Dispersion of Ripplons in Superfluid $^4$He

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Abstract

A detailed study of the dispersion law of surface excitations in liquid $^4$He at zero temperature is presented, with special emphasis to the short wave length region. The hybridization mechanism between surface and bulk modes is discussed on a general basis, investigating the scattering of slow rotons from the surface. An accurate density functional, accounting for backflow effects, is then used to determine the dispersion of both bulk and surface excitations. The numerical results are close to the experimental data obtained on thick films and explicitly reveal the occurrence of important hybridization effects between ripplons and rotons.

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I. INTRODUCTION

Superfluid helium is a unique system where undamped excitations can propagate also in the short wave length regime. This behaviour characterizes the dynamics of the bulk as well as of the surface, and is at the origin of several interesting phenomena. Hybridization between ripplons and rotons and quantum evaporation are important examples of such phenomena where the surface of helium is explicitly involved. These peculiar properties of liquid helium at low temperature have been the object of several experimental investigations in the last years. First results for the dispersion of short wave length ripplons have recently become available via neutron scattering experiments on helium films [1]. Quantum evaporation, i.e., the emission of an atom produced by a roton propagating balistically in the medium and impinging on the surface, has been also systematically investigated (see for example Ref. [2]).

The above phenomena have received attention also from a theoretical point of view. However, due to intrinsic difficulties associated with a reliable description of the statics and dynamics of strongly interacting inhomogeneous systems, the predictions have been so far only semi-quantitative. The main reason lies in the fact that both microscopic approaches, based on correlated basis functions, and phenomenological methods, mainly based on density functional theory, have been used in the framework of the so called Feynman approximation, or equivalent schemes. This approximation significantly overestimates the roton energy and this clearly rules out the possibility of a quantitative description of quantum evaporation as well as of the dynamics of energetic ripplons, since in both cases the relevant energies are of the order of the roton gap.

In order to obtain a better description it is necessary to include backflow effects in the theory. Here, following the spirit of density functional theory, we account for such effects through a new phenomenological current dependent interaction [3]. In the present work we use the new functional to provide a quantitative description of the ripplon dispersion, with special emphasis to the region near the roton threshold. The study of quantum evaporation
will be the object of a future work.

The work is organized in two parts: in Sec. II we discuss in details the mechanism of the hybridization between ripplons and rotons. In particular we show that this mechanism is governed by the properties of reflection of rotons from the free surface. In Sec. II we present numerical results for the ripplon dispersion obtained by solving the equations of time dependent density functional theory with the inclusion of backflow terms.

II. HYBRIDIZATION BETWEEN RIPPLONS AND ROTONS

The hybridization between ripplons and rotons consists of a coupling between surface and bulk excitations that takes place when the energy of ripplons is close to the one of rotons.

The physical origin of such a phenomenon is clear. Let us consider a surface excitation with energy larger than the roton gap $\Delta$. This surface mode can naturally decay into a roton if its momentum parallel to the surface is lower than the roton momentum. Indeed this process is possible because only the momentum parallel to the surface is conserved, while the orthogonal momentum can be transferred to the surface.

This decay mechanism provides a natural threshold for the energy of ripplons, given by the roton gap $\Delta$. The occurrence of this threshold has been confirmed by recent experimental data with neutron scattering and is clearly expected to influence the dispersion of energetic ripplons. Such a phenomenon was first explicitly explored in the case of helium in Ref. [4] using the formalism of Green’s functions. A similar phenomenon was discussed in Ref. [5] for the case of dielectrics where it results in a damping of surface waves.

The problem of the interaction between ripplons and bulk excitations in superfluid $^4$He was investigated several years ago by Edwards et al. [6,7]. They wrote the solution for the velocity potential of the ripplon in the form

$$\phi = A e^{i(k_x x + k_z z - \omega t)}$$

(1)
where $x$ and $z$ are parallel and orthogonal to the surface, respectively; the wave vector $k_z$ is a function of $\omega$ and $k_x$, defined by the equation

$$\omega = \epsilon((k_z^2 + k_x^2)^{1/2})$$

(2)

where $\epsilon(k)$ is the dispersion law for bulk excitations. The authors of Ref. [6,7] took only imaginary solutions of Eq. (2) for $k_z$. This corresponds to consider purely damped waves in the $z$-direction with damping length $|k_z|^{-1}$. The solution is then given by $k_z = i\sqrt{k_x^2 - k^2(\omega)}$ where $k(\omega)$ is the momentum of bulk excitations with energy $\omega$. Of course this solution exists only for $k_x > k(\omega)$. However this is not the only possibility, since Eq. (2) can have also complex solutions for $k_z$. In particular, when $\omega$ is below and close to the roton gap $\Delta$, one can use the well known approximation [8]

$$\epsilon = \Delta + \frac{(k - p_0)^2}{2\mu}$$

(3)

to the roton dispersion, yielding the following solution for $k_z$:

$$k_z \simeq p_1 + \frac{p_0}{p_1}i\sqrt{2\mu(\Delta - \omega)}$$

(4)

with $p_1 = \sqrt{p_0^2 - k_x^2}$. This solution corresponds to a penetration depth

$$\delta = \frac{p_1}{p_0 \sqrt{2\mu(\Delta - \omega)}}$$

(5)

that becomes larger and larger as $\omega$ approaches $\Delta$ at fixed $k_x$.

