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Effective Mass of an Electron Bubble in Superfluid Helium-4

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Abstract We present the results of computer simulations of the motion of an electron bubble through superfluid helium-4 when acted upon by an electric field. The simulations are based on an extended version of the Gross–Pitaevskii equation. The temperature is assumed to be sufficiently low for the drag exerted on the bubble by thermal excitations to be negligible, and the calculations are made for velocities below the critical velocitie for nucleation of vortices and roton production. We calculate the effective mass $m*$ of the bubble and obtain results in excellent agreement with the measurements of Poitrenaud and Williams, and Ellis, McClintock, and Bowley.

Keywords Superfluid helium-4 · Electron bubbles

1 Introduction

An electron in liquid helium forms a bubble state with an energy which, as a first approximation, can be considered to arise from the sum of the zero-point energy of the electron trapped in the bubble, the surface energy, and the work done against the pressure in forming the bubble. Thus,

$$E = \frac{h^2}{8mR^2} + 4\pi R^2 \sigma + \frac{4\pi R^3}{3} P. \tag{1}$$

Here R is the radius of the bubble, m is the mass of the electron, σ is the surface tension, and P is the pressure applied to the liquid. This simple expression for the energy is

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obtained by making a number of approximations. It is assumed, for example, that the potential barrier of height V preventing the electron wave function from penetrating into the liquid is sufficient to result in the wave function of the electron being very close to zero at the bubble surface. The surface energy is taken to be given by the surface area times the experimentally measured surface tension, i.e., no allowance is made for the curvature of the surface or for the possible variation of the surface tension with pressure. A more accurate theory of the energy and the structure of the electron bubble can be made using a density functional scheme to model the helium. This type of calculation has been carried out by Eloranta and Apkarian [1] and by Grau et al. [2] in order to learn about the bubble structure and to find the photon energies needed to excite the electron to higher energy states. The results of these calculations were in good agreement with the optical absorption measurements of Grimes and Adams [3,4], Zipfel [5], and Parshin and Pereversev [6–8].

Another test of the structure of the electron bubble can be made through measurement of the effective mass of the bubble when in motion through the liquid. This mass has been measured with good accuracy in beautiful experiments by Poitrenaud and Williams [9,10] and by Ellis et al. [11,12]. The Poitrenaud–Williams experiment was at zero pressure, whereas the Ellis et al. measurements were between 11 and 25 bars. For a solid sphere moving through an incompressible fluid, the effective mass m^* is the sum of the mass of the sphere plus one half of the mass of the liquid that is displaced. Since the mass of the electron is negligible, this would give

$$m^* = \frac{2\pi\rho R^3}{3} \tag{2}$$

where ρ is the density of the liquid. From the simple theory in Eq. (1), when the pressure is zero the radius at which the energy is a minimum is

$$R = \left(\frac{h^2}{32\pi m\sigma}\right)^{1/4}. \tag{3}$$

At zero temperature, the surface tension is 0.375 erg cm^{-2} [13] and Eq. (3) gives a radius of 18.91 Å. Then from Eq. (2) using the zero-temperature density of 0.14513 g cm^{-3}, the mass comes out to be $309m_4$ where m_4 is the helium atom mass [14]. This compares with the experimental result of $(243 \pm 5)m_4$ [9,10]. Similar discrepancies exist between the simple theory and the data of Ellis et al. [11,12]. To attempt a better agreement with experiment, we present here a calculation of the effective mass based on an extended version of the Gross–Pitaevskii (GP) equation [15,16].

2 Calculation

The simplest version of the GP equation to describe superfluid helium-4 is

$$i\hbar\frac{\partial\psi}{\partial t} = -\frac{\hbar^2}{2m_4}\nabla^2\psi + g\,|\psi|^2\,\psi, \tag{4}$$

