Rotons and Roton Wave Packets in Superfluid ^{4}He

D. E. Galli, E. Cecchetti, and L. Reatto

Interuniversitario di Fisica della Meteria and Dipartimento di Fisica, Università di Milano, Via Celoria 16, 20133 Milano, Italy

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We give new information on the excitations in superfluid ^{4}He. By a variational computation we obtain a very accurate description of the excitations; the energy spectrum has deviation from experiment at the level of 5%. The first microscopic study of roton wave packets is presented. R^+ and R^- rotons cannot be described as single particle excitations due to interference effects between neighboring atoms. The roton minimum corresponds to the special wave vector where this interference disappears and the local density and momentum essentially coincide with those of a single particle excitation. [S0031-9007(96)02056-X]

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Many of the properties of superfluid ^{4}He are determined by the elementary excitations of the system. If there is some general agreement on the nature of the long-wavelength small energy excitations, i.e., phonons, this is not the case for the roton excitations. A number of models have been considered, from the picture of a roton as an atomically small vortex ring put forward by Feynman and Cohen [1] and recently revived by Williams [2], to the view of a roton as a renormalized single particle excitation which goes back to Miller, Pines, and Nozieres [3] and to Chester [4]. The different temperature behavior of the neutron scattering in the phonon and in the roton region has motivated Glyde and Griffin [5] to propose that the phonon-maxon-roton excitation curve arises from two quite distinct processes, a zero sound mode at small q and a single particle mode beyond the maxon wave vector q.

The microscopic variational theory started by Feynman and Cohen [1] and developed by many workers has been able to account for the shape of the excitation spectrum $E(q)$. In spite of this the exact nature of a roton is still generally considered as not being understood [6]. This has two motivations. These computations are quite complex and basically the only outcome is the energy, an integrated quantity which hardly gives a physical picture of the excitation. Second, even the most elaborate theories [7,8] give a roton energy of order of 10 K at standard vapor pressure, more than 15% above experiment. This can be contrasted with the typical 5% or even smaller deviation for the ground state energy E_0 coming from a good variational computation. This leaves the doubt that some important physics is missing in the description of rotons.

In this Letter we present new results on rotons and more generally on the full $E(q)$. First, by improving upon previous computations [9] based on shadow wave function (SWF) we show that the excitation spectrum can be described at a level of accuracy similar to that of the ground state. Second, we present the first computation of roton wave packets built with these accurate excited states. With these localized excitations we can study local properties like the density and the momentum, we present the first detailed study of backflow at short distance, and the role of particle indistinguishability can be clearly identified.

The introduction of SWF has given a great impulse to the variational study both of the ground state and of the excited states of superfluid ^{4}He. With this type of wave function interparticle correlations of all order beyond the pair (Jastrow) level are implicitly introduced through a set of subsidiary variables, the shadows, which are integrated over. For this reason the SWF technique has been found to be very important for the helium system in which correlations between atoms are very strong and not limited to the pair level. In addition, by writing the phase factors of an excited state in terms of these subsidiary variables, backflow effects between the He atoms are implicitly introduced and terms of all order in the density fluctuations $\rho_{\vec{q}} = \sum_j \exp(i\vec{q} \cdot \vec{r}_j)$ are generated [9]. Without any variational parameter a roton energy of about 10 K was obtained. We improve the previous computations in two ways. First, we introduce in the wave function $\Psi_{\vec{q}}$ an explicit backflow contribution [10], i.e., we write

$$\Psi_{\vec{q}}(R) = \int dS\, F(R,S)\tilde{\sigma}_{\vec{q}}(S)/\mathcal{N}_q^{1/2}. \qquad (1)$$

$R = \{\vec{r}_1, \ldots, \vec{r}_N\}$ is the set of positions of N ^{4}He atoms and $S = \{\vec{s}_1, \ldots, \vec{s}_N\}$ is the set of subsidiary variables. $\mathcal{N}_q$ is the normalization constant. Interparticle correlations are introduced by $F(R,S)$ which is a product of terms, $F(R,S) = \phi_p(R)\phi_s(S)\prod_i f_{ps}(|\vec{r}_i - \vec{s}_i|)$. $\phi_p(R)$ is a Jastrow factor, $\phi_p(R) = \prod_{i<j} f_p(r_{ij})$, and similarly for $\phi_s(S)$. The momentum carrying term in (1) is

$$\tilde{\sigma}_{\vec{q}}(S) = \sum_j e^{i\vec{q}\cdot\tilde{\vec{s}}_j}, \qquad \tilde{\vec{s}}_j = \vec{s}_j + \sum_{l(\neq j)} (\vec{s}_j - \vec{s}_l)\lambda(s_{jl})\,. \qquad (2)$$