To investigate the behaviour of the ripplon dispersion near the threshold $\Delta$ one must learn more about the dynamics of slow rotons. For this we take the familiar roton Hamiltonian

$$H = \Delta + \frac{(k^2 - p_0^2)^2}{8\mu p_0^2}$$

(6)

yielding dispersion (3) for $k$ close to $p_0$. At given $k_x$ Eq. (6) can be written in the form

$$H = \Delta + \frac{(k_x^2 - p_1^2)^2}{8\mu p_1^2}$$

(7)

with $p_1$ defined above. For the description of the threshold behaviour of ripplons only rotons with energy close to $\Delta$ are important. In this case the roton wave function can be written as
\[ \Psi_r(z) = f_1(z) \exp[-ip_1z] + f_2(z) \exp[ip_1z] , \]  

(8)

where \( f_1(z) \) and \( f_2(z) \) are slowly varying function of \( z \). By neglecting higher derivatives of \( f_i \) in the Schrödinger equation one finds that the functions \( f_i \) are solutions of

\[ H f_i = \omega f_i , \quad i = 1, 2 \]  

(9)

with

\[ H_f = \Delta - \frac{1}{2m^*} \frac{d^2}{dz^2} \]  

(10)

and \( m^* = \frac{\mu p_0^2}{p_1^2} \). \[ 9 \] .

In the same scheme the surface mode, with energy close to \( \Delta \), appears as a surface bound state of rotons, whose wave function can be written as

\[ \Psi_s(z) = 2A \exp[-\kappa z] \cos(p_1z) \]  

(11)

where

\[ \kappa = \left[2m^*(\Delta - \omega)\right]^\frac{1}{2} , \]  

(12)

and we have made an explicit choice for the phase. Equation (11) corresponds to taking

\[ f_1(z) = f_2(z) = A \exp[-\kappa z] . \]  

(13)

Clearly both the scattering and the bound solutions (8) and (11) hold only far from the surface. The quantity \( \kappa \) is a function of \( k_x \), which can be found, in principle, by solving the proper Schrödinger equation in the surface region. Close to the surface, where \( |z| \) is of the order of the surface thickness \( a \), the Hamiltonian (10) has to be changed in order to account for the interaction of rotons with the surface. However for slow rotons the solutions \( f_i \) of the Schrödinger equation vary slowly and the role of the surface can be safely replaced by the imposition of suitable boundary conditions at \( z = 0 \). The general form of these boundary conditions is
\[ \left. \frac{df_1}{dz} \right|_{z=0} = -\alpha_{11} f_1(0) - \alpha_{12} f_2(0) \quad (14a) \]

\[ \left. \frac{df_2}{dz} \right|_{z=0} = -\alpha_{21} f_1(0) - \alpha_{22} f_2(0). \quad (14b) \]

The matrix \( \alpha_{ij} \) must be hermitian in order to ensure real values for \( \kappa \) in the case of bound states. Furthermore, due to time reversal invariance, one must have \( \alpha_{11} = \alpha_{22} \) and the phases of the functions \( f_1(z) \) and \( f_2(z) \) can be always chosen such that \( \alpha_{12} = \alpha_{21}^* \) is real. The quantities \( \alpha_{11} \) and \( \alpha_{12} \), fixing the boundary conditions at \( z = 0 \), are entirely determined by the properties of the surface.

Let us first apply Eq. (14) to the surface mode for \( \omega < \Delta \). In this case the functions \( f_i \) are given by expression (13) so that Eq. (14) yields

\[ \kappa = \sqrt{2m^*(\Delta - \omega)} = \alpha(\omega, k_x) \quad , \quad (15) \]

where \( \alpha(\omega, k_x) = \alpha_{11} + \alpha_{12} \). This equation has a solution describing a surface mode if \( \alpha > 0 \). This scheme provides a natural description of the dispersion near the threshold. Let us suppose, for example, that \( \alpha(\Delta, k_x) = 0 \) at some point \( k_x = k_t < p_0 \). Near this point the function \( \alpha \) can be expanded as \( \alpha(\Delta, k_x) \approx \beta(k_x - k_t) \). Thus the dispersion curve near the threshold has a parabolic form:

\[ \Delta - \omega = \frac{\beta^2}{2m^*}(k_x - k_t)^2 \quad , \quad (16) \]

approaching the point \( k_t \) with a horizontal tangent.

