Hybridization of localized and density modes for the roton spectrum of superfluid $^4$He.

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A new description is presented for the roton part of the energy spectrum of superfluid $^4$He. It is based on the assumption that in addition to the Feynman density excitations, there exist localized modes which describe vortex-core elements. The energy spectrum which results from the hybridization of these two kinds of excitations is compared to the experimental data namely the structure factor and the scattering cross-section for the single quasiparticle excitation. Another type of excitation interpreted as a vortex loop is obtained whose energy agrees both with Raman scattering and critical velocity experiments.

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In this letter we present a new theoretical description of the roton region of the excitation spectrum of superfluid $^4$He. In spite of the success obtained using the wavefunction proposed by Feynman \cite{Feynman}, a quantitative agreement with the experimental results has not yet been achieved. Subsequent refinements using more complicated variational wavefunctions were at the expenses of a simple interpretation as a pure density fluctuation. More recently, new experimental results \cite{Avetisyan} obtained in high resolution neutron scattering did show puzzling features such as the persistence of the phonon peak up to temperatures higher than $T_\lambda$ together with the decrease of the sharp peaks associated respectively to the roton and roton excitations. These features tend to indicate that the low momentum phonon mode is marginally related to superfluidity or even to the Bose-Einstein statistics, a point which was already noticed by Pines \cite{Pines} and proposed to interpret this mode as a collective zero sound just like in $^3$He. In contrast, the decrease at the transition of the other modes suggests a connection with quantum exchange effects.

In order to interpret these features we assume the existence of two kinds of excitations in the system. At large scales, there are delocalized density fluctuations while at scales of a few interatomic distances there exist localized excitations which may be associated with microscopic vortex-core elements. These two kinds of excitations are not independent but instead are hybridized in a way reminiscent of the case of excitons in dielectric crystals \cite{Hopfield}. This analogy will guide us in order to build a phenomenological Hamiltonian. This phenomenological model will allow us to derive analytical expressions for measurable quantities and to provide an interpretation for the high-momentum roton region of the spectrum where the variational approach becomes more involved.

The physical motivation leading to the assumption of the existence of localized excitations stems from the following remarks. In any attempt to reproduce quantitatively the spectrum using a variational approach more localized structure needs to be introduced into the excited-state wavefunction. In addition it is generally accepted that the superfluid supports quantized vortices with microscopic cores. In order to describe them, it is relevant to consider exchange effects associated to localized and closed exchange rings of atoms. Therefore, we view the system as being a liquid at large distances while locally, on the scale of some interatomic distances, we consider localized quantum clusters playing the role of the vortex-core elements. Since the helium atoms are indistinguishable, we cannot split them into two classes (i.e. either embedded in a long range density mode or in a localized cluster) but we suppose instead that each atom retains both characteristics. As a consequence, these two kinds of excitations are coupled and the spectrum results from this hybridization. From a methodological point of view, our approach is close to that of Hopfield \cite{Hopfield} who considered excitons in dielectric crystals as localized excitations whose interactions are mediated by the photons. Here, along the same line, the interaction between the localized excitations is mediated by the Feynman density fluctuations.

To make those qualitative remarks more precise, we first consider the Hamiltonian $H_0 = \sum_k \epsilon(k) a_k^\dagger a_k$ describing the pure density modes obtained using the Feynman ansatz \cite{Feynman} with the energy $\epsilon(k) = -\frac{\hbar^2 k^2}{2mN}$. where $m$ is the mass of the helium atoms and $S(k)$ the structure factor of the liquid. Then, we assume the localized excitations to be two-level systems of energy $\hbar\omega_0$, such that the corresponding Hamiltonian is $H_0^{\text{loc}} = \sum_k \hbar\omega_0 \left( b_k^\dagger b_k + \frac{1}{2} \right)$. The operators $a$ and $b$ obey bosonic commutation relations and commute between themselves, but for the $b$ operators the bosonic character is only approximate and holds in the limit of a low density of localized modes \cite{Hopfield}. To write down the part describing interactions between the two sets of excitations, we follow the approach of Hopfield and Anderson \cite{Hopfield} and assume that the role of the density fluctuations is to induce an effective interaction between the localized modes which within the dipolar approximation allows to write the effective Hamiltonian

