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Evaporation from superfluid helium

C. Caroli, B. Roulet, and D. Saint-James

Groupe de Physique des Solides de l'Ecole Normale Supérieure, associé au Centre National de la Recherche Scientifique, Université Paris VII, 2 Place Jussieu, 75 221 Paris-Cedex 05, France

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We calculate the spectral distribution of atoms evaporating from superfluid helium, with the help of a theory, derived from the exact treatment of tunneling, which is free from the transfer-Hamiltonian approximation. In the absence of a detailed microscopic model for He II, the current cannot be computed completely. However, it is found that the spectrum must exhibit a singularity at the energy of the roton minimum: It is shown that, contrary to earlier predictions, this is of the "cusp" or "rounded wedge" type, due to the shape of the transmission-coefficient singularity at the threshold of the roton channel.

I. INTRODUCTION

A few years ago, King and Johnston[1] reported that ^{4}He atoms evaporated from the superfluid liquid had a mean temperature exceeding that of the liquid. It is now known[2] that such a result was due to an unsuitable experimental arrangment, and more recent evaporation experiments[3,4] do not report any clear effect of that sort. However, a theoretical study of He II evaporation is of interest, on one hand in order to achieve a better understanding of the evaporation (or condensation) process itself, and on the other hand in order to make clear how the energy distribution of the current is related to the quasiparticle spectrum of the liquid.

Following a suggestion by Anderson,[5] several authors[6-8] have predicted that one should observe in the single-particle elastic emission spectrum an enhancement in the vicinity of the energy corresponding to the roton minimum ω_r of the superfluid liquid. Most of these theories rely on the assumption that the coupling between the superfluid and its vapor can be described by an effective transfer Hamiltonian

$$H_T = \sum_{\vec{p},\vec{p}'} T_{\vec{p}\vec{p}'}[a^\dagger_{\vec{p}'}c_{\vec{p}} + a_{\vec{p}'}c^\dagger_{\vec{p}}], \qquad (1)$$

where a_p and c_p are operators which destroy an atom in the superfluid and vapor phases, respectively. Assuming $T_{pp'}$ to be quasiconstant and treating H_T to lowest order, as is done is Bardeen's theory of tunneling,[9] one finds an evaporation current spectrum of the form

$$j(\omega) \propto |T|^2 \rho_L(\omega)\rho_V(\omega), \qquad (2)$$

where ρ is the density of states for excitations in the liquid (L) or atoms in the vapor (V). The enhancement then comes directly from the high density of roton states in the liquid at $\omega \sim \omega_r$.

Such a theory has been successfully applied to explain the results of Giaever's experiments on tunneling in superconductors.[10] But it is well known that it does not correctly describe tunneling between normal metals. Moreover, Griffin and Demers[11] have proven that even in the case of superconducting electrodes it is not exactly the BCS density of states which is measured by the tunneling current (even though, in practice, the difference in that case is too small to be measurable. Indeed, the use of a simplified transfer Hamiltonian (i.e., with a constant matrix element) cannot be justified in general. A detailed discussion of this point, which we will not reproduce here, is given in a paper by Caroli and Saint-James.[12] Moreover, in the present case the coupling between the two phases is obviously not small enough to justify *a priori* a first-order approximation.

The approach we develop in Sec. II. is based on Keldysh's formalism for out-of-equilibrium many-body systems. It does not rely on a transfer-Hamiltonian approximation, and treats the coupling to all orders, with the help of a method which was previously used to treat tunneling and the thermionic effect.

For a liquid maintained at a uniform temperature $T \ll T_\lambda$ emitting atoms into the vacuum, the elastic current spectrum $j(\omega)$ can then be expressed formally in the frame of well-defined approximations. The next step would be to evaluate quantitatively $j(\omega)$ for the whole range of experimentally acessible ω's. Unfortunately, there is no convincing microscopic model for superfluid helium, so that it is not possible to calculate numerically the parameters involved in the formal expression of $j(\omega)$. Nevertheless, it is possible to draw conclusive results in the immediate vicinity of the roton minimum energy ω_r: We shall show that there is no enhancement of $j(\omega)$ near ω_r, but (when interactions between excitations are neglected) a structure with a vertical tangent at ω_r and a $|\omega - \omega_r|^{1/2}$ behavior of $j(\omega)$ on both sides of this point exists.

This structure is to some extent rounded by inelastic and lifetime effects. This kind of behavior is not surprising at all; it is in fact well-known and general in other physical domains, in which a similar situation takes place, namely, the opening of a new channel at a threshold energy (here the roton channel for $\omega \geqslant \omega_r$). This corresponds to a "cusp" or a "rounded wedge" threshold behavior (as high-energy physicists call it) of a current spectrum, a phase shift, a reflectivity, or a cross section depending on the problem at hand. This will be discussed in more detail in Sec. III.

II. CALCULATION OF EVAPORATION CURRENT SPECTRUM

A. Description of model

Recently Caroli *et al.*[13] developed a microscopic theory of tunneling based on Keldysh's nonequilibrium perturbation formalism. This method does not rely on any effective-Hamiltonian approximation and gives an exact expression for the current.

In the present work we shall apply this formalism to the case of atomic emission into the vacuum from liquid maintained at a uniform temperature T ($\ll T_\lambda$).

At the very beginning of the calculation a difficulty arises which does not appear in the problems involving emission of electrons from solids. Indeed, in a solid the electron gas is restrained inside the material by the ionic potential, so that, at least in a first approximation, the confinement of the electrons to a limited region of space is due to a one-body potential. This is not at all the situation for a liquid, in which it is the interactions between the atoms themselves which are responsible for the separation into phases (and we want to study the evaporation of these atoms!); thus a correct description of the system (semi-infinite liquid + semi-infinite vacuum) would demand a microscopic description of the condensation. Unfortunately, the only tractable approximation for such a system is a generalized Hartree-Fock scheme, which, as it is well known, is unable to predict any separation of the fluid into phases.[14] In order to circumvent this difficulty, we take the existence of the liquid condensation as a starting point: we assume that the atomic density $n(x)$ is a known function of position, falling from the bulk liquid value (for $x \to -\infty$) to zero (for $x \to +\infty$) on some characteristic surface thickness of the order of the atomic radius a.

