

Quantum evaporation from superfluid ^4He : Normal incidence

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(Received 14 August 1997)

We study the scattering of atoms and quasiparticles at the surface of ^4He at $T=0$ K. Using the microscopic theory of Beliaev in a real-space formulation we derive an equation of motion for the quasiparticles valid in bulk helium, through the surface and in the vacuum. Assuming normal incidence, we solve the equation and calculate probabilities for the various surface scattering processes for a range of energies (between 7.5 and 15 K). Some of the scattering rates obtained are markedly different from those reported recently.

[S0163-1829(97)51646-8]

Quantum evaporation is one manifestation of the scattering of quasiparticles from a free liquid ^4He surface in which an incident quasiparticle, be it a roton (R^+ or R^-) or a phonon, results in the emission of a single ^4He atom.

Direct experimental evidence that the process was a quantum process was provided by the time-of-flight experiments of Baird *et al.*¹ The evaporation process is characterized by the energy conservation equation

$$\hbar\omega - |\mu_0| = \frac{\hbar^2 \mathbf{k}^2}{2m}, \quad (1)$$

where $\hbar\omega$ is the energy of the quasiparticle and lies on the phonon-roton energy spectrum, μ_0 ($=-7.16$ K) is the chemical potential, and $\hbar^2 \mathbf{k}^2/2m$ is the kinetic energy carried off by the evaporated atom. Together with this energy conservation, the momentum $\hbar\mathbf{Q}$ parallel to the surface [$\mathbf{k} = (\mathbf{Q}, k_a)$, where k_a is the component of the atom wave vector normal to the surface] is conserved because of the translational symmetry of the problem.

More generally a quasiparticle incident on the surface is expected to undergo mode conversion, reflecting either as itself or another quasiparticle or evaporating subject to the conservation laws described above.

Unfortunately despite the considerable success of the experimental studies on quantum evaporation, the probabilities of the different surface scattering processes cannot be determined experimentally using the present available techniques. Instead the best one can hope to do is to describe the experimental features via a realistic microscopic model and predict the relative probabilities of mode conversion both for the evaporation process and its inverse, the absorption of ^4He atoms into the surface. It is clear that any realistic treatment of the surface scattering problem has to take into account (i) the nonlocality of the He-He interaction, (ii) the change in the properties of the condensate through the surface region, and (iii) the finite width of the surface. We include all these in the present study.

Most of the earlier theories²⁻⁴ of quantum evaporation/condensation were not very successful. They used a perturbation method in which the quasiparticles are weakly coupled to the atoms, contrary to the experimental evidence.⁵ Maris⁶ used an ‘‘adiabatic’’ model and found that quasiparticles (phonons and rotons) with energies between the roton

minimum energy Δ and the maxon energy Δ_m do not evaporate atoms, whereas experiments^{7,8} show that R^+ rotons do contribute to quantum evaporation at energies between Δ and Δ_m .

The microscopic theory of Mulheran and Inkson⁹ predicted scattering rates for all the one-to-one surface processes. They derived an equation of motion which they solved in a WKB approximation for normal incidence and used the quantum states associated with the WKB solutions to perturbatively study the surface scattering processes. Their results were in broad agreement with experimental evidence. Stringari and co-workers¹⁰⁻¹² have recently produced scattering rates for the surface processes using a linearized density functional theory. They used a phenomenological density functional (the ‘‘Orsay-Trento’’ functional¹³) to derive equations of motion for the elementary excitations, which they solved numerically for the flux of phonons, rotons, and atoms, and used these to calculate the probabilities associated with each one-to-one surface scattering process.

