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Computer Simulation of the High-Velocity Motion of Electron Bubbles in Superfluid Helium

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Abstract We have performed computer simulations of the motion of electron bubbles through superfluid helium. The helium is modeled through the use of a modified version of the Gross-Pitaevskii equation. We find that by the time the bubble reaches the velocity at which vortex nucleation occurs the shape has changed significantly from spherical.

Keywords Electron bubble · Superfluid helium · Ion mobility

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1 Introduction

An electron injected into liquid helium forms a bubble due to its strong repulsion with the surrounding helium. The energy dissipation that takes place when the electron bubble moves through the superfluid phase has been a topic of interest for some time. A moving bubble experiences a drag force due to collisions with thermally excited phonons and rotons [1, 2]. Below 1 K this drag becomes very small, and even a modest electric field will increase the velocity up to a critical value v_c at which new mechanisms set in. There are two well-accepted mechanisms for energy loss, namely roton emission and vortex ring nucleation [3]. At zero applied pressure, the Landau velocity v_L for roton emission is about 58 $\mathrm{m\,s^{-1}}$, and the critical velocity for vortex nucleation v_{vort} is about 30 $\mathrm{m\,s^{-1}}$ in natural ^{4}He [4] and about 44 $\mathrm{m\,s^{-1}}$ in isotopically pure ^{4}He [5]. Hence, at low pressures the first mechanism to set in is vortex-ring nucleation. To observe the roton emission mechanism, one must pressurize the liquid

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thereby lowering v_L and at the same time increasing v_{vort}. Above 15 bars $v_L < v_{vort}$, Allum *et al.* [6, 7] and Ellis *et al.* [8] were able to observe roton pair production.

In the theory of the nucleation of vortices by moving electron bubbles, [9] it is assumed that the electron bubble has a shape that is close to spherical. In a previous paper, [10] the change in shape of an electron bubble was calculated based on a highly simplified model. The density of the helium was taken to change abruptly from zero inside the bubble to the bulk value outside, the penetration of the electron wave function into the helium was neglected and, probably most importantly, the liquid was taken to be incompressible. Based on this model, it was found that there was a substantial change in size and shape of the bubble by the time the velocity reached 40 m s^{-1}. In this paper, we present the results of a more complete calculation in which the approximations just mentioned are not used.

2 Simulation Model

To study the motion of an electron bubble it is essential to use a model in which the equation of state of helium is reproduced with reasonable accuracy. The standard form of the Gross-Pitaevskii (GP) equation is

$$i\hbar\frac{\partial\psi}{\partial t} = \left[-\frac{\hbar^2}{2m_{\mathrm{He}}}\nabla^2 - \mu_{\mathrm{He}} + g_0|\psi|^2\right]\psi, \tag{1}$$

where ψ is the macroscopic helium wave function, μ_{He} is the chemical potential and g_0 comes from the short range repulsion between the atoms. However, this gives an unrealistic relationship between pressure and density. For example, if we choose μ_{He} and g_0 to give the density and sound velocity equal to the experimental values at zero pressure, the pressure from (1) is 41 bars. In addition, the surface tension is incorrect. To fix this and to include the interaction between the helium and an electron we modify (1) to become

$$i\hbar\frac{\partial\psi}{\partial t} = \left[-\frac{\hbar^2}{2m_{\mathrm{He}}}\nabla^2 - \mu_{\mathrm{He}} + f_0|\phi|^2 + g_0|\psi|^2 + g_1|\psi|^4 + g_2|\psi|^6 - w_1\nabla^2|\psi|^2\right]\psi, \tag{2}$$

and take the Schrodinger equation for the electron to have the form

$$i\hbar\frac{\partial\phi}{\partial t} = \left[-\frac{h^2}{2m_e}\nabla^2 - eEz + f_0|\psi|^2\right]\phi, \tag{3}$$

where ϕ is the electron wave function, and E is the electric field applied along the negative z-direction. We add these terms so that with the choice $g_0 = -9.927 \times 10^{-38}$ erg cm^3, $g_1 = -4.995 \times 10^{-60}$ erg cm^6, $g_2 = 3.421 \times 10^{-82}$ erg cm^9, $w_1 = 6.220 \times 10^{-53}$ erg cm^5, we can produce the pressure-density relation with reasonable accuracy in the range from -9 to 25 bars, the correct sound velocity of 2.38×10^4 cm s^{-1} at the zero-pressure density $\rho = 0.14513$ g cm^{-3}, and also the correct surface tension $\sigma = 0.3755$ erg cm^{-2}. By choosing $f_0 = 7.672 \times 10^{-35}$ erg cm^3 we get the correct energy barrier of 1 eV for an electron entering uniform liquid helium at zero pressure. With this choice of the parameters, the model gives a width to

