

Possible equivalence of Feynman's backflow and spin-dependent correlations

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The topic in the title has produced debate about whether spin-dependent correlations should be used in trial wave functions for Hamiltonians that are independent of spin. We investigate this question by calculating the ground-state properties of a small system of ${}^3\text{He}$ atoms using the variational Monte Carlo method and trial wave functions, first, with explicit backflow correlations and second, with spin-dependent correlations. We review how backflow and spin-dependent correlations can be made approximately equivalent, and then give Monte Carlo results which demonstrate that spin-dependent correlations can substantially reproduce the effect of backflow correlations. [S0163-1829(97)05409-X]

Many authors¹⁻¹⁰ have recognized the importance of Feynman-Cohen backflow¹¹ correlations as well as spin-dependent correlations in the description of liquid and solid ${}^3\text{He}$. However, quantitative understanding of the relative importance of these correlations has been elusive. Attempts to investigate spin-dependent correlations have used mainly integral equation techniques^{3,4,6} with the well-known difficulties of calculating the elementary diagrams in closed form. In addition, the noncommutativity of the backflow and spin-dependent correlations requires the development of new approximations which are not well characterized, and are different for backflow and spin-dependent cases. Other studies, where the variational Monte Carlo method was employed, have used correlations which depend only on the z component of the spin. These latter correlation factors break the spin rotational symmetry, have little or no effect at all, and do not reproduce the results of backflow correlations.⁶

In this work we investigate the importance of including spin-dependent correlations in trial functions for Hamiltonians without an explicit spin dependence. We also want to show that in these systems the effect of spin-dependent correlations and backflow correlations are largely overlapping. Finally, we demonstrate that Monte Carlo calculations with a symmetrized product of spin-dependent correlations wave function for liquid ${}^3\text{He}$ are within our present computational capabilities. This work might have important consequences for other Fermi systems such as atoms, strongly correlated electrons, and nuclei.

Classical backflow is related to the flow of a fluid around a large impurity and including backflow correlations in a trial wave function gives the correct correspondence principle limit. Backflow correlations and how to include them in variational wave functions were first described by Feynman and Cohen¹¹ in their pioneering calculations of the effective mass of ${}^3\text{He}$ in liquid ${}^4\text{He}$ and of the excitation spectrum of ${}^4\text{He}$. For a single component fermion system such as ${}^3\text{He}$, both integral equation^{1,4} and Monte Carlo calculations^{12,13} have shown that the ground state is generally well described by using backflow correlations, along with three-body corre-

lations. However, this same system, shows some remarkable magnetic properties, being, in some sense, nearly ferromagnetic. In fact, most calculations have difficulty getting the spin-polarized ${}^3\text{He}$ system higher in energy than the unpolarized system. Wave functions with pairing and other correlations^{7,9} have been proposed to deal with this problem.

Just as in electronic systems where the underlying interaction is independent of spin, the magnetic effects in ${}^3\text{He}$ are produced by the Pauli principle and exchange. Even though the interaction is independent of spin, including spin exchange terms in the wave function may describe the physical correlations in a simpler way than just using spatial correlations. Obtaining the correct answer to the question implied by the title is therefore important in understanding the physics of both quantum fluids and other many-particle systems.

As a side benefit, if spin correlations can substantially reproduce backflow correlations, we would expect less effect from adding backflow correlations to wave functions of systems where spin correlations are directly induced by the Hamiltonian. Such systems include neutron matter, nuclei, and nuclear matter.

In our work we apply the variational Monte Carlo method to calculate the ground-state expectation values of 14 ${}^3\text{He}$ atoms with periodic boundary conditions. Much of the size dependence of the energy comes from the difference between the free gas energy per particle for the infinite and finite systems. For 14 particles in a cubic periodic system, this difference is only about 1.5%. Despite the small size of the system, comparisons between different forms of wave functions should be valid. By using only 14 particles, full spin summations can be carried out for a wave function with a symmetrized product of spin-dependent correlation factors.

The simplest form for a trial wave function for the ground state of liquid ${}^3\text{He}$ is

$$|\Psi_T\rangle = \prod_{i<j} f_{ij} |\Phi\rangle. \quad (1)$$

The $f_{ij}=f(r_{ij})$ is a two-body correlation factor that depends on the distance r_{ij} between particles i and j . $|\Phi\rangle$ is the uncorrelated model state, a Slater determinant of space and spin orbitals.