When \( \omega > \Delta \) the boundary conditions (14) describe the reflection of rotons at the surface. In this case the functions \( f_i \) take the form

\[ f_1 = \exp[-ik_z z] + R_1(\omega) \exp[ik_z z] \quad (17) \]

\[ f_2 = R_2(\omega) \exp[ik_z z] \quad . \quad (18) \]

By definition the coefficients \( R_1 \) and \( R_2 \) are the amplitude for change-mode reflection and normal reflection, respectively. After imposing the boundary condition (14) in the threshold
region $\omega \simeq \Delta$ and near $k_i$ where $\alpha \ll \alpha_{11}, \alpha_{12}$, we find the following results for the amplitudes $R_1$ and $R_2$:

$$R_1 = -\frac{\alpha}{ik_z + \alpha}$$

and

$$R_2 = \frac{ik_z}{ik_z + \alpha}.$$

Note that if $k_z \ll \alpha$ one has

$$R_1 \simeq -1 + i\frac{k_z}{\alpha}.$$

This equation shows that when $\omega$ approaches $\Delta$, and consequently $k_z \rightarrow 0$, the change-mode reflection amplitude approaches the value $-1$, while the normal reflection amplitude tends to zero \[10\]. In this limit the solution \[8\] of the Schrödinger equation, far from the surface, takes the form

$$\Psi_r(z) = \exp[-i(p_1 + k_z)z] - \exp[-i(p_1 - k_z)z]$$

and corresponds to the reflection of a roton $R^+$, with momentum $(k_x, 0, p_1 + k_z)$, into a roton $R^-$, with momentum $(k_x, 0, p_1 - k_z)$ (see Fig. \[4\]). Notice that the roton $R^-$ has negative velocity and, consequently, the roton scatters backwards not only in the $z$ direction, but also in the $x$ one. The occurrence of the change-mode scattering, peculiar of rotons, will be explicitly confirmed in Sec. \[III\] through the numerical solution of the equations of the time dependent density functional theory.

The theory developed above is very general. It is reasonable to assume however the interaction between ripplons and rotons in $^4$He, producing the hybridization, to be weak. In this case one can proceed further, looking for a theory which describes the crossover region between an unperturbed ripplon dispersion, entirely characterized by surface properties in the absence of interaction with bulk modes, and the dispersion near the threshold, dominated by the hybridization mechanism. Under the assumption of weak interaction one expects (see the Appendix) that the function $\alpha$ has the form
\[ \alpha(\omega, k_x) = b(k_x) + \frac{g^2}{\epsilon_0(k_x) - \omega} \]  

(23)

when \( \omega \) is close to \( \Delta \). In Eq. (23) \( \epsilon_0(k_x) \) is the dispersion law of unperturbed ripplons and \( g \) is a coupling constant. By using Eq. (23) in Eq. (15) the dispersion of the surface modes becomes

\[ \sqrt{2m^*(\Delta - \omega)} = b(k_x) + \frac{g^2}{\epsilon_0(k_x) - \omega} \].

(24)

Note that the coefficient \( g^2 \) must be positive to ensure a stable solution of Eq. (24) when the unperturbed ripplons have a damping. Different scenarios can now take place depending on the value of the coefficient \( b \):

- 1) \( b < 0 \). In this case the spectrum reaches the \( \omega = \Delta \) threshold at a point \( k_x = k_t \), as assumed in the derivation of result (16). The value of \( k_t \) is fixed by the equation

\[ \frac{g^2}{\epsilon_0(k_t) - \Delta} = -b(k_t) \].

(25)

and the coefficient \( \beta \) in Eq. (16) can be directly calculated from Eq. (24). Clearly the point \( k_t \) lies at the right of the unperturbed ripplon branch.

- 2) \( b > 0 \). Equation (24) has now a solution also for \( g = 0 \). A surface branch exists independently of the ripplon dispersion. This branch corresponds to a bound state of rotons near the surface. This scenario describes a hybridization between two surface modes, ripplons and surface rotons respectively, near the threshold for bulk modes.

- 3) If the coefficient \( b \) satisfies the condition \( |b| \ll (m^*)^{1/3}g^{2/3} \), then its role can be neglected in Eq. (24). One obtains that the ripplon dispersion approaches asymptotically the roton threshold with the law

\[ \Delta - \omega \propto \frac{g^4}{(\epsilon_0(k_x) - \Delta)^2} \].

(26)

This hybridization mechanism was previously discussed in Ref. [4]. Also note that a transition from \( b \) small and positive to \( b \) small and negative corresponds to a transition from a bound surface state to a "virtual level" (see §133).
In the next Section we will carry out a full calculation of the ripplon dispersion using a density functional approach. The numerical results will be shown to follow the behaviour predicted by the first scenario (Eqs. (16) and (25)).