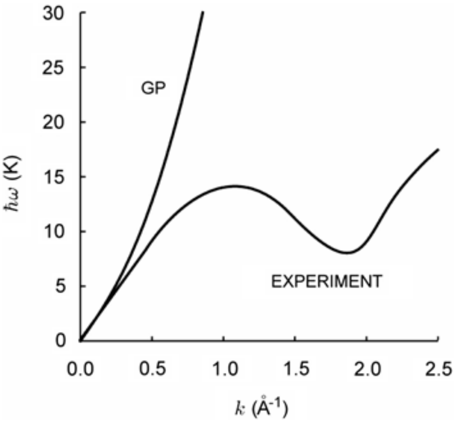

Fig. 1 Excitation dispersion relation based on the modified Gross-Pitaevskii model and from experiment

the free surface of liquid helium of 7 Å (10% to 90% density) consistent with experiment [11]. Since the model produces the correct sound velocity, it correctly describes the long wavelength part of the excitation spectrum.

Stringari and Treiner [12] have used a somewhat different scheme to modify the GP equation to give correspondence with the measured properties of helium. The coupling between the electron and the helium is the same as has been used by Berloff and Roberts [13].

Our simulation cannot correctly treat roton generation or the nucleation of vortices. As shown in Fig. 1, the model does not reproduce the roton part of the spectrum. In principle, one can adopt a nonlocal functional which does result in a roton minimum [14]. However, this would greatly increase the computation time. In addition, it is not clear that even with the correct dispersion relation roton generation would be calculated correctly. The simulation as performed so far assumes axial symmetry. However, Muirhead *et al.* [9] argue that vortex production is most likely to take place at the side of the bubble, and clearly this cannot be treated correctly if axial symmetry is assumed.

Due to the big difference between the helium and electron time scales (of the order of $m_{\mathrm{He}}/m_e \sim 7300$), to numerically evolve the coupled equations, we used the adiabatic approximation. For a given helium profile, we first find the electron ground state by evolving the electron wave function in imaginary time by 100 time steps of magnitude 0.002 fs. To time develop the helium we use a 0.002 ps time step based on fourth-order finite difference in combination with a fourth-order Runge-Kutta method. The computation grid is 400 × 800 (transverse r- and longitudinal z-direction) with a spacing of 0.5 Å. The grid is moved along to keep the electron in the center. For the helium evolution near the boundary, we put a damping coefficient into (2) that increases smoothly as the boundary is approached. Such an absorbing layer can absorb the phonons radiated from the central region and generates no reflection because of its mathematically smooth behavior. We evolve the program for about 5 ns physical time during which the electron travels between 250 and 500 nm. In a typical run, we use parallel computing with 8-cores to complete the calculation in about one week.

3 Results

Figure 2 shows a series of snapshots of the helium number density $m_{He}|\psi|^2/\rho$ at a sequence of times. In this series the bubble starts at rest ($t = 0$) in liquid at zero pressure and the applied electric field is 4 MV m^{-1}. The initial acceleration of the bubble has the value that is expected based on the applied force and the hydrodynamic mass $2\pi R^3\rho/3$ where R is the bubble radius. During the initial acceleration of the bubble, liquid in front of the bubble is compressed as shown in the image for $t = 0.12$ ns. The velocity at this time is 32 m s^{-1}.

In Fig. 3 we show a plot of the dimensions of the bubble at early times. This includes a comparison with the result obtained previously by Guo and Maris [10] using the simplified model mentioned above. It is interesting that the two calculations give similar results for the variation of the waist with velocity but the distance from pole to pole differs between the two calculations. In the present work it is found to decrease slightly as the velocity increases. We assume that this is the result of allowing for the compressibility of the liquid.

Once the velocity becomes large enough for roton generation to set in or for vortices to nucleate, we cannot expect the simulation to be quantitatively correct. However, the dynamics of the bubble are interesting and so we give a brief description. As the velocity of the bubble increases further, the shape changes dramatically from an oblate spheroid, to a shape with a narrow extension running around the equator. During this process the bubble still has a shape that has almost even parity relative to the z-axis. As the bubble deforms, the changes in the size and the shape cause the effective mass to increase and the acceleration to decrease (see $t = 1.5$ ns at which point the velocity is 47 m s^{-1}). At this time, surprisingly, there is still no energy dissipation associated with the motion. In contrast to the situation at $t = 0.12$ ns, there is now a substantial increase in the density of the liquid in front of and behind the bubble; this is due to the Bernoulli effect. We have made a separate check that there is no dissipation below this critical velocity. To do this we turned off the electric field and were able to see that the bubble continued to move at a constant speed.