Feynman-Cohen backflow correlations are introduced in $|\Psi_T\rangle$ by modifying the plane waves in $\langle R|\Phi\rangle$ so that they become

$$\exp(i\vec{k}_l \cdot \vec{r}_m) \rightarrow \exp\left(i\vec{k}_l \cdot \left[\vec{r}_m + \sum_{n \neq m} \eta_{mn} \vec{r}_{mn}\right]\right). \quad (2)$$

Standard variational wave functions for liquid He often include a three-body correlation factor product, $\prod_{i < j < k} f_{ijk}^{(3)}$, in Eq. (1). Although it is straightforward to include these terms, they are not used in the present calculations so that comparisons are easier.

In a wave function without spin-dependent correlations, the spin matrix elements can be calculated analytically and the result is that one can consider the system to be made up of nonidentical spin-up and spin-down particles. The wave function can be written as the correlation factor times two determinants of spatial orbitals: one for up spins and one for down spins. The standard variational Monte Carlo method can then be applied. The reason for this simplification is that neither the correlation operator nor the Hamiltonian can flip the spins.

The introduction of spin-dependent correlations makes this simple analysis fail. The spin correlations introduce spin exchanges which flip the spins of particles. Since the amplitude for these components changes as a function of the pair distances, the spin degrees of freedom become intimately connected with the positions of the particles and the spin sums can no longer be done analytically.

A spin-dependent wave function that includes spin-spin pair correlations and which is invariant under rotations in spin space is the symmetrized product form

$$|\Psi_{SP}\rangle = \mathcal{S} \prod_{i < j} (f_{ij}^c + f_{ij}^\sigma \vec{\sigma}_i \cdot \vec{\sigma}_j) |\Phi\rangle. \quad (3)$$

In this expression \mathcal{S} represents a symmetrizing operator that averages over all ordering of the correlations in the pair product. Here $|\Phi\rangle$ is not the product of two Slater determinants but is given by the single determinant of the $N \times N$ matrix with elements $\phi_k(\vec{r}_n) |\sigma_z\rangle_n$. For our helium system the ϕ are the plane waves without backflow correlations, $|\sigma_z\rangle_n$ the spin state of particle i , either up or down, and $R \equiv \{\vec{r}_i | i = 1, \dots, N\}$. In our calculations we expand $\langle R|\Phi\rangle$ by grouping together all terms which have the same spin assignments for the particles. Each of these terms is a determinant of the spatial orbitals of the up spin particles times a determinant of the spatial orbitals of the down spin particles,

$$\begin{aligned} \langle R|\Phi\rangle &= \sum_S (-1)^{P(S)} \det(R_{S_+}) \det(R_{S_-}) |S\rangle, \\ &= \sum_S \Phi(R, S) |S\rangle, \end{aligned} \quad (4)$$

where $|S\rangle$ is a shorthand notation for a given spin assignment to each particle, i.e., $|\sigma_z\rangle_1 |\sigma_z\rangle_2 \cdots |\sigma_z\rangle_N$. R_{S_+} and R_{S_-} stand

for the positions of the particles with spin-up and spin-down, respectively. The determinants in Eq. (4) are numbers depending only on the positions of the particles. $P(S)$ is either 0 or 1, and is chosen consistently with the ordering convention of the particles in the spin-up and spin-down determinants so that we reproduce the correct signs to assure that $|\Phi\rangle$ is antisymmetric under particle interchange.

Backflow is often described as a state dependent correlation since it can be thought of as applying a correlation factor to pairs of particles that depends on their relative momentum. Spin dependence can give a similar effect since at low relative momentum, the particles are in a relative s state which must be spatially symmetric and therefore is a spin singlet. At higher momenta, the particles can be in a relative p state which corresponds to a spin triplet state. The spin-dependent wave function, Eq. (3), gives a correlation factor of $f^c - 3f^\sigma$ for spin singlets and $f^c + f^\sigma$ for spin triplets.

To make the correspondence more concrete, we follow a method analogous to that given by Pandharipande and Itoh¹⁴ and expand the backflow and spin dependent wave functions for a pair of particles with small relative wave vector k . If we eliminate the center of mass motion, the spatial two-body wave function for the backflow case is

$$\begin{aligned} f(r) \exp\left(i \frac{\vec{k} \cdot \vec{r}}{2} [1 + 2\eta(r)]\right) \\ \approx f(r) \exp\left(i \frac{\vec{k} \cdot \vec{r}}{2}\right) [1 + i\vec{k} \cdot \vec{r} \eta(r)], \end{aligned} \quad (5)$$

TABLE I. Variational and kinetic energies at given densities and wave functions as described in the text. The calculations at $\rho = 0.01659 \text{ \AA}^{-3}$ were made with 54 particles, all ours with 14 particles. At the equilibrium density we have used the following variational parameters: $b = 2.94 \text{ \AA}$, $\lambda = 1.0$, $r_0 = 2.3 \text{ \AA}$, and $w = 1.3 \text{ \AA}$, at $\rho = 0.01797 \text{ \AA}^{-3}$, r_0 was changed to 2.4 \AA and at the freezing density to 2.6 \AA .

