J Low Temp Phys (2007) 148: 213–217
DOI 10.1007/s10909-007-9371-4

Calculation of the Cross-Section for Optical Transitions of an Electron Bubble to D States

Wei Guo · Humphrey J. Maris

Published online: 23 May 2007

Abstract The optical transitions of an electron bubble (negative ion) in liquid helium from the ground state to the 1P and 2P states have been studied in a number of experiments. For an ideal spherical bubble electric-dipole transitions can occur only to P states. Thermal or quantum fluctuations in the bubble shape make other transitions possible. In this paper we calculate the cross-sections for transitions from the 1S ground state to the 1D and 2D states. The cross-section for the 1S to 1D transition is approximately two orders of magnitude less than the cross-section for the 1S to 1P.

PACS 67.40 · 77.22-d

1 Introduction

An electron injected into liquid helium forms a spherical cavity that is almost free of helium atoms. The energy E of this electron bubble can be approximated by the expression [1, 2]

$$E_{\mathrm{el}} + 4\pi R^2\alpha + \frac{4\pi}{3}R^3 P, \tag{1}$$

where E_{el} is the ground state energy of the electron inside the spherical cavity of radius R, α is the energy per unit area of the liquid-vapor interface, and P is the applied pressure. The first term is the zero-point energy of the electron that is confined in the bubble. The energy of the electron is obtained by solution of Schrödinger's equation with a potential that is zero inside the bubble, $(r < R)$ and equal to a constant V_0 outside the bubble $(r > R)$ [3]. The second and third terms represent the surface energy of the bubble, and the work done in forming the bubble against the pressure in the liquid, respectively. Equation (1) is based on a number of approximations [4].

W. Guo · H.J. Maris (✉)
Department of Physics, Brown University, Providence, RI 02912, USA
e-mail: humphrey_maris@brown.edu

For example, it is assumed that the bubble has a sharp wall at which the density of the helium jumps discontinuously from zero to its value in bulk liquid, and the surface tension of the liquid has been taken to be independent of the curvature of the bubble surface. Since when the electron is in the ground state, the wave function penetrates a distance into the helium which is small compared to R, for many purposes one can make the further approximation that the wave function vanishes at the bubble wall, equivalently take V_0 to be an infinite barrier. A more accurate calculation could be performed treating helium using a density functional method.

In this paper we consider the absorption of light by electron bubbles. The optical absorption has been measured by Northby and Sanders [5], Zipfel and Sanders [6, 7], Parshin and Pereversev [8], and by Grimes and Adams [1]. In the initial experiments, there was some uncertainty in observed absorption line assignment. The measurements of Northby and Sanders [5] at zero pressure for photons in the energy range around 1 eV are probing transitions from the ground state 1S to states in the continuum. The sharp peak in the cross-section at around 0.5 eV seen by Zipfel and Sanders [6, 7] arises from the 1S to 2P transition. The absorption peak near to 0.1 eV studied by Parshin and Pereversev [8], and by Grimes and Adams [1] is due to the 1S to 1P transition.

These main features in the optical spectrum arise from "allowed transitions", i.e., electric-dipole transitions in which the angular momentum of the electron changes by $\hbar$. Here, we consider processes that are "forbidden" within the electric dipole approximation, specifically transitions from the 1S state to D states. For a perfectly spherical bubble the cross-section for these transitions is extremely small, i.e., less than the cross-section for the allowed transitions by a factor which is of the order of $(R/\lambda)^2$, where R is the radius of the bubble and λ is the light wavelength. However, because of thermal and quantum fluctuations, at any instant the bubble has a significant deviation from spherical shape and this greatly increases the probability of a transition to a D state.

2 Theory

In a previous paper [9] we have calculated the amplitude of these shape fluctuations. The distance $R(\theta,\phi)$ from the origin to the surface of the bubble in the direction (θ,ϕ) was written as

$$R(\theta,\phi) = R_0 + \sum_l f_l Y_{l0} + \sum_{lm} f_{lm} U_{lm} + \sum_{lm} \tilde{f}_{lm} \tilde{U}_{lm}, \tag{2}$$

where R_0 is the average radius, $U_{lm} = Y_{lm} + Y^*_{lm}$, $\tilde{U}_{lm} = -i(Y_{lm} - Y^*_{lm})$, and the sums over m go from 1 to l. The fluctuating quantities f_{lm} and $\tilde{f}_{lm}$ have average squared values of

$$\langle f_0^2 \rangle = \left[\frac{1}{2}\hbar\omega_0 + \frac{\hbar\omega_0}{\exp(\hbar\omega_0/k_B T) - 1} \right] \Big/ \left(\frac{5\pi\hbar^2}{4mR_0^4} - 2\alpha \right), \tag{3}$$

