Derivation of energy lower bound models for translation-invariant many-fermion systems



1978 J. Phys. A: Math. Gen. 11 291

(http://iopscience.iop.org/0305-4470/11/2/008)

J. Phys. A: Math. Gen., Vol. 11, No. 2, 1978. Printed in Great Britain. © 1978

# Derivation of energy lower bound models for translation-invariant many-fermion systems

R J M Carr

Department of Mathematics, Bedford College, University of London, London NW1 4NS, UK

Received 30 August 1977

**Abstract.** A derivation of the SHRIMP energy lower bound model for translation-invariant many-fermion systems is given. Previous models are obtained as special cases.

## 1. Introduction

A sequence of energy lower bound models for translation-invariant many-fermion systems: HIP, SHIP, RIP and SHRIMP, has been introduced (Carr and Post 1968, 1971, 1977). As presented the derivations of later models in this sequence depended on the derivation of previous ones. The result is that the published derivation of the SHRIMP model is obscure. Some readers have doubted the validity of the derivation of the HIP and SHIP models (Balbutsev 1976 and others by private communication). A direct detailed derivation of the SHRIMP model follows which includes the superseded models as special cases.

## 2. Derivation of lower-bound models

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

$$H=-\frac{\hbar^2}{2m}\sum_{i=1}^{N}\Delta \boldsymbol{r}_i+\sum_{i<j=1}^{N}\sum V(|\boldsymbol{r}_i-\boldsymbol{r}_j|)$$

where the $i$th particle has the position vector $\boldsymbol{r}_i$ and mass $m_i=m$.

Let us consider the class of normalised translation-invariant trial functions $\Psi(\boldsymbol{r}_1, \boldsymbol{r}_2, \ldots, \boldsymbol{r}_N)$ for the problem obeying the usual boundary conditions of quantum mechanics. Since we have a fermion system we further restrict this class to those functions which are antisymmetric with respect to the interchange of any pair of particles $1, 2, \ldots, N$. We denote this antisymmetry by writing $\Psi(\overline{\boldsymbol{r}_1, \boldsymbol{r}_2, \ldots, \boldsymbol{r}_N})$ for any member of this sub-class which we label class $L$. The ground-state energy $E_0$ for the system is given by

$$E_0=\min\,(\Psi, H\Psi)$$

the minimisation being with respect to all functions of class $L$. We are insisting on translation invariance, therefore the variables $r_1, r_2, \ldots, r_N$ are not independent. Throughout this section we have only $3N$-3 *independent* variables. Let the ground state of $H$ be $\Psi_0(\overline{r_1, r_2, \ldots, r_N}) \in L$, then

$$E_0 = (\Psi_0, H\Psi_0).$$

We express $E_0$ as the expectation value of a sum of $N$ new Hamiltonians $H_i$; thus

$$E_0 = \frac{1}{N}\left(\Psi_0, \left(\sum_{i=1}^{N} H_i\right)\Psi_0\right) = \frac{1}{N}\sum_{i=1}^{N} (\Psi_0, H_i\Psi_0) \tag{1}$$

where

$$H_i = -\frac{\hbar^2}{2m_i}\Delta r_i + \sum_{\substack{j=1\\ j\neq i}}^{N}\left(-\frac{\hbar^2}{2m_j}\Delta r_j + \frac{N}{2}V(|r_j - r_i|)\right).$$

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

Take a typical term $(\Psi_0, H_i\Psi_0)$ in the expression (1) and consider that part which depends on the masses of the particles, namely

$$\left(\Psi_0, \left(-\frac{\hbar^2}{2m_i}\Delta r_i - \sum_{\substack{j=1\\ j\neq i}}^{N}\frac{\hbar^2}{2m_j}\Delta r_j\right)\Psi_0\right).$$

Exploiting the antisymmetry of $\Psi_0$ with respect to the interchange of any pair of particles $1, 2, \ldots, N$ this may be written

$$-\frac{\hbar^2}{2}\left(\frac{1}{m_i} + \frac{N-1}{m_j}\right)(\Psi_0, \Delta r_j\Psi_0).$$