$\rho \text{ \AA}^{-3}$	$\langle E \rangle (K)$	$\langle T \rangle (K)$	WF
0.01635	-1.35 ± 0.02	12.61 ± 0.09	SP
	-1.49 ± 0.02	12.65 ± 0.04	JSB
	-1.18 ± 0.02	13.00 ± 0.03	JS
0.01659	-1.55 ± 0.04		JSB (Ref. 12)
	-1.08 ± 0.03		JS (Ref. 12)
	-1.91 ± 0.03		JTSB (Ref. 12)
0.01797	-1.10 ± 0.04	14.45 ± 0.09	SP
	-1.21 ± 0.03	14.56 ± 0.04	JSB
	-0.86 ± 0.03	14.93 ± 0.04	JS
0.01946	-0.57 ± 0.05	16.53 ± 0.10	SP
	-0.68 ± 0.03	16.44 ± 0.05	JSB
	-0.39 ± 0.03	16.87 ± 0.05	JS

where we have kept just the linear term in η since it is expected to be small. If the particle pair is in a spin singlet, the spatial wave function must be symmetric. If spin-dependent and backflow wave functions were equivalent, we would require,

$$\begin{aligned} f(r) \left[\cos\left(\frac{\vec{k}\cdot\vec{r}}{2}\right) - \vec{k}\cdot\vec{r} \eta(r) \sin\left(\frac{\vec{k}\cdot\vec{r}}{2}\right) \right] \\ = [f^c(r) - 3f^\sigma(r)] \cos\left(\frac{\vec{k}\cdot\vec{r}}{2}\right). \end{aligned} \quad (6)$$

Similarly, for a spin triplet state we would require,

$$\begin{aligned} f(r) i \left[\sin\left(\frac{\vec{k}\cdot\vec{r}}{2}\right) + \vec{k}\cdot\vec{r} \eta(r) \cos\left(\frac{\vec{k}\cdot\vec{r}}{2}\right) \right] \\ = [f^c(r) + f^\sigma(r)] i \sin\left(\frac{\vec{k}\cdot\vec{r}}{2}\right). \end{aligned} \quad (7)$$

These equation cannot be solved generally for all k values. Expanding and keeping just the lowest order term in k gives the approximate correspondence

$$f^c(r) = f(r) \left[1 + \frac{3}{2} \eta(r) \right], \quad f^\sigma(r) = \frac{1}{2} f(r) \eta(r). \quad (8)$$

Equivalence of backflow and the spin-dependent correlations should imply that $|\Psi_T\rangle$ and $|\Psi_{SP}\rangle$ with the above correspondence provide similar results.

The variational Monte Carlo method used in calculations with the backflow correlated wave function^{12,15} is now a completely standard application of the Metropolis *et al.* method.¹⁶ The spin-dependent wave function $|\Psi_{SP}\rangle$ requires a few simple modifications of the standard treatment.¹⁸ We write the spin operator using the identity

$$\vec{\sigma}_i \cdot \vec{\sigma}_j = 2E_{ij} - 1, \quad (9)$$

where E_{ij} exchanges the spins of particles i and j . For each of the spin states $|S\rangle$ in Eq. (4), we record the state that each E_{ij} produces. The multiplication of $|\Phi\rangle$ by the $N(N-1)/2$ correlation operators is then easily accomplished as a series of very sparse matrix operation — each row of the matrix representing a correlation factor in S space has only 1 or 2 nonzero elements, the diagonal element, and the pair exchanged element if the spins of the pair are different. If the spins are different, the diagonal element is $f_{ij}^c - f_{ij}^\sigma$ and the nondiagonal $2f_{ij}^\sigma$. The number of possible spin assignments gives the number of elements in our wave function. For our total spin zero wave function this is $(N!)/[(N/2)!(N/2)!]$ namely 3432 states for $N=14$. Flipping all the spins of the particles leaves the magnitude of our wave function unchanged; the sign changes for $(N/2)$ odd. We can therefore reduce the size of our problem to 1716 states by using this symmetry. It is amusing that if we were to attempt to calculate the next closed Fermi surface for the periodic cubic box, 38 particles, we would have about a factor of 10^6 more spin states.