The current study removes the WKB restrictions in the Mulheran and Inkson⁹ theory. Following Mulheran and Inkson, we neglect inelastic (rippions, phonon-decay) processes, i.e., we assume that all quasiparticles are stable and propagate ballistically. We take a real-space formulation of the quantum field theory of Beliaev¹⁴ and, from the two ‘‘coupled diagrams’’ for the quasiparticle propagators, we write down the equation of motion

$$0 = \left[\hbar\omega - \mu(\mathbf{r}) + \frac{\hbar^2}{2m} \nabla^2 \right] \phi(\mathbf{r}) - \int_{-\infty}^{+\infty} \Sigma(\mathbf{r}, \mathbf{r}', \omega) \phi(\mathbf{r}') d^3 \mathbf{r}' \quad (2)$$

for the ‘‘particle-hole’’ wave function $\phi(\mathbf{r})$ valid in bulk, through the surface and in the vacuum. The function $\mu(\mathbf{r})$ changes from 0 (in bulk) to $|\mu_0|$ (in the vacuum) across the surface. The central feature of this equation is the self-energy

$$\begin{aligned} \Sigma(\mathbf{r}, \mathbf{r}', \omega) = & \sqrt{\rho(\mathbf{r})} V(\mathbf{r}-\mathbf{r}') \sqrt{\rho(\mathbf{r}')} \\ & + \sqrt{\rho(\mathbf{r})\rho(\mathbf{r}')} \int \int_{-\infty}^{+\infty} V(\mathbf{r}-\mathbf{r}_1) \sqrt{\rho(\mathbf{r}_1)} \\ & \times G_n(\mathbf{r}_1-\mathbf{r}_2, -\omega) \sqrt{\rho(\mathbf{r}_2)} V(\mathbf{r}_2-\mathbf{r}') d^3 \mathbf{r}_1 d^3 \mathbf{r}_2, \end{aligned} \quad (3)$$

where $G_n(\mathbf{r}, \omega)$ is the “normal” Green’s function.¹⁵ The self-energy is a function of the helium density $\rho(\mathbf{r})$ and the nonlocal helium-helium interaction $V(\mathbf{r}-\mathbf{r}')$. The corresponding “hole-particle” wave function $\psi(\mathbf{r})$ is given by

$$\begin{aligned} \psi(\mathbf{r}) = & \int \int_{-\infty}^{+\infty} G_n(\mathbf{r}-\mathbf{r}_1, -\omega) \\ & \times \sqrt{\rho(\mathbf{r}_1)} V(\mathbf{r}_1-\mathbf{r}') \sqrt{\rho(\mathbf{r}')} \phi(\mathbf{r}') d^3\mathbf{r}_1 d^3\mathbf{r}'. \end{aligned} \quad (4)$$

The hole-particle wave function $\psi(\mathbf{r})$ is necessary to correctly describe the effects associated with a quasiparticle propagating through a correlated system (see, for example, Dalfovo *et al.*¹¹).

In deriving the above equations, we have allowed the condensate density $\rho(\mathbf{r})$ to vary with position and we use this to describe the free surface. Deep in bulk the density has the value of bulk superfluid condensate and high above the surface it has the vacuum value. Equation (2) has the correct limits—in bulk it is the Schrödinger equation for the quasiparticles (of energy $\hbar\omega$) and in the vacuum it is the Schrödinger equation for the free atom (of energy $\hbar\omega - |\mu_0|$).

We assume that the quasiparticles and atoms are incident normal to the surface ($|\mathbf{Q}| = \mathbf{0} \text{ \AA}^{-1}$; since momentum parallel to the surface is conserved, this reduces the problem to a one-dimensional one) and we use a Fermi function for the surface profile $\rho(z)$ (we take z to be the direction normal to the surface). We also assume that the interaction is the same as in bulk helium and use the effective potential of Brueckner and Sawada.¹⁶ The Brueckner potential gives a good fit to the experimentally observed quasiparticle excitation spectrum in bulk when used with the Bogoliubov spectrum¹⁷ and retains the nonlocality of the He-He interaction. The variation of the chemical potential is described as $\mu(z) = |\mu_0|f(z)$. The choice of $f(z)$ is required to model the change in μ across the surface. We have used both the forms $f(z) = [1 - \rho(z)]$ and $f(z) = (2\alpha a_0)^{-1} \ln\{[1 + \exp\alpha(z + a_0)] / [1 + \exp\alpha(z - a_0)]\}$ (with α chosen to give a sharper change than the first form and a_0 of the order of the range of the interatomic potential); both forms give comparable results indicating that the results are not too sensitive to this parameter.