If $\lambda = 0$, $\tilde{\sigma}_{\vec{q}}$ is simply a density fluctuation in the shadow variables and the structure of $\Psi_{\vec{q}}$ coincides with the one previously studied [9]. $\lambda(s)$ introduces an explicit backflow, and we have assumed the short range form $\lambda(s) = A[(s/r_0) - 2]^2 \exp\{-[(s - r_0)/\omega]^2\}$

for $s < 2r_0$, $\lambda(s) = 0$ for $s > 2r_0$. A, r_0, and w are the variational parameters for the excited states.

In the previous computations [9] the ground state factor $F(R, S)$ was based on simple parametrizations of the correlating factors or pseudopotentials. Recently [11], with the basis set method it has been possible to achieve the full optimization of all three correlating factors, f_p, f_s, and f_{ps}, and these are what we use here. This fully optimized SWF gives the best variational result of the *ground state* energy E_0 of ^{4}He at all densities. For instance, at ρ_{eq} $E_0 = -6.94$ K/atom, 0.2 K above experiment, and at freezing $\rho = 1.2\rho_{\text{eq}}$, $E_0 = -6.38$ K/atom, 0.18 K above experiment. The use of optimized pseudopotentials is important in order to be sure that the excitation energy is not affected by a poor choice of the ground state.

The excitation energy is computed by a Monte Carlo method as in previous computations [9] and the Aziz'79 interatomic potential is used. We have performed [12] the computation at two densities, at equilibrium $\rho_{\text{eq}} = 0.0218$ Å^{-3} and at $\rho = 1.2\rho_{\text{eq}}$. The energy spectrum $E(q)$ is shown in Fig. 1 together with the experimental result [13]. The roton energy is 9.05 ± 0.29 K at ρ_{eq} and 7.73 ± 0.25 K at $1.2\rho_{\text{eq}}$ to be compared with the experimental values [14] 8.61 ± 0.01 K and 7.3 ± 0.2 K, respectively. At ρ_{eq} the full spectrum is in very good agreement with experiment, the deviation being at the level of 5%. Similar agreement for the roton is found at higher density, and this is remarkable in view of the difficulties found by other theories to treat the high density regime. The agreement with experiment is not limited to the energy but extends to the strength Z_q of the single excitation peak in the dynamical structure factor $S(q, \omega)$. The result for the relative strength of this peak, i.e., $f(q) = Z(q)/S(q)$ where $S(q)$ is the static structure factor, is compared with experiment in Fig. 2. There is a very good agreement with recent results [15], and this is important because this quantity is rather sensitive to the structure of the wave function. $f(q)$ in the roton region is almost density independent, but in the maxon region there is a significant decrease of $f(q)$ at the higher density. This is exactly what is found experimentally [15].

The energy of the single excited state (1) is in significant disagreement with experiment in two cases: at large q above ~ 2.5 Å^{-1} and in the maxon region for the higher ρ. In both cases the experimental $E(q)$ is about twice the roton energy so that we might expect that these excitations are a mixture of single and double excitations. To prove that this is relevant we have extended our computation to a double roton excited state, $\Psi_{\vec{k},\vec{q}-\vec{k}}$. This is obtained by replacing in (1) $\tilde{\sigma}_{\vec{q}}$ by $\tilde{\sigma}_{\vec{k}}\tilde{\sigma}_{\vec{q}-\vec{k}}$, k and $|\vec{q} - \vec{k}|$ being the roton wave vector. The results for a few values of q are also shown in Fig. 1. We indeed find that in these two regions the energy of a double excitation is below the one of the single excitation and close to experiment. This proves that under these conditions (1) is not a good representation of the excited state and a mixture of states should be considered.

