Excited States in ^{4}He Described by a Shadow Wave Function

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The idea of the shadow wave function, which incorporates quantum delocalization of particles in the description of quantum liquids and solids, is applied to excited states of liquid ^{4}He. With a simple Feynman shadow wave function we compute the phonon-roton excitation spectrum by a Monte Carlo method at three different densities. The variation of the excitation energy with density is consistent with the behavior of the experimental data. The energy near the roton minimum is in excellent agreement with experiment at all densities.

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If the ground-state properties of liquid ^{4}He can be considered as reasonably well understood, our understanding of the excited states of the system, in particular, roton and vortex excitations, is incomplete and uncertain. Consider how little quantitative progress has been achieved in the computation of the roton energy since the pioneering work of Feynman and Cohen [1] (FC). A recent elaborate computation [2] in which the wave function of a roton includes contributions up to fourth order in density fluctuations $\rho_{\mathbf{k}}=\sum_j e^{i\mathbf{k}\cdot\mathbf{r}_j}$ (FC is second order) gave an energy which is about 15% higher [3] than the experimental value. It showed even larger deviations in the strength $Z(k)$ of the single-excitation peak of the dynamical structure factor $S(k,\omega)$. The systematic study of the excitation spectrum from perturbation theory based on correlated basis functions has given [4] useful insight into the problem but a computation of this sort taken to high order requires approximations for correlation functions beyond the pair level with a resulting uncertainty on the results.

In this Letter we introduce a new form for the wave function of these excited states based on the use of subsidiary variables. Such a shadow wave function, which we will shortly define, was first introduced [5] to describe the ground state Ψ_0 of ^{4}He. It made a number of important contributions, for instance to our understanding of solidification. Here we show how to generalize this form for excited states. Within the new framework provided by the shadow wave function we use the basic idea of constructing an excited state by modulating the coordinates of the shadow particles. This is conceptually a very simple approach and in its simplest form leads to a function for an excited state with no new variational parameters. We find that the trial function, with momentum $\hbar\mathbf{k}$, gives a very good value for the energy at the roton minimum. It also gives an equally good description of the density dependence of the energy of a roton. We believe that these very good results clearly demonstrate that the shadow wave function provides a powerful, and practical, new approach for the description of boson systems.

The shadow wave function for the ground state [5] couples the positions $\{\mathbf{r}_i\}$ of He atoms by a Bijl-Jastrow product times a factor that couples the particles by Gaussians to subsidiary variable $\{\mathbf{s}_i\}$. These variables are in turn correlated by a pair product factor. Since the $\{\mathbf{s}_i\}$ are integrated out, there are many-body couplings among the $\{\mathbf{r}_i\}$ beyond the pair level.

A physical motivation for this choice of Ψ_0 comes from Feynman's path-integral formulation of the density matrix over discrete imaginary time [6]. As is well known, to each particle position $\mathbf{r}_i$ we can associate, in this formalism, a sequence of positions $\mathbf{r}_i^{(\mu)}$. In this context we can think of particles as being represented by a kind of "polymer" where the $\mathbf{r}_i^{(\mu)}$ are the monomer coordinates. For the purpose of the present discussion, cross-linking of the polymers related to Bose statistics is not important because the hard-core interaction prevents frequent cross-linking. Both particles and associated monomers interact with each other, so correlations between particles occur both directly and indirectly via the polymers. This last mechanism induces correlations beyond the two-body level. In other words, due to the quantum uncertainty, the particles are delocalized and high-order correlations arise. As the intrapolymer interaction in the path integral is harmonic, it is reasonable to expect that the monomers have a Gaussian-like distribution about the center of mass of its polymer. From this picture the shadow wave function emerges. The subsidiary variables have the role of the centers of mass of the polymers, and the interpolymer correlations are represented by an effective interaction between these centers of mass, i.e., between the subsidiary (shadow) variables.