III. PREDICTIONS OF DENSITY FUNCTIONAL THEORY

In this section we present the results of a calculation of the dynamics of inhomogeneous liquid helium obtained using time dependent density functional theory. In the density functional approach the internal energy is assumed to be a functional of the one-body densities in the form

\[ E = \int d\mathbf{r} \mathcal{E}[\Psi^\ast \Psi] \]  

(27)

where the wave function \( \Psi \), for a Bose system at zero temperature, is written as

\[ \Psi(\mathbf{r}, t) = \Phi(\mathbf{r}, t) \exp(iS(\mathbf{r}, t)) \]  

(28)

The real function \( \Phi \) is related to the particle density by \( \rho = \Phi^2 \), while the phase \( S \) is related to the velocity \( \mathbf{v} \) of the fluid by

\[ \mathbf{j} = \rho \mathbf{v} = \frac{i}{2m} (\Psi \nabla \Psi^\ast - \Psi^\ast \nabla \Psi) = \frac{\rho}{m} \nabla S \]  

(29)

where \( \mathbf{j} \) is the current density, and \( m \) is the mass of the \(^4\text{He}\) atoms.

The formalism of time dependent density functional has been already applied to describe the surface excitations of superfluid helium [12, 13]. In Ref. [13] the effective Hamiltonian has been derived microscopically starting from the interatomic potential in the framework of the hypernetted chain scheme. Vice-versa the functionals employed in Refs. [14,15] are of phenomenological type.

The equations of motion of time dependent density functional theory can be derived starting from the least action principle

\[ \delta \int_{t_1}^{t_2} dt \int d\mathbf{r} \left[ \mathcal{E}[\Psi^\ast \Psi] - \Psi^\ast \frac{\partial \Psi}{\partial t} \right] = 0 \]  

(30)
making variations with respect to \( \Phi \) and \( S \) \cite{[13]}, or, equivalently, with respect to \( \Psi^* \). In the latter case one finds a Schrödinger-like equation of the form

\[
\tilde{H}\Psi = i \frac{\partial}{\partial t} \Psi ,
\]

where \( \tilde{H} = \delta \mathcal{E}/\delta \Psi^* \) is an effective Hamiltonian. If one looks for linearized solutions

\[
\Psi(\mathbf{r}, t) = \Psi_0(\mathbf{r}, t) + \delta \Psi(\mathbf{r}, t)
\]

the Hamiltonian \( \tilde{H} \) takes the form

\[
\tilde{H} = \tilde{H}_0 + \delta \tilde{H} .
\]

The static Hamiltonian \( \tilde{H}_0 \) is fixed by the equilibrium state \( \Psi_0(\mathbf{r}, t) = e^{-i\mu_4 t} \sqrt{\rho(z)} \) (\( \mu_4 \) is the chemical potential) through the equation \( \tilde{H}_0 \Psi_0 = \mu_4 \Psi_0 \). The term \( \delta \tilde{H} \) is linear in \( \delta \Psi \) and accounts for changes in the Hamiltonian induced by the collective motion of the system. Since \( \tilde{H} \) depends explicitly on the wave function \( \Psi \), the Schrödinger equation \((31)\) has to be solved using a self-consistent procedure, even in the linear limit considered in the present work. The formalism then coincides with the one of the Random Phase Approximation (RPA) for Bose systems. Of course this theory, which is basically a mean field theory, accounts for collective and single particle excitations, but cannot account for multiphonons excitations.

In the bulk \( \Psi_0 \) is constant and \( \delta \Psi \) can be expanded in plane waves, corresponding to the propagation of the phonon-roton mode. In the presence of a free surface, orthogonal to the \( z \)-coordinate, one can write \( \Psi \) as

\[
\Psi(x, z, t) = \Psi_0(z, t) + e^{-i\mu_4 t} \left( \Phi_1(z)e^{-i(\omega t - k_x x)} + \Phi_2(z)e^{i(\omega t - k_x x)} \right) ,
\]

where the structure of \( \Phi_1 \) and \( \Phi_2 \) allows to distinguish between bulk and surface modes. The linear variation of the density (transition density), associated with the solution \((34)\), is given by

\[
\delta \rho = 2 |\Psi_0(z)| \Phi^+(z) \cos(\omega t - k_x x)
\]
with $\Phi^* = \Phi_1 + \Phi_2$.

From the equation of motion (31) we obtain linear equations for the functions $\Phi_1(z)$ and $\Phi_2(z)$, which, without any loss of generality, can be chosen real. These functions are expanded on a basis of eigenstates of the static one-body Hamiltonian $\hat{H}_0$ in order to get a matrix equation which is solved numerically by direct diagonalization.

In order to write the RPA equations one needs the explicit form of the functional $\mathcal{E}$. The functionals used so far in liquid helium have the form [12,14–16]

$$\mathcal{E}_0 = \frac{1}{2m} |\nabla \Psi|^2 + \mathcal{V}[\rho],$$

(36)

where $\mathcal{V}[\rho]$ is a velocity independent functional. An accurate phenomenological functional of this form [17] (hereafter named Orsay-Paris functional) has been used, for instance, in Ref. [15] to study the dispersion of collective modes in helium films. The same functional has proven to be quite reliable in the study of the equilibrium configuration of several helium systems, such as the free surface [17], films [18], droplets [19], and vortices [20].

With functionals of the form (36) the dispersion law predicted by Eq. (31) has the form

$$\omega^2 = \frac{k^2}{m|\chi(k)|},$$

(37)

where $\chi$ is the static response function. The quantity $\chi(k)$ is a key ingredient for calculations with density functional theory at zero temperature. A major advantage of liquid $^4$He is that $\chi(k)$ is well known experimentally [21].