The symmetrized product wave function requires that we average over all the orderings of the correlation operators. We choose to do this averaging by Monte Carlo sampling of the orders. In principle this could lead to a sign problem in the Monte Carlo method because the order of the operators on the left and right wave functions in the Monte Carlo integration are not the same, and there is no guarantee that their product is positive. In practice we have not encountered any negative signs. If a few were produced, they would not contribute significantly to the variance, and could be dealt with by sampling from the absolute value and including the sign in the averaging.

The expectation value of the energy is

$$\langle H \rangle = \frac{\sum_{\text{orders}}^{\text{pair}} \int dR \sum_{SS'} \langle S' | \Phi(R, S') \prod_{mn} (f_{mn}^c + \vec{\sigma}_m \cdot \vec{\sigma}_n f_{mn}^\sigma) H \prod_{mn} (f_{mn}^c + \vec{\sigma}_m \cdot \vec{\sigma}_n f_{mn}^\sigma) \Phi(R, S) | S \rangle}{\sum_{\text{orders}}^{\text{pair}} \int dR \sum_{SS'} \langle S' | \Phi(R, S') \prod_{mn} (f_{mn}^c + \vec{\sigma}_m \cdot \vec{\sigma}_n f_{mn}^\sigma) \prod_{mn} (f_{mn}^c + \vec{\sigma}_m \cdot \vec{\sigma}_n f_{mn}^\sigma) \Phi(R, S) | S \rangle}. \quad (10)$$

The sums over S and S' are done explicitly. The sums over the pair operator orderings and the integration over the spatial coordinates R are done using the Metropolis method. The Hamiltonian includes only a pairwise potential and is

$$H = -\frac{\hbar^2}{2m} \sum_{i=1}^N \nabla_i^2 + \sum_{i<j} v(|\vec{r}_{ij}|). \quad (11)$$

Results for the energies of our 14 particle model helium liquid with periodic boundary conditions and the HFDHE2 potential¹⁷ are shown in Table I. Figure 1 shows a comparison of two-body distribution functions. In our calculations we use $f(r) = \exp[-\frac{1}{2}(b/r)^5]$ together with $L/2$ corrections,

where L is the side of the simulation cell.¹² We present results for the Jastrow-Slater trial function modified by backflow correlations (JSB)

$$\eta(r) = \lambda \exp[-(r-r_0)^2/w^2] \left(\frac{L/2-r}{L/2} \right)^3, \quad (12)$$

and for the spin-dependent symmetrized-product (SP) wave function with $f^c(r)$ and $f^\sigma(r)$ given by the relations in Eq. (8). At all densities, we have optimized the trial energy obtained with JSB with respect to r_0 , the parameter of $\eta(r)$ that most affects the trial energy. Calculations have been done at the equilibrium density, at freezing and at an intermediate density. We also give results for a simple Jastrow-Slater (JS) wave function. For completeness, we report

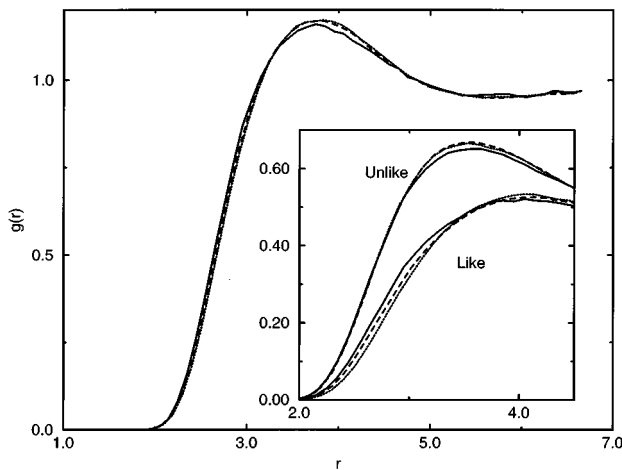


FIG. 1. The SP (solid), JS (dotted), and JSB (dashed) two-body distribution functions are shown at equilibrium density $\rho=0.01635 \text{ \AA}^{-3}$. The insert displays the contributions for like and unlike spin pairs.

results¹² at a density very near the equilibrium density for a system of 54 ^3He atoms. In this case, three different trial functions were considered: the JS and JSB forms, and the Jastrow-triplet-Slater with backflow (JTSB) form. Comparing the JS and JSB results for 14 and 54 atoms one can see that finite size effects are not dramatic.

