavy independent particle) model. Comparing with the lower bound shell model of paper VI we see that the new SHIP shell model has the same energy levels but an extra particle, the whole multiplied by a factor $(N-1)/N$. Thus $S > \mathscr{E}$ always.

The angular momentum theorem of § 2 still applies to the new SHIP lower bound shell model. For the exact problem the internal angular momentum is given by

$$\boldsymbol{L} = \sum_{i=1}^{N} \boldsymbol{r}_i \times \boldsymbol{p}_i$$

for states ψ which are translation invariant, whereas for the new SHIP shell model the angular momentum is given by

$$\boldsymbol{L}_s = \sum_{i=1}^{N} \boldsymbol{r}_i \times \boldsymbol{p}_i.$$

If we restrict ourselves to translation invariant states ψ of the exact problem, then the ψ are eigenstates of L_s^2 and L_{s_3}, and the result follows. Solutions of the exact problem which are not translation invariant have algebraically higher energy than corresponding translation invariant states and the theorem holds *a fortiori*.

4. Calculations with the improved lower bound (SHIP model)

We continue the policy of paper VI and examine spatially antisymmetric problems in one and three dimensions for simple central force interactions.

4.1. *Hooke's interaction*

Figure 1 compares the improved lower bound shell model SHIP ground state energy S with the exact ground state E_0, for $V_{ij} = k^2(x_i - x_j)^2$ and $N = 2(1)20$ in the case of one dimension. The previous HIP lower bound $\mathscr{E}$ of paper VI is shown dotted. The improved SHIP lower bound is given by $S = N(N-1)(\frac{1}{2}N)^{1/2}k'$, where $k' = (\hbar^2/2m)^{1/2}k$. This new SHIP lower bound improves monotonically as N increases in the sense that $(E_0/S)_N > (E_0/S)_{N+1}$ for all N.

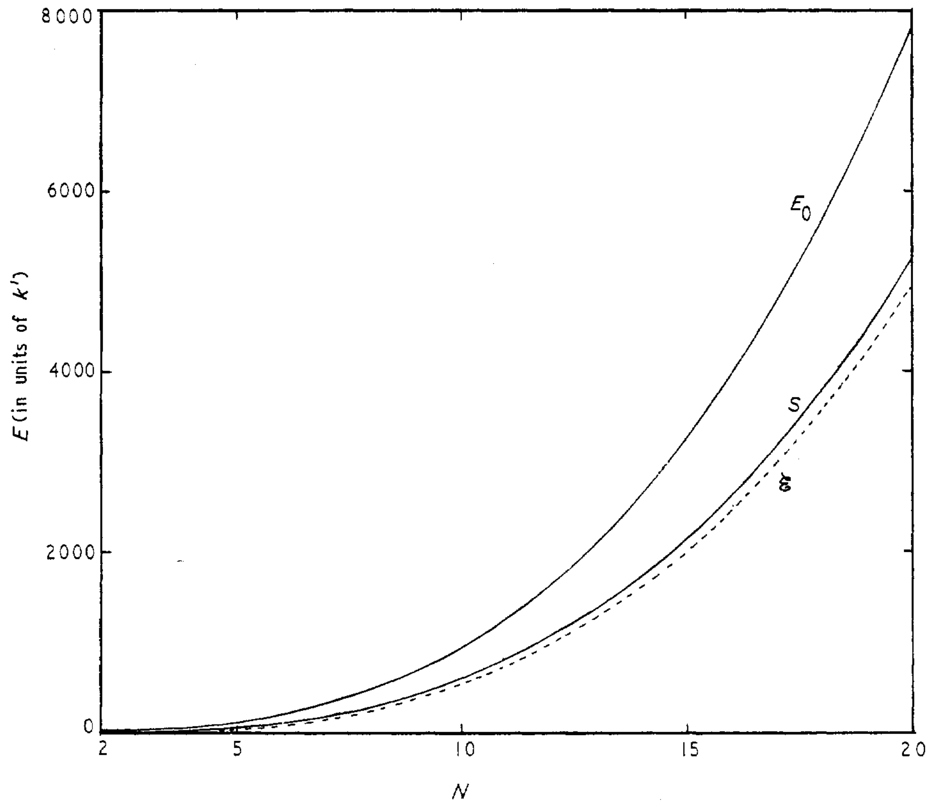

Figure 1. N particles in one dimension interacting by Hooke's forces ($V_{ij} = k^2x_{ij}^2$), E (in units of $k' = (\hbar^2/2m)^{1/2}k$) against N; E_0 is the lowest spatially antisymmetric state of the exact problem; S is the new SHIP shell model lower bound; $\mathscr{E}$ is the HIP lower bound of paper VI.