The total current density induced by the departure from equilibrium (owing to the zero pressure maintained in the vacuum region) is

$$\vec{j}(\vec{r},t) = (\hbar/2m)(\vec{\nabla}_{\vec{r}'} - \vec{\nabla}_{\vec{r}})G^{+}(\vec{r},t;\vec{r}',t)\big|_{\vec{r}'=\vec{r}}\,, \qquad (3)$$

where $G^{+}(\vec{r},t;\vec{r}',t')$ is the "occupation propagator" for the entire out-of-equilibrium system,

$$G^{+}(\vec{r},t;\vec{r}',t') = i\langle\psi^{\dagger}(\vec{r}',t')\psi(\vec{r},t)\rangle. \qquad (3a)$$

$\psi^{\dagger}$ and ψ are, respectively, the atom creation and destruction operators. Without entering into the details described at length in a series of papers on tunneling,[13, 15] let us first recall the principle of the method used to calculate this G^{+} in the simple case where interaction effects can be neglected. The system is cut into two subsystems (which, here, would be the "liquid," $x<0$, and the "vacuum," $x>0$); to zeroth order the semi-infinite subsystems are both treated as completely isolated (bounded by an infinite potential) and separately at equilibrium, each with its own chemical potential. Then the coupling between these two subparts, which originates from the kinetic-energy term of the total Hamiltonian, is reintroduced and *treated to all orders*, with the help of Kjeldysh's perturbation formalism for out-of-equilibrium systems.

When interactions cannot be neglected, which is precisely the case here, the procedure is slightly more complicated. It is described in detail in Ref. 16, and we will here state only its principle. One again defines semi-infinite subsystems, but these are not strictly isolated. Indeed, they are described by Green's functions g in which a bare particle cannot go across the separation plane ($x=0$), but particles can cross that cut way and back *within a self-energy inclusion*. That is, the functions g are given by the following "pseudo-Dyson equation":

$$g = g_0 + g_0\Sigma g, \qquad (4)$$

where g_0 is the free-particle propagator in the isolated subsystem and $\Sigma(x,x')$ is that part of the self-energy of the complete system (in the presence of the current) which does not couple the two sides of the cut ($xx'>0$). Thus a given g can connect only two points on the same side of the cut, but it is not exactly the propagator of an isolated semi-infinite medium at equilibrium, which would have a particle density $n'(x)$ different from $n(x)$ in the surface layer (in particular, one would have $n'(0)=0$ on the cutting plane) and, in general, a self-energy term σ different from Σ.

In the case of tunneling,[16] since the quantity $\Sigma(x,x')$ appearing in Eq. (4) is, by definition, nonzero only when x and x' lie in the same electrode, and since the transmission coefficient of the tunneling barrier is very small, it is clear that the difference between Σ and σ is very small—except possibly at a distance from the cut of atomic order. In particular, for the same reason, the effect on Σ of the departure from equilibrium (i.e., of the current flow itself) is obviously small enough to be neglected.

In the present case, only excitations with energies above the vacuum level contribute to the evaporation current; particles do not tunnel through any barrier, but are simply "refracted," so that one does not expect the transmission coefficients of interest to be particularly small. One may then wonder about the magnitude of the effect on Σ of the current flow. However, one can make the following remark: the evaporation process affects the population of excitation levels essentially only in the range of energy $L_0 < \omega < L_0 + \Delta E$, where $\Delta E \sim kT$ and the energy of the vacuum level L_0 is equal to the latent heat of evaporation (Fig. 1). Since we are considering low-temperature evaporation only, the equilibrium population $[\sim \exp(-L_0/kT)]$ in that range is very small, and so is, *a fortiori*, the change of this population owing to the current flow. On the other hand, the self-energy Σ_ω is made up of the contributions of all the interaction processes consistent with the conservation laws. That is, Σ_ω results from a sum on phase space involving the non-current-carrying states ($\omega < L_0$) as well as the "evaporation range." The population change in that range can therefore induce only a small modification of the self-energy (i.e., of lifetimes and of the shape of the dispersion curve), with respect to that of the semi-infinite liquid at equilibrium, at least at distances from the surface larger than the space range ($\sim a$) of Σ itself.

Of course, since we are dealing with a superfluid liquid phase, it is understood that our system is characterized not only by a particle density function, but also by a condensate wave function $\langle \psi(x) \rangle$. This, as well as $n(x)$, is, even in the absence of the current, different from the corresponding quantity in the isolated semi-infinite liquid at equilibrium. Moreover, it is also modified by the current flow. Again, by the above argument, we can assume that this last effect is small, and it is clear that this remains true as long as the temperature T is small enough for the evaporation current J to be much smaller than the critical current J_S. Thus we will from now on assume that the subsystems can be considered as completely isolated and separately at equilibrium, each of them being characterized by a given value of the chemical potential ($\mu = \mu_L$ for the liquid, $\mu = -\infty$ for the vacuum).

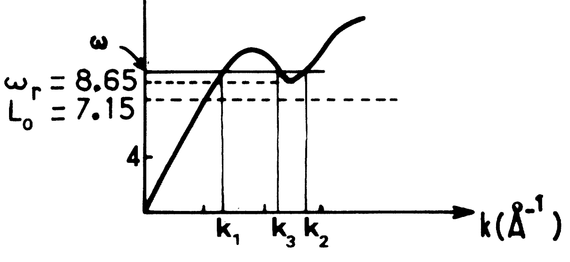

FIG. 1. Dispersion curve for quasiparticles in superfluid helium below T_λ. L_0 is the heat of evaporation of the liquid.