The total energy per atom determined with the spin-dependent symmetrized product trial function is significantly better than the one obtained with a wave function of the Jastrow-Slater form. This calculation was performed within the variational Monte Carlo framework and thus subject only to statistical uncertainties. It demonstrates that spin-dependent correlations can account for a fraction of the energy defect that we have when a simple wave function of the Jastrow-Slater form is used, even if the system Hamiltonian does not depend explicitly on spin.

The overall agreement between the total energy per atom obtained with the spin-dependent symmetrized product and

the Jastrow-Slater-Backflow trial functions is good. This situation shows that spin-dependent correlations and backflow correlations produce effects that are largely overlapping. Figure 1 shows that the spin dependent correlations change the two-body distribution more than backflow correlations although the differences are small. We want to emphasize again that we have not optimized the spin-dependent correlations. This situation could very well account for the fact that the JSB form of the wave function provides slightly better energies. The result that effects of spin-dependent correlations and backflow correlations are similar for spin independent Hamiltonians can help us understand the role of these two different correlations on observable properties of the system, and may show how to include backflow correlations in problems where so far the efforts to introduce them have not been successful. The major advantage to using backflow correlations is that they are computationally much cheaper.

The overlapping effects of spin and backflow correlations may be relevant for other systems. In nuclear physics, where spin and isospin dependent correlations are already required by the form of the Hamiltonian, our results indicate that little will be gained by including additional backflow correlations. In atomic and molecular physics, calculations with backflow correlations have not been successful in improving the trial wave functions. Spin-dependent correlations may give a clue that will help understand both the physical correlations and how to include them in electronic structure calculations.

In conclusion, this work, which reports Monte Carlo calculations with a symmetrized product of spin-dependent correlations wave function for liquid ^3He , shows that spin-dependent correlations defined to be equivalent to backflow correlations at low relative momenta, produce similar effects. Besides giving a better understanding of the underlying physics of the quantum many-body problem, our results may prove useful in other fields.

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¹K. E. Schmidt and V. R. Pandharipande, Phys. Rev. B **19**, 2504 (1979).

²K. E. K urten and C. E. Campell, J. Low Temp. Phys. **44**, 149 (1981).

³J. C. Owen and G. Ripka, Phys. Rev. B **25**, 4914 (1982).

⁴E. Manousakis, S. Fantoni, V. R. Pandharipande, and Q. N. Usmani, Phys. Rev. B **28**, 3770 (1983).

⁵E. Krotscheck, in *Quantum Fluids and Solids, Sanibel, Florida, 1983*, Proceedings of the Symposium on Quantum Fluids and Solids, edited by E. D. Adams and G. G. Ihas (AIP, New York, 1983), p. 132.

⁶K. E. K urten and J. W. Clark, Phys. Rev. B **30**, 1342 (1984).

⁷J. P. Bouchaud and C. Lhuillier, Europhys. Lett. **3**, 1273 (1987).

⁸M. Viviani, E. Buendia, S. Fantoni, and S. Rosati, Phys. Rev. B **38**, 4523 (1988).

⁹J. P. Bouchaud and C. Lhuillier, in *Spin Polarized Quantum*

Systems, edited by S. Stringari (World Scientific, Berlin, 1989).

¹⁰F. Pederiva, S. A. Vitiello, K. Gernoth, S. Fantoni, and L. Reatto, Phys. Rev. B **53**, 15 129 (1996).

¹¹R. P. Feynman and M. Cohen, Phys. Rev. **102**, 1189 (1956).

¹²K. E. Schmidt, M. A. Lee, M. H. Kalos, and G. V. Chester, Phys. Rev. Lett. **47**, 807 (1981).

¹³R. M. Panoff and J. Carlson, Phys. Rev. Lett. **62**, 1130 (1989).

¹⁴V. R. Pandharipande and N. Itoh, Phys. Rev. A **8**, 2564 (1973).

¹⁵K. E. Schmidt and D. M. Ceperley, in *The Monte Carlo Method in Condensed Matter Physics*, edited by K. Binder (Springer-Verlag, Berlin, 1992).

¹⁶N. Metropolis, A. W. Rosenbluth, H. Rosenbluth, A. Teller, and E. Teller, J. Chem. Phys. **21**, 1087 (1953).

¹⁷R. A. Aziz, V. P. S. Nain, J. S. Carley, W. L. Taylor, and G. T. McConville, J. Chem. Phys. **70**, 4330 (1979).

¹⁸J. Lomnitz-Adler, V. R. Pandharipande, and R. A. Smith, Nucl. Phys. A **361**, 399 (1981).