Figure 2 gives corresponding results for three dimensions, where $V_{ij} = k^2(\boldsymbol{r}_i - \boldsymbol{r}_j)^2$. The improved SHIP lower bound is given by

$$S = \frac{N-1}{N}(3+5+5+5+\ldots)\left(\frac{N}{2}\right)^{1/2} k'$$

to N terms in the bracket. Again $(E_0/S)_N > (E_0/S)_{N+1}$ for all $N \geqslant 2$, we have monotonic improvement as N increases.

4.2. *Square-well interaction*

Figure 3 compares the SHIP lower bound S' with the lowest spatially antisymmetric state of the exact problem E_0' for two particles in one dimension, where

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

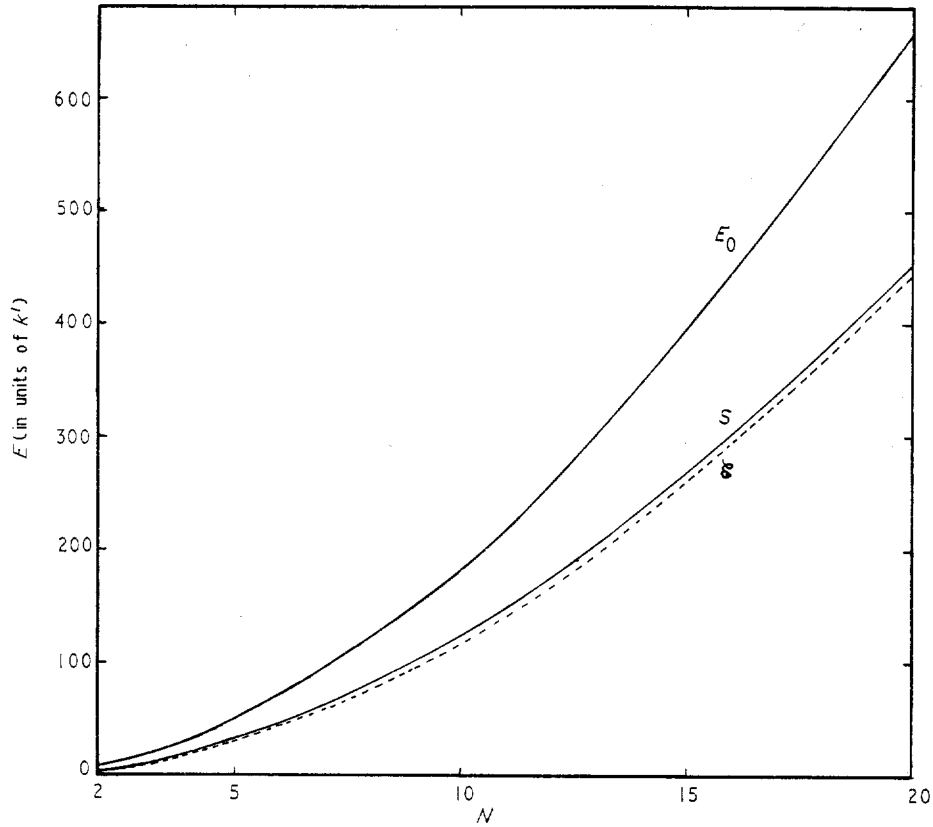

Figure 2. N particles in three dimensions interacting by Hooke's forces. E (in units of k') against N; E_0 is the exact solution; S is the new SHIP lower bound; $\mathscr{E}$ is the previous HIP lower bound.