At this point, a problem remains: We have to choose a model to account for the space variation (which takes place mostly in the layer $|x| \lesssim a$) of the quantities [particle density $n(x)$, condenstate wave function $\langle \psi(x) \rangle$, self-energy $\Sigma(x, x')$] which characterize our total system. Since we are not able to calculate them from first principles, we choose to represent them by the simplest possible approximation: The liquid is completely restrained to the $x < 0$ region, with the same characteristic functions as the infinite liquid, namely,

$$n(x) = n_L \Theta(-x), \quad \langle \psi(x) \rangle = \langle \psi \rangle_L \Theta(-x), \qquad (5)$$
$$\Sigma(x, x') = \Sigma_L(x - x') \Theta(-x) \Theta(-x'),$$

where $\Theta(x)$ is the unit step function which is zero for negative arguments. That is, we neglect the direct coupling between the liquid and vacuum regions via self-energy terms, and therefore assume that the transfer primarily derives from the kinetic-energy coupling.[15] This model is obviously not self-consistent in a layer of atomic thickness along the interface, but describes correctly bulk properties. It therefore does not permit one to obtain reliable quantitative results for the current. But as we shall see, our qualitative conclusions about the variation of j close to ω_r derive only from the structure of the bulk spectrum. Thus the present approximation, which affects only the "matching properties" at the interface, does not limit their validity.

B. Formal expression of evaporation current

In order to go further and get a formal expression for the current from Eq. (3), we must define the Green's functions involved in the problem. First of all, we are dealing with a superfluid Bose system, which brings in anomalous functions; each Green's function (in Kjeldysh's sense) becomes a 2×2 matrix $\hat{G}$,

$$\hat{G} = \begin{pmatrix} G & F \\ \tilde{F} & \tilde{G} \end{pmatrix} \qquad (6)$$

defined in the usual way.[17] For example, the causal Green's-function matrix is defined by

$$\hat{G}^c(\vec{r}t;\vec{r}'t') = -i\langle T[\hat{\Phi}(\vec{r},t)\hat{\Phi}^\dagger(\vec{r}',t')]\rangle,$$

where

$$\hat{\Phi}(\vec{r}t) = \begin{pmatrix} \varphi(\vec{r},t) \\ \varphi^\dagger(\vec{r},t) \end{pmatrix} \tag{7}$$

and

$$\varphi(\vec{r},t) = \psi(\vec{r},t) - \langle\psi(\vec{r},t)\rangle .$$

In the following, we will use the four matrices $\hat{G}^+$, $\hat{G}^-$, $\hat{G}^a$, $\hat{G}^r$:

$$\begin{aligned} \hat{G}^+(\vec{r}t;\vec{r}'t') &= -i\langle\hat{\Phi}^\dagger_T(\vec{r}'t')\hat{\Phi}_T(\vec{r},t)\rangle , \\ \hat{G}^-(\vec{r}t;\vec{r}'t') &= -i\langle\hat{\Phi}(\vec{r}t)\hat{\Phi}^\dagger(\vec{r}'t')\rangle , \\ \hat{G}^r(\vec{r}t;\vec{r}'t') &= -i\theta(t-t')\langle\hat{\Phi}(\vec{r}t)\hat{\Phi}^\dagger(\vec{r}'t') \\ &\qquad - \hat{\Phi}^\dagger_T(\vec{r}'t')\hat{\Phi}_T(\vec{r}t)\rangle , \\ \hat{G}^a(\vec{r}t);\vec{r}'t') &= i\theta(t'-t)\langle\hat{\Phi}(\vec{r}t)\hat{\Phi}^\dagger(\vec{r}'t') \\ &\qquad - \hat{\Phi}^\dagger_T(\vec{r}'t')\hat{\Phi}_T(\vec{r}t)\rangle , \end{aligned} \tag{8}$$

where $\hat{\Phi}_T$ is the transpose of $\hat{\Phi}$.

The above Green's functions refer to the whole system. We also define the corresponding Green's matrices $\hat{g}^+(\vec{r},t;\vec{r};t')$, $\hat{g}^-(\vec{r},t;\vec{r}'t')$, $\hat{g}^a(\vec{r},t;\vec{r}',t')$, and $\hat{g}^r(\vec{r},t;\vec{r}'t')$ for the zero-order system (no coupling between liquid and vacuum). Note that the $\hat{g}$'s vanish when $\vec{r}$ and $\vec{r}'$ belong to the two different subsystems and that in the vacuum region (x and $x'>0$) they reduce to diagonal matrices (the condensation amplitude being zero in that region). Moreover, we are dealing with a continuous system, so that the technique described in detail in Ref. 15 has to be worked out. We introduce an infinite set of points on the x axis,

$$x_n = -\tfrac{1}{2}\epsilon + n\epsilon \quad \text{with } n = 0, \pm 1, \pm 2, \ldots ,$$

and we consider the above Green's functions only between points of the discretized set. Then the coupling between the two subsystems must be introduced; it links point x_0 to point x_1 and is represented in the above matrix formulation by a 2×2 matrix

$$\hat{T} = \begin{pmatrix} \tau & 0 \\ 0 & \tau \end{pmatrix},$$

where $\tau = -\hbar^2/2m\epsilon^2$. At the end of the calculation, the $\epsilon\to 0$ limit has to be taken.

Following Ref. 15, the total current flowing out of the whole surface can be written[18]

$$J_x = \lim_{\epsilon\to 0}\left(-\frac{\tau}{\hbar}\int\frac{d\omega}{2\pi}\int\frac{d^2k_\parallel}{(2\pi)^2}[G^+_\omega(x_1,x_0;\vec{k}_\parallel) - G^+_\omega(x_0,x_1;\vec{k}_\parallel)]\right), \tag{9}$$

with

$$G^+_\omega(x,x';\vec{k}_\parallel) = \int d^2\rho\, dt\, G^+(\vec{r}t;\vec{r}'t') \times \exp[i\vec{k}_\parallel\cdot(\vec{\rho}-\vec{\rho}') - i\omega(t-t')]. \tag{10}$$

$\vec{\rho} = (y,z)$ and $\vec{k}_\parallel$ are vectors lying in a plane parallel to the surface.

