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Behavior of an ion in a bubble in the ground state

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Deuterons might be trapped in a bubble embryo which occurs due to statistical fluctuation in heavy water. The size of the bubble embryo is expected to be an order of a small molecule. The ground state energy level which the deuteron may occupy in the bubble is calculated by solving the Schroedinger equation, and by considering the interaction between the trapped deuteron by a spherical bubble and the surrounding polarized liquid medium (heavy water). From the dependence of the energy eigenvalue of the ground state on the bubble radius, the

pressure exerted on the bubble wall is obtained. It is found that the pressure is negatively very large if the bubble radius is about the molecular size (3 to 7 Å). From extrapolating this result to larger sizes, we expect that a bubble would quickly collapse if enough energy is supplied and never grows to a stable bubble when the deuteron is trapped in the ground state.

BEHAVIOR OF AN ION IN A BUBBLE IN THE GROUND STATE

by

JOUNG HOON OH

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INTRODUCTION

One of the possible models of the so called "cold fusion" is deuterons enclosed in a small bubble. This is the motivation of the present thesis problem.

Historically, a bubble with an electron inside is found to be stable in liquid helium and has been treated theoretically and experimentally (Briscoe, Choi, and Stewart 1968; Burdick 1965). Since the dielectric constant of liquid helium is about unity in the high frequency region, the potential energy of a fast moving electron in a bubble is vanishingly small; therefore the electron can be considered as if it moves freely in a bubble. If the bubble is spherical, then the energy eigenfunction is a spherical Bessel function (Merzbacher 1970), and the ground state energy eigenvalue is given by

$$E = \frac{1}{2\cdot\mu}\cdot\left[\frac{\hbar\cdot\pi}{a}\right]^2 \qquad (1)$$

where μ is the electron mass, a is the radius of the bubble, and $\hbar$ is Planck's constant. The pressure exerted by the electron on the bubble wall can then be given as

$$P = \frac{-1}{4\cdot\pi\cdot a^2}\cdot\left[\frac{dE}{da}\right] = \frac{\hbar^2\cdot\pi^2}{4\cdot\mu\cdot a^5} \qquad (2)$$

This pressure is just enough to sustain the bubble of radius about 15 Å against the atmospheric pressure P_{atm} and the surface tension τ at the bubble wall. Namely,

$$P = P_{atm} + \frac{2 \cdot \tau}{a} \qquad (3)$$

assuming that helium vapor contributes a negligibly small pressure.

The present problem of this thesis is, as stated before, to treat the motion of a deuteron in a bubble, which is in practice a bubble embryo which occurs due to statistical fluctuation in the heavy water. But we may call the bubble embryo simply a bubble, since stable bubbles are hardly expected in heavy water at room temperature, unless there is some mechanism favorable for the bubble formation.

If such a bubble appears in contact with a deuteride metal(palladium), since deuterons are Bosons, two or more deuterons may move from the metal to the same bubble in the same, say, ground level, leading to the possibility of cold fusion. But, treatment of two or more interacting particles in a small bubble is not easy, so for simplicity that we will consider the case of one deuteron in a bubble to obtain some insight.

Since protons are Fermions, they behave statistically differently compared to deuterons, so that we need not pay attention to the behavior of protons in a bubble. But, as long as treatment is limited to a single particle, there is no essential difference between a deuteron and a proton. However, ions other than deuterons and protons usually have complex structures consisting of many particles which introduce complex interactions with surroundings. When considering cold fusion, deuterons seem to be the most interesting particles.

The interaction energy is assumed to be the electrostatic interaction between a point charge on the deuteron and the polarizable medium (which is assumed to be continuous, linear, isotropic, homogeneous, and not to chemically react with a deuteron). This potential energy is obtained by solving Poisson's equation, while ignoring the retardation that is caused by moving ion in a bubble. The bubble-heavy water interface is assumed to be a clean surface without impurities and ions, and the shape of the interface is spherical with a definite radius.

When the dielectric constant of the surrounding medium is infinitely large (a perfect conductor), the polarization charge can be represented by a point image charge. Then, then the potential energy of the deuteron in a bubble can be easily obtained. The Schroedinger equation with this potential energy cannot be analytically solved. Approximate methods, like a WKB approximation, are available. But they still need a numerical computation. In the case of a finite dielectric constant, the potential energy cannot be obtained by an image method and may be expressed in an infinite series. Then, it definitely needs a numerical solution. The trapped deuteron moves rapidly within the bubble and the frequency of the motion is in the order of molecular vibration or lattice vibration of a solid, namely in the range of the infrared light. Thus, the dielectric constant of heavy water to be used for the calculation is assumed to be 2.25 .

The energy eigenfunction in the ground state is usually spherically symmetric for a central field. Thus, we can assume

consistently that the bubble is spherical and the deuteron is present in the ground state. Stability of a thermodynamic system may be discussed by using the free energy. But, when the thermodynamic state of the liquid is far away from a boiling or superheated state, bubble formation is more easily considered in terms of a pressure balance, while ignoring the small vapor pressure. The heavy water is at room temperature, not close to the boiling point. In this thesis, only the pressure exerted by the deuteron on the bubble wall is computed. Then, we qualitatively discuss the stability.

We have found that a similar calculation for an electron in a bubble is numerically much easier, so that the results for an electron is also given in this thesis for comparison.

