# $R^-$ Rotons and Quantum Evaporation

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We apply Beliaev's theory to superfluid $^4$He with a free surface at $T = 0$ K to derive equations of motion valid in bulk helium, through the surface, and in the vacuum. We solve the equations and calculate probabilities for the one-to-one surface scattering processes as a function of energy, both for fixed parallel momenta and fixed angles of incidence. In particular, in contrast with the recent calculations of Stringari and co-workers, we show that $R^-$ rotons *do* quantum evaporate atoms in the presence of phonons. We also compare our quantum evaporation results with those of experimental simulations. [S0031-9007(99)09007-9]

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There have been a number of studies, both experimental [1–3] and theoretical [4–10], of quantum evaporation and the reverse process of quantum condensation in $^4$He over the years. It has been established experimentally [1–3] that the evaporation of atoms by bulk excitations is essentially a one-to-one process, where a bulk quasiparticle incident on the surface ejects an atom. This process can be represented by the energy conservation equation $\hbar\omega - |\mu_0| = \hbar^2\mathbf{k}^2/2m = \hbar^2(\mathbf{Q}^2 + k_a^2)/2m$, where $\hbar\omega$ is the energy of the quasiparticle and $\hbar^2\mathbf{k}^2/2m$ [$\mathbf{k} = (\mathbf{Q}, k_a)$, where $k_a$ is the component of the atom wave vector normal to the surface] is the kinetic energy of the evaporated atom. $\mu_0$ ($= -7.16$ K) is the chemical potential of the system. Because of the translational invariance of the system in a direction parallel to the surface, the momentum $\hbar\mathbf{Q}$ parallel to the surface is also conserved. The energy threshold for quantum evaporation is $|\mu_0| + \hbar^2\mathbf{Q}^2/2m$.

Neglecting inelastic processes, several channels are open to a bulk excitation incident on the surface, subject to the energy and momentum conservation requirements: it can either reflect as itself, undergo a mode-change reflection, or evaporate an atom. The microscopic theory of Mulheran and Inkson [4] gave quantitative predictions for all the one-to-one surface scattering processes, but their results were confined to normal incidence ($\mathbf{Q} = \mathbf{0}$ Å$^{-1}$). Stringari and coworkers [6–10] have recently studied the problem in the framework of a linearized time-dependent density functional theory and have calculated probabilities for the various processes. The equations of motion they derive do not have the expected symmetry in the surface region and, as a result, some of their normal-incidence probabilities [8] $P_{ij}$ (the probability of state $i$ scattering into state $j$, where $i, j =$ atom $a$, phonon $p$, $R^-$ roton$-$, $R^+$ roton$+$) are surprising and possibly unphysical (see [9] for a discussion). In particular, their atom-atom and phonon-phonon reflectivities are identically zero, i.e., $P_{aa} = 0 = P_{pp}$ at all energies, even at energies just above the atom threshold $-\mu_0$, and therefore, as a consequence of unitarity and time-reversal symmetry, $P_{ap} = 1 = P_{pa}$ for bulk quasiparticle energies $\hbar\omega$ between $-\mu_0$ and the roton minimum energy $\Delta$ ($\sim 8.7$ K). Unless an unknown implicit symmetry or other conservation law is operating, it is difficult to see how this can arise. At oblique incidence, their main result [8,10] is that $R^-$ rotons quantum evaporate atoms only in the phonon-forbidden regions (i.e., at energies and parallel momenta for which the conservation laws exclude phonons from the surface scattering processes), whereas preliminary analysis of the recent experiments of Tucker and Wyatt [11] shows that $R^-$ rotons *do indeed* evaporate atoms in regimes which do not exclude phonons.

In a recent article [9], Sobnack and Inkson reported the results of their study of quantum evaporation at normal incidence, where, in particular, their numerical results showed that the atom reflection $P_{aa}$ ($= P_{pp}$, the phonon-phonon reflection probability) is finite for $-\mu_0 < \hbar\omega < \Delta$ and that the atom-phonon scattering probability $P_{ap} = P_{pa} < 1$ there. The purpose of this Letter is to report the results of the extension of the work to the case of oblique incidence (lengthy details are omitted here—these will be published separately).

As before [9], we assume that all the quasiparticles have long mean free paths with respect to the surface scale lengths and travel ballistically. We neglect inelastic (multiphonon, ripplons) processes. Using Beliaev's [12] formalism in a real-space formulation, we derive equations of motion for the "particle-hole" wave function $\psi(\mathbf{r})$ and the "hole-particle" wave function $\phi(\mathbf{r})$ [Eqs. (2) and (4) of [9], respectively].