The contribution to the evaporation current owing to atoms of energy ω and parallel wave vector $\vec{k}_\parallel$ can be deduced immediately from Eq. (9),

$$j_x(\omega,\vec{k}_\parallel) = -[\tau/(2\pi)^3\hbar][G^+_\omega(x_1,x_0;\vec{k}_\parallel) - G^+_\omega(x_0,x_1;\vec{k}_\parallel)], \tag{11}$$

where the $\epsilon\to 0$ limit is understood.

Making extensive use of the recipes described at length in Refs. 13 and 15, we calculate the G^+'s in terms of the g's with the help of the Dyson equation for the $\hat{G}$ matrices,

$$\begin{aligned} \hat{G}^+(x_1,x_0;\vec{k}_\parallel) &= [\hat{g}_\omega(x_1,x_1;\vec{k}_\parallel)\hat{T}\hat{G}_\omega(x_0,x_0;\vec{k}_\parallel)]^+ \\ &= \hat{g}^r_\omega(x_1,x_1;\vec{k}_\parallel)\hat{T}\hat{G}^+_\omega(x_0,x_0;\vec{k}_\parallel) \\ &\quad + \hat{g}^+_\omega(x_1,x_1;\vec{k}_\parallel)\hat{T}\hat{G}^a_\omega(x_0,x_0;\vec{k}_\parallel) \end{aligned} \tag{12}$$

and

$$\begin{aligned} \hat{G}^+_\omega(x_0,x_1;\vec{k}_\parallel) &= \hat{G}^+_\omega(x_0,x_0;\vec{k}_\parallel)\hat{T}\hat{g}^a_\omega(x_1,x_1;\vec{k}_\parallel) \\ &\quad + \hat{G}^r_\omega(x_0,x_0;\vec{k}_\parallel)\hat{T}\hat{g}^+_\omega(x_1,x_1;\vec{k}_\parallel). \end{aligned} \tag{13}$$

Using the fact that the chemical potential of the vacuum is $\mu_V = -\infty$, which implies that

$$\hat{g}^+_\omega(x_1,x_1;\vec{k}_\parallel) = 0 \tag{14}$$

and that

$$g^r_\omega(x_1,x_1;\vec{k}_\parallel) - g^a_\omega(x_1,x_1;\vec{k}_\parallel) = g^-_\omega(x_1,x_1;\vec{k}_\parallel), \tag{15}$$

we find

$$j_x(\omega,\vec{k}_\parallel) = -[\tau^2/(2\pi)^3\hbar]g^-_\omega(x_1,x_1;\vec{k}_\parallel)G^+_\omega(x_0,x_0;\vec{k}_\parallel). \tag{16}$$

We thus have to calculate $G^+_\omega(x_0,x_0;\vec{k}_\parallel)$. Using once again the matrix form of Dyson's equation, we easily find

$$\hat{G}^+_\omega(x_0,x_0;\vec{k}_\parallel) = [\hat{I} - \hat{T}^2\hat{g}^r_\omega(x_0,x_0;\vec{k}_\parallel)\hat{g}^r_\omega(x_1,x_1;\vec{k}_\parallel)]^{-1} \times\hat{g}^+_\omega(x_0,x_0;\vec{k}_\parallel)\times[\hat{I} - \hat{T}^2\hat{g}^a_\omega(x_1,x_1;\vec{k}_\parallel)\hat{g}^a_\omega(x_0,x_0;\vec{k}_\parallel)]^{-1}, \tag{17}$$

where $\hat{I}$ is the unit matrix.

Before calculating explicitly G_ω^+ from Eq. (17), it is convenient to take the $\epsilon \to 0$ limit of Eq. (17). Once again following Ref. 15, we get

$$
\begin{aligned}
&\hat{g}_\omega^{r(a)}(x_0, x_0; \vec{k}_\parallel) \cong (1/\tau)[\hat{I} + \epsilon\, \hat{\gamma}_0^{r(a)}(\omega, \vec{k}_\parallel)],\\
&\hat{g}_\omega^{r(a)}(x_1, x_1; \vec{k}_\parallel) \cong (1/\tau)[\hat{I} + \epsilon\, \hat{\gamma}_1^{r(a)}(\omega, \vec{k}_\parallel)],\\
&\hat{g}_\omega^{+}(x_0, x_0; \vec{k}_\parallel) \cong (\epsilon/\tau)\, \hat{\gamma}_0^{+}(\omega, \vec{k}_\parallel),\\
&\hat{g}_\omega^{-}(x_1, x_1; \vec{k}_\parallel) \cong (\epsilon/\tau)\, \hat{\gamma}_1^{-}(\omega, \vec{k}_\parallel),
\end{aligned}
\tag{18}
$$

where the $\hat{\gamma}$ matrices are independent of ϵ and finite. Setting

$$
\hat{\gamma} = \begin{pmatrix} \gamma & u \\ \tilde{u} & \tilde{\gamma} \end{pmatrix}
\tag{19}
$$

and using Eqs. (16)–(18), we finally obtain

$$
j_x(\omega, \vec{k}_\parallel) = \frac{1}{(2\pi)^3 \hbar}\, \gamma_1^- \, \frac{\gamma_0^+ |\tilde{\gamma}_0^r + \tilde{\gamma}_1^r|^2 + \tilde{\gamma}_0^+ u_0^r \tilde{u}_0^a - u_0^+ \tilde{u}_0^a(\tilde{\gamma}_0^r + \tilde{\gamma}_1^r) - \tilde{u}_0^+ u_0^r(\tilde{\gamma}_0^a + \tilde{\gamma}_1^a)}{|(\gamma_0^r + \gamma_1^r)(\tilde{\gamma}_0^r + \tilde{\gamma}_1^r) - u_0^r \tilde{u}_0^r|^2}\,,
\tag{20}
$$

where it is understood that all of the functions involved have arguments $(\omega, \vec{k}_\parallel)$.

Let us recall that the above result is valid only in the approximation, described in Sec. II. B, where direct coupling via self-energy terms is neglected. At this point, and even in our very simplified model, a full calculation of $j_x(\omega, \vec{k}_\parallel)$ from Eq. (20) would demand a complete microscopic model for superfluid helium. We will therefore study only the shape of the j-vs-ω curve in the immediate vicinity of the roton minimum.