POTENTIAL ENERGY

We assume that the bubble has a spherical shape. The potential energy V of a deuteron at $\vec{r}$ in a bubble surrounded by a polarizable medium can be written as

$$V = \frac{q}{2} \Phi_{induced} \tag{4}$$

where 1/2 comes from the fact that $\Phi_{induced}$ is the potential at $\vec{r}$ due to polarization charges induced by the point charge q of the deuteron. A point charge q in a bubble is depicted in Figure 1.

The potential can be obtained by solving Poisson's equation with the source q at $\vec{d}$. We assume that the dielectric constant of the polarizable medium is K, and that the dielectric constant inside the bubble unity. Using the spherical coordinate system with the origin at the center of the bubble, the observation point and the source point are denoted by respectively $\vec{r}=(r,\theta,\phi)$ and $\vec{d}=(r,0,0)$. Then the general solution can be written in Gaussian units system, and it follows (Jackson 1975).

For r<a,

$$\Phi_{in} = q \cdot \sum_j \frac{r_<^j}{r_>^{j+1}} \cdot P_j(\cos(\theta)) + \sum_j A_j \cdot r^j \cdot P_j(\cos(\theta)) \tag{5}$$

where $r_<$ ($r_>$) the smaller (larger) between r and d. $P_j(\cos(\theta))$ is

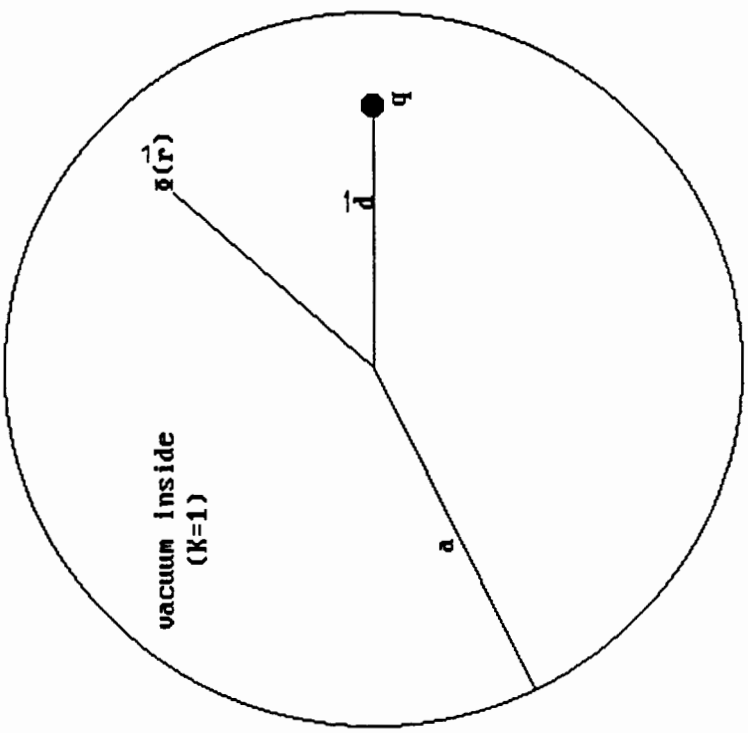

Figure 1. Diagram for an ion in a bubble.

the Legendre polynomial of order j, and θ is an angle between $\vec{r}$ and $\vec{d}$.

For a<r,

$$\Phi_{out} = \sum_j B_j \cdot r^{-(j+1)} \cdot P_j(\cos(\theta)) \tag{6}$$

For r<d, $r_< = r$ and $r_> = d$.

$$\Phi_{in} = q \cdot \sum_j \frac{r^j}{d^{j+1}} \cdot P_j(\cos(\theta)) + \sum_j A_j \cdot r^j \cdot P_j(\cos(\theta)) \tag{7}$$

For d<r, $r_< = d$ and $r_> = r$.

$$\Phi_{in} = q \cdot \sum_j \frac{d^j}{r^{j+1}} \cdot P_j(\cos(\theta)) + \sum_j A_j \cdot r^j \cdot P_j(\cos(\theta)) \tag{8}$$

The coefficients A_j and B_j can be found by applying the boundary conditions at r=a. They are given by

$$\frac{d\Phi_{in}}{dr} = K \cdot \frac{d\Phi_{out}}{dr} \quad \text{and} \quad \frac{d\Phi_{in}}{d\theta} = \frac{d\Phi_{out}}{d\theta} \tag{9}$$

By solving these, we find that

$$A_j = -q \cdot \frac{d^j}{a^{2j+1}} \cdot \frac{(j+1)(K-1)}{K(j+1)+j} \tag{10}$$

$$B_j = -q \cdot d^j \cdot \frac{2j+1}{K(j+1)+j} \tag{11}$$

The second term of Eq.(5) is due to polarization charges and is equivalent to $\Phi_{induced}$. In Eq.(4), this induced

potential is evaluated at the point charge q. Finally, we obtain an expression for the potential energy for the deuteron with a charge q at $\vec{r}=\vec{d}$ inside the bubble. It is thus given by

$$V = \frac{q^2}{2\cdot a}\cdot\sum_j \left[\frac{r}{a}\right]^{2j}\cdot\left[\frac{2j+1}{K(j+1)+j} - 1\right], \qquad 0 \le r < a \qquad (12)$$

Note for the clarification, that the position of a deuteron is denoted by $\vec{r}$ instead of $\vec{d}$, from now on, and this potential energy is central.