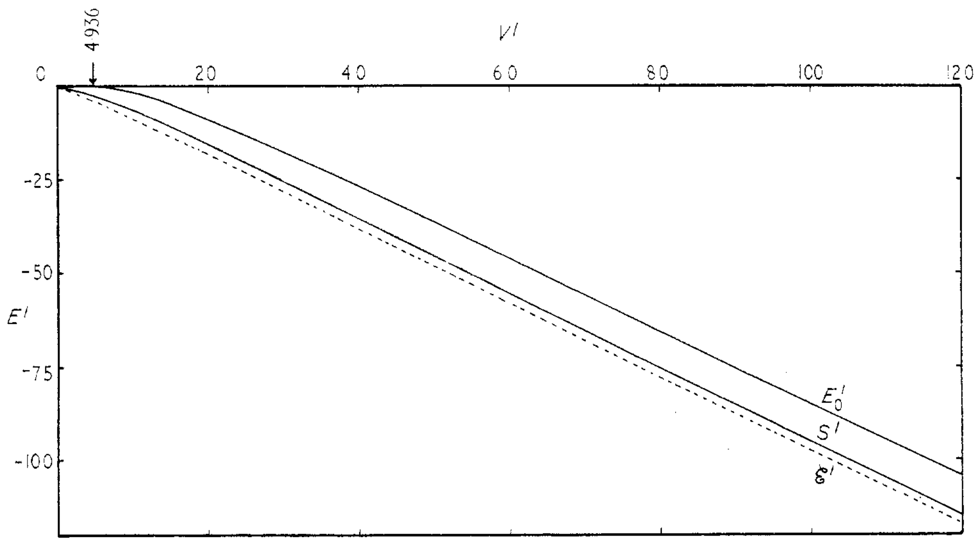

Figure 3. 'Square well' interaction in one dimension, two particles; E' ($= 2mEa^2/\hbar^2$) against V' ($= 2mV_0a^2/\hbar^2$) for lowest spatially antisymmetric states: E_0' is the exact solution; S' is the new SHIP lower bound; $\mathscr{E}'$ is the previous HIP lower bound.

Energies are expressed in dimensionless quantities such that $E' = 2mEa^2/\hbar^2$ etc. The previous HIP lower bound $\mathscr{E}'$ of paper VI is shown dotted. The SHIP lower bound improves as we deepen the well in that E_0/S increases as V' increases.