C. Behavior of $j_x(\omega, \vec{k}_\parallel)$ near ω_r

We will now show that the qualitative behavior of $j_x(\omega, \vec{k}_\parallel)$ near the roton minimum ω_r, as deduced from Eq. (20), does not depend on the specific microscopic model used to describe superfluid helium, but only on the well-known shape of the bulk dispersion equation $\omega = \omega(k)$ depicted in Fig. 1. In order to study this behavior, we express the $\hat{g}$'s (and then the $\hat{\gamma}$'s) in terms of the Green's functions $\hat{G}^\infty$ of the infinite liquid. Neglecting as above the self-energy terms linking points on different sides of the cut,[20] we immediately obtain

$$
\begin{aligned}
&\hat{g}_\omega^r(x_0, x_0; \vec{k}_\parallel)\\
&\qquad = \hat{G}_\omega^{\infty, r}(x_0, x_0; \vec{k}_\parallel)[\hat{I} + \hat{T}\hat{G}_\omega^{\infty, r}(x_1, x_0; \vec{k}_\parallel)]^{-1}.
\end{aligned}
\tag{21}
$$

Performing the matrix product, taking the $\epsilon \to 0$ limit, and using (for the sake of simplicity of the following analytic expression) the two relations, which are easily proved by integrating the equations of motion of G^∞ and F^∞,

$$
\begin{aligned}
&\lim_{\epsilon \to 0^+} \left(\frac{\partial}{\partial x} G_\omega^{\infty, r}(x, x'; \vec{k}_\parallel) \right)_{x = x' - \epsilon} = \frac{m}{\hbar^2},\\
&\lim_{\epsilon \to 0^+} \left(\frac{\partial}{\partial x} F_\omega^{\infty, r}(x, x'; \vec{k}_\parallel) \right)_{x = x' - \epsilon} = 0,
\end{aligned}
\tag{22}
$$

and, finally, noting that $F_\omega^{\infty, r}(x, x'; \vec{k}_\parallel) = \tilde{F}_\omega^{\infty, r}(x, x'; \vec{k}_\parallel)$, we obtain

$$
\gamma_0^r = (m/\hbar^2)\tilde{G}_\omega^{\infty, r}(0, 0; \vec{k}_\parallel)[\Delta^r(\omega, \vec{k}_\parallel)]^{-1},
\tag{23}
$$

$$
\tilde{\gamma}_0^r = (m/\hbar^2)G_\omega^{\infty, r}(0, 0; \vec{k}_\parallel)[\Delta^r(\omega, \vec{k}_\parallel)]^{-1},
\tag{24}
$$

$$
u_0^r = \tilde{u}_0^r = (m/\hbar^2)F_\omega^{\infty, r}(0, 0; \vec{k}_\parallel)[\Delta^r(\omega, \vec{k}_\parallel)]^{-1},
\tag{25}
$$

where

$$
\begin{aligned}
\Delta^r(\omega, \vec{k}_\parallel) = {}& G_\omega^{\infty, r}(0, 0; \vec{k}_\parallel)\tilde{G}_\omega^{\infty, r}(0, 0; \vec{k}_\parallel)\\
&- [F_\omega^{\infty, r}(0, 0; \vec{k}_\parallel)]^2,
\end{aligned}
\tag{26}
$$

from which the other quantities of interest are easily deduced, with the help of the thermodynamic relations

$$
\gamma_0^+ = -\, 2iB(\omega)\, \mathrm{Im}\gamma_0^r\,,
\tag{27a}
$$

$$
\tilde{\gamma}_0^+ = -\, 2iB(\omega)\, \mathrm{Im}\gamma_0^r\,,
\tag{27b}
$$

$$
u_0^+ = \tilde{u}_0^+ = -\, 2iB(\omega)\, \mathrm{Im}\, u_0^r\,,
\tag{27c}
$$

where $B(\omega)$ is the Bose-Einstein function

$$
B(\omega) = \{\exp[(\omega - \mu_L)/kT] - 1\}^{-1}.
\tag{27d}
$$

$G_\omega^{\infty, r}(x, x'; \vec{k}_\parallel)$ and $F_\omega^{\infty, r}(x, x'; \vec{k}_\parallel)$ are now expressed in terms of their Fourier transforms,

$$
G_\omega^{\infty, r}(x, x'; \vec{k}_\parallel) = \int \frac{dk_x}{2\pi} \exp[ik_x(x - x')]G_\omega^{\infty, r}(\omega, \vec{k}),
\tag{28}
$$

with a similar expression for $F_\omega^{\infty, r}$; k_x is the component of the momentum vector $\vec{k}[\equiv (k_x, \vec{k}_\parallel)]$ in the direction transverse to the surface. $G^{\infty,r}(\omega,\vec{k}_\parallel)$ and $F^{\infty,r}(\omega,\vec{k}_\parallel)$ are usually written[17]

$$G^{\infty,r}(\omega,\vec{k})=\tilde{G}^{\infty,r}(-\omega,-\vec{k})$$

$$=\frac{\omega+\epsilon_k-\mu_L+S(\omega,k)-A(\omega,k)}{D(\omega,k)}\equiv\frac{N(\omega,k)}{D(\omega,k)}, \tag{29}$$

$$F^{\infty,r}(\omega,\vec{k})=-C(\omega,k)/D(\omega,k), \tag{30}$$

with

$$D(\omega,k)=[\omega+i\eta-A(\omega,k)]^2-[\epsilon_k-\mu_L+S(\omega,k)]^2+c^2(\omega,k) \tag{31}$$

and $\epsilon_k=\hbar^2k^2/2M$. $S(\omega,k)$ and $A(\omega,k)$ are, respectively, an even and an odd function of ω. Owing to the rotational invariance of the infinite liquid, all of these functions depend only on $|\vec{k}|=(k_x^2+\vec{k}_\parallel^2)^{1/2}$. The excitations of the infinite liquid are defined by the solutions of the equation $D(\omega,k)=0$. They, of course, have finite lifetimes. However, in the superfluid phase and in the energy range of interest here ($\omega\sim\omega_r$), these lifetimes are long enough for the dispersion relation (Fig. 1) to be measurable experimentally. Therefore as a first approximation we will, for the time being, assume that the solutions of the $D=0$ equation are completely real. This neglects at the same time the widths of the quasiparticle peaks and the incoherent background in the spectral density.