When K=1, V must vanish, as expected, since there is no polarization charge. On the other hand, for K=∞, V is reduced to the potential energy for a spherical cavity in a perfect conductor as follow

$$V = \frac{-q^2}{2\cdot a}\cdot\left[\frac{a^2}{a^2 - r^2}\right] \qquad (13)$$

which can be easily obtained by an image method.

SCHROEDINGER EQUATION

The motion of a deuteron in the bubble is found by solving the time independent Schroedinger equation,

$$\frac{-\hbar^2}{2\cdot\mu}\nabla^2\Psi + V\Psi = E\Psi \tag{14}$$

The deuteron is located at $\vec{r}$ from the center of the bubble. Since the electrostatic potential energy V is central and the bubble is spherical, the solution of Schroedinger equation can be expressed by a product of the radial part and a spherical harmonics (Merzbacher 1970). The spherical harmonics is well known, therefore, we only need to be concerned with the following radial part of the Schroedinger equation.

$$R''(r) + \frac{2}{r}\cdot R'(r) + \frac{2\mu}{\hbar^2}\cdot(E - V)\cdot R(r) - \frac{\ell(\ell+1)}{r^2}\cdot R(r) = 0 \tag{15}$$

This equation can be simplified by transformation,

$$R = \frac{X}{r} \tag{16}$$

Then, the radial equation can be written as

$$X''(r) + \frac{2\mu}{\hbar^2}\cdot(E - V)\cdot X(r) - \frac{\ell(\ell+1)}{r^2}\cdot X(r) = 0 \tag{17}$$

We note that, for the ground state, $\ell = 0$. Then the radial equation can be written simply as

$$X''(r) + \frac{2\mu}{\hbar^2} \cdot (E - V) \cdot X(r) = 0 \qquad (18)$$

By solving this equation, with the boundary conditions that X=0 both at r=0 and r=a, we can find the energy eigenvalue for the spherically symmetric state.

NUMERICAL COMPUTATION

We non-dimensionalize the radial equation Eq(17). For $\ell=0$, it can be written as

$$X''(\rho) + 2\,\alpha\,(\epsilon - v)\,X(\rho) = 0 \qquad (19)$$

where dimensionless parameters are defined by

$$\alpha = \frac{a}{a_o}, \qquad V_o = \frac{q^2}{a}, \qquad \rho = \frac{r}{a}, \qquad \epsilon = \frac{E}{V_o}, \qquad v = \frac{V}{V_o}$$

$$a_o = \frac{\hbar^2}{\mu \cdot q^2}$$

It is easy to see that the dimensionless potential energy is given by

$$v = \frac{1}{2} \cdot \sum_{j=0}^{\infty} \rho^{2j} \cdot \left[\frac{2j + 1}{K(j + 1) + j} - 1 \right], \qquad 0 \le \rho < 1 \qquad (20)$$

Dimensionless potential energy v is plotted for the different dielectric constants in Figure 2. Note that the potential energy drops very rapidly near the bubble wall. When K approaches 1, the potential energy vanishes.

Since the dimensionless potential energy v is expressed in infinite series, an analytical solution is not possible. Even in its numerical analysis, the equation is hard to handle unless we use some approximation to the series. If j is large, approximately