and for $l \neq 0$

$$\langle f_0^2 \rangle = \langle f_{lm}^2 \rangle = \langle \tilde{f}_{lm}^2 \rangle$$
$$= \left[\frac{1}{2}\hbar\omega_l + \frac{\hbar\omega_l}{\exp(\hbar\omega_l/k_B T) - 1} \right] \Big/ \left[\alpha(l^2 + l - 2) + \frac{\pi\hbar^2}{2mR_0^4}(1 + \pi S_l) \right], \quad (4)$$

where ω_l is the frequency of the l-th vibrational mode of the bubble, and S_l is a coefficient given in terms of derivatives of Bessel functions [9].

For light of frequency Ω that is polarized along the z-axis, the cross-section for a transition from the ground state 0 to a state i is

$$\sigma(\Omega) = \frac{4\pi^2 e^2 \Omega}{c} |z_{0i}|^2 \delta(E_0 + \hbar\Omega - E_i), \quad (5)$$

where z_{0i} is the matrix element of z between the ground state and the state i, and E_0 and E_i are the energies of these states. The shape fluctuations modify both the energies of the different quantum states as well as the matrix elements between the states. We have used perturbation theory to calculate the shift in the energy level of the 1D states to first order in the amplitude of the fluctuations. The result is most conveniently expressed in terms of the dimensionless parameters and ε_{lm} and $\tilde{\varepsilon}_{lm}$ defined by

$$\varepsilon_{lm} \equiv \frac{f_{lm} - i\tilde{f}_{lm}}{R_0\sqrt{2}}, \qquad \tilde{\varepsilon}_{lm} \equiv (-1)^m \frac{f_{lm} + i\tilde{f}_{lm}}{R_0\sqrt{2}}. \quad (6)$$

We write the wave function of the perturbed D states in the form

$$\psi = \sum_{m=-2}^{2} A_m \psi_m, \quad (7)$$

where ψ_m is the m-th unperturbed D state. Let the shift in the energy level of the 1D state be ΔE_{1D} and let

$$x \equiv \Delta E_{1D}/E_{1D}. \quad (8)$$

Then following the method as in [8], we find that the eigen-equation for x becomes

$$2 \sum_{m'=-2}^{2} \sum_{l_0 m_0} \varepsilon_{l_0 m_0} \int Y_{2m}^* Y_{2m'} Y_{l_0 m_0} d\Omega A_{2m'} = -x A_{2m}. \quad (9)$$

From this equation we can obtain the shift $\Delta E_{1D}^{(M)}$ and amplitude of the wave function components in the $A_m^{(M)}$ in the Mth D state for any particular set of values of the ε_{lm} and $\tilde{\varepsilon}_{lm}$ parameters. Using the properties of the spherical harmonics, we find that the energy shifts of the 1D states have contributions from shape deformations of the bubble with $l = 0$, 2, and 4, and that the matrix elements only involve $l = 3$.

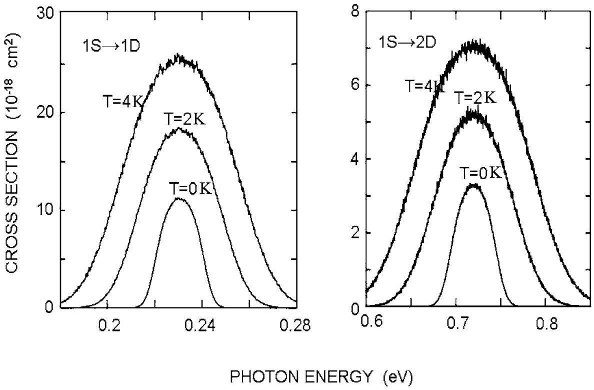

Fig. 1 Calculated cross-section for the 1S to 1D and 1S to 2D transitions for electron bubbles in helium at zero pressure

The matrix element between the perturbed 1S and the Mth perturbed 1D state can be written as

$$I = \langle 1\mathrm{S}'|z|1\mathrm{D}^{(M)}\rangle = \sum_{m=-2}^{2} C_m A_m^{(M)}, \tag{10}$$

where the coefficients C_m are given by

$$\begin{aligned} C_m = & -\frac{\pi \varepsilon_{3,m}}{\sqrt{3}} \frac{j_0'(\pi)}{j_3(\pi)} \int_0^{R_0} j_3\left(\frac{\pi r}{R_0}\right) j_2\left(\frac{\alpha_2 r}{R_0}\right) r^3 dr \int Y_{2,m}^* Y_{3,m} Y_{1,0} d\Omega \\ & - \frac{\alpha_2 \varepsilon_{3,-m}}{\sqrt{3}} \frac{j_2'(\alpha_2)}{j_1(\alpha_2)} \int_0^{R_0} j_0\left(\frac{\pi r}{R_0}\right) j_1\left(\frac{\alpha_2 r}{R_0}\right) r^3 dr \\ & \times \int Y_{1,0}^* Y_{2,m} Y_{3,-m} d\Omega, \end{aligned} \tag{11}$$

where j_l denotes a spherical Bessel function, and α_2 is the first zero of j_2. A similar expression can be derived for the 1S to 2D transition.