In order to study $j_x(\omega,\vec{k}_\parallel)$ near ω_r we must expand the Green's functions $\hat{G}^\infty$ in powers of $(\omega-\omega_r)$. As is clear from Eq. (28), their behavior is controlled by the positions of the zeros of $D(\omega,k)$. Developing the dispersion equation in the vicinity of $\omega=\omega_r$, we can write the following:

(i) Near (ω_r,k_1), where k_1 is the momentum of the photon of energy ω_r (i.e., on the phonon branch of the spectrum),

$$D(\omega,k)\cong(\omega-\omega_r)\left(\frac{\partial D}{\partial\omega}\right)_{\omega=\omega_r,\,k=k_1}+(k^2-k_1^2)\left(\frac{\partial D}{\partial(k^2)}\right)_{\omega=\omega_r,\,k=k_1}, \tag{32}$$

that is, for a given energy ω and parallel momentum $\vec{k}_\parallel$, there are two possible phonons with transverse wave vectors $k_x=\pm p_1(\omega,k_\parallel)$, propagating in opposite directions,

$$p_1^2=k_1^2-k_\parallel^2+b(\omega-\omega_r), \tag{33}$$

with

$$b=-\left(\frac{\partial D}{\partial\omega}\Big/\frac{\partial D}{\partial(k^2)}\right)_{\omega=\omega_r,\,k=k_1}>0.$$

(ii) Near (ω_r,k_r), where k_r is the momentum of the rotons of minimum energy (i.e., on the roton branches),

$$D(\omega,k)=(\omega-\omega_r)\left(\frac{\partial D}{\partial\omega}\right)_{\omega=\omega_r,\,k=k_r}+\tfrac{1}{2}(k^2-k_r^2)^2\left(\frac{\partial^2D}{\partial(k^2)^2}\right)_{\omega=\omega_r,\,k=k_r}, \tag{34}$$

i.e., for given $\vec{k}_\parallel$ and ω, there are four roton modes, with transverse wave vectors $\pm p_2(\omega,k_\parallel)$, $\pm p_3(\omega,k_\parallel)$ given by

$$\begin{aligned}p_2^2&=k_r^2-k_\parallel^2+[a(\omega-\omega_r)]^{1/2},\\ p_3^2&=k_r^2-k_\parallel^2-[a(\omega-\omega_r)]^{1/2},\end{aligned} \tag{35}$$

with

$$a=-2\left(\frac{\partial D}{\partial\omega}\Big/\frac{\partial^2D}{\partial(k^2)^2}\right)_{\omega=\omega_r,\,k=k_r}>0.$$

Clearly, two cases must be considered: $\omega>\omega_r$ and $\omega<\omega_r$. For $\omega\gtrsim\omega_r$, the largest possible value of $k_\parallel$ (which corresponds to grazing emission) is

$$k_\parallel^{\max}=[(2M/\hbar^2)(\omega_r-L_0)]^{1/2}, \tag{36}$$

where M is the free-atom mass. With $\omega_r=8.65$ °K and $L_0=7.15$ °K, one finds that $k_\parallel^{\max}\simeq0.5$ Å^{-1}. This value is slightly smaller than the phonon wavevector k_1, and *a fortiori*, $k_\parallel^{\max}<k_r$. Therefore whatever the direction of emission, p_1, p_2, and p_3 are real functions of ω. In other words, at the energies of interest, atoms are refracted from the vacuum into the liquid; there is no total reflection. The retarded propagator must be analytic in the upper ω-half-plane. This imposes the restriction that the poles which contribute to expression (28) are $p_1\,\mathrm{sgn}(x-x')$, $p_2\,\mathrm{sgn}(x-x')$, and $-p_3\,\mathrm{sgn}(x-x')$. That is, causality implies that only excitations with a group velocity in the x direction v_{gx} satisfying $\mathrm{sgn}v_{gx}\equiv\mathrm{sgn}(x-x')$ contribute to $G^{\infty,r}$. Thus

$$G_\omega^{\infty,r}(0,0;\vec{k}_\parallel)=\frac{i}{2}\Bigg[\frac{N(\omega,[k_1^2+b(\omega-\omega_r)]^{1/2})}{p_1(\omega,k_\parallel)[\partial D/\partial(k^2)]_{\omega=\omega_r,\,k=k_r}}+\frac{1}{[a(\omega-\omega_r)]^{1/2}[\partial^2D/\partial(k^2)^2]_{\omega=\omega_r,\,k=k_r}}$$

$$\times\left(\frac{N(\omega,\{k_r^2+[a(\omega-\omega_r)]^{1/2}\}^{1/2})}{p_2(\omega,k_\parallel)}+\frac{N(\omega,\{k_r^2-[a(\omega-\omega_r)]^{1/2}\}^{1/2})}{p_3(\omega,k_\parallel)}\right)\Bigg], \tag{37}$$

$$F_\omega^{\infty,r}(0,0;\vec{k}_\parallel)=-\frac{i}{2}\left[\frac{C(\omega,[k_1^2+b(\omega-\omega_r)]^{1/2})}{p_1(\omega,k_\parallel)[\partial D/\partial(k^2)]_{\omega=\omega_r,\,k=k1}}+\frac{1}{[a(\omega-\omega_r)]^{1/2}[\partial^2 D/\partial(k^2)^2]_{\omega=\omega_r,\,k=k_r}}\right.$$
$$\left.\times\left(\frac{C(\omega,\{k_r^2+[a(\omega-\omega_r)]^{1/2}\}^{1/2})}{p_2(\omega,k_\parallel)}+\frac{C(\omega,\{k_r^2+[a(\omega-\omega_r)]^{1/2}\}^{1/2})}{p_3(\omega,k_\parallel)}\right)\right]. \tag{38}$$

