J Low Temp Phys (2007) 148: 207–211
DOI 10.1007/s10909-007-9372-3

Calculation of the Shape of S-State Electron Bubbles in Liquid Helium

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Published online: 24 May 2007

Abstract We consider the shape of electron bubbles in liquid helium. Grinfeld and Kojima (Phys. Rev. Lett. **91**, 105301, 2003) have shown that the in a certain pressure range the 2S electron bubble is unstable against small distortions with $l = 3$ and loses its spherical symmetry. We report more detailed calculations of this effect and also study the behavior of the 3S and 2P bubbles.

PACS 67.40 · 77.22-d

1 Introduction

Electron bubbles in liquid helium have a size and shape that is dependent on the quantum state of the electron and on the pressure P in the liquid [1–4]. The total energy E of this electron bubble can be approximated by the expression [5, 6]

$$E = E_{\mathrm{el}} + \alpha A + PV, \tag{1}$$

where E_{el} is the ground state energy of the electron inside the cavity, α is the energy per unit area of the liquid-vapor interface, P is the applied pressure, A and V are the surface area and the volume of the bubble respectively. The form of the bubble is such as to minimize the total energy, i.e., the sum of the energy E_{el} of the electron, the surface energy αA and the volume energy PV. In discussion of these bubbles, it is convenient to label the different quantum states in the following way. First consider an electron inside a spherical cavity. The quantum state of the electron can then be specified by a radial quantum number n ($n = 1, 2, 3, \ldots$), an angular momentum l and the azimuthal quantum number m. Then allow the shape of the bubble to change so as to lower the energy until the system reaches a stable state. Because this change

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in shape may destroy the spherical symmetry of the wave function, the angular momentum is no longer a conserved quantity. However, it is convenient to continue to label the states by n and l.

In previous work [1–4] the shape of bubbles has been calculated based on the assumption that the bubbles have axial symmetry. The equilibrium shape of 1S, 2S, 1P, 2P, and 1D states at zero applied pressure was determined and for some of these states the change in shape with pressure was investigated. As expected, the nS states remained spherical but became smaller as the pressure was increased. The 1P state at zero pressure was shaped like a peanut and when the pressure was increased to around 10 bars, the "waist" of the peanut shrank to have dimensions of only a few interatomic spacings. To investigate such a situation in more detail would require the use of density functional techniques, rather than simple approximations in which the energy of the bubble surface is taken to be the area multiplied by the surface tension. Interesting results were obtained for the 2P state [4]. At pressures above 1.53 bars, it was determined that no stable state could be found, i.e., the shape of the bubble could be changed so as to continuously lower the energy to a state in which the bubble broke into two pieces.

In a very interesting paper, Grinfeld and Kojima (GK) [7] obtained the surprising result that except in a small pressure range, the nS states with $n \geq 2$ were unstable against distortions with $l = 3$ and thus lost their spherical symmetry. For the 2S state the spherical bubble was unstable against $l = 3$ above a pressure of -1.23 bars. Above this pressure the bubble has tetrahedral (T) symmetry. At some higher, but unspecified pressure, GK mentioned that a second instability set in and the bubble shape and wave function evolved into a 1D state.

2 Investigation of the 2S State

The GK investigation [7] included both an analysis of the stability of the spherical bubble against small-amplitude fluctuations and also finite element calculations of the shape of the equilibrium bubble after the instability had occurred. We have repeated their numerical calculations for the T state using a different method. We first write the radius of the bubble in the direction (θ, ϕ) as

$$r(\theta, \phi) = \sum_{l,i} A_l^{(i)} f_l^{(i)}(\theta, \phi), \tag{2}$$

where $A_l^{(i)}$ are some coefficients, and the functions

$$f_l^{(i)}(\theta, \phi) = \sum_m B_{lm}^{(i)} Y_{lm}(\theta, \phi) \tag{3}$$

are linear combinations of the spherical harmonics $Y_{lm}(\theta, \phi)$ that have tetrahedral symmetry [8, 9]. We solve the Schrödinger equation for the electron with the boundary condition that $\psi = 0$ on the bubble surface using for ψ an expansion in terms of a set of functions with T symmetry, i.e., with angular dependence given by the $f_l^{(i)}(\theta, \phi)$ functions. Typically, the shape was expanded using functions up to $l = 6$,

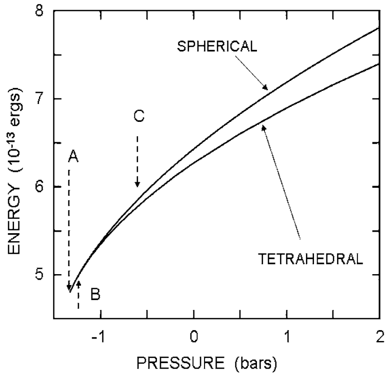

Fig. 1 Energy of the 2S electron bubble as a function of pressure. Below A the bubble becomes unstable against uniform radial expansion. Above B the spherical bubble becomes unstable and takes on a tetrahedral shape. At C the tetrahedral bubble becomes unstable