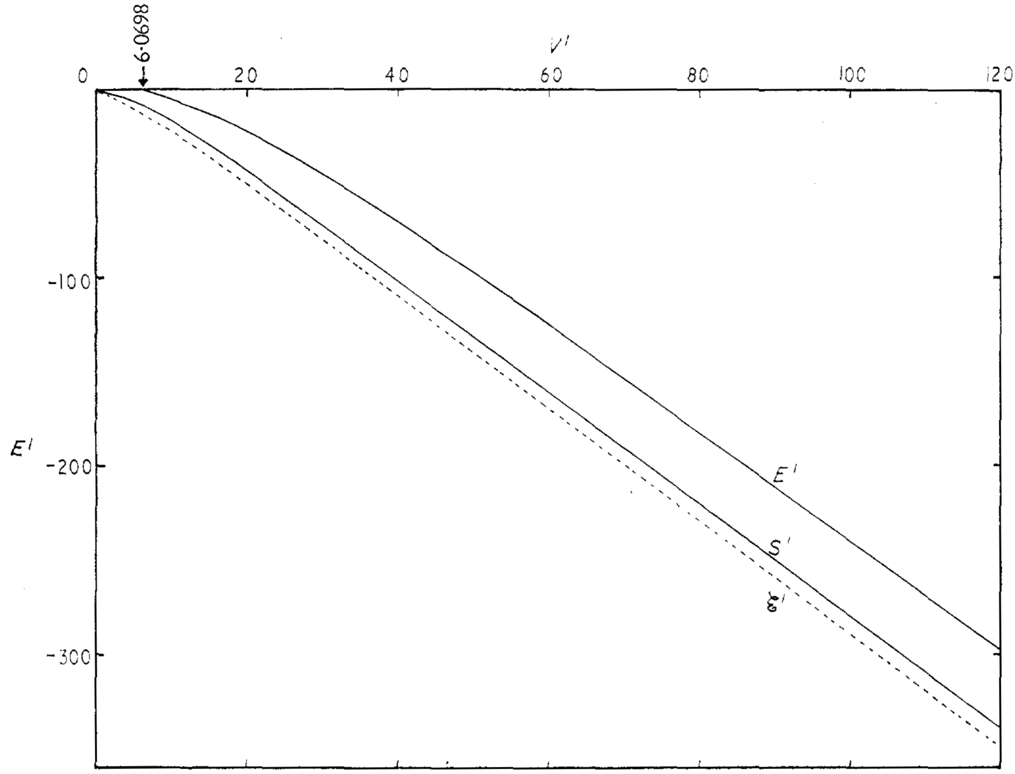

Figure 4. 'Square well' interaction in three dimensions, two particles. E' against V' for lowest spatially antisymmetric states; E' is the upper bound obtained by numerical minimization; S' is the new SHIP lower bound; $\mathscr{E}'$ is the previous HIP lower bound.

Corresponding results for three particles are shown in figure 4. In this case E' is the upper bound described in paper VI, obtained by numerical minimization with a translation invariant and spatially antisymmetric trial function. E/S increases as V' increases.

The quality of the SHIP lower bound S' appears to be better for two particles in the sense that $(E_0/S)_2 > (E/S)_3$ for $V' = 10(10)120$. As before in paper VI, we have failed to demonstrate improvement with increasing N in this case.

For deep wells we compare our SHIP lower bound S' with E_c', the 'collapsed state' upper bound given in paper VI. As $V' \to \infty$, $E_c/S \to 1$ for all N.

Figure 5 compares the 'collapsed state' upper bound E_c' of paper VI for N particles in three dimensions in the case of $V' = 200$, with $\mathscr{S}'$, a lower bound to S'. To obtain $\mathscr{S}'$, lower bounds on the single particle shell model energies ϵ_i' were obtained by the method given in paper VI. We have monotonic improvement in the sense that $(E_c/\mathscr{S})_N < (E_c/\mathscr{S})_{N+1}$ for $N = 2(1)20$ in this case. For $V' \to \infty$, $(E_c/\mathscr{S}) \to 1$ for all N.

In paper VI table 4 indicates that the upper bound E_c' is poor. We expect $\mathscr{S}'$ to be closer to the exact energy than E_c'.