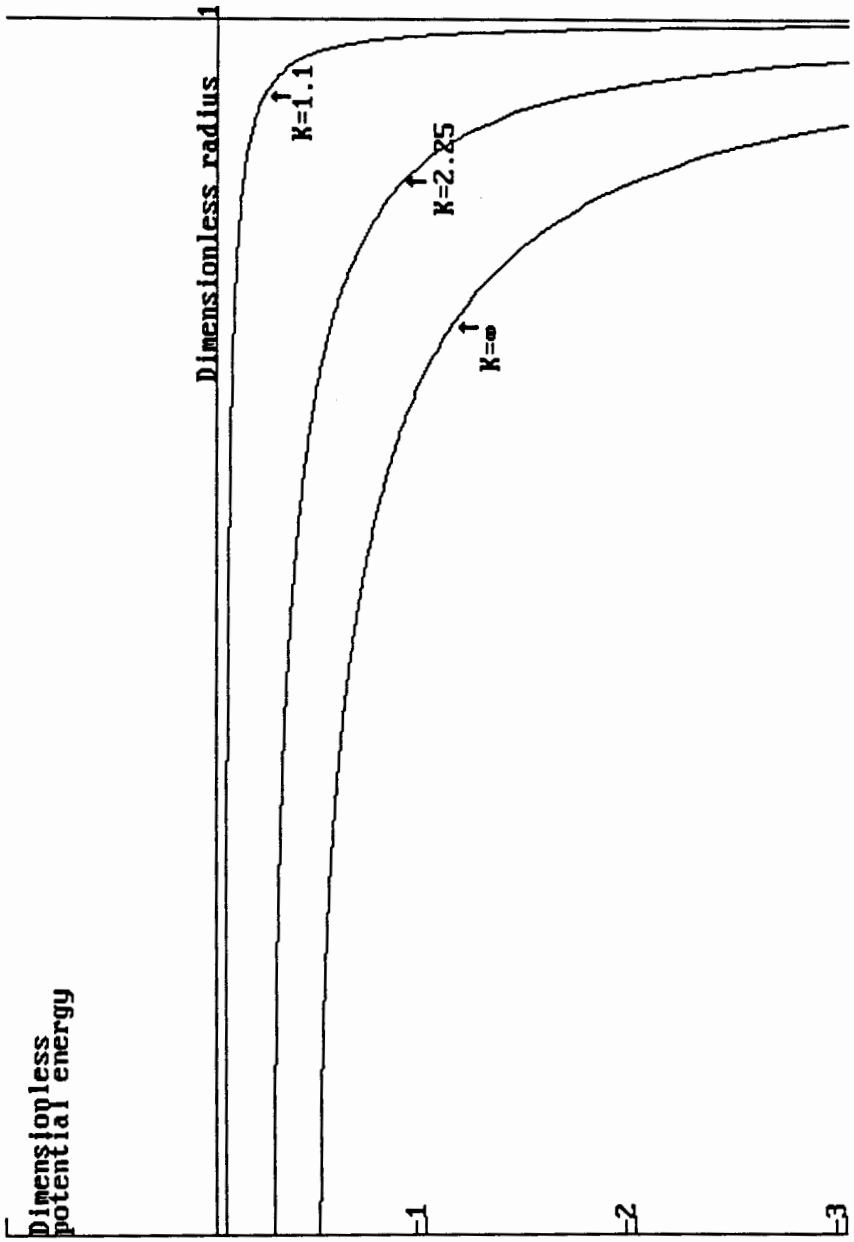

Figure 2. Behavior of potential with different K.

$$\frac{2j + 1}{K(j + 1) + j} \approx \frac{2}{K + 1} \tag{21}$$

If n is a large number, we have approximately

$$v \approx \frac{1}{2} \sum_{j=0}^{n} \frac{2j + 1}{K(j + 1) + j} \cdot \rho^{2j} + \frac{1}{2} \left[\frac{2}{K + 1} \cdot \rho^{2(n+1)} - 1 \right] \cdot \frac{1}{1 - \rho^2} \tag{22}$$

The series of the dimensionless potential energy v terminates at a finite term. n is set equal to 1 in the actual numerical computation in order to limit the long computing time. The maximum error of about 3.5% occurs at about ρ=0.93 due to the truncation as shown in TABLE I. Fortunately this error does not introduce a serious problem in the energy eigenvalue, since the classical turning point occurs at a much large value of ρ for the bubble radius larger 3 Å.

Before proceeding in the numerical computation of Eq.(19), we note a difficulty, which is expected in the computation. If the charge q is +e, α in the is order of 10000. The size of a bubble to be considered is in the order of a few Å. The magnitude of the coefficient of the second term of Eq.(19), 2 α (ϵ - v), is about a million, if (ϵ - v) is -100. In the classically forbidden region, the solution of Eq.(19) then behaves roughly as

$$X \approx \exp\left[\sqrt{\text{million}} \cdot \rho\right] \tag{23}$$

which is out of the range of the number handling capability of the ordinary computer, if ρ is larger than 0.1. Thus, the solution of Eq.(19) easily overflows as ρ increases. One way to avoid the difficulty is to use numerically solve the radial wave equation along increasing ρ, until the solution is near overflow.

TABLE I

ERROR ESTIMATION OF POTENTIAL ENERGY
DUE TO THE TRUNCATED SERIES

Radius	v(n=1)	v(n=1000)	Error(%)
0	-.277778	-.277778	0
.1	-.28007	-.280072	7.90495e-4
.2	-.287189	-.287225	1.26116e-2
.3	-.299944	-.300135	6.35043e-2
.4	-.320002	-.32064	.198916
.5	-.350622	-.352308	.478615
.6	-.398538	-.402437	.968803
.7	-.479677	-.488075	1.72065
.8	-.642036	-.659874	2.7033
.9	-1.12594	-1.16709	3.52566
.9	-1.12594	-1.16709	3.52566
.91	-1.23314	-1.27848	3.54635
.92	-1.36707	-1.41726	3.5417
.93	-1.53916	-1.59506	3.50467
.94	-1.76849	-1.83123	3.42578
.95	-2.08941	-2.16053	3.29184
.96	-2.5706	-2.65239	3.08354
.97	-3.37231	-3.4684	2.77062
.98	-4.97531	-5.09244	2.30012
.99	-9.78344	-9.93825	1.55767
.99	-9.78344	-9.93825	1.55767
.991	-10.8519	-11.0125	1.45899
.992	-12.1874	-12.3546	1.35386
.993	-13.9045	-14.0792	1.24141
.994	-16.1939	-16.3774	1.12048
.995	-19.3991	-19.5929	.989558
.996	-24.2068	-24.4135	.846499
.997	-32.2197	-32.4429	.688033
.998	-48.2453	-48.4919	.508407
.999	-96.3223	-96.6067	.294363
.9999	-961.707	-962.058	3.64493e-2
.99991	-1068.54	-1068.9	3.29064e-2
.99992	-1202.09	-1202.44	2.93417e-2
.99993	-1373.79	-1374.15	2.57549e-2
.99994	-1602.73	-1603.09	2.21456e-2
.99995	-1923.25	-1923.6	1.85136e-2
.99996	-2404.01	-2404.37	1.48585e-2
.99997	-3205.3	-3205.66	.01118
.99998	-4807.86	-4808.22	7.4776e-3
.99999	-9615.55	-9615.91	3.75106e-3

Then, we arbitrarily reduce the magnitude and slope of the solution at that point by a same factor and restart the computation following the same procedure of solving the equation, and so on. In order to eliminate this complicated method, another procedure is possible as illustrated in APPENDIX A. However, for the case of an electron instead of a deuteron, Eq.(19) is unlikely to introduce overflow in the numerical analysis unless the bubble size is very large.