It is worth noticing that the dispersion law (37) does not reproduce correctly the experimental phonon-roton dispersion, especially in the roton region. This is due to the fact that functional (36) ignores backflow effects. To understand better this point it is useful to rewrite Eq. (37) as the ratio between the energy weighted and the inverse energy weighted moments of the dynamic structure function: $\omega^2 = m_1(k)/m_{-1}(k)$, where

$$m_1(k) = \int d\omega \, S(k,\omega) \, \omega = \frac{k^2}{2m},$$

(38)

is the f-sum rule, and
\[ m_{-1}(k) = \int d\omega \ S(k,\omega) \ \omega^{-1} = -\frac{1}{2} \chi(k) \]  (39)

is the compressibility sum rule. The analysis of the spectra of neutron scattering experiments [21] shows that, due to the \( \omega^{-1} \) factor in the integrand, the collective phonon-roton mode almost exhausts the compressibility sum rule for all wave lengths up to about 2.2 \( \text{Å}^{-1} \). On the contrary, it gives only a fraction (\( \simeq 1/3 \)) of the energy weighted sum rule, the remaining part being exhausted by high energy multiphonon excitations. This explains why functionals of the form (36), yielding the dispersion law (37), significantly overestimate the roton energy.

To overcome this difficulty we add a current-current interaction term to the functional (36):

\[ \mathcal{E} = \mathcal{E}_0 - \frac{m}{4} \int dr' \ V_J(|r-r'|) \ \rho(r)\rho(r')(\mathbf{v}(r) - \mathbf{v}(r'))^2 . \]  (40)

The new term is Galilean invariant and depends on local changes in the fluid velocity field. The new dispersion of bulk excitations, obtained by solving Eq. (31), takes the form

\[ \omega^2 = \frac{k^2}{m|\chi(k)|} \left[ 1 - \rho(V_J(k) - V_J(0)) \right] , \]  (41)

where \( V_J(k) \) is the Fourier transform of the current interaction \( V_J(r) \) of Eq. (40). Notice that the new term in Eq. (41) does not modify the static response function \( \chi(k) \), which is completely fixed by \( \mathcal{E}_0 \). Notice also that the dispersion law (41) is not affected by the new term in the \( k \to 0 \) hydrodynamic regime, where it coincides with the traditional phonon law \( \omega = k/\sqrt{m|\chi(0)|} \). This is an important feature ensured by Galilean invariance.

Equation (41) explicitly shows that the inclusion of the current term in the density functional can provide a reduction of the phonon-roton contribution to the moment \( m_1 \), thereby improving the description of the dispersion law. The fact that the new functional no longer satisfies the \( f \)-sum rule (38) points out in a clear way that the time dependent density functional theory, or equivalently the RPA, does not account for multiphonon excitations which provide the remaining fraction of the \( f \)-sum rule. A similar separation between collective and multiphonon excitations, in the context of linear response theory, has been developed by Pines and collaborators (see for example Ref. [22]).
Let us briefly discuss the criteria used to choose the new functional, whose explicit form and parametrization is discussed in Ref. [3]. The static part $\mathcal{V}$ has a form similar to the one of the Orsay-Paris functional [17]. It contains a two-body Lennard-Jones interaction and a phenomenological density dependent term accounting for short range correlations. The density dependent term of the Orsay-Paris functional has been changed in order to reproduce more accurately the experimental value of the static response function $\chi(k)$ in the roton region. The current-current interaction $V_J$ is then chosen to reproduce phenomenologically the phonon-roton dispersion in bulk liquid [23] through Eq. (41). Its form is shown in Fig. 2.

After fixing the density functional to reproduce the bulk spectrum, one can solve the equations of motion in systems with non uniform density. We will focus here on the problem of the free surface. We choose, for numerical convenience, a slab geometry (liquid between two parallel surfaces) and look for solutions of the form (34). All the states are confined in a box larger than the slab thickness, and, consequently, even the continuum of states outside the slab is discretized. We take typically a basis of more than 50 eigenstates of $\tilde{H}_0$, to cover all the relevant part of the spectrum.

The main features of the spectrum, extrapolated to the semi-infinite system, are shown in Fig. 3. The dispersion of bulk phonon-roton modes is the upper solid line; the agreement with the experimental data follows from the choice made for $V_J$. The surface mode corresponds to the lowest solid line. An important feature emerging from the present calculation is the deviation of the ripplon dispersion from the hydrodynamic law. This is in agreement with the experimental data for surface excitations in helium films [1]. The horizontal line corresponds to the threshold for rotons having energy close to $\Delta = 8.65$ K and propagating at different angles. The dispersion of the surface mode reaches the roton threshold at about $1.15$ Å$^{-1}$. The threshold $\omega = |\mu_4| + k_x^2/2m$ for creating excited states outside the liquid, at zero temperature, is also shown. The value at $k_x = 0$ coincides with the experimental chemical potential, $|\mu_4| = 7.15$ K.