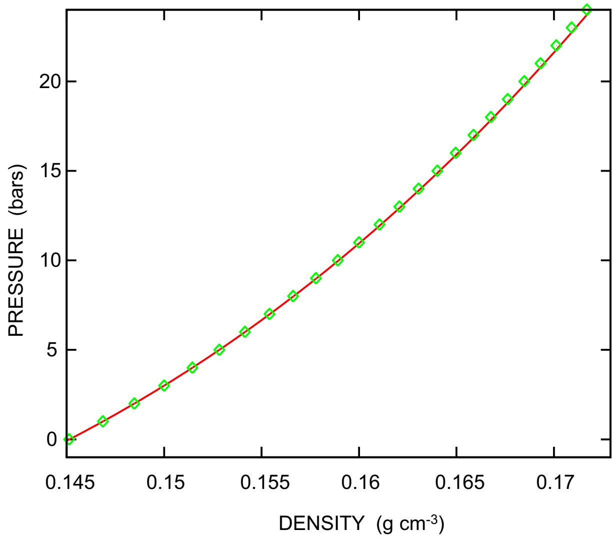

Fig. 1 Pressure as a function of density . The *solid line* is from Eq. (6), and the *diamonds*are the experimental results from Ref. [13] (Color figure online)

where there is assumed to be a short-range repulsion between helium atoms of strength governed by g. The number density of helium atoms at position $\vec{r}$ is $|\psi|^2$. In Eq. (4), g is the only parameter that can be adjusted to give the correct properties of liquid helium. As a result, no matter how g is chosen, Eq. (4) cannot provide a good approximation to the measured equation of state, the surface tension, and the variation of the liquid density near to a free surface. To fit all of these quantities, it is necessary to add extra terms to Eq. (4). Jin [17,18] has proposed the equation

$$i\hbar\frac{\partial\psi}{\partial t} = -\frac{\hbar^2}{2m_4}\nabla^2\psi + g_0\,|\psi|^2\,\psi + g_1\,|\psi|^4\,\psi + g_2\,|\psi|^6\,\psi - w_1\nabla^2\,|\psi|^2\,\psi, \quad (5)$$

where the parameters have the values $g_0 = -9.927\times10^{-38}$ erg cm^3, $g_1 = -4.995\times10^{-60}$ erg cm^6, $g_2 = 3.421\times10^{-82}$ erg cm^9, and $w_1 = 6.220\times10^{-53}$ erg cm^5. The parameters g_0, g_1, and g_2 are chosen so that Eq. (5) leads to a good approximation to the equation of state, and to the sound velocity as a function of density. For example, the pressure in uniform liquid is related to the number density by

$$P = \frac{1}{2}g_0n^2 + \frac{2}{3}g_1n^3 + \frac{3}{4}g_2n^4. \quad (6)$$

In Fig. 1, we show a comparison between Eq. (6) and the measured pressure as a function of density [19]. The parameter w_1 is chosen to give the correct value for the surface tension, and it can be shown that this value of w_1 results in a width of the liquid/vacuum interface which is consistent with the experimentally measured width [20]. Equation (5) does not lead to the correct dispersion relation for excitations of large momentum; there is no roton minimum, for example. Note that the values of the

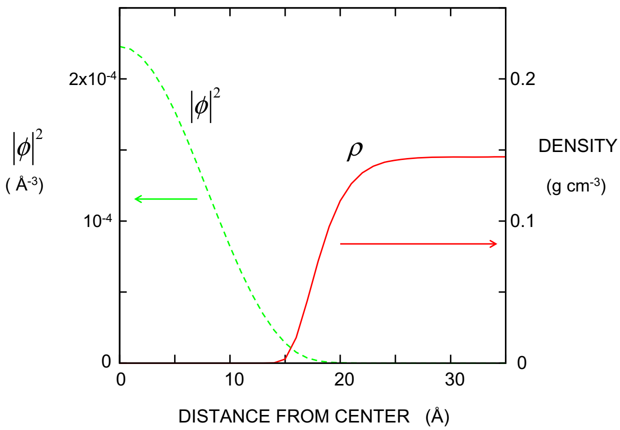

Fig. 2 *Dashed line* shows the square of the wave function of an electron in the ground state as a function of the distance r from the center of the bubble. *Solid line* is the helium density. The pressure is zero (Color figure online)

parameters used in the present paper are the same as were proposed in previous work by Jin; no adjustments to the parameters were made in order to fit the effective mass data.