The potential energy has a singularity at $\rho=1$. Therefore, in numerically solving Eq.(19), the series expansion method may be used around $\rho=1$. Then the solution of radial part of the wave function obtained by starting from the origin, $\rho=0$, is smoothly connected to the expansion near singularity at $\rho=1$. The series expansion around the singularity can be written as

$$X(\rho) = a0\cdot(1-\rho) + a1\cdot(1-\rho)^2 + a2\cdot(1-\rho)^3 \quad ..... \quad (24)$$

If ρ is close enough to 1, then second, and higher terms of the series expansion can be neglected, so that we have

$$X(\rho) = a0\ (1-\rho) \quad (25)$$

where a0 is associated with the normalization constant but not with ϵ.

For numerical computation, the 5th-order stepsize control Runge-Kutta-Fehlberg (RKF) method (Gerald and Wheatley 1984) was used. The computer program written in True Basic is listed in APPENDIX B.

In this program, the bubble radius a, which is unity in the dimensionless expression, is divided into many small divisions, each of which may be called a step. The size of each

step is controlled by the relative difference between the 4th- and 5th-order-solution. Then the error can be given by

For |5th_order_solution| ≥ |4th_order_solution|,

$$\text{Error} = 1 - \left|\frac{\text{4th\_order\_solution}}{\text{5th\_order\_solution}}\right| \tag{26}$$

For |4th_order_solution| > |5th_order_solution|,

$$\text{Error} = 1 - \left|\frac{\text{5th\_order\_solution}}{\text{4th\_order\_solution}}\right| \tag{27}$$

We assume that the denominators in Eq.(26) and Eq.(27) are not zero. The value of the error is compared with a critical number (tolerance) chosen in order to secure a desired number of significant digits. The value of the tolerance is 10^(-N), where N is a given number. And the number N is in between 6 to 10 depending on the case in question (an electron, or a deuteron bubble size). If the tolerance is met, then the stepsize is increased by 1.4 times, and the 5th-order-solution gives desired solution. If the tolerance is not met, then the stepsize is decreased by 1.4 times, and the solutions are recalculated until the tolerance is met. A "double precision" method was used throughout. In this way, the number of significant digits in eigenvalue was kept to be more than seven or eight in many cases. Such a precision seems to be required for finding pressures exerted by the deuteron on the bubble wall.

The numerical calculation of pressure of the bubble of radius a was made by using the relation,

$$\text{Pressure} = -\left[\frac{1}{4\cdot\pi\cdot a^2}\right]\cdot\left[\frac{E(a+\delta a) - E(a)}{\delta a}\right] \tag{28}$$

where E(a) and E(a + δa) are the energy eigenvalues for the values of the radius a and a + δa, respectively. δa is a small change of the radius. The change δa was chosen to be $\pm$0.001 for the most cases. If the results in pressure with δa= $\pm$0.001 are not nearly the same at least in the order of magnitude, the size of δa may be made smaller and the precision in computation of E(a) and E(a + δa) is increased.

RESULT AND DISCUSSION

In the case of the deuteron in a bubble, TABLES II and III give energy eigenvalues and pressures for the different bubble sizes. In case of an electron in a bubble, TABLE IV gives the energy eigenvalues and pressure as a function of the different bubble size. The pressure is plotted with respect to in Figure 3. Plotting gets difficult when it comes to the deuteron as an ion, because the change of energy or pressure is very steep with respect to the change of bubble size.

The general behavior of a deuteron in the ground state may be suggested by that for an electron in a bubble. When the bubble size increases to infinity, the energy eigenvalue approaches zero. As the bubble size decreases, the energy eigenvalue very slowly decreases to a minimum (-2.252 eV at 13.5 Å for an electron) and then the energy eigenvalue increases rather rapidly as the size further decreases.

Since the pressure exerted by the electron on the bubble wall is closely related to the slope of the energy profile plotted against the bubble radius, the behavior of the pressure should follow the similar profile with exhibition of a minimum at a certain bubble radius.

The behavior of the energy profile also reflects on the free energy of the system. The equilibrium condition at constant temperature is roughly given by

TABLE II

ENERGY EIGENVALUE AND PRESSURE FOR A BUBBLE OF DIFFERENT SIZE WITH A DEUTERON

1st column is written in the unit of Å.
2nd column is written in the unit of eV.
3rd column is written in the unit of atm.

Bubble size(Å)	Energy(eV)	Pressure(atm)
5.30005e-5	3.54155e+6	6.15723e+24
1.73753e-3	8.27017	8.59092e+16
2.99695e-3	-883.926	1.98786e+15
3.71005e-3	-924.363	7.82573e+12
3.73651e-3	-924.351	-1.60643e+13
3.76305e-3	-924.27	-3.82977e+13
3.89551e-3	-922.957	-1.27369e+14
.004081	-919.007	-2.05154e+14
4.25628e-3	-913.573	-2.44806e+14
5.30005e-3	-865.827	-2.28445e+14
5.30053e-2	-506.887	-3.8377e+10
.530005	-466.151	-3.949e+6
1.59053	-462.924	-61790.6
2.64947	-461.971	-13579.
3.71053	-461.209	-6639.9
5.30053	-459.999	-3705.52
7.95053	-457.538	-2096.26

TABLE III

ENERGY EIGENVALUE AND PRESSURE FOR A BUBBLE OF DIFFERENT SELECTED SIZE WITH A DEUTERON

1st column is written in the unit of Bohr radius(0.53 Å).
2nd column is written in the unit of Å.
3rd column shows the energy in the unit of eV.
4th column shows the pressure in the unit of atm.