To appreciate the effect of the backflow term included in the functional, the spectrum obtained without backflow ($V_J \equiv 0$) is plotted in Fig. 4. The roton minimum is pushed up
significantly, from 8.65 K to about 14 K, as follows from Eq. (41), while the dispersion of the surface mode is less affected by backflow. As a consequence the branch of the surface mode reaches $\Delta$ near the roton minimum. The spectrum in Fig. 4 is similar to the one of previous calculations on slabs \cite{24,15} and films \cite{13,15}. We note however that, even without backflow, density functional theory, once the value of $\chi(k)$ is properly accounted for, gives better predictions than the original Feynman approximation. The latter, in fact, gives the roton minimum at about 20 K. The reason is that the phonon-roton dispersion in Feynman approximation is fixed by the ratio $\omega = m_1(k)/m_0(k)$ between the energy weighted and non energy weighted moments of the dynamic structure function. This ratio should be compared with prediction (B7) of density functional theory without backflow. The moment $m_0$ is more affected than the inverse energy weighted moment $m_{-1} = -(1/2)\chi(k)$ by multiphonon excitations. It then follows that the density functional approach gives a significantly lower value for the energy of the collective mode (14 K at the roton minimum).

Due to the finite thickness of the slab, with parallel surface at $z = \pm L$, one can distinguish between odd and even states. In Fig. 5 we show a typical spectrum with the excited states of a slab of thickness $2L = 50$ Å. For simplicity, only even states are shown in the figure. Each state, at given energy and parallel wave vector, is a stationary superposition of bulk excitations, surface excitations and free atoms, with the proper matching conditions. For instance, the almost orizontal lines are mainly bulk rotons reflecting at the slab surfaces; the gap between these states is fixed by the slab thickness. The oscillations of the roton lines, below the maxon region, are peculiar of the slab geometry; they originate from a periodic splitting of even and odd states. The period of such oscillations is predicted by the theory of roton scattering developed in Sect. II to be $\Delta k_x \simeq p_1 \pi/(2Lk_x)$. The energy of the surface mode is instead practically independent of $L$. Above the ripplon mode there is also an excited surface mode, whose dispersion reaches the roton threshold at about $k_x = 0.7$ Å$^{-1}$.

The solution of the RPA equations also allows to compute the dynamic structure function, defined by
\[ S(k, \omega) = \sum_n |\langle n|\rho_k^\dagger|0\rangle|^2 \delta(\omega - \omega_{n0}) \]  

where \( \rho_k^\dagger = \sum_j \exp[i \mathbf{k} \cdot \mathbf{r}_j] \) is the usual density operator, and \( k \equiv (k_x, 0, k_z) \). An example is given in Fig. 6 where we show the results for \( k_x = 0.8 \text{ Å}^{-1} \) and \( k_z = 0 \) in a slab 50 Å thick. The ripplon corresponds to the peak at lowest energy. The other peaks are excited surface modes, as the one at about 9 K, and bulk modes, the most important one being the high energy phonon at about 13 K. The figures reveals that, even for a rather thick slab, the contribution of the surface mode to the total strength is significant. It is also interesting to explore the dependence of the relative strength on the scattering angle, i.e. as a function of \( k_z \) for a fixed \( k_x \). In Fig. 6 the relative contribution of the surface mode to the total strength is shown for \( k_x = 0.8 \text{ Å}^{-1} \). One notes that the most favorable condition for exciting ripplons is to induce momentum transfer parallel to the surface (\( k_z = 0 \)).

In Fig. 7 the quantity \( \Phi^+ \), characterizing the transition density (see Eq. (35)), is plotted in three cases: a surface mode (a), free atoms coupled to high energy phonons (b), free atoms coupled to rotons (c). In Fig. 7 we show in detail what happens to the surface mode when its energy approaches the energy of the lowest roton mode. The surface mode transforms continously in a bulk mode, and vice-versa. The gap between the two levels tends to vanish when the slab thickness increases. The resulting hybridization mechanism then agrees with the predictions of the scenario (1) discussed in Section II (see Eqs. (16) and (25)), with \( k_t \simeq 1.15 \text{ Å}^{-1} \).

In Sec. II we have shown that rotons close to \( \Delta \), according to Eqs. (20) and (21), are totally reflected with a change-mode reflection, as in Fig. 1. The roton wave function for energy close to \( \Delta \) is explicitly written in Eq. (22). In the slab geometry one has to account for \( R^+ \) and \( R^- \) rotons propagating in both directions and reflecting on two surfaces, at \( z = \pm L \). The corresponding roton wave function is particularly simple at \( k_x = 0 \), where it takes the form

\[ \Psi_r(z) \propto \cos(p_0 z) \cos\left(\frac{\pi z}{2L}\right). \]  

This picture is well confirmed by the numerical solution of the equations of motion. The
comparison between the result of the numerical calculation and formula (43) is shown in Fig. 10. The two curves are almost indistinguishable, showing that the density functional approach properly accounts for the change-mode reflection of rotons on the free surface.