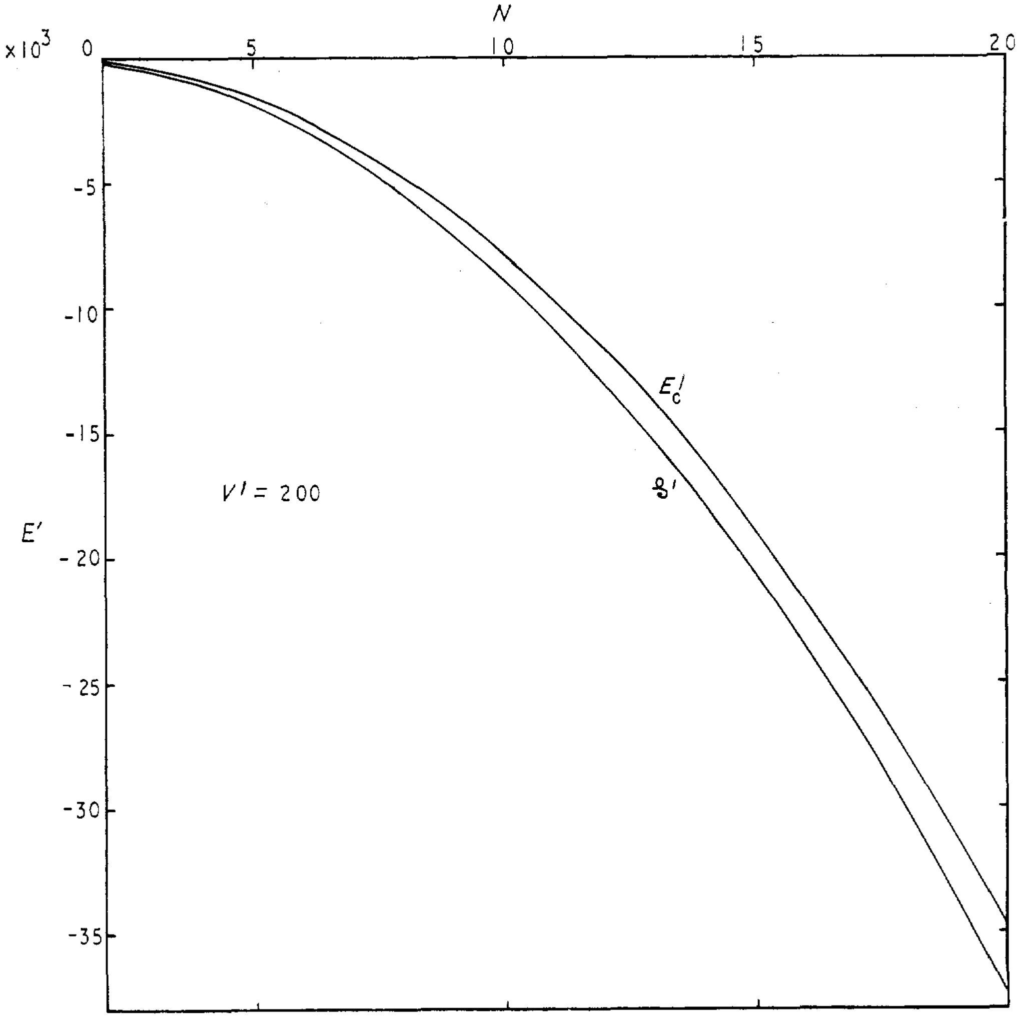

Figure 5. 'Square well' interaction in three dimensions, N particles; $V' = 2mV_0a^2/\hbar^2 = 200$; E' against N for lowest spatially antisymmetric states; E_c', collapsed state upper bound; $\mathscr{S}'$, lower bound to the SHIP shell model energy S'. The previous HIP lower bound lies close to $\mathscr{S}'$ and is omitted for clarity.

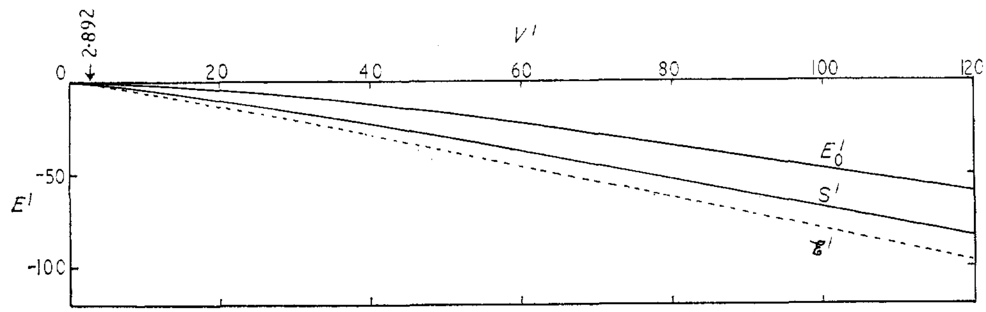

Figure 6. Exponential interaction in one dimension, two particles, $E'(=2mEa^2/\hbar^2)$ against V' $(=2mV_0a^2/\hbar^2)$ for lowest spatially antisymmetric states; E_0' is the exact solution; S' is the new SHIP lower bound; $\mathscr{E}'$ is the previous HIP lower bound.

4.3. *Exponential interaction*

Figure 6 compares the SHIP lower bound S' with the lowest spatially antisymmetric state of the exact problem E_0' for two particles in one dimension, where $V_{ij} = -V_0 \exp(-|x_{ij}|/a)$. The units of energy are the same as for the square-well interaction. The previous HIP lower bound $\mathscr{E}'$ of paper VI is shown dotted. We have improvement as the well deepens in the sense that E_0/S increases with V'.