$$H_{\text{loc}} = \sum_k (\hbar\omega_0 + X(k)) \left( b_k^\dagger b_k + \frac{1}{2} \right)$$
$$+ \sum_k X(k) \left( b_k^\dagger b_{-k}^\dagger + b_k b_{-k} \right) \quad (1)$$

where $X(k)$ is a (real and negative) matrix element which depends on the microscopic details of the dipolar interaction. The dipolar approximation is the simplest limit for which the resulting Hamiltonian can be analytically worked out. Moreover, it corresponds to the physical picture of the localized-modes as vortex-core elements. Such
microscopic line-elements may be treated as local dipolar defects with respect to the surrounding fluid. As we shall see later, in this limit, the knowledge of the exact expression of $X(k)$ is not necessary. The coupling between the phonons and the localized modes is described by the Hamiltonian

$$ \mathcal{H}_c = \sum_k (\lambda(k,\omega_0) b_k + \mu(k,\omega_0) a_k) (a_k^\dagger + a_{-k}) + \hbar c. \quad (2) $$

where the two functions $\lambda$ and $\mu$ are given by $\lambda(k) = i\hbar \omega_0 (-3X(k))/2\epsilon(k)$ and $\mu(k) = -\hbar \omega_0 (3X(k))/2\epsilon(k)$. $H_{\text{loc}}$ is diagonalized using the Bogoliubov transformation $\beta_k = u(k)b_k + v(k)b^\dagger_{-k}$, which the resulting spectrum

$$ E = \sqrt{\hbar \omega_0 (\hbar \omega_0 + 2X(k))} \quad (3) $$

The two functions $u(k)$ and $v(k)$ are given by $u^2(k) = 1/2(\hbar \omega_0 + X(k)/E(k)) + 1$ and $v^2(k) = 1/2(\hbar \omega_0 - X(k)/E(k) - 1)$. The Hamiltonian $H_0 + H_{\text{loc}}^2 + H_c$ is quadratic and is diagonalized by means of the canonical transformation $\alpha_k = Aa_k + Bb_k + C a^\dagger_{-k} + D b^\dagger_{-k}$ and $\delta_k = B a_k + A b_k + D a^\dagger_{-k} + C b^\dagger_{-k}$. The corresponding dispersion relation is

$$ \frac{\omega^2(k)}{E^2(k)} = 1 - \frac{6}{\hbar \omega_0} \frac{X(k)}{(E(k)/(\hbar \omega_0))^2} \quad (4) $$

We first notice that taking the coupling $X(k)$ between the two sets of modes to zero, we obtain, as expected, the two solutions $E(k) = \epsilon(k)$ describing a pure density mode and $E = \hbar \omega_0$ for the localized two-levels. A non zero coupling hybridizes these two sets of excitations. We take for the energy $\hbar \omega_0$ the highest value of the phonon-roton spectrum i.e. where it terminates, namely $\hbar \omega_0 = 2\Delta$ where the energy $\Delta$ corresponds to the roton minimum. New experimental results at higher values of $k$ confirm this behaviour at the termination point $k_{\text{max}}$.

To solve for the dispersion relation and to obtain the phonon part of the spectrum, we use (3) into (4). This gives $E(k) = \frac{1}{2} \epsilon(k)$ i.e. an expression independent of the matrix element $X(k)$. Using now this latter expression into (4), we obtain the other branch describing the hybridized local modes at $E = 2\hbar \omega_0 = 4\Delta$ which is as well independent of $X(k)$. We emphasize again that this is a consequence of the particular choice of the dipolar approximation which is manifested in the expressions for the coupling functions $\lambda$ and $\mu$. As a result of the hybridization, the energy spectrum of the density fluctuations is shifted by a factor two towards lower energies relatively to the Feynman ansatz, and the localized modes still have a constant energy although twice the original value.