In an excited state, particles undergo additional motion but the delocalization of the particles, producing what we call quantum holes, should appear not only in the ground state but also in these excited states. This hole should be

essentially unaltered for excitations of low energy. Guided by this idea we have constructed our trial functions for excited states. For a state with momentum $\hbar\mathbf{k}$ we write the unnormalized function in the form

$$\Psi_{\mathbf{k}}(R)=\psi_r(R)\int dS\prod_i\theta(\mathbf{r}_i-\mathbf{s}_i)\psi_s(S)\sigma_{\mathbf{k}}\,, \tag{1}$$

where

$$\sigma_{\mathbf{k}}=\sum_{i=1}^{N}e^{i\mathbf{k}\cdot\mathbf{s}_i}\,, \tag{2}$$

$$R\equiv\{\mathbf{r}_1,\mathbf{r}_2,\ldots,\mathbf{r}_N\},\quad S\equiv\{\mathbf{s}_1,\mathbf{s}_2,\ldots,\mathbf{s}_N\}\,,$$

$$\psi_r(R)=\prod_{i<j}\exp[-\tfrac{1}{2}(b/|\mathbf{r}_i-\mathbf{r}_j|)^n]\,,$$

$$\theta(\mathbf{r}_k-\mathbf{s}_k)=\exp[-C(\mathbf{r}_k-\mathbf{s}_k)^2]\,,$$

and

$$\psi_s(S)=\prod_{i<j}\exp[-(b_s/|\mathbf{s}_i-\mathbf{s}_j|)^5]\,.$$

Except for $\sigma_{\mathbf{k}}$, all terms in Eq. (1) are identical to those in the trial wave function for the ground state [5]. The values of the variational parameters b, n, C, and b_s are those that best describe the ground state.

The trial function Ψ_k has essentially a Feynman form [7] but the density fluctuation appears in the subsidiary variables via $\sigma_{\mathbf{k}}$. That this $\Psi_{\mathbf{k}}$ should be superior to the standard Feynman form is inferred from the fact that it already includes backflow effects. In fact, by expanding the integrand in (1) with respect to $\mathbf{r}_i\cdot\mathbf{s}_i$ to lowest order in the width of the Gaussian θ, one finds exactly the FC form [1] with a dipolar backflow function. Its spatial dependence is not the hydrodynamic r^{-2} form, however, but is determined by the form of $\psi_s(S)$. On the other hand, for a finite width of θ the expansion leads to terms of all order in powers of $\rho_{\mathbf{k}}$. Therefore our $\Psi_{\mathbf{k}}$ has a nonpolynomial structure in $\rho_{\mathbf{k}}$. An additional insight on our wave function is obtained if the expansion mentioned above is transformed in a cumulant expansion of the average of $e^{i\mathbf{k}\cdot(\mathbf{s}_i-\mathbf{r}_i)}$ with respect to the shadow variables. In this case the term of lowest order has the FC form in the exponential form. Therefore in our computation we are able to handle implicitly for the first time the backflow in the exponential form and this can be important for excitations in the maxon and roton regions where the short-range structure is important as well.

It is significant to note that the trial function of Eq. (1) has no free parameters and the amount of backflow is determined by the ground-state correlations. One can, however, easily generalize that function so that it contains a variable amount of backflow. This new function $\Psi_{\mathbf{k}}^{(\alpha)}$ is the same as Eq. (1) but $\sigma_{\mathbf{k}}$ is replaced by

$$\sigma_{\mathbf{k}}^{(\alpha)}=\sum_{j=1}^{N}e^{i\mathbf{k}\cdot\mathbf{s}_j+i\alpha\mathbf{k}\cdot(\mathbf{s}_j-\mathbf{r}_j)}\,, \tag{3}$$

where α is a variational parameter. Since $\sigma_{\mathbf{k}}^{(-1)}=\rho_{\mathbf{k}}$, the trial function $\Psi_{\mathbf{k}}^{(-1)}$ is just the standard Feynman form when the ground state is the shadow function. The quantity $\alpha+1$ is a measure of the amount of backflow.