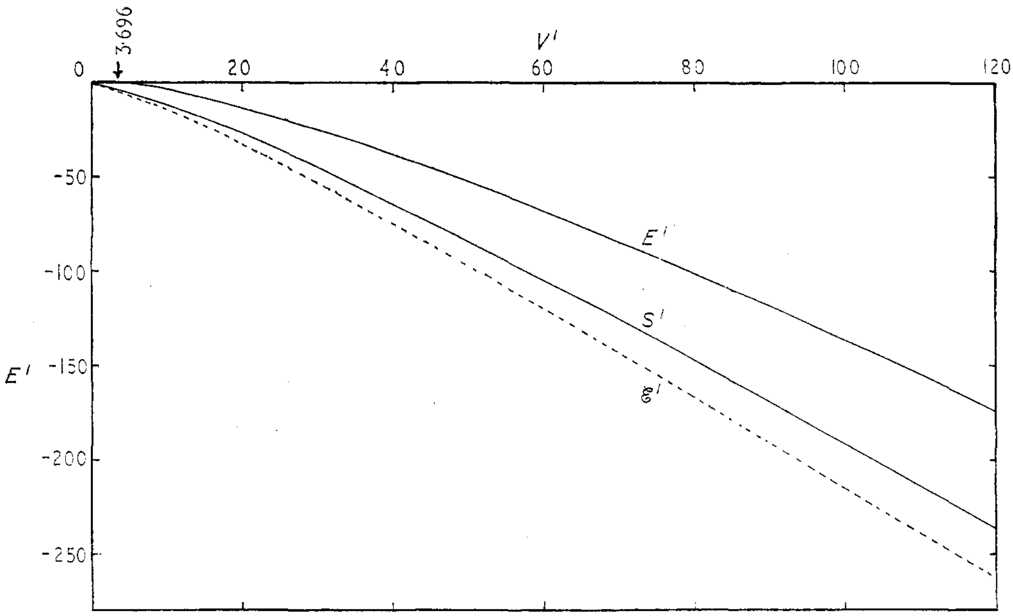

Figure 7. Exponential interaction in one dimension, three particles, E' against V' for lowest spatially antisymmetric states; E' is the upper bound obtained by numerical minimization ; S' is the new SHIP lower bound; $\mathscr{E}'$ is the previous HIP lower bound.

Corresponding results for three particles are shown in figure 7. The upper bound E' is obtained by numerical minimization with a translation invariant and spatially antisymmetric trial function in paper VI. E/S increases as V' increases.

The lower bound is better for three particles in that $(E_0/S)_2 < (E/S)_3$ for $V' = 10(10)120$. For this case also we have improvement as N increases.

4.4. *Inverse-square interaction*

Table 1 compares the lower bounds S' and $\mathscr{E}'$ with E_L', the upper bound of Levy-Leblond (1969) for $N = 2, 3, 4$ in three dimensions when $V_{ij} = -k/r_{ij}$. On comparing the upper bound E_L' with the exact solution E_0' for two particles, the upper bound appears rather poor, and hence probably exaggerates unduly the error of the shell model energy for $N = 3$ and for $N = 4$.

To obtain an explicit expression for the lower bound we follow the method used by Levy-Leblond and over fill the shell model levels to give closed shells for which energy bounds may easily be deduced. We obtain

$$S' > \mathscr{S}' = -\tfrac{1}{8}N^{4/3}(N-1)k'^2$$

and

$$\mathscr{E}' > \mathscr{L}' = -\tfrac{1}{8}N^2(N-1)^{1/3}k'^2.$$

For the upper bound

$$E_{\mathrm{L}}' = \frac{-1}{3\pi^2 2^6} N^{1/3}(N-1)^2 k'^2.$$

Again in the sense that $(E/\mathscr{S})_N < (E/\mathscr{S})_{N+1}$ we have monotonic improvement as N increases.

Table 1

	$N = 2$	$N = 3$	$N = 4$
Levy-Leblond upper bound E_{L}'	0·00067	0·00305	0·00754
Exact ground state E_0'	0·0313	—	—
SHIP shell model energy S'	0·156	0·563	1·313
HIP lower bound $\mathscr{E}'$	0·25	0·703	1·50
Lower bound $\mathscr{S}'$	0·315	1·082	2·38
Lower bound $\mathscr{L}'$	0·50	1·417	2·89

Energy is in units of $-k'^2$, where $k' = 2mk/\hbar^2$.

For large N all the bounds become proportional to $N^{7/3}$. It is plausible to assume that the exact solution 'sandwiched' between E_{L}' and $\mathscr{S}'$ has the same N-dependence.