Thus if we increase $m_i$ at the same time decreasing the $m_j$ so as to keep $(1/m_i) + (N-1)/m_j$ constant we have the relation

$$(\Psi_0, H_i\Psi_0)_{m_i > m} = (\Psi_0, H_i\Psi_0)_{m_i = m}. \tag{2}$$

We introduce relative coordinates $\rho_1, \rho_2, \ldots, \rho_N$ as follows. The particle masses are absorbed by a change of scale. Let $r'_j = m_j^{1/2} r_j$, $j \neq i$; and $r'_i = m_i^{1/2} r_i$. The transformation is

$$\rho'_i = \left(\frac{m_i}{M}\right)^{1/2} r'_i + \sum_{\substack{j=1\\ j\neq i}}^{N}\left(\frac{m_j}{M}\right)^{1/2} r'_j, \tag{3a}$$

centre-of-mass coordinate, and

$$\rho'_j = \left(\frac{m_i}{m_i + m_j}\right)^{1/2} r'_j - \left(\frac{m_j}{m_i + m_j}\right)^{1/2} r'_i \tag{3b}$$

$j = 1, 2, \ldots, N$; $j \neq i$. $M$ is the total mass, $M = m_i + (N-1)m_j$. Let $\rho'_i = M^{1/2}\rho_i$ and $\rho'_j = m_j^{1/2}\rho_j$, $j \neq i$. Then from (2) we have

$$(\Psi_0, H_i\Psi_0) \equiv (\Psi_0, H'_i\Psi_0) \tag{4}$$

where

$$H'_i = -\frac{\hbar^2}{2M}\Delta\rho_i - \sum_{\substack{j=1\\ j\neq i}}^{N}\frac{\hbar^2}{2m_j}\Delta\rho_j - \sum_{\substack{j<k=1\\ j,k\neq i}}^{N}\sum\frac{\hbar^2}{m_i + m_j}\nabla_{\rho_j}\cdot\nabla_{\rho_k} + \frac{N}{2}\sum_{\substack{j=1\\ j\neq i}}^{N} V\left(\left(\frac{m_i + m_j}{m_i}\right)^{1/2}\rho_j\right).$$

It should be noted that $\boldsymbol{\rho}_i$ is the centre-of-mass coordinate and is orthogonal to all the $\boldsymbol{\rho}_j$, $j \neq i$. Initially we took $\Psi_0$ to be translation invariant. $\Psi_0$ can be expressed solely in terms of the $\boldsymbol{\rho}_j$, $j \neq i$, when $m_i, m_j \neq m$. The only term in $H_i'$ which contains $\boldsymbol{\rho}_i$ is the kinetic energy term for the centre of mass. Thus from (4) for any $m_i \geqslant m$, with the $m_j$ suitably adjusted, we have

$$(\Psi_0, H_i'\Psi_0) = (\Psi_0, H_i''\Psi_0) \tag{5}$$

where

$$H_i'' = \sum_{\substack{j=1\\ j\neq i}}^{N} -\frac{\hbar^2}{2m_j}\Delta\boldsymbol{\rho}_j - \sum_{\substack{j<k=1\\ j,k\neq i}}^{N}\sum \frac{\hbar^2}{m_i+m_j}\nabla_{\boldsymbol{\rho}_j}\cdot\nabla_{\boldsymbol{\rho}_k} + \frac{N}{2}\sum_{\substack{j=1\\ j\neq i}}^{N} V\left(\left(\frac{m_i+m_j}{m_i}\right)^{1/2}\rho_j\right). \tag{6}$$

From (4) and (5) we have

$$(\Psi_0, H_i\Psi_0) = (\Psi_0, H_i''\Psi_0) \tag{7}$$

thus (2) becomes

$$(\Psi_0, H_i''\Psi_0)_{m_i>m} = (\Psi_0, H_i''\Psi_0)_{m_i=m}. \tag{8}$$

Now let $m_i \to \infty$ on the left-hand side of equation (8) retaining the function $\Psi_0$ and such that $(1/m_i)+(N-1)/m_j$ remains constant. From ($3a$) and ($3b$) and adjacent relations $\boldsymbol{\rho}_i \to \boldsymbol{r}_i$ and $\boldsymbol{\rho}_j \to \boldsymbol{r}_j - \boldsymbol{r}_i$, $j \neq i$. But $\boldsymbol{r}_i$ is the centre-of-mass coordinate of an infinitely massive system and therefore represents a fixed point. To emphasise this let $\boldsymbol{r}_i = \boldsymbol{a}_i$ (constant). We introduce orthogonal coordinates $\bar{\boldsymbol{\rho}}_j = \boldsymbol{\rho}_j + \boldsymbol{a}_i = \boldsymbol{r}_j$, $j \neq i$. In the limit $m_j \to m(N-1)/N$ and (8) becomes

$$\lim_{m_i\to\infty} (\Psi_0, H_i''\Psi_0) = (\Psi_0, H_i''\Psi_0)_{m_i=m}. \tag{9}$$

