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LETTER TO THE EDITOR

Incorrect lower bounds for the *N*-fermion problem

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Abstract. The symmetrised versions of the Carr and Post lower bounds for *N*-fermion systems are examined. It is shown that both formulae, known also as the SHIP and SHRIMP models, are incorrectly derived.

1. Introduction

Recently the author has shown (Manning 1978) that several lower bound results derived variously by Post and by Hall, can all be derived from a common formalism. This was done by introducing a reduced density operator for the interparticle separation, which in fact leads to an improved bound. All the bounds derived in this approach clearly arise by relaxing the constraint that the wavefunction be antisymmetric in all particle coordinates. Furthermore there seems to be no way in which the SHIP and SHRIMP bounds due to Carr and Post (1971, 1977, 1978) can be obtained via the reduced density operator formalism. These two lower bound formulae are the only ones which maintain the antisymmetry of the wavefunction.

As a result of this observation the derivation of the SHIP and SHRIMP models will now be re-examined. It will be shown that their derivation is incorrect and that although no counter examples are known the SHIP and SHRIMP models cannot be regarded as proven lower bounds.

2. Analysis of the SHRIMP model

We will consider the derivation of the SHRIMP model given in the most recent paper by Carr (1978). In order to focus attention on the error in this work the derivation is not re-stated here in any detail. It is assumed that the reader is familiar with Carr's arguments and the notation used here is identical with Carr (1978).

The first step in deriving the SHRIMP model is to rearrange the Hamiltonian

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

as

$$H=\frac{1}{N}\sum_{i=1}^{N}H_i$$

where

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

The ground state wavefunction is written Ψ_0 and the ground state energy of interest is

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

Taking a typical term on the right-hand side of (1) it is shown that, by defining relative and centre-of-mass coordinates $\boldsymbol{\rho}$, and by letting the mass $m_i \to \infty$,

$$(\Psi_0, H_i\Psi_0) = \left(\Psi_0, \left(-\frac{N}{N-1}\frac{\hbar^2}{2m}\sum_{\substack{j=1\\ j\neq i}}^{N}\Delta\boldsymbol{\rho}_j + \frac{N}{2}\sum_{\substack{j=1\\ j\neq i}}^{N} V(\boldsymbol{\rho}_j)\right)\Psi_0\right) \qquad (2)$$

where

$$\boldsymbol{\rho}_j = \boldsymbol{r}_j - \boldsymbol{r}_i, \qquad j \neq i.$$

At this point the following statement is made: '$\boldsymbol{r}_i$ is the centre-of-mass coordinate of an infinitely massive system and therefore represents a fixed point.' This is not true. The coordinate $\boldsymbol{r}_i$ is defined by its role in the N-particle configuration space on which Ψ_0 acts. The coordinates do not derive their significance from the transformed form of the Hamiltonian as Carr seems to assume. In fact, it would only be meaningful to regard $\boldsymbol{r}_i$ as fixed in terms of wavefunctions specific to the transformed problem with $m_i = \infty$. Such wavefunctions are no longer antisymmetric among the N particles, while it is essential for later parts of Carr's argument that we continue to use the fully antisymmetric wavefunction Ψ_0.

The statement that has been quoted above is used by Carr to justify the replacement of $\boldsymbol{r}_i$ in (2) by a constant $\boldsymbol{a}_i$. It is then argued, on the grounds that Ψ_0 is translationally invariant, that $\boldsymbol{a}_i$ can be replaced by the coordinate origin. In view of what has been said above, this procedure is not justified. Furthermore the inconsistency of the results of this procedure can be seen directly. In equation (11) of his paper Carr appears to have shown that

$$E_0 = \left(\Psi_0, \left(-\frac{\hbar^2}{2m}\sum_{i=1}^{N}\Delta\boldsymbol{r}_i + \sum_{i<j=1}^{N}\sum V(|\boldsymbol{r}_i - \boldsymbol{r}_j|)\right)\Psi_0\right)$$

$$= \left(\Psi_0, \sum_{i=1}^{N}\left(-\frac{\hbar^2}{2m}\Delta\boldsymbol{r}_i + \frac{N-1}{2}V(\boldsymbol{r}_i)\right)\Psi_0\right).$$

Note that at this stage the only properties of Ψ_0 that have been used are that it is antisymmetric in the N coordinates and that it is translationally invariant. In particular, the fact that Ψ_0 is the ground state of H has not been used. Cancelling the kinetic energy terms in this 'equality' we have apparently that

$$\left(\Psi_0, \sum_{i<j=1}^{N}\sum V(|\boldsymbol{r}_i - \boldsymbol{r}_j|)\Psi_0\right) = \frac{N-1}{2}\left(\Psi_0, \sum_{i=1}^{N} V(\boldsymbol{r}_i)\Psi_0\right)$$

for all antisymmetric translation invariant wavefunctions Ψ_0 and all interaction potentials V. This clearly cannot be the case, in fact if it were there would be no many-body problem!

3. Conclusion

The derivations of the SHIP and SHRIMP models are very similar and both use the erroneous procedure discussed above. They must therefore be regarded as unproven. In contrast, the RIP and HIP bounds can be proven quite rigorously from (2) above. The situation is then that all the rigorous lower bounds for the many-fermion problem arise by relaxing the constraint of antisymmetry in the wavefunction.

Finally, it must be mentioned that there are no known situations in which the exact ground state energy falls below the value of the SHIP or SHRIMP models. One might conjecture then that the model does provide a lower bound and that a proper proof may be forthcoming. On the other hand, the improvement obtained by symmetrising the HIP and RIP bounds is fairly small and both these bounds are generally rather poor. The lack of a counter example is therefore not surprising.

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