We solve the full equation (2) numerically at a given energy $\hbar\omega$ for the wave function $\phi(z)$ in a box of size $2L$ ($z = -L - s$ to $z = L - s$, with the surface centred at $z = 0$ and with bulk helium in $z < 0$). $\psi(z)$ is then evaluated using Eq. (4). To calculate the various probabilities, we need several solutions at the same energy. These are obtained by keeping $\hbar\omega$ fixed and solving the equation for different values of s .

We take the surface to have a 90–10% width of 6.5 \AA , which is within the accepted experimental estimate (see, for example, Ref. 18). Figures 1(a) and 1(b) show the wave functions $\phi(z)$ and $\psi(z)$, respectively, at $\hbar\omega = 11.5 \text{ K}$. At this energy, in bulk, both $\phi(z)$ and $\psi(z)$ have three Fourier components $k = k_p, k_-, k_+$, corresponding to phonons, R^- rotons, and R^+ rotons, respectively, at precisely the wave vectors expected from the excitation spectrum. In the vacuum $\phi(z)$ has a single component $k = k_a$ in agreement

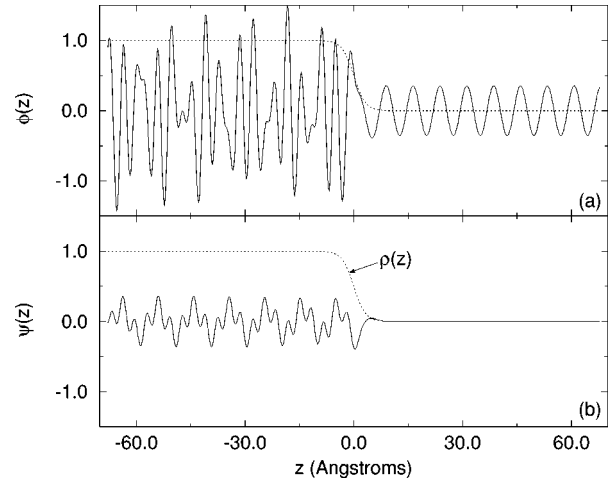


FIG. 1. The wave functions $\phi(z)$ (a) and $\psi(z)$ (b) at $\hbar\omega = 11.5 \text{ K}$. The dashed line is the surface profile. The surface is centered at $z = 0$ ($L = 67.8 \text{ \AA}$ and $s = 0$).

with the value calculated from $\hbar\omega = |\mu_0| + \hbar^2 k_a^2 / 2m$, whereas $\psi(z)$ is zero. $\phi(z)$ can be fitted with functions of the form

$$\phi(z < 0) = \sum_{i=p,-,+} \phi_i \cos(k_i z + \theta_i),$$

$$\phi(z > 0) = \phi_a \cos(k_a z + \theta_a),$$

where θ_i is a phase and i labels the quasiparticles, atom a , phonon p , R^- roton $-$, R^+ roton $+$. The “hole-particle” wave function $\psi(z)$ can be fitted with a function similar to the first one for $z < 0$ and $\psi_a = 0$ for $z > 0$. The difference in behavior stems directly from the condensate nature of the liquid and the noncondensate form of the vacuum. “Hole” states are not supported by the vacuum and therefore no excitation is possible. A small evanescent penetration of the vacuum by the liquid hole states can be seen in Fig. 1(b) in the region where a low-density liquid remains. The (real) amplitudes ϕ_i and ψ_i extracted from the fits are used to calculate the current j_i associated with each quasiparticle/atom from

$$j_i = \frac{1}{2} v_i^g (\phi_i^2 - \psi_i^2),$$

where v_i^g ($i = a, p, -, +$) is the group velocity of the elementary excitation i , and from these currents we calculate the various scattering probabilities. We omit the details here as they can be found elsewhere (see, for example, Ref. 11).