To compare our results with the experimental data we shall consider first two independent sets of results namely the measurements of the energy spectrum and of the structure factor $S(k)$. We obtain from (4) the relation

$$ E(k) = \frac{\hbar^2 k^2}{4mS(k)} \quad (5) $$

for the lower branch which we compare to the experimental results obtained for two different pressures both for $E(k)$ [13] and $S(k)$ [14] (Figs.1 and 2). The main discrepancy is obtained in the low momentum region ($k \leq 1\AA^{-1}$), i.e. below the maxon momentum. As $k \to 0$ the experimental data is close to the Feynman result i.e. twice the value we obtain in (5). This signals a failure of the dipolar approximation for long wavelengths. Our description becomes meaningless when the phonon-roton branch terminates since the Feynman spectrum approaches that of a free particle. Around the roton minimum, and over a large range of momentum the result (5) provides a good fit to the experimental results. Feynman himself in his original paper noticed the factor 2 discrepancy between his ansatz and the experimental results around the roton minimum. Here we deduce this factor from an exact analytical solution. This interpretation of the roton excitation as resulting from the dipolar hybridization of two separate excitations, to be compared with the approach of Glyde and Griffin [14] which uses a dielectric formalism to describe hybridized phonons and free-particle excitations.

The neutron scattering intensity is a direct measure of the density fluctuations in the liquid and is obtained from the dynamical structure factor $S(k,\omega)$. It is accepted since the work of Miller, Pines and Nozieres [15] that we can split $S(k,\omega)$ into two parts, $S(k,\omega) = N Z \delta \rho \delta (\hbar \omega - \epsilon_k) + S^{(1)}(k,\omega)$ where the first term accounts for single quasi-particle excitations while the second describes multiparticle excitations. This separation is quite easy to justify at low temperature and low momentum, typically for $k \leq 0.5\AA^{-1}$ where we obtain $Z(k) = S(k)$, which results also from the Feynman theory. The comparison with the experimental data [16] shows that although it works in the low momentum regime mentioned above, it fails to describe the behavior at higher momentum, except perhaps for the position of the maximum. In contrast to this, we do not consider here a precise decomposition of the structure factor. Since the density fluctuations are hybridized with the localized modes, we expect the differential cross-section $Z(k)$ for the excitation of a single quasi-particle to be proportional to $\langle b_k^\dagger b_{-k}^\dagger \rangle = u_k v_k$, where the expectation value is calculated in the ground state of the Bogoliubov pairs. Then, $Z(k) = 4\pi k^2 I_0 u_k v_k$ where $I_0$ is a normalization constant. Using our previous expression for $u_k$ and $v_k$ we obtain $u_k v_k = \frac{1}{2} \frac{X(k)}{E(k)}$ which together with (3) and (5) gives

$$ Z(k) = \pi k^2 I_0 \frac{\hbar \omega_0}{E(k)} \left( \frac{E(k)}{\hbar \omega_0} \right)^2 - 1 \quad (6) $$

From the two independent measures of $E(k)$ and $S(k)$ we obtain using (6) a theoretical expression of the differential cross-section which fits well the experimental results as shown in Fig.3. In particular from (6) it follows that the intensity of the single quasi-particle branch vanishes when $E(k) \to 2\Delta$ which is a new result. Moreover, in the low momentum limit, we recover the expected proportionality between $S(k)$ and $Z(k)$. 