For the bubble size 2.65 Å

Bubble size		Energy	Pressure
5.000	2.65000	-461.970699	
5.005	2.65265	-461.968591	-14426.3561
5.001	2.65053	-461.970303	-13535.7092
4.999	2.64947	-461.971095	-13578.9793
4.998	2.64894	-461.971498	-13694.3349

For the bubble size 3.71 Å

Bubble size		Energy	Pressure
7.000	3.71000	-461.209755	
7.001	3.71053	-461.209375	-6639.8961
6.999	3.70947	-461.210135	-6642.0774

For the bubble size 5.3 Å

Bubble size		Energy	Pressure
10.000	5.30000	-459.99944	
10.001	5.30053	-459.99901	-3705.5235
9.999	5.29947	-459.99987	-3716.1246

For the bubble size 7.95 Å

Bubble size		Energy	Pressure
15.000	7.95000	-457.5388334	
15.001	7.95053	-457.5382826	-2096.2646

TABLE IV

ENERGY EIGENVALUE AND PRESSURE FOR A BUBBLE OF DIFFERENT SIZE WITH AN ELECTRON

1st column is written in the unit of Å.
2nd column shows the energy in the unit of eV.
3rd column shows the pressure in the unit of atm.

For the bubble size 1 Å

Bubble size	Energy	Pressure
1	31.9529026	
.99999	31.95359916	8879101.53
1.00001	31.95220621	8878650.10

For the bubble size 7 Å

Bubble size	Energy	Pressure
7	-.075177149	
6.99990	-.075166715	271.45478
6.99999	-.075176105	271.44409
7.00001	-.075178192	271.44171
7.00010	-.075187582	271.43111

For the bubble size 12 Å

Bubble size	Energy	Pressure
12	-.24791465126	
12.00001	-.247914701	4.417728844
11.99999	-.247914601	4.417763320

For the bubble size 12.5 Å

Bubble size	Energy	Pressure
12.5	-.24991215927	
12.50001	-.249912190	2.50859812
12.49999	-.249912128	2.50862235

TABLE IV

ENERGY EIGENVALUE AND PRESSURE FOR A BUBBLE OF DIFFERENT SIZE WITH AN ELECTRON (continued)

1st column is written in the unit of Å.
2nd column shows the energy in the unit of eV.
3rd column shows the pressure in the unit of atm.

For the bubble size 13.5 Å

Bubble size	Energy	Pressure
13.5	-.25151637239	
13.50001	-.251516375	.23893208
13.49999	-.251516368	.23894752

For the bubble size 14.2 Å

Bubble size	Energy	Pressure
14.2	-.251279900	
14.20001	-.251279891	-.59933230
14.19999	-.251279910	-.59931170

For the bubble size 15 Å

Bubble size	Energy	Pressure
15	-.25007951123	
14.99999	-.250079531	-1.12650101
15.00001	-.250079491	-1.12653235

For the bubble size 18 Å

Bubble size	Energy	Pressure
18	-.24105203386	
17.99999	-.241052069	-1.41543921
18.00001	-.241051997	-1.41546694

TABLE IV

ENERGY EIGENVALUE AND PRESSURE FOR A BUBBLE OF DIFFERENT SIZE WITH AN ELECTRON (continued)

1st column is written in the unit of Å.
2nd column shows the energy in the unit of eV.
3rd column shows the pressure in the unit of atm.

For the bubble size 20 Å

Bubble size	Energy	Pressure
20	-.23366303	
19.9999000	-.23366341	-1.1866355
19.9999900	-.23366307	-1.1866194
20.0000001	-.23366303	-1.1866057
20.0000100	-.23366300	-1.1866237
20.0001000	-.23366266	-1.1866220

For the bubble size 30 Å

Bubble size	Energy	Pressure
30	-.2024277845	
30.00001	-.2024277605	-.340645170

For the bubble size 60 Å

Bubble size	Energy	Pressure
60	-.16483998543	
59.999990	-.16483999182	-.022611762
60.000001	-.16483998479	-.022611849
60.000010	-.16483997905	-.022611961

For the bubble size 200 Å

Bubble size	Energy	Pressure
200.0	-.13761866565	
200.00001	-.13761866506	-.00018794