Figures 2, 3, and 4 show our calculated probabilities P_{ij} , respectively, for a range of energies between $\hbar\omega = 7.5 \text{ K}$ and $\hbar\omega = 15 \text{ K}$ (all energies relative to the zero in bulk) for atoms, phonons, and R^+ rotons incident on the surface. Note that, because of the form of the energy spectrum, only phonons are present in bulk for $\hbar\omega < \Delta \sim 8.7 \text{ K}$ and only R^+ rotons are present for $\hbar\omega > \Delta_m \sim 14 \text{ K}$. As expected $P_{ij} = P_{ji}$ (a consequence of unitarity and time-reversal symmetry) and, for each i , the probabilities do satisfy the unitarity condition $\sum_j P_{ij} = 1$ ($i, j = a, p, -, +$) to within numerical accuracy.

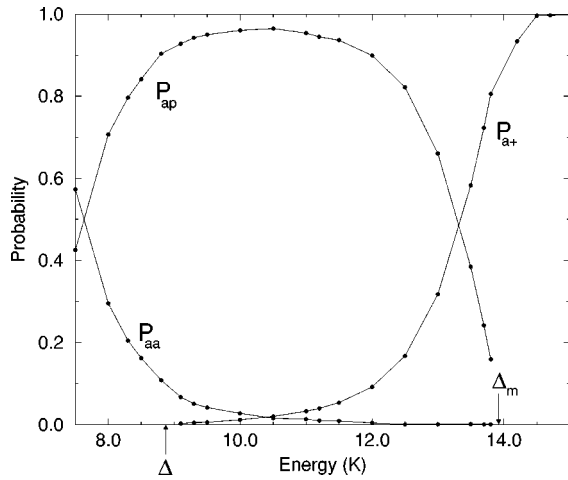


FIG. 2. The various scattering probabilities P_{aj} as a function of bulk energy for an atom incident on the surface. Δ and Δ_m are, respectively, the roton minimum energy and the maxon energy. P_{aa} —reflection of a ^4He atom from the surface; P_{ap} —absorption of a ^4He atom into a phonon mode, and P_{a+} —absorption of a ^4He atom into an R^+ roton mode. $P_{a-}=0$.

Consider now the three principal processes.

Evaporation. We note that, at normal incidence, R^- rotons do not evaporate atoms (i.e., $P_{-a}=0$). This is readily understood if one considers the large momentum change involved at the surface during the process remembering that R^- rotons have a negative “phase momentum.” Since the “extra” momentum has to be absorbed/provided by the surface, the processes that involve smaller changes in momentum are more likely to take place. R^+ rotons, on the other hand, are efficient at evaporating atoms. The probability P_{+a} is finite as soon as the roton channel opens up at the roton minimum (Fig. 4), increases monotonically with energy, and the $R^+ \rightarrow$ atom evaporation process becomes the dominant one near the maxon. The probability P_{pa} (Fig. 3) of a phonon evaporating an atom is small at small energies ($\hbar\omega$ near $|\mu_0|$), increases with energy to a maximum of about 0.9, and then decreases to zero (near Δ_m). This is in sharp contrast, as