We have from (6), (7) and (9)

$$(\Psi_0, H_i\Psi_0) = \lim_{m_i\to\infty} (\Psi_0, H_i''\Psi_0) = (\Psi_0, \mathscr{H}_i(\boldsymbol{a}_i)\Psi_0) \tag{10}$$

where

$$\mathscr{H}_i(\boldsymbol{a}_i) = \sum_{\substack{j=1\\ j\neq i}}^{N}\left(-\frac{N}{N-1}\frac{\hbar^2}{2m}\Delta\boldsymbol{r}_j + \frac{N}{2}V(|\boldsymbol{r}_j - \boldsymbol{a}_i|)\right) = \sum_{\substack{j=1\\ j\neq i}}^{N} h_j(\boldsymbol{a}_i)$$

$$h_j(\boldsymbol{a}_i) = -\frac{N}{N-1}\frac{\hbar^2}{2m}\Delta\boldsymbol{r}_j + \frac{N}{2}V(|\boldsymbol{r}_j - \boldsymbol{a}_i|).$$

Applying (10) to each term in (1) we replace $(\Psi_0, H_i\Psi_0)$ by $(\Psi_0, \mathscr{H}_i(\boldsymbol{a}_i)\Psi_0)$, $i = 1, 2, \ldots, N$, which gives

$$E_0 = \frac{1}{N}\sum_{i=1.}^{N} (\Psi_0, \mathscr{H}_i(\boldsymbol{a}_i)\Psi_0)$$

$$= \frac{1}{N}\left(\Psi_0, \left(\sum_{j\neq 1} h_j(\boldsymbol{a}_1) + \sum_{j\neq 2} h_j(\boldsymbol{a}_2) + \ldots + \sum_{j\neq N} h_j(\boldsymbol{a}_N)\right)\Psi_0\right).$$

Now since $\Psi_0$ is translation invariant

$$(\Psi_0, h_j(\boldsymbol{a})\Psi_0) = (\Psi_0, h_j(\boldsymbol{b})\Psi_0)$$

when $\boldsymbol{a} \neq \boldsymbol{b}$. In particular

$$(\Psi_0, h_j(\boldsymbol{a}_i)\Psi_0) = (\Psi_0, h_j(\mathbf{0})\Psi_0), \qquad i = 1, 2, \ldots, N; j \neq i.$$

Let $h_j(\mathbf{0}) = h_j$. We may then write

$$E_0 = \frac{1}{N}\left(\Psi_0, \left(\sum_{j\neq 1} h_j + \sum_{j\neq 2} h_j + \ldots + \sum_{j\neq N} h_j\right)\Psi_0\right) = \left(\Psi_0, \left(\frac{N-1}{N}\sum_{j=1}^{N} h_j\right)\Psi_0\right)$$

since $\Psi_0$ is antisymmetric in $\boldsymbol{r}_1, \boldsymbol{r}_2, \ldots, \boldsymbol{r}_N$. Thus

$$E_0 = (\Psi_0, H_s\Psi_0) \tag{11}$$

where

$$H_s = \frac{N-1}{N}\sum_{i=1}^{N} h_i = \sum_{i=1}^{N}\left(-\frac{\hbar^2}{2m}\Delta\boldsymbol{r}_i + \frac{N-1}{2}V(r_i)\right)$$

and

$$h_i = -\frac{N}{N-1}\frac{\hbar^2}{2m}\Delta\boldsymbol{r}_i + \frac{N}{2}V(r_i).$$