When a time of 2.72 ns is reached the velocity has reached approximately 50 m s^{-1}. At this velocity the surface of the bubble becomes slightly irregular (this is hard to see in the figure). These irregularities fluctuate in time resulting in sound radiation into the liquid. The wavelength of the radiated sound is of the order of 10 Å, and the sound is radiated into a large solid angle in the forward and backward directions relative to the direction of motion. After this time the bubble evolves in an interesting manner. The rate of energy loss from the bubble increases to a large value and the velocity of the bubble decreases. The plot for $t = 3.06$ ns shows a typical form of the helium density during this phase of the motion. Once the bubble has slowed to a velocity around 43 m s^{-1}, the rate of energy dissipation decreases dramatically and the appearance is as shown for $t = 3.48$ ns. The velocity then increases again and the cycle repeats.

The dissipation associated with this mechanism is remarkably strong and has the consequence that the time average of the velocity $\langle v \rangle$ is almost independent of the applied electric field. In Fig. 4 we show $\langle v \rangle$ as a function of pressure. One can see that increasing the field from 2 MV m^{-1} to 10 MV m^{-1} increases the average velocity by

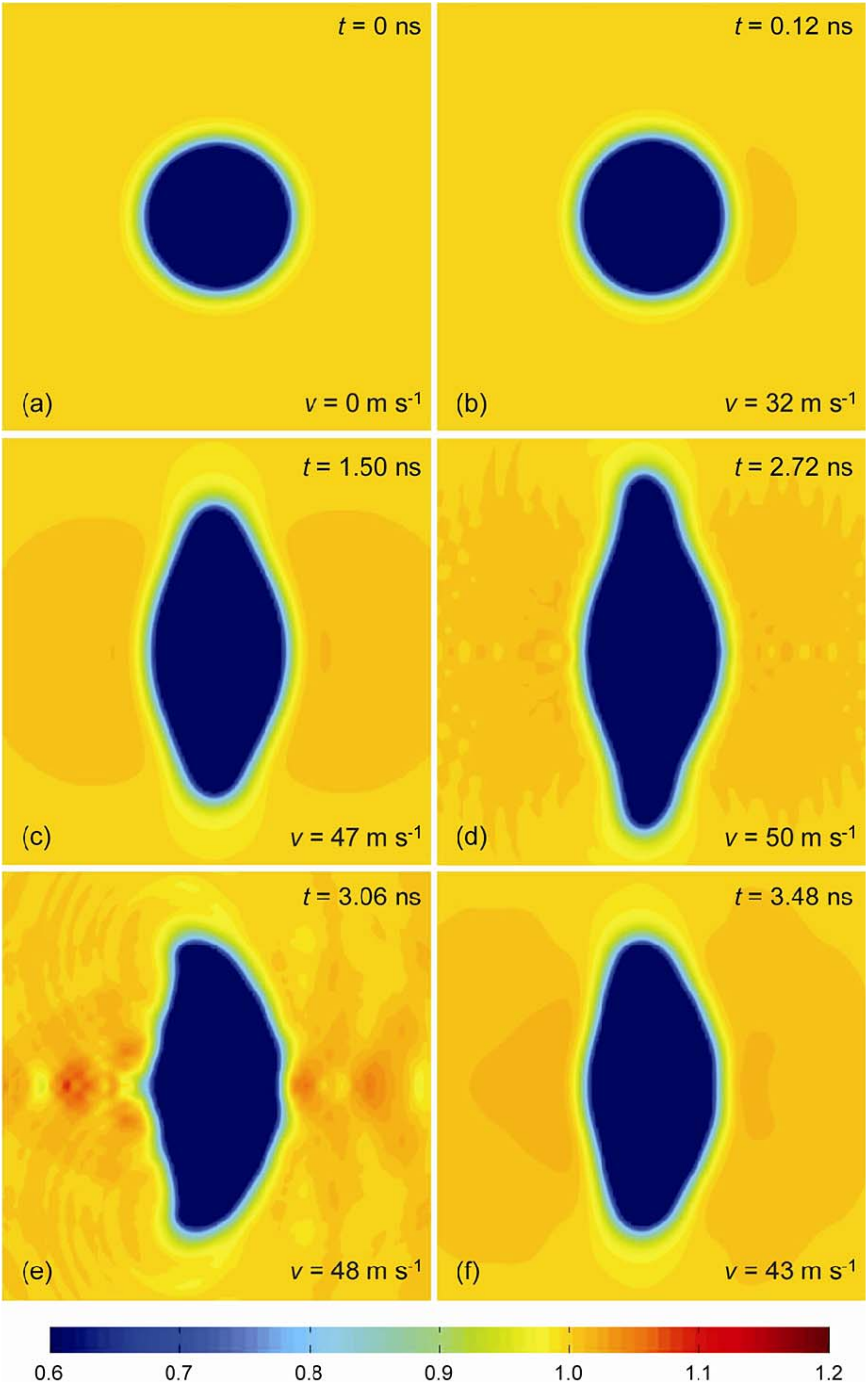

Fig. 2 (Color online) Plot of the helium number density $m_{\mathrm{He}}|\psi|^2/\rho$ surrounding an electron bubble at different times. The side of each square is 120 Å. The pressure $P = 0$

