Effect of roton backflow on quantum evaporation from superfluid ^{4}He

M. B. Sobnack
Department of Physics, Loughborough University, Loughborough, Leicestershire LE11 3TU, United Kingdom
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We investigate the effect of roton backflow on the scattering of atoms, rotons, and phonons at the free surface of superfluid ^{4}He at $T=0$ K by including backflow semiphenomenologically in the form of a backflow potential in the theory of Sobnack, Inkson, and Fung [M. B. Sobnack, J. C. Inkson, and J. C. H. Fung, Phys. Rev. B **60**, 3465 (1999)]. We assume that all the surface scattering processes are elastic and that the quasiparticles and atoms are incident with fixed parallel momenta to the free surface. We calculate probabilities for the various one-to-one surface scattering processes allowed for a range of energies and compare the scattering rates with those obtained when backflow is neglected.

When an elementary excitation of superfluid ^{4}He impinges on the free surface, it may eject an atom in a one-to-one process by exchanging single quanta of energy. This process is called quantum evaporation. The reverse process, in which an atom from the vapor hits the free surface and excites the available quasiparticle channels, is called quantum condensation. The processes conserve energy and momentum parallel to the surface.

Despite the considerable success of the experimental studies on quantum evaporation and quantum condensation, the probabilities of the different surface scattering processes cannot in general be determined experimentally using the present available techniques (one notable exception is the atomic reflectivity experiments of Edwards *et al.*[1]), emphasizing the need for quantitative theoretical work. Over the years there have been several theoretical studies[2–10] of quantum evaporation and quantum condensation with varied degrees of success (see Ref. 11 for a full discussion). Recently, Sobnack *et al.*[11–13] adapted Beliaev's theory[14] to the inhomegeneous superfluid ^{4}He system with a free surface at $T=0$ K and calculated probabilities for the one-to-one surface scattering processes as a function of energy. In particular, they showed that R^- rotons *do* quantum evaporate atoms in the presence of phonons. This was subsequently confirmed experimentally by Tucker and Wyatt.[15] However, use of their calculated probabilities in simulations of experiments[11,13,16] showed that while the calculated probability of evaporation by phonons show very good agreement with experiments, the calculations underestimate the evaporation efficiencies of R^+ rotons — the probabilities were too small at low roton energies, thus highlighting the need for a better description of the roton and for a better theory.

The theory of Sobnack *et al.*[11–13] did not take into account roton backflow correlations. The concept of roton backflow was first introduced by Feynman and Cohen[17] when they realized that current was not conserved in the transport of rotons in the earlier Feynman theory.[18] It has subsequently become accepted that roton backflow has to be included to provide both a quantitative and a physical understanding of the (transport of) excitations in superfluid ^{4}He.

The current work is an extension of the earlier study[11–13] by including the important physics of roton backflow. We study the effects of roton backflow on the scattering of atoms and bulk quasiparticles at the free surface of superfluid ^{4}He at $T=0$ K.

The polarization potential (PP) theory of Aldrich and Pines[19] was an attempt to describe the elementary excitations in superfluid ^{4}He by accounting for contributions from roton backflow and from multiphonon processes. The additional contribution manifests itself as a renormalized single-particle effective mass m^* and one finds that the strength of the backflow potential is proportional to the extra mass $\Delta m = m^* - m$.

Here we assume that the multiphonon contributions in the PP theory do not affect the quantum evaporation process. This is a reasonable assumption, given the evidence[20] that the process is one to one. In the Bogoliubov limit,[21] inclusion of the PP backflow is equivalent[22,23] to replacing the effective He-He potential $V(\mathbf{k})$ by $V(\mathbf{k})+\hbar^2\omega^2 W(\mathbf{k})$, where $W(\mathbf{k})=\Delta m/\hbar^2\mathbf{k}^2$. Lengthy details are omitted here—these will be published separately. We assume that the effective mass is wave-vector independent. The single-particle Green's functions of the superfluid system then have poles at $\hbar\omega=\pm E_B$, where E_B is the ''new'' Bogoliubov spectrum[21,22]

$$E_B(\mathbf{k})=\left[\frac{\hbar^4\mathbf{k}^4}{4mm^*}+2\rho_0\frac{\hbar^2\mathbf{k}^2}{2m}V(\mathbf{k})\right]^{1/2}, \qquad (1)$$

where ρ_0 is the condensate density. Inclusion of the backflow potential is equivalent to replacing the factor m^2 in the denominator of the first term on the right-hand side of Eq. (2) of Ref. 11 by the product mm^*. The Bogoliubov spectrum, with the choice $V_0=15.2\,\mathrm{K}\,\mathrm{\AA}^{-1}$ and $a_0=2.1$ Å for the effective Brueckner potential[24]

$$V(k)=a_0V_0\frac{\sin a_0k}{a_0k},$$

together with $m^*=1.4m$, gives a very good fit to the experimentally measured excitation spectrum of ^{4}He.[22]