We have computed the excitation energy $\bar{\varepsilon}_k$ corresponding to $\Psi_{\mathbf{k}}^{(\alpha)}$ from the expression

$$\bar{\varepsilon}_k=\frac{\langle\sigma_{-\mathbf{k}}'^{(\alpha)}\sigma_{\mathbf{k}}^{(\alpha)}(H\Psi_T)/\Psi_T\rangle}{\langle\sigma_{-\mathbf{k}}'^{(\alpha)}\sigma_{\mathbf{k}}^{(\alpha)}\rangle}-\left\langle\frac{H\Psi_T}{\Psi_T}\right\rangle, \tag{4}$$

where the first term is the total energy of the excited state and the second term is the ground-state energy. H is the Hamiltonian, Ψ_T is the ground state, i.e., Eq. (1) without the factor $\sigma_{\mathbf{k}}$, and the averages (denoted by the angular brackets) are taken with respect to the normalized function

$$p(R,S,S')=\frac{\Xi(R,S)\Xi(R,S')}{\int dR\,dS\,dS'\Xi(R,S)\Xi(R,S')}\,. \tag{5}$$

Here $\Xi(R,S)=\psi_r(R)\prod_i\theta(\mathbf{r}_i-\mathbf{s}_i)\psi_s(S)$, and $\sigma_{\mathbf{k}}'^{(\alpha)}$ in Eq. (4) stands for Eq. (3) with $\mathbf{s}_i'$ in place of $\mathbf{s}_i$. The $9N$-dimensional integrals in Eq. (4) are evaluated by the Metropolis Monte Carlo algorithm.

In our computation we have used the interatomic pair potential of Aziz *et al.* [8], the ground-state factors ψ_r, θ, and ψ_s are the ones determined in Ref. [5], and the excitation energy is computed for moments corresponding to the Born–von Karman wave vectors consistent with the periodicity of the simulation cell (108 particles in the present computation).

In Fig. 1 we show the excitation energy as a function of α for a single value of the wave vector, at $k=1.843$ Å^{-1}, the value nearest to the roton minimum. At $\alpha=-1$ the energy is of order of 20 K, a typical value of the roton energy given by the standard Feynman wave function. It is clear that there is a dramatic decrease of the energy with increasing value of α and that somewhere near $\alpha=0$ there

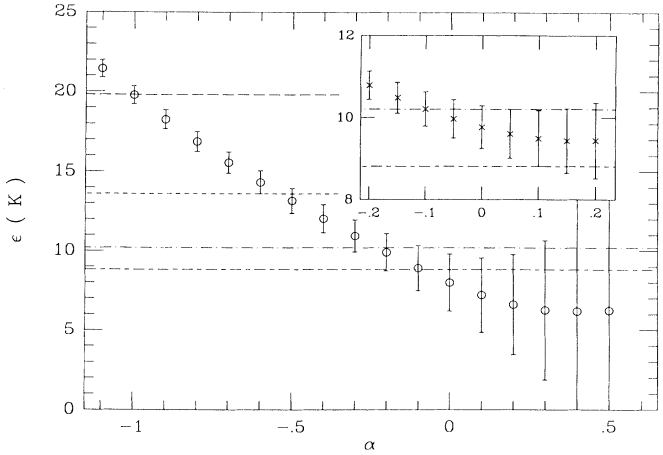

FIG. 1. Excitation energy of liquid ^{4}He at equilibrium density as a function of α for $k=1.843$ Å^{-1} for runs of 150000 attempted moves per particle and per shadow. The bars represent the statistical fluctuation. Inset: The results of runs 10 times longer. The horizontal lines represent, respectively, the experimental value (short-dash–long-dashed), the Bijl-Feynman value [2] (long-dashed), the FC value [2] (short-dashed), and the second-order perturbation result [2] with FC states (dot-dashed).