Our wave function has the same structure at all q. What is changing with q is only the strength A of the backflow which changes in a continuous way and it turns out to be maximum for the roton. For instance, at ρ_{eq} $A = 0.3$ for the roton and $A = 0.15$ for the maxon. The length parameters r_0 and w are insensitive to q. Therefore the uniform agreement of our $E(q)$ with experiment gives no hints of the possible different nature [5] of the excitations at small and at large q, at least at small temperatures. The question remains, *what is a roton?* In order to throw some light on this we have considered Gaussian-like wave packets built with the states (1). For a packet centered at

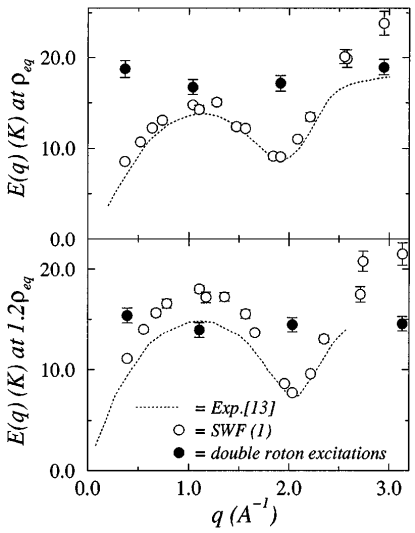

FIG. 1. Energy spectrum for single excitations and double roton excitations at ρ_{eq} and $1.2\rho_{\text{eq}}$ and experimental results.

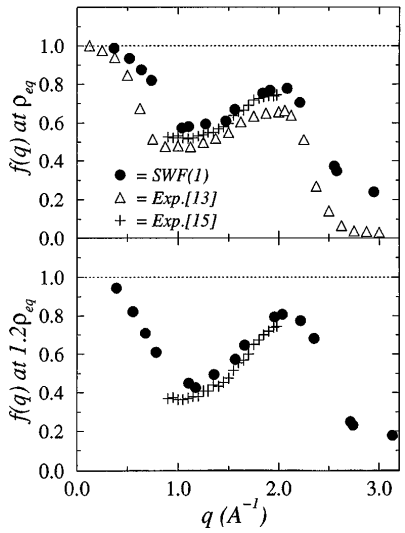

FIG. 2. Theoretical and experimental $f(q) = Z(q)/S(q)$ at ρ_{eq} and $1.2\rho_{\text{eq}}$; for a Feynman wave function $f(q) = 1$.

$\vec{r}_0$ we take as wave function $\Psi_{\vec{r}_0,\vec{q}_0,\Delta}(R)$ the form (1) with $\tilde{\sigma}_{\vec{q}}$ replaced by

$$\tilde{\sigma}_{\vec{r}_0,\vec{q}_0,\Delta}(S) = \sum_j f(|\tilde{\vec{s}}_j - \vec{r}_0|) \exp[i\vec{q}_0 \cdot (\tilde{\vec{s}}_j - \vec{r}_0)], \quad (3)$$

with $f(s) = e^{-\Delta^2 s^2} + e^{-\Delta^2(s-L)^2} - 2e^{\Delta^2(L/2)^2}$ for $s < L/2$, $f = 0$ for $s > L/2$. $\vec{q}_0$ and Δ determine, respectively, the characteristic wave vector and spread of the wave packet in momentum space. This modified Gaussian shape $f(s)$ has been introduced so that the packet complies with the periodic boundary condition. The system is no longer uniform, and we have computed the local density $\langle\rho(\vec{r})\rangle$ and the local momentum $\langle\vec{p}(\vec{r})\rangle$. We center the packet at $\vec{r}_0 = 0$, the center of the simulation box of side L. If we choose $\vec{q}_0$ in the z direction, due to the symmetry of the problem $\langle\rho(\vec{r})\rangle = \rho(z, r_\perp)$ where $r_\perp = \vec{q}_0 \cdot \vec{r}/q_0$. Similarly $\langle\vec{p}\rangle$ is function of z and of $r_\perp$.