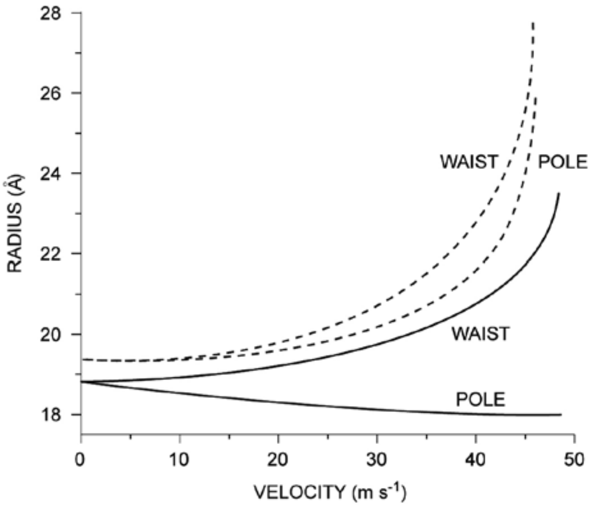

Fig. 3 Radius of the waist of the bubble and distance from the center to the pole as a function of velocity. The pressure $P = 0$. *Solid lines* from the present calculation and *dotted lines* from Ref. [10]

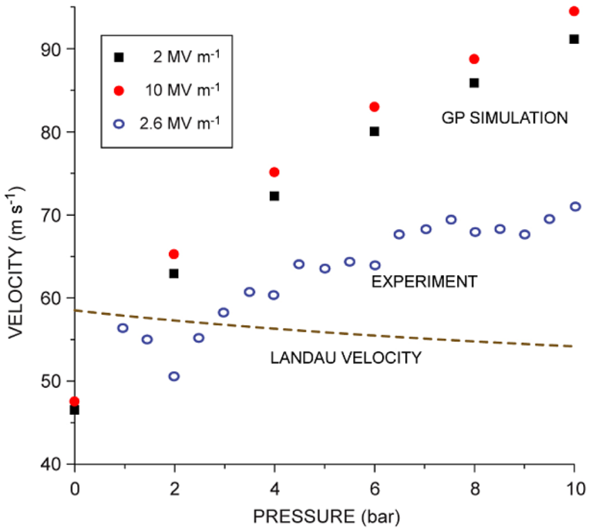

Fig. 4 (Color online) Bubble velocity as a function of liquid pressure. The *solid symbols* are from the computer simulation described in the text. The *open circles* are the experimental results of Nancolas *et al.* [15]

at most a few meters per second. In Fig. 4 we have included the experimental results of Nancolas *et al.* [15] who applied a field of 2.6 MV m^{-1}. Except near zero pressure, the average velocity measured by Nancolas *et al.* is below our calculated values, thereby implying that either the roton or vortex generation mechanism becomes a strong dissipation mechanism *before* the energy loss mechanism that we have found sets in. In future work, we plan to investigate whether this is still true when our model is extended to allow for non-axially symmetric motion and the dispersion relation is modified to include the roton minimum.

4 Summary

We have found that a moving electron bubble undergoes a significant change in shape as the velocity increases towards the value at which vortices nucleate. It would be interesting to try to modify the theory of the vortex nucleation to allow for this shape change.

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