To calculate the cross-section we consider a Gaussian distribution of values of each of the ε_{lm} and $\tilde{\varepsilon}_{lm}$ parameters with average squared values as given by (3) and (4). The results for the cross-section for the 1S to 1D and 1S to 2D transitions as a function of photon energy at zero applied pressure are shown in Fig. 1. These cross-sections decrease rapidly with increasing pressure. As an example, Fig. 2 shows the cross sections at 2 K for several pressures. In Fig. 3 we show the integral of the cross-section over photon energy as a function of temperature.

Note that the results for the 2D transition have limited accuracy because the energy of the electron in the 2D state is approaching the height of the energy barrier provided by the helium and so to make a more accurate theory, the penetration of the wave function into the helium should be taken into account.

3 Discussion

The calculated cross-sections are between two and three orders of magnitude less than the cross-sections for the allowed 1S→1P and 1S→2P transitions calculated earlier.

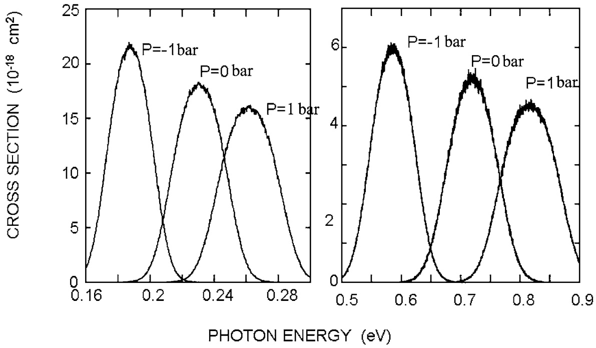

Fig. 2 Calculated cross-section for the 1S to 1D and 1S to 2D transitions at $T = 2$ K for several pressures

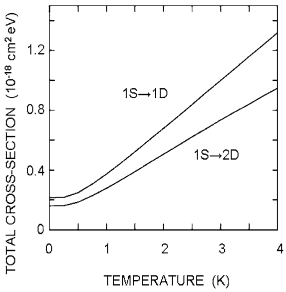

Fig. 3 Calculated total cross-section for the 1S to 1D and 1S to 2D transitions as a function of temperature. The pressure is zero

Nevertheless, these cross-sections are sufficiently large that it should be possible to measure them by the methods that were used earlier to study the allowed transitions. In fact, it is interesting to note that in the measurements of Northby and Sanders [5] a weak peak was detected at 0.75 eV. They attributed this to a transition to a "bound P state", presumably the 2P state. It is now clear that the transition to the 2P state occurs for a photon energy of ~0.5 eV for $P = 0$ K. Consequently, there is a possibility that the peak seen at 0.75 eV by Northby and Sanders is due to the $1S \rightarrow 2D$ transition. To test this possibility, it would be important to make a quantitative measurement of the magnitude of the cross-section; the measurements of Northby and Sanders do not provide this information.

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

References

1. C.C. Grimes, G. Adams, Phys. Rev. B **41**, 6366 (1990)
2. C.C. Grimes, G. Adams, Phys. Rev. B **45**, 2305 (1992)
3. W.T. Sommer, Phys. Rev. Lett. **12**, 271 (1964)
4. A.L. Fetter, in *The Physics of Liquid and Solid Helium*, ed. by K.H. Benneman, J.B. Ketterson (Wiley, New York, 1976), Chap. 3
5. J.A. Northby, T.M. Sanders, Phys. Rev. Lett. **18**, 1184 (1967)
6. C.L. Zipfel, Ph.D. thesis, University of Michigan, 1969, unpublished
7. C.L. Zipfel, T.M. Sanders, in *Proceedings of the 11th International Conference on Low Temperature Physics*, ed. by J.F. Allen, D.M. Finlayson, D.M. McCall, p. 296 (St. Andrews University, St. Andrews, 1969),
8. A. Ya, Parshin and S.V. Pereversev, Pis'ma Zh. Eksp. Teor. Fiz. **52**, 905 (1990); JETP Lett. **52**, 282 (1990)
9. H.J. Maris, W. Guo, J. Low Temp. Phys. **137**, 491 (2004)