5. Accuracy of models and approach to shell theory

As explained in the introduction, a derivation of shell theory requires a relative location of the relevant actual energy levels to an accuracy greater than the spacing of these levels in the model. Apart from a determination of an upper estimate of the 'error' of taking the various lower-bound models as actual values in the case of each individual interaction by a straightforward calculation of an upper bound, pessimistic estimates of the 'errors' corresponding to the OP and SHIP models may be obtained for any interaction in general from the following theorems respectively:

(i) In the N-boson case we can immediately give the exact value to a stated accuracy for any Hamiltonian H:

$$E_0 = \tfrac{1}{2}(N-1)(e_0+e_{\mathrm{g}}) \pm \tfrac{1}{2}((\varphi-g), h(\varphi+g))$$

where e_0 is the ground state energy of the equivalent one-particle problem corresponding to the one-particle wave function φ, as obtained by the OP method in paper II, and e_{g} is the expectation value of the equivalent one-particle Hamiltonian h using the Gaussian state function g (the normalized Hermite function of order zero).

Thus we see that the deviation of the equivalent one-particle state function from the Gaussian form is a measure of the inaccuracy of this method ('symmetry requirement effect').

(ii) In the N-fermion case, we may compare the lower bound obtained by the SHIP model, with an upper bound obtained as the expectation value of the true Hamiltonian of the problem, for the state function corresponding to the 'empty shell' model, that is, for the state function corresponding to N particles in shell states corresponding to the central interaction of the SHIP model. This latter (upper bound) expectation value is given by

$$\left(\Phi_s\overline{(\boldsymbol{r}_1, \boldsymbol{r}_2, \ldots, \boldsymbol{r}_N)}, \left[-\sum_{i=1}^{N} \frac{\hbar^2}{2m}\Delta_{r_i} + \sum_{i<j=1}^{N}\sum V_{ij}\right] \Phi_s\overline{(\boldsymbol{r}_1, \boldsymbol{r}_2, \ldots \boldsymbol{r}_N)}\right). \tag{9}$$

The former is given by

$$S = (\Phi_s\overline{(\boldsymbol{r}_1, \boldsymbol{r}_2, \ldots, \boldsymbol{r}_N)}, H_s\Phi_s\overline{(\boldsymbol{r}_1, \boldsymbol{r}_2, \ldots, \boldsymbol{r}_N)}) \tag{10}$$

where

$$H_s = \sum_{i=1}^{N}\left(-\frac{\hbar^2}{2m}\Delta_{r_i} + \tfrac{1}{2}NV_i\right)$$

is the Hamiltonian corresponding to an 'atom' of 'nuclear charge' $N/2$ with N non-interacting 'electrons'. The difference between the right hand side of (9) and (10) is the first order perturbation value of the potential energy in an atom of N 'electrons' and 'nuclear charge' $N/2$. This is a (pessimistic) measure of the inaccuracy of this method. For the HIP model see Post (1968).

The pessimistic estimates of errors resulting from these techniques are in general too large to derive a shell theory. Shell theory would be established if we could show that in going from the two- to the N-particle case the difference in the errors in successive levels is not reversed to an amount greater than the level spacing in the shell.

For interaction by Hooke's forces in three dimensions ($V_{ij} = k^2 r_{ij}^2$) the SHIP shell model ground state S has precisely the same sequence of angular momenta with N as that found in the exact problem. This may be seen by comparing the SHIP shell model with the exact solution given in paper I. We have N particles in each case to fill the same sequence of single particle levels.

This exact correspondence between the angular momenta of the model and the angular momenta of the exact ground states would hold generally if the *specific isotope shift* (Hughes and Eckart 1930) were zero. We are in a sense increasing the mass of one particle in going from the exact problem to our lower bound shell model (at least in the case of the HIP model).

In general all we require is that the levels corresponding to the lowest energies of different angular momenta do not cross as we change the mass of one (or all) particle(s). We do not have a *general* law supporting this required hypothesis. Familiar non-crossing rules relate to states of the same angular momentum.

In a later paper it will be shown that while our lower bound methods would be expected to give poor estimates of actual values in the case of saturating interactions, the HIP and SHIP models can be applied to produce saturation. Indeed, it may be argued that certain types of saturation go hand-in-hand with shell formation: the cocktail of four parts of Majorana with one part of Wigner interaction saturates precisely because it reduces inter-shell interaction to zero.