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. As before,[11–13] we use the quantum field theory

Beliaev.[14] With the inclusion of the backflow potential $\hbar^2\omega^2 W(\mathbf{k})$, the two Beliaev ''coupled diagrams'' for the two propagators of the superfluid ^{4}He system — the usual single-particle Green's function $G(\mathbf{k},\omega)$ and the ''anomalous'' Green's function $F(\mathbf{k},\omega)$, which describes the effects associated with a quasiparticle propagating in a correlated system — give, in real space, the equations of motion

$$\left[\hbar\omega-\mu(\mathbf{r})+\frac{\hbar^2}{2m^*}\nabla^2\right]\phi(\mathbf{r})-\sqrt{\rho(\mathbf{r})}\int_{-\infty}^{+\infty}[V(\mathbf{r}-\mathbf{r}')+\hbar^2\omega^2W(\mathbf{r}-\mathbf{r}')]\sqrt{\rho(\mathbf{r}')}\times[\phi(\mathbf{r}')+\psi(\mathbf{r}')]d^3\mathbf{r}'=0,$$

$$\left[-\hbar\omega+\mu(\mathbf{r})+\frac{\hbar^2}{2m^*}\nabla^2\right]\psi(\mathbf{r})-\sqrt{\rho(\mathbf{r})}\int_{-\infty}^{+\infty}[V(\mathbf{r}-\mathbf{r}')+\hbar^2\omega^2W(\mathbf{r}-\mathbf{r}')]\sqrt{\rho(\mathbf{r}')}\times[\phi(\mathbf{r}')+\psi(\mathbf{r}')]d^3\mathbf{r}'=0 \quad (2)$$

for the ''particle-hole'' wave function $\phi(\mathbf{r})$ (associated with G) and the ''hole-particle'' wavefunction $\psi(\mathbf{r})$ (associated with F) valid in bulk, through the surface and in the vacuum. The hole-particle wave function $\psi(\mathbf{r})$ is necessary to correctly describe the effects associated with a quasiparticle propagating through a correlated system. In the bulk, along the lower part of phonon branch of the excitation spectrum $\psi(\mathbf{r})=O[\phi(\mathbf{r})]$; $\psi(\mathbf{r})=o[\phi(\mathbf{r})]$ along the roton branch (near the roton threshold $\Delta\sim 8.7$ K) and $\psi(\mathbf{r})\to 0$ at very high $\hbar\omega\gg\Delta$. In the vacuum, $\psi(\mathbf{r})$ vanishes identically.

The above equations have the appearance of one-body Schrödinger equations with a nonlocal potential, reflecting that this is a many-body problem. The function $\mu(\mathbf{r})$ describes the variation of the binding energy. It changes from 0 (in bulk) to $|\mu_0|$ (in the vacuum) across the surface. $\mu_0=-7.16$ K is the condensate chemical potential. In deriving the above equations, we have allowed the condensate density $\rho(\mathbf{r})$ to vary with position so that the equations may be used to tackle the general inhomogeneous problem such as the free surface. Deep in bulk, the density has the value of bulk superfluid condensate, i.e., $\rho=\rho_0$ (const), and high above the surface it has the vacuum value $\rho=0$. We take $m^*=m+\Delta m\rho(\mathbf{r})/\rho_0$. With these prescriptions, the equations have the expected limits — in bulk they are the Schrödinger equations for the quasiparticles (of energy $\hbar\omega$) and in the vacuum the Schrödinger equations for the free atom (of energy $\hbar\omega-|\mu_0|$).

As in Ref. 11, 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,[25] which is within the experimentally accepted estimate. We use a Fermi function for the surface profile. 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

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

where $\mathbf{R}=(x,y)$. For a given bulk quasiparticle energy $\hbar\omega$ and parallel momentum $\hbar\mathbf{Q}$, we solve the full Eqs. (2) numerically — we look for (real) standing-wave solutions $\phi(z)$ and $\psi(z)$. Because of the geometry we need to extract the appropriate parameters for the dynamic scattering processes: we fit $\phi(z)$ with functions of the form

$$\phi(z<0)=\sum_i \phi_i\cos(k_{zi}z+\theta_i) \quad\text{and}\quad \phi(z>0)=\psi_a\cos(k_{za}z+\theta_a)$$