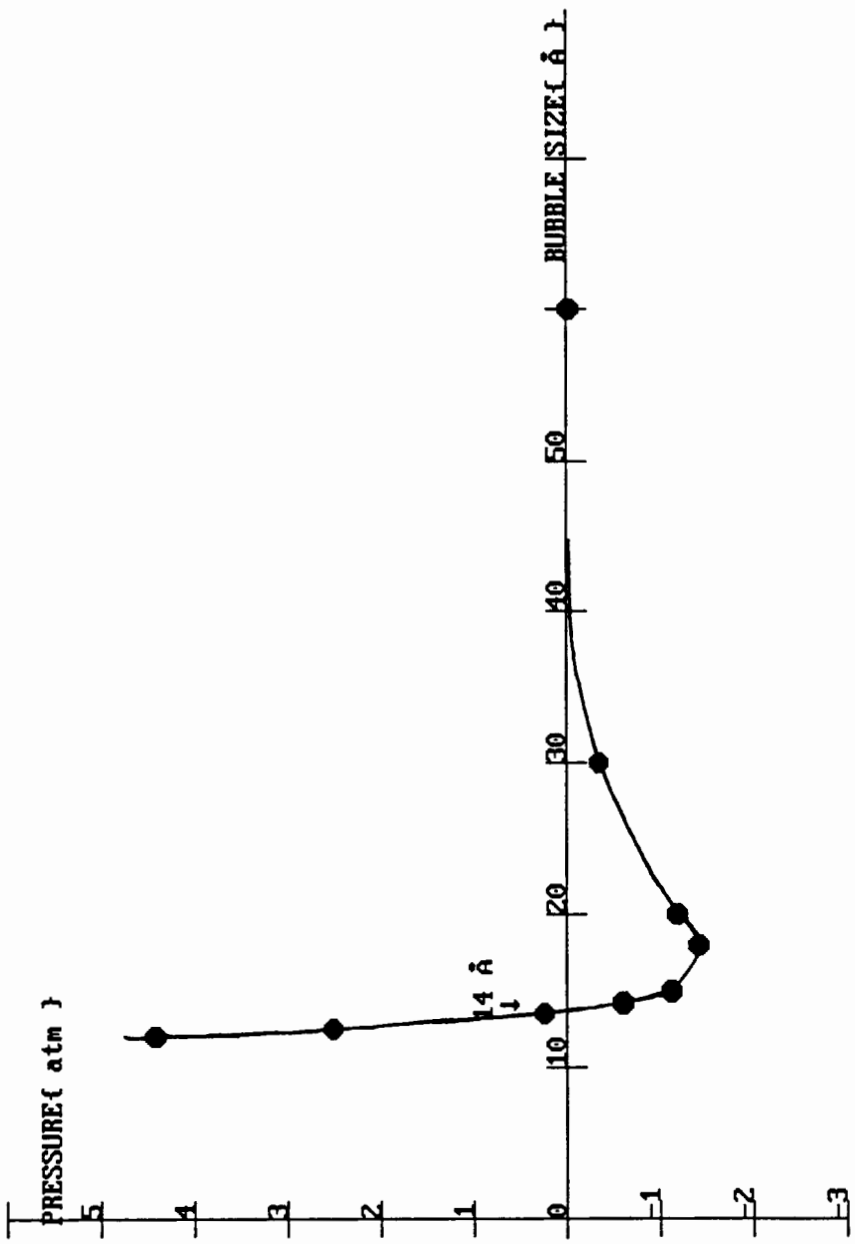

Figure 3. Pressure vs bubble size for an electron in a bubble.

$$P_{electron} = P_{atm} + \frac{2 \cdot \tau}{a} \qquad (29)$$

by ignoring the vapor pressure of the liquid. This relation may be satisfied at a certain bubble size analogous to the system of an electron in a bubble in liquid helium. For heavy water with an electron, the bubble can be stable at the radius where the free energy is minimum. But a stable bubble with an electron may not occur because electrons are more likely to attach to the surrounding molecules (except for the case of helium).

The equilibrium condition for a deuteron in heavy water does not occur in practice due to another reason. The predicted stable size is too small (0.0037 Å). Namely, if one deuteron is present in a practical bubble embryo, the bubble will collapse if enough energy is supplied; it will never grow to a stable bubble. However, if two or more deuterons, which are Bosons, are present somehow in the same bubble, the situation might change due to the Coulomb repulsion among the deuterons. At the same time, if the pressure remains negatively and large for the many-deuteron case, the negative pressure confines the deuterons in a small volume. Of course, this model may need the presence of an electron or electrons inside the bubble to neutralize to some extent the repulsive force among the deuterons.

The classical turning point for the motion of a deuteron in the bubble of a molecular size(3 to 7 Å) is located very close to the bubble wall as shown in TABLE V. The deuteron within this narrow region moves fast. This feature will enhance confining of many deuterons in a small region.

TABLE V

DISTANCE BETWEEN THE CLASSICAL TURNING POINT AND THE BUBBLE WALL WITH THE DEUTERON

Bubble size	Non-Tp	Tp	Trap distance
1.59	.998112	1.587	3.00122e-3
2.65	.998867	2.647	3.00346e-3
5.3	.999431	5.29699	3.01335e-3
7.95	.999619	7.94697	3.02856e-3

1st column is written in the unit of Å.
2nd column shows the dimensionless classical turning point.
3rd column shows the classical turning point, and is written in the unit of Å
4th column shows the distance between the classical turning point and the bubble wall, and is written in the unit of Å.

CONCLUSION

We have treated a model of an electron or a deuteron in a bubble. The surrounding medium has a finite dielectric constant (K=2.25). For simplicity, we treated only the case of a spherical symmetry, so that the bubble is spherical, and the system is in the spherically symmetric ground state (ℓ=0). For a deuteron case, energy level is about -460 eV and pressure exerted by the particle on the bubble is negatively so high that the bubble collapses if enough energy is supplied. For an electron case, energy level is about -0.25 eV and pressure is zero around the bubble size of 14 Å.