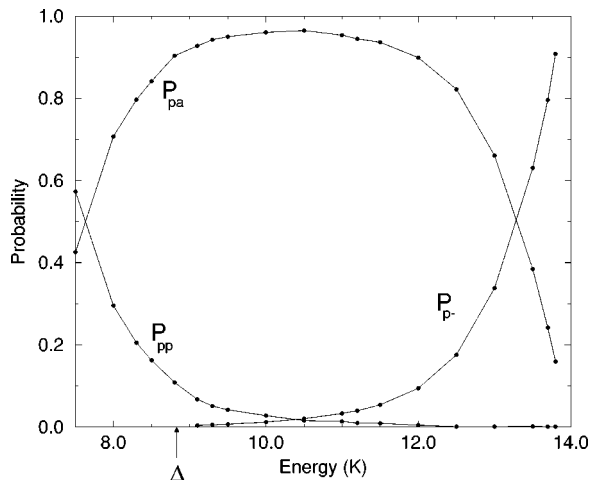


FIG. 3. The probabilities P_{pj} as a function of energy for an incident phonon. P_{pp} —reflection of a phonon from the surface, P_{pa} —evaporation of a ^4He atom by a phonon, and P_{p-} —reflection of a phonon mode into an R^- roton mode. $P_{p+}=0$.

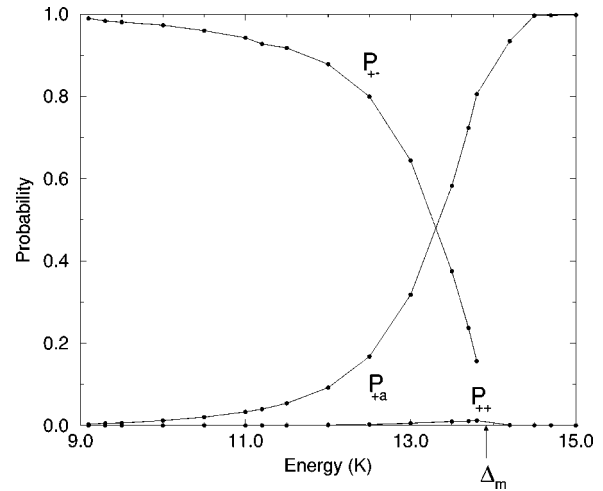


FIG. 4. The transition probabilities for an incident R^+ roton as a function of energy. P_{++} —reflection of an R^+ roton from the surface, P_{+a} —evaporation of a ^4He atom by an R^+ roton, and P_{+-} —reflection of an R^+ roton into an R^- roton. $P_{+p}=0$.

discussed later, with the results of Stringari *et al.*¹⁰ who found that $P_{pa}=1$ at small energies and then decreases monotonically to zero.

The evaporation probabilities for R^+ rotons can be related to the results of the experiments at normal incidence of Forbes and Wyatt.¹⁹ Agreement in terms of the trends (i.e., P_{+a} increases monotonically from 0 to 1 as $\hbar\omega$ increases from the roton minimum energy to the maxon energy) is good (as indeed are those of Stringari *et al.*¹⁰).

Condensation. Figure 2 shows the probabilities (as a function of bulk energy) of the various transitions possible when an atom is incident on the surface. The atom reflectivity P_{aa} is large at low (atom) energies ($\hbar\omega$ near $|\mu_0|$) in agreement with basic scattering theory and drops rapidly to zero as $\hbar\omega$ increases. The experiment of Edwards *et al.*⁵ showed that the experimental P_{aa} falls much faster as k_a ($\hbar^2 k_a^2/2m = \hbar\omega - |\mu_0|$) increases. However, we would expect the calculated reflectivity also to decrease much faster if we were to include multiple phonon excitation processes [atom $\rightarrow n(>1)$ low energy phonons] or even riplons, both excluded from the present calculation. Again our atom reflectivity results are in contrast with the results of Stringari *et al.*,¹⁰ who found that $P_{aa}=0$ at all energies in conflict with both experiments and simple physical considerations.