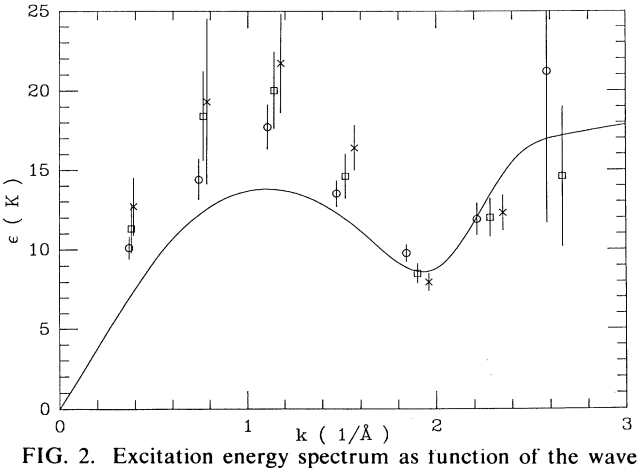

FIG. 2. Excitation energy spectrum as function of the wave vector when $\alpha=0$. The solid line is a least-squares spline fit to neutron-scattering data [13] obtained at the equilibrium density ρ_0. The circles are our results at this last density. The squares stand for our data at $\rho=1.1\rho_0$. The crosses show our results at a density $\rho=1.2\rho_0$ close to freezing.

is a minimum with an energy of order of 9.5 K. The minimum is not well determined, however, even for the longer runs we have made (corresponding to the data in the inset in Fig. 1). In fact, this computation is very demanding because we are interested in an energy difference and because we have to deal with very fast oscillating phases when evaluating the energy of the excited states. Typically our runs take more than 40 h on the IBM 3090. In any case we are able to conclude on the basis of the present computation that the shadow Feynman form gives an energy much better than the FC value (around 14 K) and even lower than a second-order perturbation computation with FC states which gives [2,3] 10.3 K. The fact that α is close to zero at the minimum of the excitation energy verifies our hypothesis that the quantum hole for low-energy excitations is essentially unchanged with respect to the ground state.

The excitation energy for the other values of k has a similar trend as function of α but since the minimum with respect to α is ill determined, we show in Fig. 2 the results for $\alpha=0$, i.e., for the wave function given by (1) and (2). The shape of the spectrum as a function of k is given correctly but the deviation from experiment in the maxon region is substantially larger than in the roton region. It is known [2], however, that the maxon energy is very dependent on the form used for the ground state. So, the maxon energy we get could be affected by the specific choice [5] of the ground-state shadow function and a careful optimization of the correlating factors contained in Ψ_T is required for a full assessment of our results for the maxon energy.

Experimentally, the excitation spectrum has an important density dependence, the maxon energy going up with density, whereas the roton energy goes down and the roton minimum is displaced to a larger k value. We have performed the computation of $\bar{\varepsilon}_k$ at higher densities up to freezing and the results for $\alpha=0$ are also shown in Fig. 2. It is clear that the trend of $\bar{\varepsilon}_k$ with density is exactly the experimental one and in Table I we present the excitation energies and their errors for the momentum value nearest to the roton minimum. Also in this table we quote estimates of the experimental values [9,10] at the given momenta. There is a remarkable agreement, particularly when we keep in mind that the wave function (1) has no variational parameter. From our computation there is a clear indication that the position of the roton minimum moves to a larger wave vector as we increase the density. The drawback of a computational simulation like ours is that we can only compute $\bar{\varepsilon}_k$ for a finite set of wave vectors. The size of the system in the present calculation is too small to allow an estimate of the location of the roton minimum and of the effective mass. In this respect the development of analytically based treatment of the present wave function would be very useful.

TABLE I. Excitation energy near the roton minimum at the densities displayed in the first column. The second column shows the value of the wave vector which in our computation is closest to the roton minimum. In the last two columns we present our results and estimates of the experimental energies for the indicated k values. At the highest density, the experimental result is at $\rho=0.0256$ Å^{-3}.

ρ (Å^{-3})	k (Å^{-1})	$\bar{\varepsilon}_k$ (K)	ε_k (K) (Expt.)[a]
0.0219	1.843	9.77 ± 0.52	8.90
0.0240	1.901	8.51 ± 0.59	8.04
0.0262	1.960	7.97 ± 0.55	7.74

[a]References [9] and [10].