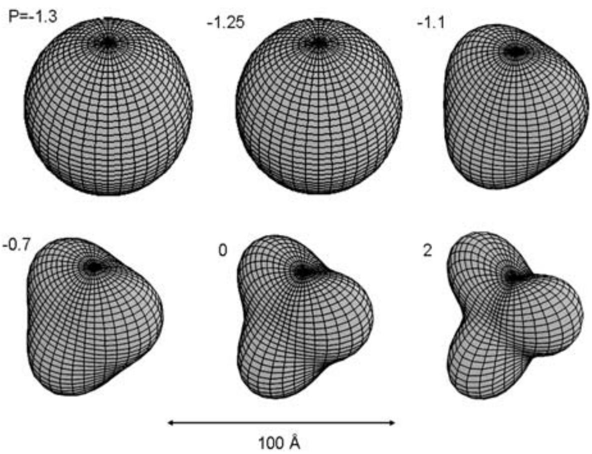

Fig. 2 Shape of the 2S electron bubble at several pressures. The shapes shown for 0 and 2 bars are stable against fluctuations with tetrahedral symmetry but are unstable against other fluctuations

and up to $l = 9$ for ψ. In Fig. 1, we show the energy of the spherically-symmetric (SS) 2S state as a function of pressure along with the energy of the bubble when deformations with T symmetry are allowed. We find that the instability leading to T symmetry occurs at -1.23 bars, in agreement with the earlier results of GK. In Fig. 2, we show the shape of the 2S bubble at a series of pressures. It can be seen that the distortion of the bubble shape from spherical increases rapidly as the pressure is increased.

We do not have any simple physical explanation for the instability of the 2S spherical state against tetrahedral distortion. However, we note that the numerical simulations show that the T state has larger electron and volume energy, but significantly lower surface energy.

We then considered the T state at each pressure and examined whether the energy of the state could be lowered if the radius in the direction (θ, ϕ) was allowed to be of the more general form

$$r(\theta, \phi) = \sum_{lm} C_{lm} Y_{lm}(\theta, \phi), \tag{4}$$

where the complex C_{lm} coefficients are restricted only by the requirement that $r(\theta, \phi)$ be real. The wave function was also allowed to have a general symmetry. The result was that the T state was found to be stable up to a pressure of −0.65 bars. Above this pressure, it was possible to vary the C_{lm} coefficients so as to lower the energy by a large amount below the T state, i.e., the T-state became unstable.

It is important to recognize that these calculations simply search for equilibrium states, i.e., the numerical program repeatedly varies the C_{lm} coefficients to see if the energy can be lowered. However, this calculation does not determine what actually happens to a T-state bubble in helium when the pressure is increased so as to make the bubble unstable. To study such a situation requires the analysis of the dynamics of the bubble wall and the resulting motion of the surrounding liquid. To do this it would be necessary to include the effects of dissipation in the liquid due to the thermal excitations, the radiation of sound, and other effects. Thus, it is possible that the final state of a bubble after it has become unstable is different at different temperatures.

3 Investigation of the 3S and 2P States

We have also considered the 3S bubble. Grinfeld and Kojima [7] show that the nS state becomes unstable against fluctuations with l-symmetry if the quantity f_{nl} defined by

$$f_{nl} = \frac{(l-1)(l+2)}{4n^2\left(l - 1 - \frac{n\pi J_{l-1/2}(n\pi)}{J_{l+1/2}(n\pi)}\right)} \tag{5}$$

is positive *and* if the pressure is such that the bubble radius is *less* than a critical radius

$$R_c = \left(\frac{h^2}{32\pi m\alpha f_{nl}}\right)^{1/4}. \tag{6}$$

Based on these equations we find that a spherical 3S bubble can be unstable against fluctuations with $l = 3$ or $l = 5$. The critical pressures are −0.92 bars ($l = 3$) and +1.72 bars ($l = 5$). In addition, the bubble becomes unstable against uniform expansion when the pressure is below −1.08 bars. Thus, the SS state is stable for $-1.08 < P < -0.92$ bars. We have confirmed by numerical calculations that the SS state becomes unstable against T deformations above −0.92 bars.

The 3S bubble has a much more complex behavior and we have not been able to make a complete study. At some pressures, the bubble can have more than one shape that is stable against small amplitude fluctuations. Thus, for example, immediately above $P = -0.92$ bars, we have found two stable states with T symmetry. For $P = -0.90$ bars these shapes are shown in Fig. 3. They are both stable against further tetrahedral deformations, and have energies that differ by only a few K. For state A, the distortion from spherical tends to zero as $P \to -0.92$ from above, while B retains its T symmetry even below −0.92 bars.

These results naturally lead to questions about the stability of other states such as nP, and nD. The investigation of these states is more difficult because there is no obvious way to do a linear stability analysis as GK did for the nS states. So far

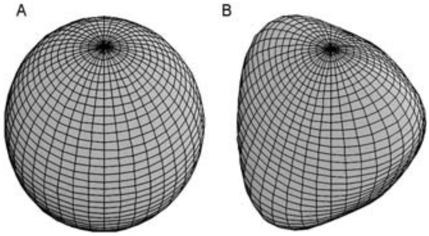

Fig. 3 Two stable shapes of the 3S electron bubble at $P = -0.9$ bars

we have investigated only the 2P state using numerical methods. We do not find any evidence of an instability of the axially-symmetric state in the pressure range up to $+1.53$ bars at which point the state becomes unstable against axially-symmetric fluctuations as already known. We hope to report on more detailed investigations at a later date.

Acknowledgement This research was supported by NSF Grants DMR-0305115 and DMR-0605355.

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