$\Psi_0$ will not in general be an eigenstate of $H_s$. We minimise with respect to normalised functions obeying the usual boundary conditions of quantum mechanics and antisymmetric with respect to the interchange of any pair of particles $1, 2, \ldots, N$. Equation (11) becomes an inequality

$$E_0 \geqslant (\Phi_s, H_s\Phi_s) \tag{12}$$

where $\Phi_s$ is the lowest eigenstate of $H_s$ subject to the above constraints†, an antisymmetrised product (Slater determinant) formed from the first $N$ eigenstates of $h_i$. Let $h_i\phi_n(\boldsymbol{r}_i) = \epsilon_n\phi_n(\boldsymbol{r}_i)$, we take $\phi_n$ to be normalised to unity. The inequality (12) becomes

$$E_0 \geqslant \frac{N-1}{N}\sum_{i=0}^{N-1}\epsilon_i = S.$$

We have an $N$-particle shell model retaining antisymmetry in all $N$ particles, which we call the SHRIMP (symmetrised heavy reduced independent many particle) model.

Another lower-bound shell model retaining antisymmetry in only $N-1$ particles may be obtained as follows. From (1), (2) and (10) we have that

$$\begin{aligned} E_0 &= (\Psi_0, H_1\Psi_0)_{m_1=m} = (\Psi_0, H_1\Psi_0)_{m_1>m} \\ &= (\Psi_0, \mathscr{H}_1(\boldsymbol{a}_1)\Psi_0) = (\Psi_0, \mathscr{H}_1\Psi_0) \end{aligned} \tag{13}$$

where $\mathscr{H}_i = \mathscr{H}_i(\mathbf{0})$. We minimise the expectation value of $\mathscr{H}_1$ with respect to functions of class $M$ defined as follows. Class $M$ consists of those functions which satisfy the conditions of class $L$ except that the restriction of antisymmetry with respect to the interchange of particle 1 with any of the particles $2, 3, \ldots, N$ is dropped ($L \subset M$). Thus

$$E_0 \geqslant (\Phi_R(\overline{\boldsymbol{r}_2, \ldots, \boldsymbol{r}_N}), \mathscr{H}_1\Phi_R(\overline{\boldsymbol{r}_2, \ldots, \boldsymbol{r}_N})) = \mathscr{E}$$

† We assume such an eigenstate exists.

where $\Phi_R$ is the ground state of $\mathscr{H}_1$ in class $M$, an antisymmetrised product formed from the first $N-1$ eigenstates of $h_i$ giving a lower bound

$$\mathscr{E} = \epsilon_0 + \epsilon_1 + \ldots + \epsilon_{N-2}.$$

We have a shell system of $N-1$ independent particles interacting with a fixed centre of force which we call the RIP (reduced independent particle) model.

Lower-bound models were originally obtained by the procedure of letting $m_i \to \infty$ keeping the $m_j = m$ (constant) (see Carr and Post 1968, 1971). The relation (10) is then an inequality

$$(\Psi_0, H_i\Psi_0) > \lim_{m_i \to \infty} (\Psi_0, H_i''\Psi_0)$$

$$= (\Psi_0, \mathscr{H}_i(\boldsymbol{a}_i)\Psi_0) = (\Psi_0, \mathscr{H}_i\Psi_0)$$

giving lower-bound shell models for which

$$h_i = -\frac{\hbar^2}{2m}\Delta \boldsymbol{r}_i + \frac{N}{2} V(r_i).$$

We call the model corresponding to the SHRIMP model when the $m_j$ are kept constant in the limiting procedure the SHIP (symmetrised heavy independent particle) model and that corresponding to the RIP model the HIP (heavy independent particle) model.

## 3. Conclusion

Comparing the RIP with the SHRIMP model we see that the RIP model has the same energy levels apart from a factor $N/(N-1)$ but one less particle. Thus $S > \mathscr{E}$ always. However, having one less particle gives the RIP model an advantage in the discussion of angular momenta. When constructing the allowed total angular momentum values there is one less angular momentum vector in the sum which leads to a restricted set of values (Carr and Post 1971).

For the HIP and SHIP models $h_i$ has no factor $N/(N-1)$ in the kinetic energy which leads to weaker lower bounds compared with RIP and SHRIMP respectively. Thus HIP and SHIP are superseded.

## Acknowledgments

The author would like to thank Professor H R Post and Mr G Horton for many useful discussions, help and encouragement.

## References

Balbutsev E B 1976 *Dubna Preprint* JINR E4-9841
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
—— 1977 *J. Phys. A: Math. Gen.* **10** L59–61