Assuming that $N(\omega,k)$, $C(\omega,k)$, and $\gamma_1(\omega,k_\parallel)$ are well-behaved functions of ω and k, and using the relation

$$D(\omega,k)=-N(\omega,k)\tilde{N}(\omega,k)+C^2(\omega,k), \tag{39}$$

we obtain easily the expansion of the γ_0's and u_0's in the vicinity of ω_r, with the help of formulas (23)–(27). Inserting them into Eq. (20), we get

$$j_x(\omega,k_\parallel)\cong j_x(\omega_r,k_\parallel)[1+\alpha_>(k_\parallel)(\omega-\omega_r)^{1/2}],\quad \omega>\omega_r. \tag{40}$$

For $\omega\lesssim\omega_r$, $p_2(\omega,k_\parallel)$ and $p_3(\omega,k_\parallel)$ are now complex quantities (roton waves are evanescent) but the same kind of expansion can be worked out; it gives

$$j_x(\omega,k_\parallel)\cong j_x(\omega_r,k_\parallel)[1+\alpha_<(k_\parallel)(\omega_r-\omega)^{1/2}],\quad \omega<\omega_r. \tag{41}$$

It is not difficult, although lengthy, to obtain the formal expressions of the two coefficients $\alpha_>(k_\parallel)$ and $\alpha_<(k_\parallel)$. We do not write them here explicitly, because they are complicated combinations of $N(\omega_r,k_i)$, $C(\omega_r,k_i)$, $D(\omega_r,k_i)$ [where $\vec{k}_i=(p_{1,2,3},\vec{k}_\parallel)$], and their derivatives. These coefficients cannot be simplified (even by using sum rules) in the absence of a detailed microscopic model, so that their expressions are of no practical interest. Moreover, owing to the lack of such a model, (i) we cannot derive any simple relationship between $\alpha_>$ and $\alpha_<$; and (ii) there is no way to decide on their signs: each of them can, *a priori*, be either positive or negative; signs may change at some values of $k_\parallel$. In the vicinity of ω_r, $j_x(\omega,k_\parallel)$ may therefore vary with one of the four possible shapes (all characterized by a vertical tangent at $\omega=\omega_r$) depicted in Fig. 2, depending on the signs of $\alpha_>$ and $\alpha_<$. It is even possible that the shape of the j-vs-ω curve could be of different types in different ranges of values of $k_\parallel$.

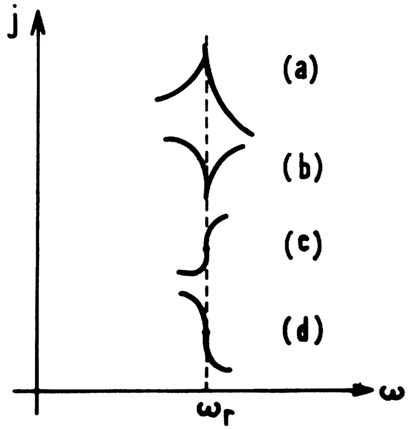

FIG. 2. (a) and (b) Cusp and (c) and (d) rounded wedge singularities in $j_x(\omega,k_\parallel)$ near ω_r.

The energy distribution of the total current $J_x(\omega)$ can be easily inferred from $j_x(\omega,k_\parallel)$,

$$J_x(\omega)=\int d^2k_\parallel\, j_x(\omega,k_\parallel). \tag{42}$$

Since the value of ω at which $j_x(\omega,k_\parallel)$ has a square-root singularity is independent of $k_\parallel$, the total current will exhibit a singularity of the same type at the same energy, namely ω_r,

$$\begin{aligned}J_x(\omega)&\cong J_x(\omega_r)[1+\beta_>(\omega-\omega_r)^{1/2}]\quad \text{if } \omega>\omega_r,\\ J_x(\omega)&\cong J_x(\omega_r)[1+\beta_<(\omega_r-\omega)^{1/2}]\quad \text{if } \omega<\omega_r.\end{aligned} \tag{43}$$

Again, the respective values and signs of the numerical coefficients $\beta_>$ and $\beta_<$ could be obtained only from a complete microscopic calculation.

III. DISCUSSION

As shown in Sec. II, our calculation cannot provide a full quantitative expression for the evaporation spectrum, but only a prediction about its (singular) shape in the vicinity of the roton minimum. This situation results from two physical difficulties (which are, in our opinion, very hard to overcome):

(i) We do not know the values of all of the parameters involved in our calculation. More exactly, a complete description, even in the simplified model used in Sec. II, would require that we know not only the dispersion relation, but the full Green's functions (or equivalently, the self-energies) of the *infinite liquid*, for all values of ω and k.

(ii) Even if condition (i) were realized, the simple model used here to describe the coupling between the "liquid" and "vacuum" subsystems would not give an accurate numerical value of $J_x(\omega)$.

Indeed, for the sake of practical feasibility of calculation, we have neglected the coupling across the surface via self-energy terms and kept only the coupling due to the kinetic-energy (one-body) term. This approximation amounts to matching, at the interface, free-atom wave functions, not with the true wave functions Ψ of quasiparticles of the liquid, but with approximate "bare" functions. That is, the continuity at the surface of that part of the Ψ's which corresponds to the presence of a dressing cloud is not assured by our approximation. In other words, it is not possible, in the case of helium, to calculate simply an exact value of the excitation- (phonon- roton-) atom transmission coefficients. This stems from the fact that the (atomic) range of nonlocal (dressing) effects is of the same order of magnitude as all of the other characteristic lengths, including the coherence distance ξ, so that the equations of motion of the excitations are irreducibly nonlocal. This contrast with the case of superconductors,[11] for which, since $\xi \gg a$, nonlocal effects are negligible, and the transmission coefficients of Bogoliubov excitations can be obtained from standard local matching equations.