The Schrodinger equation for the wave function ϕ of the electron in liquid helium is taken to be

$$i\hbar \frac{\partial \phi}{\partial t} = -\frac{\hbar^2}{2m} \nabla^2 \phi + f_0 \left|\psi\right|^2 \phi. \tag{7}$$

An electron in bulk helium of uniform density at zero pressure has an energy of approximately 1 eV due to the repulsion of the helium atoms. This fixes the value of f_0 to be 7.672×10^{-35}erg cm^3. This interaction results in a corresponding term $f_0 \left|\phi\right|^2 \psi$ on the right hand side of Eq. (5).

The first step in the calculation is to find the wave function of the electron and the helium when the electron is in its ground state and there is no applied electric field. We have done this by numerically integrating Eqs. (5) and (7) in imaginary time. After sufficient time, the wave functions converge to the ground state with the electron confined to a bubble. The position of the bubble is, of course, arbitrary. We use a mesh of spacing 1 Å and a time step of 5×10^{-5} ps. The results for the helium mass density $m_4 \left|\psi\right|^2$ and the electron wave function $\left|\phi\right|^2$ at zero pressure are shown in Fig. 2. We add a term $-eEz\phi$ to the right hand side of Eq. (7) corresponding to an electric field in the negative z direction and then numerically integrate in real time. The position of the electron bubble is calculated from the electron wave function as the expectation value $< z >$. Figure 3 shows results obtained for helium at zero pressure, 10 bars, and 20 bars with a field of 2 kV cm^{-1}. The calculations were performed with the volume of helium being a cylindrical cell of length 241 Å and radius 121 Å. The initial position of the electron bubble was at the center of the cell.

When the velocity is sufficiently small the acceleration should be a constant and so the displacement should be

$$< z > = \frac{eEt^2}{2m^*} \tag{8}$$

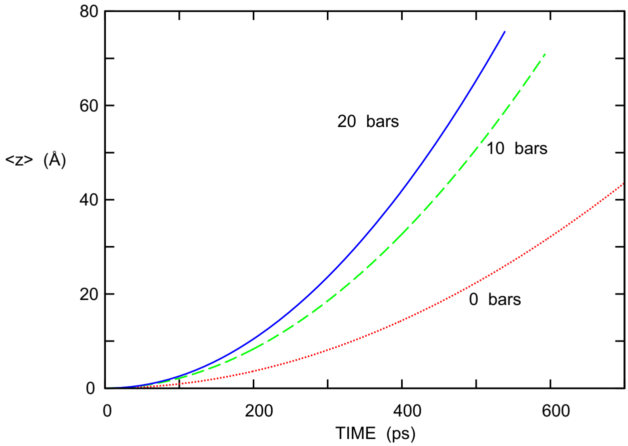

Fig. 3 Expectation value $< z >$ of the z coordinate of the electron as a function of time after application of an electric field. Results are for pressures of 0, 10, and 20 bars. The field is 2000 V cm^{-1} (Color figure online)

Ellis et al. [12] found that there were some small deviations from this relation and proposed that this could be understood by taking the energy of a bubble with momentum p to be

$$\varepsilon = \frac{p^2}{2m^*}\left(1 - \alpha p^2/2\right), \tag{9}$$

giving

$$< z >= \frac{eEt^2}{2m^*}\left(1 - \alpha \frac{e^2E^2t^2}{2}\right) \tag{10}$$

They did not report specific values found for α or indicate its approximate magnitude. To find m^* and α from the simulation results, we make a least squares fit of $< z >$ as a function of t using Eq. (10). A good fit is obtained apart from a small deviation in the first few picoseconds. We have not investigated this in detail but assume that it may arise from the sudden small change in the shape of the bubble when the electric field is applied. The uncertainty in m^* obtained from the fit is very small, i.e., of the order of m_4, but the values obtained for α have a typical uncertainty of 10–20 %.