representing the bulk $(z<0)$ and the vacuum $(z>0)$ limiting wave functions, respectively. The summation is over the different bulk excitations—phonons (p), R^- rotons $(-)$, R^+ rotons $(+)$—allowed at the given energy and parallel momentum. The hole-particle wave functions $\psi(z)$ are similarly fitted (with $\psi_a=0$). The real amplitudes ϕ_i and ψ_i, the normal (z) component k_{zi} of the wave vectors and the phases θ_i $(i=p,-,+,a)$ are extracted from the fits, and the current associated with each quasiparticle or atom is calculated from

$$\mathbf{j}_i=\frac{1}{2}\mathbf{v}_i^g(\phi_i^2-\psi_i^2).$$

It can be shown that now, because of the (extra) energy-dependent backflow potential, the total current $\Sigma_i\mathbf{j}_i$ is conserved provided one defines $\mathbf{v}_i^g$ as

$$\mathbf{v}_i^g=\frac{m}{m^*}\nabla_{\mathbf{k}}\omega(\mathbf{k}),$$

instead of the usual group velocity $\mathbf{v}_i^g=\nabla_{\mathbf{k}}\omega(\mathbf{k})$. (Full details will be published separately.) From these currents we calculate the various scattering probabilities P_{ij} $(i,j=a,p,-,+)$.

We have calculated P_{ij} as a function of (bulk) energy for several values of the parallel momentum $\hbar\mathbf{Q}$. For a given parallel momentum, one or more quasiparticles may be excluded from the surface scattering processes at certain energies by conservation of energy and momentum parallel to the surface. Below we present our results for $|\mathbf{Q}|=0.75$ Å^{-1} to enable direct comparison with the results reported in Ref. 11. At this parallel wave vector, phonons are excluded from the

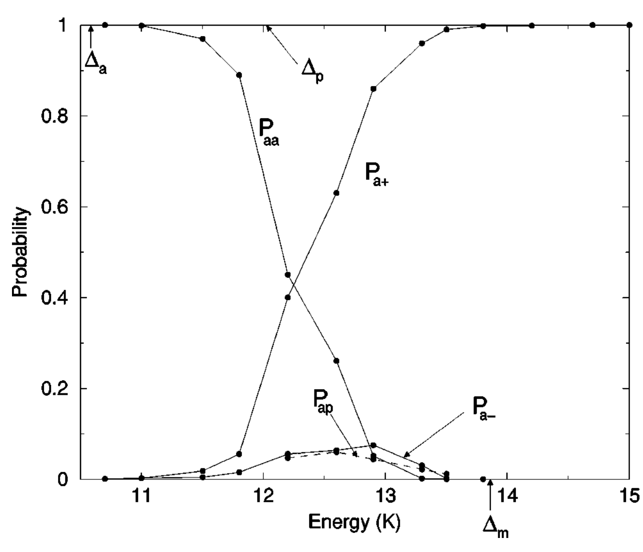

FIG. 1. The various scattering probabilities P_{aj} as a function of bulk energy for an atom incident on the surface. Δ and Δ_m are, respectively, the roton minimum energy and the maxon energy. $|\mathbf{Q}|=0.75$ Å^{-1}.

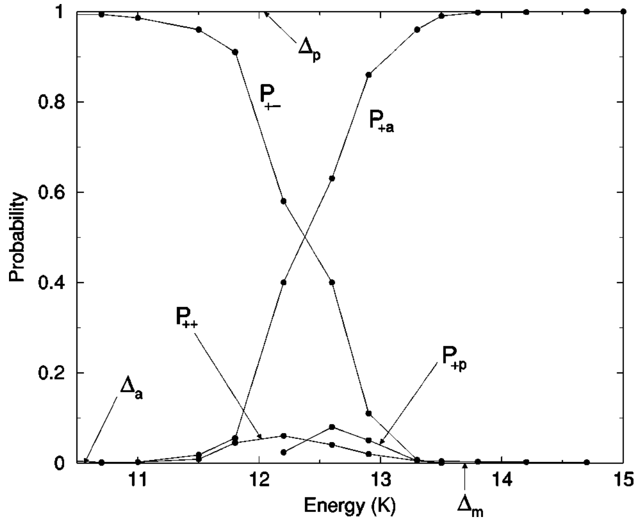

FIG. 2. The probabilities P_{+j} as a function of energy for an incident R^+ roton. $|\mathbf{Q}|=0.75$ Å^{-1}.