Contrary to the predictions of various previous theories (see, for example, Ref. 6) our results show that the atom reflectivity probability P_{aa} is continuous across the roton minimum. This is in agreement with the experimental observations of Edwards *et al.*⁵ However, they deduced from the absence of any discontinuity in P_{aa} at Δ that multiexcitation or ripplon processes are dominant over the single excitation process at the roton threshold. The present study shows that even without inelastic processes P_{aa} would still be continuous at the roton threshold; so the absence of a discontinuity should not be taken as evidence for the dominance of inelastic processes.

The coupling of atoms to R^+ rotons increases with energy and P_{+a} reaches unity above the maxon where the only available bulk quasiparticle states are the R^+ rotons. On the other hand, atoms do not couple to R^- rotons at normal

incidence ($P_{a-}=0$), a result again easily understood if one considers the momentum change involved in the process. Below the roton minimum the only transition to bulk modes available to the incident atom is condensation as a phonon. As expected from time reversal, the probability P_{ap} for the process has the same energy dependence as the evaporation probability P_{pa} .

Reflection. We note from Figs. 3 and 4 that phonons do not reflect as R^+ rotons and vice versa and that R^+ rotons do not reflect as R^+ rotons. These processes involve a large change in momentum which has to be absorbed at the surface and it is not surprising that they are suppressed. The surprising result is that there is a small range of energy near Δ_m where $P_{++}\neq 0$. At energies near the roton minimum, R^+ rotons reflect as R^- rotons (and vice versa) with essentially unit probability ($P_{+-}=P_{-+}\sim 1$). These are the reflection processes that require the smallest momentum changes. At energies approaching Δ_m the equivalent mode change reflection $R^- \rightarrow$ phonons dominates. We also note from Figs. 2 and 3 that $P_{pp}=P_{aa}$ as indeed they should be, at least for $|\mu_0| < \hbar\omega < \Delta$ following from unitarity and time-reversal symmetry. The surprising result is that the equality holds (to within numerical accuracy) even across Δ where the roton channels open up.

We would expect the phonon reflectivity P_{pp} to fall off more rapidly as the energy is increased from $|\mu_0|$ if we were to include inelastic phonon processes in our model—in practice, because of the anomalous phonon dispersion, phonons with energies up to about 10 K have a small mean free path

and decay inelastically into smaller energy phonons.^{20–22} Our phonon reflectivity is again in contrast with the results of Stringari *et al.*,¹⁰ who found that $P_{pp}=0$ at all energies, itself possibly a consequence of their unphysical P_{aa} result.

In searching for the reason behind the discrepancies between our results and those of Stringari *et al.*,¹⁰ we note that the system of equations (2) and (4) can be rewritten as a pair of coupled equations for the wave functions $\phi(\mathbf{r})$ and $\psi(\mathbf{r})$, each with the self-energy $\Sigma(\mathbf{r},\mathbf{r})=\sqrt{\rho(\mathbf{r})}V(\mathbf{r}-\mathbf{r}')\sqrt{\rho(\mathbf{r}'})$. The coupled equations derived by the Trento group¹¹ are identical in form but have $\Sigma(\mathbf{r},\mathbf{r})=\rho(\mathbf{r}')V(\mathbf{r}-\mathbf{r}')$, and thus their helium-helium interaction is different from ours in the surface region. This is principally where their unphysical results stem from. We have calculated P_{ij} using their self-energy and indeed P_{aa} ($=P_{pp}$) is now smaller and, correspondingly P_{ap} ($=P_{pa}$) is larger. Although the difference in self-energies is apparently small, our version follows directly from the Beliaev equations¹⁴ and importantly retains the non-local character of the condensate wave function and also the required symmetry in \mathbf{r},\mathbf{r}' . It is surprising, however, that such a small difference makes such a marked change in the results.

The work presented here is for normal incidence, but the study lays the groundwork for the case of oblique incidence. Work for $\mathbf{Q}\neq 0 \text{ \AA}^{-1}$ is in progress.

The authors would like to acknowledge financial support from the EPSRC.

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