To improve the calculation, we have found a different method in which no field is applied. We maintain the wave function of the helium on the boundaries of the simulation cell constant in time, and with an amplitude corresponding to the density of bulk helium and a phase gradient corresponding to a chosen fixed velocity $\vec{v}$ in the z- direction. We then perform a time development in imaginary time to find the flow field in the vicinity of the bubble and, once this has converged to a constant value, calculate the kinetic energy K of the flow in the frame moving at velocity $\vec{v}$. It is straightforward to show that including contributions up to v^4 this energy is

$$K = \frac{1}{2}m^*v^2\left(1 + \frac{3m^{*2}\alpha}{2}v^2\right) \tag{11}$$

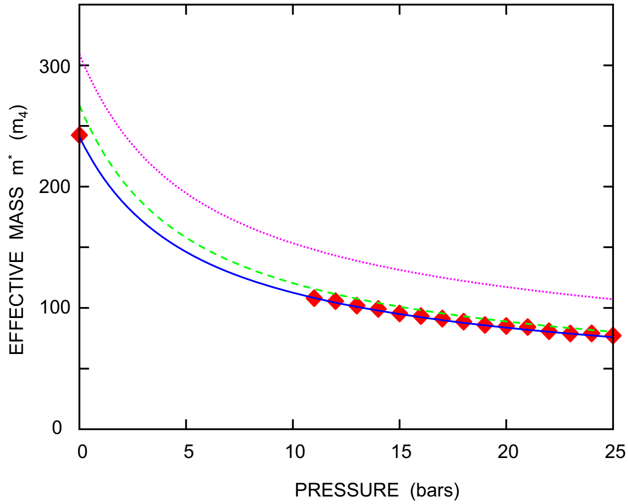

Fig. 4 Effective mass m^* of the electron bubble as a function of pressure. The measured value at zero pressure is from Refs. [9,10], and the other data points are from Ref. [12]. The *dotted curve* is the mass obtained using the simple theory Eqs. (1) and (2). The *dashed curve* shows the results obtained from the GP simulation with an applied field of 2000 V/cm. The *solid curve* incorporates the correction to allow for the polarization energy (Color figure online)

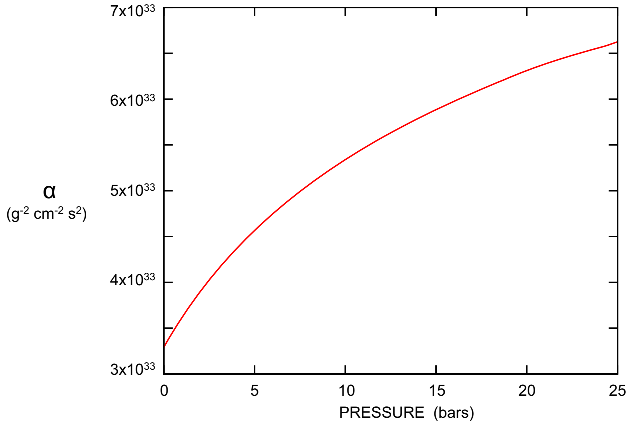

Fig. 5 The variation of the parameter α with pressure as found from the simulations (Color figure online)

Calculation was performed for velocities up to $3\,\mathrm{m\,s^{-1}}$. We then used Eq. (11) to fit the values of K found in the simulation. The best fit values of m^* and α are shown as the dashed curves in Figs. 4 and 5. This method gives much more precise values of α than were found by the first method. Figure 4 also includes as the dotted curve the effective mass calculated from Eqs. (1–3).

We have performed a number of simple checks on the GP simulation. The result for m^* was found to not change significantly due to changes in the simulation volume or the time step. The mesh spacing was 0.5 Å; an increase to 1 Å resulted in an increase of m^* at zero pressure by about 1 %.

The GP simulation we have performed does not include the effect of the polarization of the helium due to the field of the electron. To include this effect within the simulations is difficult because the potential acting on helium at position $\vec{r}$ has to include an integral over all possible positions $\vec{r}\prime$ of the electron. We have used the following method to estimate the effect of the polarization interaction.