We note however that result (21), yielding change-mode reflecton, is not valid when \( \alpha(\omega, k_x) = 0 \). We can study the behaviour of rotons also in this case using the arguments of Sect. II. In fact, for \( \omega > \Delta \), the line where \( \alpha = 0 \) is fixed by the equation

\[
\frac{g^2}{\varepsilon_0(k_x) - \omega} = -b(k_x) .
\]

(44)

It starts at the point \( k_t \) and corresponds to the continuation of the ripplon dispersion above \( \Delta \) (this continuation is clearly visible in our numerical results of Fig. 5). This line is singular for the reflection of rotons at the surface. It is clear from Eqs. (19) and (20) that, when \( \alpha = 0 \), one has

\[
R_1 \simeq 0 , \quad R_2 \simeq 1 .
\]

(45)

Thus the normal reflection dominates near the singular line.

We note again that in a slab of finite thickness \( 2L \) the roton levels are discretized. For the lowest levels near \( \Delta \) and far enough from the singular line \( \alpha = 0 \), the change-mode reflection is dominant. The condition of energy quantization has the form

\[
2k_z L + 2\delta = n\pi , \quad n = 1, 2, 3, \ldots
\]

(46)

where \( \delta \) is a phase shift at the reflection, defined by

\[
R_1(\omega) = -|R_1| \exp[2i\delta] .
\]

(47)

In the region under consideration \( R_1(\omega) \simeq -1 \) and one can choose \( \delta = 0 \). Approaching the singular line \( \alpha = 0 \) the quantization condition (46) is no longer valid. However, one can easily discuss the behaviour of the phase during the crossing of this line. In fact, comparing Eq. (47) with Eq. (19), one can write

\[
\tan(2\delta) = -\frac{k_z}{\alpha} .
\]

(48)
Crossing the singular line from left to right $\alpha$ changes sign, the change-mode reflection amplitude is again equal to $-1$, but the phase $\delta$ has increased by $\pi/2$. This means that the horizontal line $\omega(n)(k_x)$ for a roton on the left is matched to the line $\omega(n+1)(k_x)$ on the right of the singular line $\alpha = 0$. These jumps are clearly seen in Fig. 5, just above the point where the ripplon branch reaches $\Delta$.

We finally note that excited states in the region between the minimum roton energy and the maxon energy have a finite amplitude outside the slab, resulting from the coupling between rotons and evaporated atoms (see Fig. 8). A detailed analysis of this coupling can be done following the stabilization method recently proposed in Ref. [25]. One solves the eigenvalue problem in a large box of variable size, containing the slab. The energy of the excited states varies with the box size. From the analysis of such energy dependence one can extract information about the width of states localized in the slab, i.e., of rotons. A typical picture is given in Fig. 11. The change of slope of each curve corresponds to the coupling between free atoms and rotons, related to the phenomenon of quantum evaporation. A detailed study of this problem is in progress.

IV. CONCLUSIONS

In this work we have provided a detailed discussion of the ripplon dispersion of superfluid $^4$He in the regime of short wave lengths. The main results can be summarized as follows:

a) We have shown that the hybridization mechanism between ripplons and rotons is dominated by the reflection properties of rotons from the surface. We have discussed different scenarios for the behaviour of the ripplon dispersion near the threshold $\omega = \Delta$, where $\Delta$ is the usual roton gap.

b) We have calculated numerically the dispersion of ripplons by solving the equations of time dependent density functional theory in thick slabs. A phenomenological backflow term has been included in the functional in order to provide a realistic dispersion of bulk rotons. The resulting ripplon dispersion turns out to be in reasonable agreement with experiments.
Our calculations confirm in an explicit way the general reflection mechanism exhibited by rotons.

An extension of the present analysis to investigate higher energy processes associated with the phenomenon of quantum evaporation will be the object of a future paper.

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APPENDIX:

In this appendix we provide a simple argument to derive expression (23) for $\alpha(k_x, \omega)$. To this purpose one must solve the Schrödinger equation for the roton wave function $f_i$ in the domain $z \ll \kappa^{-1}$ including the boundary. For simplicity, since the wave function $\Psi_r$ can be chosen real, we take $f = f_1 = f_2^*$, so that

$$\alpha(\omega, k_x) = -\left. \frac{f''(z)}{f(z)} \right|_{z=0}. \quad (A1)$$

The Schrödinger equation for $f$ has the form

$$(H_f - \Delta)f = 0, \quad (A2)$$

where the Hamiltonian $H_f(k_x)$ contains the interaction with the surface. Notice that in Eq. (A2) we have put $\omega = \Delta$ since the $\omega$-dependence of the solution is smooth and can be ignored in first approximation. Let the value of $\alpha$ predicted by Eq. (A2) be $b(k_x)$.  

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The ripplon dispersion is defined by the Schrödinger equation for the ripplon wave function \( \phi \)

\[
(H_\phi - \omega)\phi = 0 \tag{A3}
\]

whose solutions define the unperturbed ripplon dispersion \( \epsilon_0(k_x) \).