The strength $Z^{(\alpha)}(k)$ of the single-excitation peak of the dynamical factor $S(k,\omega)$ computed using the shadow wave function is obtained through the equation

$$Z^{(\alpha)}(k)=\frac{\langle\sigma'^{(-1)}_{-\mathbf{k}}\sigma^{(\alpha)}_{\mathbf{k}}\rangle^2}{\langle\sigma'^{(\alpha)}_{-\mathbf{k}}\sigma^{(\alpha)}_{\mathbf{k}}\rangle}. \tag{6}$$

In Fig. 3 we show our results for $Z^{(\alpha)}(k)$ at the equilibrium density together with its experimental value [11]. When $\alpha=-1$ we have $Z^{(-1)}(k)=S(k)$, the ground-state structure factor given by the shadow wave function. The value of $Z^{(0)}(k)$ is substantially lower than the computed value of $S(k)$ and is in much better agreement with experimental values. This gives further support to our wave function because it produces a reasonable description of the amount of the single-excitation contribution to $S(k,\omega)$ compared to the multiple-excitation contribution. In the roton region we still overestimate the experimental $Z(k)$ by about 50% and our results are roughly comparable to those given by the second-order perturbation calculation based on FC states [2], but a detailed comparison cannot be done for the reason already mentioned in Ref. [3]. It should be noticed that $Z(k)$ is directly related to the correlation functions of our wave function Ψ_T of the *ground state*. Again a full assessment of the result for $Z(k)$ needs a careful optimization of the

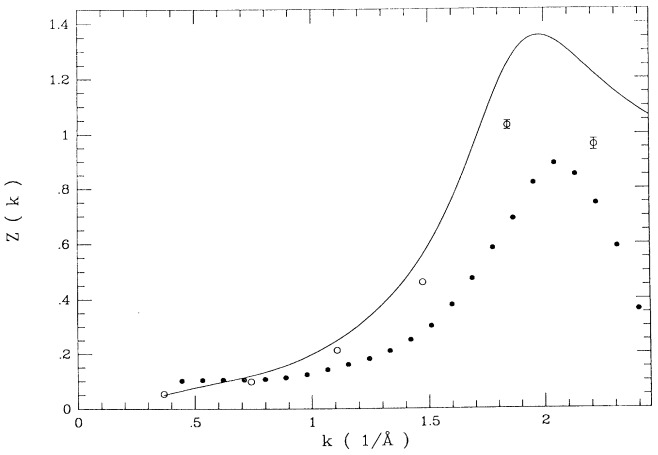

FIG. 3. Single-excitation peak intensity $Z(k)$ as a function of the wave vector. The solid line gives the result for $\alpha=-1$, that is $S(k)$ when the ground state is described by Ψ_T. The circles are our results for $\alpha=0$. Where not visible, the statistical error of our result is below the symbol size. The solid circles show the experimental data [11].

correlating factors present in Ψ_T.

In conclusion, we have shown that shadow wave functions are important not only for ground-state properties but also for excited states. With no variational parameters in a Feynman shadow function, we obtain the best theoretical estimate so far of the roton energy, having a deviation from experiment in the range of 0.5–0.8 K at all densities. The fact that we predict the correct density dependence of $\bar{\varepsilon}_k$ is particularly significant. An improved form of the shadow wave function for the *ground state* should improve the result for the excitation energy $\bar{\varepsilon}_k$. We see two important aspects by which the present wave functions differ from the traditional ones. We guarantee that the quantum hole present in the ground state is present also in the excited states. Thus many-body correlations are induced between particles, and the wave function does not have a polynomial structure in the density fluctuation variables $\rho_{\mathbf{k}}$ of the particles. It is also clear that our wave function can be expanded in powers of $\rho_{\mathbf{k}}$ and, presumably, at small k only few low-order terms will be relevant. Whether this is also the case in the roton region or whether the excellent result we get for the roton energy is due to the fact that implicit in our computation is a backflow structure in an exponential form is an important issue, and the clarification of this point can also give useful insight on the perturbative approach. We believe that aspects related to the quantum hole will be relevant to other properties of Bose fluids and also in the cases of quantum solids and of fermion systems, at least those with a hard core. As a further application of this idea, we have shown [12] that it is possible to write down a shadow wave function for a vortex excitation which has distributed vorticity and either a hollow or a filled core. A variational computation with this wave function is in progress.

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