We show the results for three wave packets at ρ_{eq}. The first is centered at $\bar{q} = q_R = 1.93$ Å^{-1}, the roton wave vector, the second is a R^+ roton with $\bar{q} = 1.99$ Å^{-1}, and the third is a R^- roton with $\bar{q} = 1.86$ Å^{-1}. The half width at half maximum is 0.25 Å^{-1}. The density profiles as a function of z for some values of $r_\perp$ are shown in Fig. 3. The vectorial representation of $\langle\vec{p}\rangle$ is displayed in Fig. 4. It is clear from the figures that something special happens at the roton minimum: at q_R the wave packet does not disturb the local density and within the noise $\langle\rho(\vec{r})\rangle = \rho_{\text{eq}}$. This happens only when the optimal backflow is used. When we move out of the minimum, $\langle\rho(\vec{r})\rangle$ has a modulation in the direction of $\vec{q}$. This happens for a R^- as well as for a R^+ roton, the modulation being somewhat larger for a R^- roton. The roton excitation has a well defined signature also in terms of the local momentum. The wave packet with $\bar{q} \simeq q_R$ displays in a nice way a backflow pattern: along the z axis $\langle\vec{p}\rangle$ points in the direction of $\vec{q}$ but as we move out of the axis $\langle\vec{p}\rangle$ gets a very significant transverse component. The backflow pattern is strong up to about 6 Å. At a larger distance from the axis $\langle\vec{p}\rangle$ becomes rather small and has a tendency to point in the opposite direction to $\vec{q}$: we clearly see a dipolar flow. An R^+ and an R^- roton have a different pattern of $\langle\vec{p}\rangle$: one still recognizes a backflow pattern but, in addition, there is a strong modulation in the direction of $\vec{q}$. Again an R^- roton has a stronger modulation than an R^+ roton. This modulation of the momentum density is not explained by the modulation of $\langle\rho(\vec{r})\rangle$, but it is a much larger effect. By performing some computations for the same wave packets, although with a larger number of particles, we have verified that the size dependence of these results is small. The absence of a density modulation and the simple dipolar flow pattern beautifully confirm Feynman's intuitive idea of a roton. We find that the curl of the velocity field is nonzero in a ring-shaped region around the center of the roton and its maximum is on a circle of radius $r_\perp \simeq 3.4$ Å $\simeq 2\pi/q_R$. This behavior is what could be expected for a vortex ring scaled down to atomic size and with a core of radius of order 1–2 Å. This analogy, however, is true only at $q = q_R$, and the behavior is much more complex for $q \neq q_R$.

$\langle\rho(\vec{r})\rangle$ and $\langle\vec{p}(\vec{r})\rangle$ at q_R are similar to what could be expected for a single particle excitation in a dense medium. In order to verify this we have considered one of the ^{4}He atoms, say atom 1, as a distinguishable particle. This is similar to an impurity of ^{3}He in ^{4}He, but we keep the same mass. The trial excited state has the same form (1) but now $\tilde{\sigma}_{\vec{q}}$ contains just one term, $\exp[i\vec{q} \cdot \tilde{\vec{s}}_1]$. The backflow parameter A has been determined by minimization of the excitation energy $E_{\text{dist}}(q)$. It turns out that at $q = q_R$ the values of A for the distinguished particle and for the collective excitation are the same within the statistical uncertainty. This is

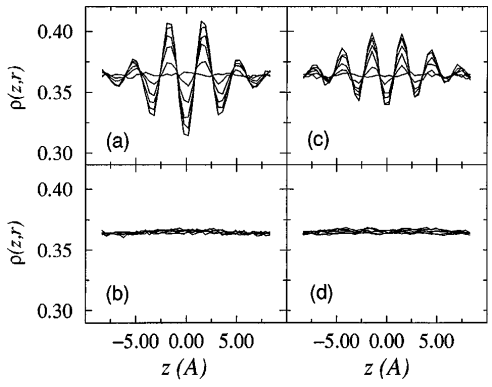

FIG. 3. Local density $\langle\rho(z, r_\perp)\rangle$ in σ units ($\sigma = 2.556$ Å) for an R^- (a), roton (b), R^+ (c), and distinguished particle (d) wave packet at ρ_{eq}, plotted for $r_\perp \simeq 0.7$, 2.1, 3.15, 4.3, 5.95, and 8.15 Å. The density fluctuations decrease monotonically with $r_\perp$ in (a) and (c).

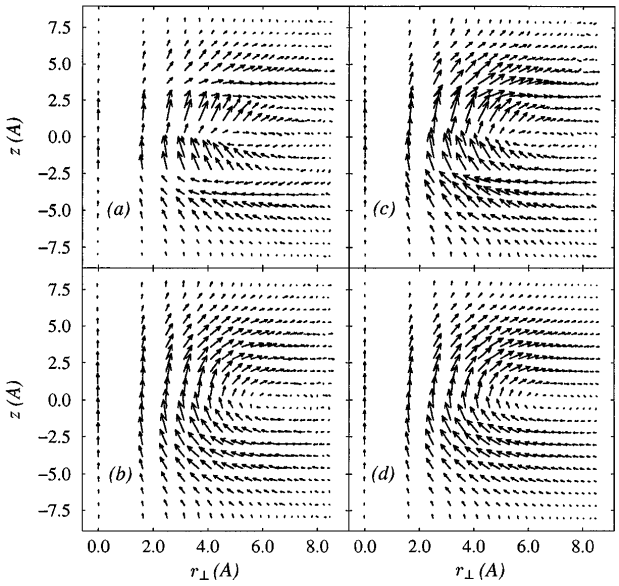

FIG. 4. The vectors represent the local momentum $\langle\vec{p}(z, r_\perp)\rangle$ when $r_\perp = 0$ and $\langle\vec{p}(z, r_\perp)\rangle \times r_\perp$ when $r_\perp \neq 0$, computed for the same wave packets of Fig. 3.