As in [9], we use a Fermi function for the surface profile and use the effective potential of Brueckner and Sawada [13] for the helium-helium interaction. We use this semiempirical approach for two reasons: first, it allows us to fit to the experimental dispersion curve and hence connect to experiments and, secondly, it avoids the problem of calculating the surface density distribution—a ground state problem of major magnitude and not directly relevant to the present analysis. We take the surface to lie in the $x$-$y$ plane (centered at $z = 0$ and with bulk helium in $z < 0$) and to have a 90%–10% width of 6.5 Å [14].

Since the momentum $\hbar\mathbf{Q}$ parallel to the surface is conserved, we look for solutions $\phi(\mathbf{r})$ and $\psi(\mathbf{r})$ of the form

$$\phi(\mathbf{r}) = e^{i\mathbf{Q}\cdot\mathbf{R}}\phi(z), \qquad \psi(\mathbf{r}) = e^{i\mathbf{Q}\cdot\mathbf{R}}\psi(z),$$

where $\mathbf{R} = (x, y)$. For a given bulk quasiparticle energy $\hbar\omega$ and parallel momentum $\hbar\mathbf{Q}$, we solve Eq. (2) of [9] numerically for (real) $\phi(z)$ for the same finite geometry as in [9]. Equation (4) of [9] then gives $\psi(\mathbf{r}) = e^{i\mathbf{Q}\cdot\mathbf{R}}\psi(z)$. Depending on $\hbar\omega$ and $\hbar\mathbf{Q}$, one or more elementary excitations may now be excluded from the surface scattering processes.

Because of the geometry we need to extract the appropriate parameters for the dynamic scattering processes. To do this we use a numerical procedure to fit sinusoidal functions of the form

$$\sum_i \phi_i \cos(k_{zi}z + \theta_i) \quad \text{and} \quad \sum_i \psi_i \cos(k_{zi}z + \theta_i)$$

(where the summation is over the different excitations—phonons, $R^-$ rotons, $R^+$ rotons, atoms—allowed at the given energy and parallel momentum) to the calculated (standing wave) wave functions $\phi(z)$ and $\psi(z)$, respectively, to extract the real amplitudes $\phi_i$ and $\psi_i$, the normal ($z$-) component $k_{zi}$ of the wave vectors and the phases $\theta_i$ in bulk and in the vacuum (with $\psi_a \equiv 0$—the atoms are free in the vacuum). From these parameters, one can then construct the current associated with each excitation (see [9], and references therein), and these are used to calculate the various scattering probabilities.

We have calculated $P_{ij}$ for all the one-to-one surface scattering processes allowed as a function of (bulk) energy both for fixed angles of incidence and fixed parallel wave vector and we only present the results relevant for this Letter below. Time-reversal symmetry and unitarity of the "scattering matrix" require that $P_{ij} = P_{ji}$ and that $\sum_j P_{ij} = 1$ for each $i$. Our results satisfy both requirements to within numerical accuracy.

*Fixed angle of incidence.*—In experiments on quantum evaporation, the bolometer producing the quasiparticle is fixed at a given position in bulk helium and the beam of quasiparticles is collimated so that all bulk excitations are incident to the surface at the same (fixed) angle $\theta_0$: at a given energy $\hbar\omega$, different elementary excitations $i$ have different parallel momenta $\hbar\mathbf{Q}_i = \hbar\mathbf{Q}_i[\theta_0, k_i(\omega)]$, with $|\mathbf{Q}_i| = k_i(\omega)\sin\theta_0$, where $k_i$ is the magnitude of the wave vector $\mathbf{k}_i$ of elementary excitation $i$, $k_i = |\mathbf{k}_i|$.

We will concentrate on just two aspects of our calculations: $R^-$ roton scattering and the measured quantum evaporation signals.

We first consider $R^-$ roton evaporation where the recent results of Stringari *et al.* [8,10] claim that $R^-$ rotons quantum evaporate only in the phonon-forbidden regions. Figure 1 shows the probabilities $P_{-j}$ ($j = a, p, +$) as a function of energy in the range roton minimum energy $\Delta < \hbar\omega <$ maxon energy $\Delta_m$ for all the possible channels into which an incoming $R^-$ roton, incident at $\theta_0 = 14°$ (dotted line) and $\theta_0 = 25°$ (solid line), can scatter.