For all of these reasons, there is little hope of obtaining reliable quantitative predictions about the complete evaporation spectrum. However, the qualitative result about the singular behavior of $j(\omega)$ around ω_r, obtained in Sec. II, is completely general, and by no means an artifact of the aforementioned approximations. We found that $j(\omega)$ must exhibit a structure with a vertical tangent at $\omega = \omega_r$, taking either a cusp [Fig. 2(a) or 2(b)] or rounded-wedge [Fig. 2(c) or 2(d)] shape, depending on the respective signs of the coefficients $\beta_{\gtrless}$. This is, indeed, a well-known scattering phenomenon which occurs, each time a new "channel" opens, at the corresponding threshold energy (the opening channel is here the roton one, with threshold $\omega = \omega_r$).[21] It has been studied extensively in high-energy physics, where it gives rise to singularities of the inelastic scattering cross sections near a reaction threshold. It can be shown directly that our evaporation problem may be recast into the language of multichannel scattering theory, leading to the same final result as the one obtained in Sec. II, under the single condition that interactions between excitations of the liquid be negligible. (This, together with transmission singularities for solids, is the subject of a separate paper.[22]) In other words, the fact that in the present paper we have neglected nonlocal effects in the vicinity of the surface does not affect the validity of our result. This is quite understandable when one considers the physical reasons for the occurrence of the threshold singularity:

(i) For $\omega < \omega_r$, only phonons can propagate in the liquid. However, close below ω_r, there also exist, near the surface, evanescent roton waves, the space range of which increases as $(\omega_r - \omega)^{-1/2}$. A phonon wave packet, before being transmitted into vacuum, spends, in the roton evanescent state, a time which increases as the range of that state. This phenomenon, which is obviously independent of the details of the (pseudo) potential in the surface layer, is what gives rise to the $(\omega_r - \omega)^{1/2}$ behavior of the phonon-atom transmission coefficient below the roton threshold.

(ii) For $\omega > \omega_r$, roton channels open, the flux carried by the rotons of energy ω varies as $(\omega - \omega_r)^{1/2}$ (and this, again, whatever the detailed properties of the surface layer). This together with the condition of flux conservation entails the square-root variations of all transmission coefficients.

Such a singularity has already been observed in one case involving a transmission problem: the optical reflectivity of CdS exhibits a cusp at the minimum energy of the upper polariton branch.[23] Note that this is an experimental proof that the predicted threshold behavior is not modified by nonlocal short-range effects; indeed, polariton modes are a superposition of photons and excitons. Excitons obviously have a finite radius, so that nonlocal effects are present in the polariton problem as well as in the case of helium.

All of the above calculation and discussion have neglected lifetime effects, or, equivalently, interactions between quasiparticles. These appear in two ways:

(i) They give rise to imaginary self-energy terms coupling points on the two sides of the surface. These are the terms responsible for inelastic transmission processes (for example, a phonon at energy ω decomposes, at the surface, into a transmitted atom of energy $\omega' < \omega$ and a reflected phonon $\omega - \omega'$, or, two phonons ω_1 and ω_2 combine at the surface into an atom $\omega_1 + \omega_2$, etc.). As has been argued by Anderson,[5] and substantiated by recent reflection measurements,[19] the phase space available for such processes is very small, so that the corresponding inelastic current can be safely neglected.

(ii) They limit the lifetimes of the bulk excitations. The finiteness of these lifetimes can be taken into account (at least approximately) by letting, in the calculation of Sec. II, the momenta $p_i(\omega, k_\parallel)$ of the excitation have finite imaginary parts. This straightforwardly results in a rounding of the roton threshold singularity, on a width $\Delta\omega \sim \hbar/\tau$ (where τ is some average of the lifetimes of the excitations of energy $\omega \sim \omega_r$). The same intuitive conclusion is also obtained from general scattering theory arguments. The different low-temperature lifetimes for roton-roton, phonon-roton, and phonon-phonon scattering are larger than, typically, 10^{-7} sec.[24] Thus $\hbar/\tau \ll \omega_r$.

Therefore, finally, the observability of the threshold singularity depends only, in practice, on the order of magnitude of the β coefficients. In the absence of a complete microscopic calculation, we must rely on dimensional arguments. In superfluid helium, all of the characteristic energies of interest are of the same order, $\sim \omega_r$, which also gives the scale of the variations of the various quantities involved in the expression of the α and β coefficients. One then finds that $\beta_{<>} \sim \omega_r^{-1/2}$. Thus it seems that one can reasonably hope that the predicted singularity is observable experimentally (especially if it turns out to be of the cusp type).

No such effect has yet been observed in evaporation experiments. However, of course, the idealized experiment considered above is not realizable as such. Most actual experiments[3,4] use a heat pulse to create an excess population of excitations in the liquid, so that the relevant occupation factor is not the thermal one, but a quantity depending on the characteristics of the pulse, the impedance of the contact between the liquid and the heating resistor, the distance between this and the surface, and the details of the thermalization processes in He II.

Since all of these quantities are very poorly known, it is difficult to extract detailed informations from the spectra thus obtained. Although it is not impossible that evaporation experiments can lead to the observation of the above predicted effect, there seems to be more hope, at least in the near future, of exploiting data about the spectrum of He atoms reflected from superfluid liquid He. Moreover, the reflection technique would probably be more appropriate since, as proved in Ref. 19, at energies of order ω_r the reflected current j_R is much smaller than the transmitted current j_T ($j_R \sim 10^{-3} j_T$) which induces a corresponding enhancement of the relative amplitude of the singularity of j_R with respect to the one of j_T. Such an experiment has recently been performed by Edwards *et al.*.[19] However, the experimental uncertainty of $j(\omega)$ is relatively large in the range $\omega \sim \omega_r$, so that further refinements are needed in order to draw a definite conclusion.

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[18] This implies that the parallel wave vector $\vec{k}_\parallel$ is conserved in the evaporation process, i.e., that the surface remains a perfect plane and that ripplon effects are negligible. That assumption is substantiated by the experimental results of Edwards *et al.*, Ref. 19.

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