only true at $q = q_R$, for other values of q the two excitations have different backflow amplitudes. $E_{\rm dist}(q)$ of the distinguished particle excitation is almost quadratic in q, and it can be described by a slightly q-dependent effective mass $\mu(q)$: $E_{\rm dist}(q) = \hbar^2 q^2/2m_4\mu(q)$. At small q we find $\mu \simeq 1.8$ and at $q = q_R$, $\mu \simeq 2.1$. At $q = q_R$ the energies of the two excitations are similar, $E_{\rm dist}(q_R) = 9.9 \pm 0.8$ K which is close to the roton energy. The same happens at $\rho = 1.2\rho_{\rm eq}$ where $E_{\rm dist}(q_R) = 8.2 \pm 0.6$ K [$\mu(q_R) \simeq 3.1$]. We have constructed wave packets also starting from these excited states for a distinguished particle and computed $\langle \rho(\vec{r}) \rangle_{\rm dist}$ and $\langle \vec{p}(\vec{r}) \rangle_{\rm dist}$. For all values of $\bar{q}$, $\langle \rho(\vec{r}) \rangle_{\rm dist}$ is essentially a constant equal to the average density [in Fig. 3(d) the case $\bar{q} = q_R$ is shown]. $\langle \vec{p}(\vec{r}) \rangle_{\rm dist}$ for the wave packet with $\bar{q} = q_R$ [Fig. 4(d)] is essentially the same of the roton excitation [Fig. 4(b)] and on the scale of Fig. 4 one cannot distinguish between the two flow patterns. The pattern of $\langle \vec{p} \rangle_{\rm dist}$ for the distinguished particle does not change shape when $\bar{q}$ is moved away from q_R. Therefore the equivalence of these local quantities for an excitation of a distinguished particle and of a collective excitation is true only in the immediate neighborhood of q_R. As we move out from the roton minimum the collective excitation gets a typical spatial modulation which is absent for the excitation of the distinguished particle. The computation at the higher density confirms all the findings at $\rho_{\rm eq}$.

The interpretation of these results is that at $q = q_R$ the interference effects between neighboring atoms cancel out due to the close matching between the wavelength of the excitation and the average distance between these particles. Therefore a roton is essentially the same as a single particle excitation. However, there is a fundamental difference between these two excitations: a roton has zero group velocity but this is nonzero for the distinguished particle. This arises because when q differs from q_R an interference pattern sets in the case of the collective excitation, whereas this pattern is absent for the distinguished particle. In a certain way our findings vindicate the view [3,4] of a roton as a single particle excitation. What was absent in these earlier works is a clear identification of the role of interference between different particles which immediately modifies the properties of the collective excitation as q moves away from q_R. The strength of the roton peak in $S(q, \omega)$ derives from the excitation of particles out of the condensate as well as of particles above the condensate [3]. In our computation we cannot separate out the two contributions but our result of the almost identical behavior of a roton ($q = q_R$) and of a distinguished particle gives evidence that the second contribution is the dominant one. This is supported by an earlier computation [16] which showed that, depending on density, one needs to excite five to ten rotons in order to deplete the condensate by one particle.

We have presented a truly accurate description of the excitation spectrum of superfluid ^{4}He with the law of interatomic interaction as the only input. We have performed the first microscopic study of wave packets built with such wave functions. Such computations have thrown light on the nature of the roton excitations. A roton is in many respects similar to a single particle excitation as one would build for a distinguishable particle, but as one moves away from the roton minimum the excitation is quite distinct from a single particle excitation due to interference effects between atoms. Therefore the picture of the full roton minimum as quasiparticle excitations does not agree with our results. Our computation vindicates many arguments of Feynman and gives them a quantitative basis. Exactly at $q = q_R$ a simple dipolar flow due to backflow is present like in a small vortex ring.

An open problem is to reach a similar understanding at a local level of the maxon excitations and of how high frequency phonons join with the rest of the excitation spectrum. This seems feasible but it will require the study of substantially larger systems. Another open problem is the evolution with temperature up to T_λ of the excitations.

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