We have distinguished between shell theory, requiring a strict derivation, and the mere postulation of a shell model. We may further distinguish between ramified shell models, introducing spin–orbit coupling etc., and 'bare' shell models. It may be of interest to point out that the rule

$$N_l \geqslant N_{l+1}$$

where N_l is the number of states of angular momentum l below any arbitrary energy value, must hold not only for any two-particle system, but for any bare shell models for which the l, the angular momenta of the individual particle states, are defined at all (such as Feenberg and Hammack 1949), since for any such bare shell models the independent particle spectra are just superimposed, and the rule $N_l \geqslant N_{l+1}$ is inherited.

A more detailed sequence of levels is given by our theory (an example of a 'bare' shell theory) for any specific interaction. But unmodified 'bare' shell theory only yields *unique* total angular momenta for N corresponding to filled shells, or to such a number ± 1. Additional correlation requirements, such as a form of an anti-Hund rule (for attractive interactions), possibly strengthened by some spin interactions, are necessary to yield unique angular momenta (destroying degeneracy) in the most general case. Even present-day ramified shell theory does not provide such predictions in general.

However, we are not here interested in ramifications of 'bare' shell theory, or in the (straightforward) introduction of spin. We are concerned in the present paper to outline a derivation of a 'bare' shell theory, to explain why there are shells at all.

6. Conclusion

We have extended the HIP method of paper VI to give separate energy bounds $\mathscr{E}$ for states of any given angular momentum. A new shell model (SHIP) has been devised yielding an energy lower bound S, which is always better than $\mathscr{E}$ for ground states. This new SHIP model also provides separate lower bounds for any given angular momentum.

In general more information may be obtained about angular momentum by considering both HIP and SHIP models. For a given N the scheme of single particle levels to be filled is the same in each case but for the HIP lower bound $\mathscr{E}$ we have $N-1$ particles to assign, while for the SHIP lower bound S we have N particles. This often leads to a greater (or different) choice of allowed angular momentum values for the SHIP lower bound S, in which case $\mathscr{E}$ may yield additional information, depending on the particular level spacing of the problem. The angular momentum for the two models is connected by the simple relation

$$\text{angular momentum for } \mathscr{E}_N = \text{angular momentum for } S_{N-1}.$$

For ground states the improvement in the lower bound when using the new SHIP shell model is moderate. The improvement appears to be greatest in situations where the previous HIP lower bound was poor, in particular for the case of small numbers of particles. The real importance of the SHIP shell model is theoretical in that we now have an *N-particle* shell model. This brings us closer both to the exact problem and to the shell theory of nuclear physics. The new SHIP lower bound model already has the correct symmetry. The states of the SHIP shell model are 'ready made' trial functions for the exact problem, the exact solution being a state of the same space. The method of error estimation given by Post (1968) becomes neater (see § 5). We no longer have to 'throw away' one particle.

Fermion lower bounds involving a sum over $N-1$ energies have been devised by Fisher and Ruelle (1966), Calogero and Marchioro (1969) and Hall (1967a), in increasing order of quality (F. Calogero 1968, private communication). The new N-particle SHIP model lower bound S appears to be superior to all these for small numbers of particles. For large N all these lower bounds tend to the same limit.

The better known variational methods for obtaining lower bounds such as that by Temple (1928), require a knowledge of the first excited state of the exact problem.

Since this must be assumed, these methods do not in general yield lower bounds rigorously.

For the nonsaturating interactions studied we observe the same general trend of improvement (ratio-wise) with increasing N and V' for the SHIP model as in the previous HIP lower bound shell model. Indeed there is a loose analogy between the effects of increasing V' and N. (For bosons these are identical.) We have found improvement with increasing V' in all cases and expect an overall improvement with increasing N to hold generally for nonsaturating interactions. The apparent counter-example to this hypothesis in the case of interaction by square well forces in one dimension for $N = 2$ and 3 need not be serious as we should not expect monotonic improvement—consider the case of interaction in three dimensions by Hooke's forces in paper VI (HIP model), where $(E_0/\mathscr{E})_N > (E_0/\mathscr{E})_{N+1}$ except when N gives a closed shell for the exact problem†. Local fluctuations may be caused by a particular level spacing but will not affect the overall trend.

In all previous papers in this series we have explicitly made use of the principle that dropping a restriction lowers the energy or at least leaves it unaffected. We have not appealed to such a principle in § 3.

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† With the SHIP lower bound for Hooke's forces there is monotonic improvement with increasing N.