Hybridization means that on the right hand side of Eqs. (A2) and (A3) we should add terms linear in \( \phi \) and \( f \), respectively:

\[
(H_f - \Delta)f = g L \phi \tag{A4}
\]

\[
(H_\phi - \omega)\phi = g L_1 f \tag{A5}
\]

where \( L \) and \( L_1 \) are some operators, while \( g \) is a coupling constant. Clearly the last equation has a pole when \( \omega \) is equal to the eigenvalue \( \epsilon_0(k_x) \) of \( H_\phi \). Near the pole one can write the solution as

\[
\phi \simeq \frac{g}{\epsilon_0(k_x) - \omega} L_2 f \tag{A6}
\]

where the quantity \( L_2 f \) has no dependence on \( \omega \). Equation (A4) then becomes

\[
(H_f - \Delta)f = \frac{g^2}{\epsilon_0(k_x) - \omega} L_2 f . \tag{A7}
\]

The solution of Eq. (A7), needed to calculate \( \alpha(\omega, k_x) \), is difficult in general. However it is evident a priori that the solution depends on \( \omega \) only through the combination \( g^2/(\epsilon_0(k_x) - \omega) \). One can finally calculate \( \alpha(\omega, k_x) \) by treating the contribution of the right hand side in Eq. (A7) as a perturbation. We then obtain the desired result

\[
\alpha(\omega, k_x) = b(k_x) + \frac{g^2}{\epsilon_0(k_x) - \omega} , \tag{A8}
\]

used in Sect. \[\text{I}\].

A non perturbative approach to the same result can be also formulated using Green’s function techniques.
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[8] Note that $\hbar = 1$ in this work.

[9] Clearly Hamiltonian (10) is not applicable to the point $k_x = p_0$, where $1/m^*$ vanishes. This case should be treated separately.

[10] This result is valid in general when $k_z \rightarrow 0$ and holds also when the rotons are damped by the process of quantum evaporation of atoms. The damping process can be taken into account by simply introducing an imaginary part in $\alpha$. The limiting value $-1$ of the change-mode reflection amplitude will be the same also in this case, so that the probability of evaporation tends to zero for $\omega \approx \Delta$.

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FIGURES

FIG. 1. Schematic picture of the change-mode reflection. A roton with positive group velocity ($R^+$) reaches the free surface and transforms in a roton with negative group velocity ($R^-$).

FIG. 2. Effective current-current interaction (adimensional) entering functional (40)

FIG. 3. Dispersion relation of bulk and free surface excitations. The present result for the surface mode (lowest solid line) is compared with the experimental data on films [1] (squares) and with the hydrodynamic dispersion of ripplons (dots). The bulk phonon-roton branch (upper solid line) is compared with the experimental one (circles). The threshold for roton states with different $k_x$ is shown as the horizontal line. The threshold for the emission of atoms into the vacuum is also shown (dot-dashed curve).

FIG. 4. Same as in Fig. 2 but with the bulk and surface mode dispersions calculated without the current-current interaction in the density functional ($V_J \equiv 0$).

FIG. 5. Dispersion relation of the excited states of a slab 50 Å thick, as a function of the parallel wave vector.

FIG. 6. Dynamic structure function (in arbitrary units) for $k_z = 0$ and $k_x = 0.8$ Å$^{-1}$ in a slab 50 Å thick. The ripplon mode corresponds to the peak at lowest energy.

FIG. 7. Ratio between the strength of the surface mode and the total strength at $k_x = 0.8$ Å$^{-1}$ as a function of $k_z$.

FIG. 8. Three examples of excited states of a slab 50 Å thick. The dashed line is the static density profile. The solid line corresponds to the numerical solution of the equations of motion, at given values of energy and parallel wavevector. The three states have the same $k_x$ but different energy: a) the lowest energy surface mode; b) free atoms outside the slab coupled to phonons; c) free atoms outside the slab coupled to rotons.
FIG. 9. Detail of the repulsion between the surface mode and the bulk roton mode near the threshold energy $\Delta$, for a slab 50 Å thick. The form of the lowest eigenstate at two different values of $k_x$ is also shown in the upper part of the figure.

FIG. 10. Wave function of the first excited state above the roton threshold at $k_x = 0$. It corresponds to a superposition of $R^+$ and $R^-$ rotons which undergo a change-mode reflection at the surface. Solid line: numerical solution of the equations of motion. Dashed line: analytic expression (43). Short dashed line: static density profile.

FIG. 11. Energy of the excited states at $k_x = 0.4$ Å$^{-1}$ as a function of the size of the computational box, containing a slab of fixed thickness (50 Å). The almost horizontal part of each curve corresponds to roton-like states inside the slab; the part with negative slope (proportional to $L_{\text{box}}^{-2}$) corresponds to free atom states outside the slab. The form of the level repulsion is connected to the probability for a roton to decay by ejecting a free atom from the liquid. The energy of the surface modes (not shown in the figure) is practically independent on $L_{\text{box}}$. 