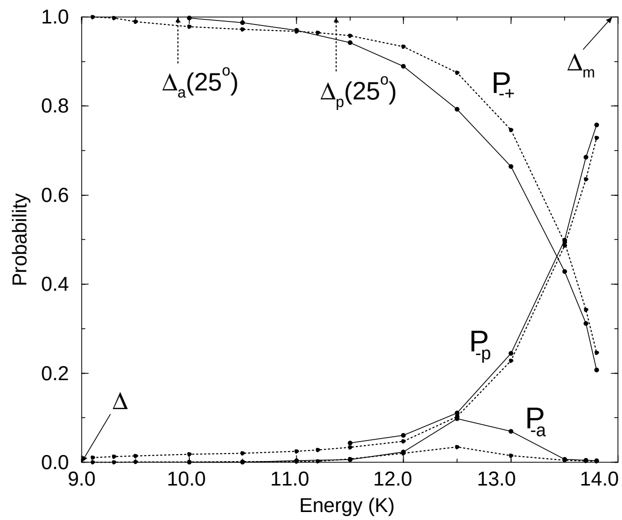


FIG. 1. The various scattering probabilities $P_{-j}$ as a function of bulk energy for an $R^-$ roton incident on the surface at $\theta_0 = 14°$ (dotted lines) and $\theta_0 = 25°$ (solid lines). $\Delta_a(25°)$ and $\Delta_p(25°)$ are, respectively, the atom and phonon threshold when $R^-$ rotons are incident at 25°. $\Delta$ and $\Delta_m$ are the roton minimum energy and the maxon energy, respectively.

At $\theta_0 = 25°$, atoms with energies less than the atom cutoff $\Delta_a(25°) \simeq 9.8$ K (with respect to the zero in bulk) and phonons with energies less than the phonon threshold $\Delta_p(25°) \simeq 11.4$ K do not propagate, and are thus excluded from the scattering processes.

For both angles of incidence shown, the probability $P_{-a}$ for this process is very small at energies just above the roton minimum, increases with energy, and then decreases as the energy is further increased ($\hbar\omega \rightarrow \Delta_m$). For $\theta_0 = 25°$, we note that $P_{-a}$ is nonzero at energies above the phonon threshold $\Delta_p(25°)$, showing that $R^-$ rotons *do* evaporate atoms in the presence of phonons in contrast with the results of Stringari *et al.* [8,10]. It is clear from Fig. 1 and from other angles of incidence we have investigated that $R^-$ rotons become increasingly efficient at emitting atoms as the angle of incidence increases (provided the transition $R^-$ roton $\rightarrow$ atom is allowed by the energy and parallel momentum conservation requirements).

Figure 1 also shows that, at these angles, $R^-$ rotons do not significantly reflect as $R^-$ rotons ($P_{--} \simeq 0$). This process involves a large change in normal momentum which has to be absorbed at the surface, and it is not surprising that it is suppressed. The dominant transition at energies near the roton minimum energy $\Delta$ is the mode-change reflection $R^-$ roton $\rightarrow R^+$ roton. With increasing energy, the probability $P_{-+}$ for this process decreases, approaching zero as the energy of the incident $R^-$ roton approaches the maxon energy $\Delta_m$ and the mode-change reflection $R^-$ roton $\rightarrow$ phonon becomes the dominant process.

There are no direct measurements of quantum evaporation probabilities for emission of atoms by phonons ($P_{pa}$) and rotons ($P_{ra}$) with which to compare our results. This is because the published experiments inject a distribution $n_i(k)$ of ballistic excitations $i$ in the liquid by pulsing a thin-film heater and, by detecting evaporated atoms, measure the relative size of the product $P_{ia}(k)n_i(k)$ [2]. Recently the distribution $n_p(k)$ of phonons has been measured independently for high-energy phonons ($\hbar\omega \sim 10$ K) [15] and this has prompted a reanalysis of the experiments and the elimination of some sources of systematic error [16]. For high-energy phonons the corrected model, which assumes that $P_{pa}(k)$ is constant ($\sim$0.3), agrees with the mechanical accuracy of the experiments. Use of our calculated phonon evaporation probabilities $P_{pa}$ [shown as a function of energy in Fig. 2(a)] changes the solid curve in Fig. 2(b) [16] by an insignificant amount, although finer details [16] show that our calculation probably overestimates the phonon-atom probability. A proper test of our calculated phonon evaporation probabilities will require a direct measurement of the evaporation probability, or a source that generates a much wider phonon spectrum.