We found a second branch of excitations at the constant energy $E = 4\Delta$. It describes localized excitations of energies twice the bare vortex core energy. It is suggestive to interpret this mode as a single vortex loop whose radius can be calculated using a Feynman-type formula for the energy of the circulating current of a vortex-loop

$$E_{\text{vortex-loop}} = 2\pi^2 \rho \frac{h^2}{m^2} \ln \left( \frac{R}{a} \right)$$

(7)

where at $T = 0$, the density of the superfluid is $\rho = \rho_s$ and $a$ is the core size equal to the atomic radius, namely $a \simeq 1.4\AA$. The radius $R$ is obtained taking $E_{\text{vortex}} = 4\Delta = 34.4K$. This gives $R \simeq 5.0A$ which is the expected size for the smallest vortex-loop. A further experimental evidence in favour of this interpretation is provided by critical velocity experiments in phase-slippage studies of the critical velocity through an orifice, the critical velocity is driven by the thermal nucleation of vortex-loops. The corresponding energy $E_s$ is determined by the nucleation rate $\Gamma$ which, using the Arrhenius law $\Gamma = \Gamma_0 \exp \left( \frac{E_c}{k_B T} \right)$, is found to be $E_s \simeq 33 \pm 5K$, which is indeed very close to our result $4\Delta = 34.4K$. Finally, the upper critical velocity $v_c$ may be estimated as the velocity of the vortex-loop itself namely $v_c = \frac{2a}{\ln (\frac{2a}{L})} \simeq 20m/s$, a value close to the largest measured critical velocity.

Another relevant set of experiments we consider is provided by the Raman scattering around $k = 0$. It has been found that besides a peak at $E = 2\Delta$, there is an additional contribution at $E = 4\Delta$ which we associate to the vortex-loop. The peak at $2\Delta$ is usually interpreted as a two-roton excitation and therefore the additional contribution is viewed as a four-roton excitation. This interpretation suffers nevertheless from the fact that there is no three-roton peak. In our model, the lowest excitation energy of a vortex-core is given by $2\Delta$ and not by $\Delta$ so that we do not expect any contribution at $3\Delta$. The peak at $2\Delta$ which does not appear in the hybridized spectrum will be discussed elsewhere.

In conclusion, we have shown that the roton region of the excitation spectrum of superfluid $^4He$ can be described quantitatively by assuming the existence of two kinds of excitations. One is provided by the delocalized density fluctuations given by the Feynman variational ansatz. In contrast, the second set of excitations describes the short range order in the system around a microscopic vortex-core element. We have assumed that these excitations are coupled in a way reminiscent from the case of excitons in dielectric systems. By writing a phenomenological Hamiltonian together with the dipolar approximation for the coupling, we obtained an excitation spectrum which involves two sets of hybridized modes. One corresponds to phonons shifted by a factor of two towards lower energies relatively to the Feynman result. The second set is interpreted as the intrinsic quantized vortex-loop modes of the superfluid. This picture provides analytical expressions which describe quantitatively a broad range of experimental results. In addition, it may help understanding the persistence of the phonon peak above $T_\Delta$ which appears to be shifted upwards in energy together with a sharp drop of both the maxon and roton peaks. Since the localized excitations depend on the superfluid order, they will vanish at the transition to the normal state, while the Feynman density modes will remain unaffected and only shifted upwards in energy in the absence of dipolar coupling $X(k)$. Our model provides a new picture of the nature of the roton excitation and may allow for a unified treatment of the phonon-roton elementary excitations and of the quantized vortex-loops excitations which are both unique to the superfluid phase.

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FIG. 1. Comparison between the experimental energy spectrum [10,11] (points) and the theoretical expression (5) (solid line) where the structure factor $S(k)$ is obtained from independent measurements [12,13]. (a) and (b) correspond respectively to the saturation vapor pressure and to $P=24$ atm. The dashed line at $4\Delta$ indicates the position of the branch of the vortex-loop excitations.

FIG. 2. Comparison between the experimental structure factor $S(k)$ (points) and the expression (5) (solid line) for the same two pressures as in fig.(1) where the energy $E(k)$ is obtained from independent measurements [10,11]. (a) circles [12], squares [14], (b) circles [13].

FIG. 3. Comparison between the experimental scattering cross-section [10] $Z(k)$ of single quasi-particle excitations (points) at 1.1 K and the theoretical expression (6). The two curves are obtained using respectively in (6) the experimental results for $S(k)$ [12] (dashed line) and for the energy $E(k)$ [11] (solid line).