We note that the polarization results in two distinct changes in the structure of the bubble. The first is an increase in the density of the helium *outside* the bubble giving an increase in m^*. The increase $\Delta\rho$ in the density at distance r from the center of the bubble is [21]

$$\frac{\Delta\rho}{\rho} = \frac{(\varepsilon - 1)\, e^2}{8\pi B\varepsilon^2 r^4}, \tag{12}$$

where ε is the dielectric constant and B is the bulk modulus. This formula is based on the approximation that the electron is localized at the center of the bubble so that the field in the liquid near to the bubble is given by $e/\varepsilon r^2$ (see discussion below). For simplicity, we assume that the velocity field $\vec{v}\,(\vec{r})$ is unchanged by the variation in the density with distance from the bubble so that the change in the effective mass is simply

$$\Delta m^* = \int \Delta\rho v^2 \mathrm{d}V \Big/ \int \rho v^2 \mathrm{d}V \tag{13}$$

where the integrals are over the volume around the bubble. The flow field around the moving bubble falls off with distance as the cube of the distance [22], and it follows that the change in density of Eq. (12) results in a change in effective mass of

$$\frac{\Delta m^*}{m^*} = \frac{3\,(\varepsilon - 1)\, e^2}{56\pi B\varepsilon^2 R^4}, \tag{14}$$

where R is the bubble radius. At zero pressure, the bubble radius based on Eq. (1) is 18.91 Å, the bulk modulus is $8.24 \times 10^7 \mathrm{g\ cm^{-1} s^{-2}}$, and the dielectric constant is 1.057 [23], and so the increase in m^* due to polarization is 0.19 %. Under pressure, the magnitude increases due to the decrease in R, but this is offset by an increase in the bulk modulus. The calculation could be improved by allowing for the fact that the electron is not localized at the center of the bubble but has a probability distribution of positions governed by the wave function. It is straightforward to allow for this but does not seem worthwhile considering the very small magnitude of the effect.

The second effect of polarization is a reduction in the bubble size and a consequent decrease in the effective mass. To obtain an estimate of this effect, we use the simple model of Eq. (1) in which the helium has uniform density outside of a radius R and zero density inside the bubble, and ignore the penetration of the electron wave function into the region occupied by the helium. If the electron is taken to be localized at the center of the bubble the polarization energy is

$$-\frac{(\varepsilon - 1)\, e^2}{2\varepsilon R}. \tag{15}$$

where $\varepsilon = 1.0573$ [20]. If allowance is made for the fact that the electron is distributed over the volume of the bubble with a probability distribution $|\phi|^2$, then it can be shown that the polarization energy is changed to [24]

$$-1.345\frac{(\varepsilon - 1)\,e^2}{2\varepsilon R} \tag{16}$$

This energy contribution will make the size of the bubble smaller. To make a correction to allow for this, we use the simple model of Eq. (1) to estimate the bubble radius R_0 without the polarization energy, and the radius R_p when the polarization energy as given by Eq. (16) is included. We then multiply the result for the effective mass found from the Gross–Pitaevskii calculation by the factor $(R_\mathrm{p}/R_0)^3$. This correction is largest at low pressure; at zero pressure there is a 9 % decrease in the effective mass. The result of applying this correction is shown as the solid curve in Fig. 4. It can be seen that the corrected values of m^* are in extremely good agreement with the experimental values. The measurement of m^* by Poitrenaud and Williams [9,10] has an uncertainty of ±2 %, and Ellis et al. [12] consider that there may be a systematic error as large as 2 % in their results.

The measurements of Ellis et al. [12] were made at ∼ 70 mK so it is appropriate to use a version of the GP equation which has been constructed to give the correct surface tension at zero temperature, as we have done. The experiment of Poitrenaud and Willams was performed at approximately 750 mK where the surface tension is about 1 % less than the zero-temperature value. Allowance for this would increase the bubble radius by 0.25 % (see Eq. 3) and the effective mass by 0.75 %. We have not included this in the results shown in Fig. 4.

We have not attempted to apply a correction for the polarization energy to the result for α since we do not know how α depends on the radius. It seems likely that the α term in Eqs. (9) and (11) results from an expansion of the bubble coming from the reduction in liquid pressure at the bubble surface due to the Bernoulli effect; this will make the bubble slightly non-spherical.

3 Summary

The results of the calculation of m^* are in remarkably good agreement with the experimental results of Poitrenaud and Williams [9,10] and Ellis et al. [12]. Both of these groups estimate that their measurements have an uncertainty of ±2 %. Our simulations give results for m^* which are in agreement with the experiment values when allowance is made for the experimental uncertainty. The main effect of pressure is to reduce the bubble size, but it may also change the way in which the density of the liquid goes from zero inside the bubble to the bulk density outside.

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