For $R^+$ rotons incident at an angle $\theta_0 = 14°$, the calculated quantum evaporation probability $P_{+a}$ increases monotonically from 0 at the roton minimum energy $\Delta$ to 1 just above the maxon energy $\Delta_m$ [Fig. 3(a)]. Unfortunately there have been no successful attempts to measure the distribution $n_+(k)$ of injected $R^+$ rotons. Experiments have been modeled [2] by assuming that

$$n_+(k)\,dk \propto \frac{k^\lambda\,dk}{\exp(\hbar\omega/T_{\rm eff} - 1)} \quad \text{with} \quad \lambda = 2\,.$$

The shape of this distribution is dominated by the value of the parameter $T_{\rm eff}$, which lies within the range 1.0 to 1.5 K [16]. Figure 3(b) [16] shows the results of the simulation using two values of $T_{\rm eff}$. In the figure, atoms detected at large bolometer angles have been evaporated by $R^+$ rotons with relatively low energies. The thin lines assume $P_{+a} = 1$ and the thick lines use our calculated evaporation probabilities. The shift in the angular distribution between the two suggests that our results are too small at small energies. This highlights the need for a better description of the roton in our model—possibly the inclusion of roton backflow.

There are no experimental $R^-$ roton-to-atom signals with which to compare our $R^-$ evaporation results. Wyborn and Wyatt [3] reported a strong $R^-$ roton-to-atom signal, but they no longer stand by the analysis of the results [17].

*Fixed parallel momenta.*—Figure 4 shows our calculated probabilities as a function of energy for scattering into the various channels available to an $R^-$ roton incident on the helium/vacuum interface with a parallel momentum $\hbar\mathbf{Q}$, $|\mathbf{Q}| = 0.75$ Å$^{-1}$. The thresholds for atoms and phonons, i.e., the energies below which atoms and phonons are excluded from the scattering processes by the conservation laws, are, respectively, $\Delta_a \sim 10.6$ K and $\Delta_p \sim 12.8$ K.

As for the case of fixed angles of incidence, at low energies the probability $P_{-a}$ of an $R^-$ roton evaporating an atom is very small. It increases as the energy $\hbar\omega$ of the incoming $R^-$ roton increases, reaches a maximum 0.25–0.3, and then decreases to zero as $\hbar\omega$ approches the maxon energy. Again we note that, even at energies

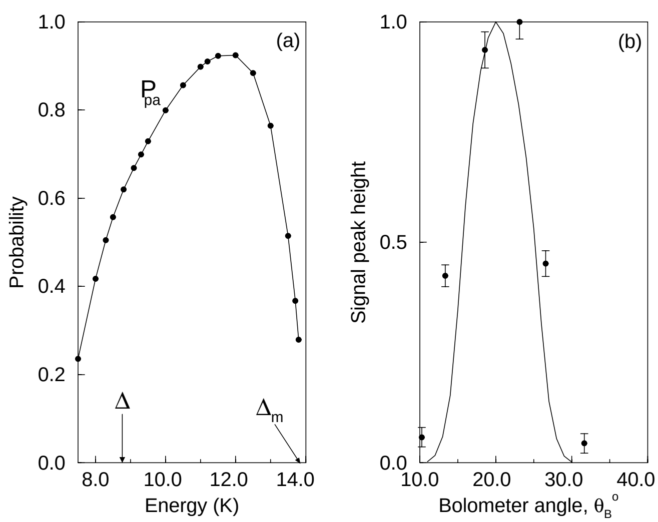


FIG. 2. (a) The calculated probability $P_{pa}$ of evaporation by phonons incident at $\theta_0 = 25°$ as a function of bulk energy. $\Delta$ is the roton minimum energy and $\Delta_m$ the maxon energy. (b) The angular dependence of the peak height of the measured (points) and simulated (curve) phonon $\rightarrow$ atom signals for an angle of incidence of $\theta_0 = 25°$. Each distribution is normalized to the maximum data point (after Williams [16]). See also Fig. 6 of [2].