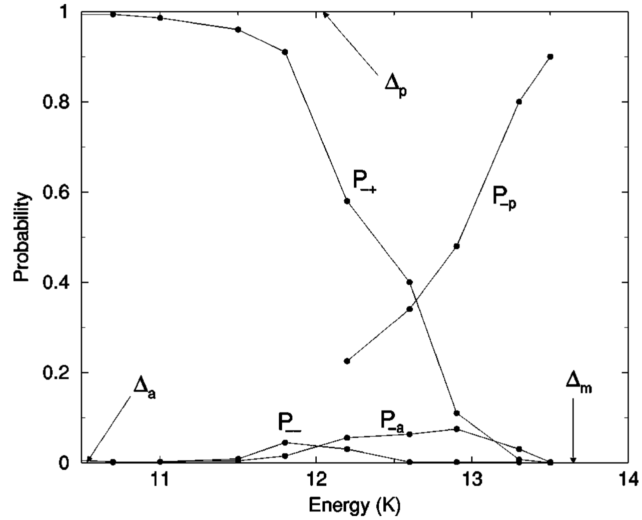

FIG. 3. The transition probabilities, as a function of energy, for an R^- roton incident on the free surface with $|\mathbf{Q}|=0.75$ Å^{-1}.

scattering processes for all energies less than the phonon threshold $\Delta_p \sim 12.1$ K. Similarly there is a cut-off for propagating atom states at $\Delta_a \sim 10.6$ K (relative to bulk).

Figures 1, 2, and 3 show the calculated probabilities P_{ij} as a function of energy of the different transitions available to atoms, R^+ rotons, R^- rotons incident on the free surface with $|\mathbf{Q}|=0.75$ Å. The roton minimum energy and the maxon energy are, respectively, $\Delta \sim 8.7$ K and $\Delta_m \sim 13.7$ K. As in our earlier studies[11,13], the probabilities P_{ij} $(i,j=a,-,+)$ around the energy Δ_p at which the phonon channel opens show some structure on top of fairly smooth trends. The structure is due to the existence of a surface barrier[11] to evaporation by phonons.

The probabilities shown in Figs. 1–3 have the same qualitative dependence as those obtained when backflow is neglected (Figs. 8–10 of Ref. 11). The striking differences between Fig. 1 and the corresponding figure with backflow neglected (Fig. 8 of Ref. 11) is that the probability P_{a+} of atoms condensing as R^+ rotons rises much faster with energy, reaching unity just below Δ_m and that the probability (P_{a-}) of atoms condensing as R^- rotons, though still finite (reaching about 0.1 at $\hbar\omega \sim 12.8$ K), is not as large as in Ref. 11. Further the atomic reflectivity P_{aa} show improved agreement with the experiments.[1]

It is instructive to compare the probabilities P_{+a} of quantum evaporation by R^+ rotons shown in Fig. 2 with those in Fig. 10 of Ref. 11. Use of the latter in simulations of experiments by Williams[16] showed that the calculations underestimated the evaporation efficiencies of R^+ rotons at low roton energies. With the inclusion of backflow, P_{+a} is much larger at low energies (compare, for example, $P_{+a} \sim 0.25$ at $\hbar\omega \sim 12.0$ K and $P_{+a} \sim 0.88$ at $\hbar\omega \sim 13.0$ K with $P_{+a} \sim 0.08$ and $P_{+a} \sim 0.3$ without backflow) with improved agreement with simulations of experiments.

Figure 3 shows that the evaporation efficiency P_{-a} of R^- rotons is smaller with the inclusion of backflow, but still finite, even at energies above the phonon threshold Δ_p. This result is in agreement with recent experiments[15]. Further, the ratio of P_{+a}/P_{-a} at energies where $P_{-a} \neq 0$ is more in line with the estimates of Tucket and Wyatt.[26]

We have presented an improved theory of quantum evaporation by incorporating roton backflow semiphenomenologically into our earlier theory of quantum evaporation.[11–13] The theory shows that backflow increases the evaporation efficiencies of R^+ rotons. In particular, at small roton energies, the probabilities P_{+a} are several factors larger than those with backflow neglected, in agreement with simulations of experiments. Backflow also decreases the quantum evaporation efficiencies P_{-a} of the negative phase momentum R^- rotons, but P_{-a} is still nonzero in regimes which allow phonons to participate in the surface scattering processes, in agreement with experiments.[15]

We would like to stress again that the work presented here is a study of one-to-one scattering processes. Liquid ^{4}He is a dynamic, many-body system. Incident particles may produce excited states, corresponding to inelastic processes, which may result in the emission of particles in states other than the elastic channel. Recently, Campbell, Krotscheck, and Saarela[27] have used a variational wave-function method to study the transmission of ^{4}He atoms through a helium slab, and found that the scattering processes are dominated by multiparticle events. Indeed, as we remarked in our previous work,[11–13] inclusion of inelastic processes (phonon decay processes, ripplon processes) would change some of the probabilities presented here. Work along this direction is currently under way.

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