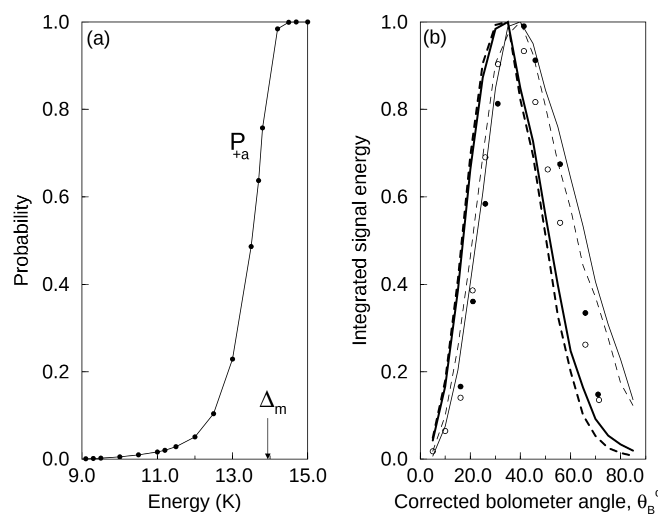


FIG. 3. (a) The calculated probability $P_{+a}$ of evaporation by $R^+$ rotons incident at $\theta_0 = 14°$ as a function of bulk energy. (b) The angular dependence of the integrated $R^+ \rightarrow$ atom signal energy. The angle of incidence is $\theta_0 = 14°$. The signals are integrated up to 160 $\mu$s after the start of the heater input pulse. The points are experiments using two different heater powers, $-27$ dB (full circles) and $-24$ dB (open circles). The curves are simulations using injected-roton spectra at two characteristic temperatures, $T_{\rm eff} = 1.0$ K (solid lines) and $T_{\rm eff} = 1.5$ K (dashed lines). The thin lines assume $P_{+a}$ = constant and the thick lines use our calculated values (after Williams [16]). See also Fig. 8 of [2].

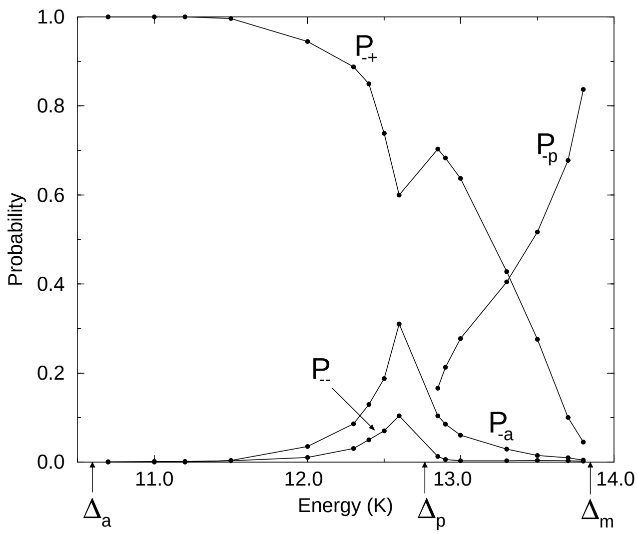


FIG. 4. The various scattering probabilities $P_{-j}$ as a function of bulk energy for an $R^-$ roton incident on the surface with parallel wave vector $\mathbf{Q}$, $|Q| = 0.75$ Å$^{-1}$. $\Delta_m$ is the maxon energy, and $\Delta_a$ and $\Delta_p$ are, respectively, the atom and phonon thresholds.

above the phonon threshold $\Delta_p$, the probability is finite. Calculations with other values of parallel wave vector $\mathbf{Q}$ confirm this and show that $P_{-a}$ is strongly dependent on the parallel momentum $\hbar\mathbf{Q}$, increasing with increasing parallel momentum. Further, the evaporation probability is continuous at the phonon threshold, a result significantly different from that of Stringari *et al.* [8,10], who reported that $P_{-a}$ is discontinuous at $\Delta_p$, dropping to zero as soon as the phonon channel opens up and remains zero at all energies thereafter. What we find instead is that all the calculated probabilities show a structure at $\Delta_p$ and then go back to the values expected from the initial trends. We believe the origin of this structure to be the existence of a surface barrier to evaporation by phonons (more details of this will be presented in a future paper).

In this Letter we have reported some of the results of the extension of our recent work [9] to the case of oblique incidence. Our $R^-$ rotons-to-atoms evaporation results show that $R^-$ rotons *do* quantum evaporate at energies and parallel momenta which do not exclude phonons from the scattering processes, in agreement with the recent experimental results of Tucker and Wyatt [11], and in contrast with the results of Stringari *et al.* [8,10]. Our calculated $P_{-a}$ also show a strong dependence on the angle of incidence (and hence parallel momenta) of the incoming $R^-$ roton, again in contrast with the results of Dalfovo *et al.* [6,7]. Use of our calculated probabilities in simulations of experiments has shown that our calculations overestimate the evaporation efficiencies of phonons and underestimate, at low energies, those of $R^+$ rotons.

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