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APPENDIX A

TRANSFORMATION OF SCHROEDINGER EQUATION

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TRANSFORMATION OF SCHROEDINGER EQUATION

In order to avoid the overflow and underflow, we introduce the transformation into the Schroedinger equation that is written as follow

$$X'' + 2\,\alpha\,(\epsilon - v(\rho))\,X = 0$$

By transforming

$$X = \rho\,\exp(Y)$$

where $Y = \ln(\,b0 + b1\,\rho + b2\,\rho^2 \ldots\ldots\,)$. Then, the transformed Schroedinger equation can be written as

$$\rho\,Y'' + \rho\,(Y')^2 + 2\,Y' + 2\,\alpha\,(\epsilon - v(\rho))\,\rho = 0$$

with the initial conditions $Y=\ln(b0)$ and $Y'=0$ at $\rho=0$. By taking another transformation

$$W = \frac{dY}{d\rho}$$

A first order non-linear differential equation can be obtained as follow

$$\rho\,W' + \rho\,W^2 + 2\,W + 2\,\alpha\,\rho\,(\epsilon - V(\rho)) = 0$$

with the initial condition at $W=0$ at $\rho=0$. The above equation can be treated more easily in the numerical computation, since the growing exponential part is eliminated.

APPENDIX B

COMPUTER PROGRAM

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COMPUTER PROGRAM

```
SET MODE"80"
DECLARE DEF ASM,POT
DIM Y1(0:5000),Y2(0:5000),T(0:5000)
DECLARE DEF F1,F2
!-------------------------------------------------------
LET TOLR=10                              !TOLR=TOLERANCE CONTROL
                                              FOR RKF
LET TI=0                                 !TI=INITIAL DIMENSIONALESS
                                             RADIUS
LET MTF=0

LET TF=0.99999                           !TF=FINAL DIMENSIONALESS
                                             RADIUS
LET BAL=1                                !BAL=FACTOR FOR AVOIDING
                                              OVERFLOW
LET YI=0                                 !YI=INITIAL POSITION AT TI
LET YF=ASM(TF)                           !YF=FINAL POSITION AT TF
LET T(0)=TI
LET Y1(0)=YI                             !Y1(0)=INITIAL POSITION
LET Y2(0)=2.8346485574616*10^4           !Y2(0)=INITIAL SLOPE
LET EIG=-0.2381610614444919              !EIG=DIMENSIONLESS ENERGY
!-----------------------------
LET A0=10^(5)                            !A0=NORMALIZATION CONSTANT
LET K=2.25                               !K=DIELECTRIC CONSTANTS
LET Q=4.80325*10^(-10)                   !Q=CHARGE ;{ESU}
LET AE=0.53*10^(-8)                      !AE=BOHR RADIUS{ANGSTROM}
LET ALPHA=3674.7685*0.007001             !ALPHA=DIMENSIONLESS
                                                BUBBLE  SIZE
LET A=ALPHA*AE/3674.7685                 !A=BUBBLE SIZE
!-------------------------------------------------------
CALL ADPMTF(T(),MTF,TF,BAL,Y1(),Y2(),MM,EIG,TOLR)
CALL PRINA(T,Y1,Y2,MM,TOLS,TOLR)
CALL SOLUTION(A,AE,EIG,Q,K)
!-------------------------------------------------------
DEF F1(V1,V2,T,EIG)=V2
DEF F2(V1,V2,T,EIG)
    LET F2=-2*ALPHA*[EIG -POT(T,K)]*V1
END DEF
!-------------------------------------------------------
DEF ASM(R)
    LET ASM=A0*(1-R)
END DEF
!-------------------------------------------------------
DEF POT(TA,K)                            !POT=POTENTIAL ENERGY
    LET AAA=0
    LET n=1
    FOR S=0 TO n
        LET AOLD=AAA
```

```
        LET AAA=(2*S+1)/(K*(S+1)+S)*TA^(2*S)
        LET AAA=AAA+AOLD
    NEXT S
    LET GG2=[ 2/(K+1)*TA^(2*(n+1))  -1]/(1-TA^2)
    LET POT=(AAA+GG2)*0.5
END DEF
!-------------------------------------------------------------
SUB ADPMTF(T(),MTF,TF,BAL,Y1(),Y2(),MM,N1,TOLR)
    CALL ADP_DD2(T(),MTF,Y1(),Y2(),M,N1,TOLR)
    LET T(0)=MTF
    LET Y1(0)=Y1(M)/BAL/BAL
    LET Y2(0)=Y2(M)/BAL/BAL
    CALL ADP_DD2(T(),TF,Y1(),Y2(),MM,N1,TOLR)
END SUB
!-------------------------------------------------------------
SUB ADP_DD2(T(),TF,Y1(),Y2(),M,N1,TOLR)
    IF TF=T(0) THEN EXIT SUB
    LET H=ABS(TF-T(0))/100
    LET J=0
    DO WHILE T(J) < TF
       CALL ARKFDD2(T,Y1(),Y2(),H,J,UFO1,UFO2,N1)
       IF ABS(UFO1)<=ABS(UFO2) THEN
          LET ERROR=[ 1-ABS(UFO1/UFO2) ]
       ELSE
          LET ERROR=[ 1-ABS(UFO2/UFO1) ]
       END IF
       !-----------------------------
       IF ERROR<10^(-TOLR) THEN
          LET J=J+1
          LET T(J)=T(J-1)+H
          LET H=H*1.4
          LET Y1(J)=UFO2
       ELSE
          LET H=H/1.4
       END IF
    LOOP
    LET M=J
    LET HT=TF-T(M-1)
    LET T(M)=TF
    CALL ARKFDD2(T,Y1,Y2,HT,M-1,0,UFO2,N1)
    LET Y1(M)=UFO2
END SUB
!-------------------------------------------------------------
SUB ARKFDD2(T(),Y1(),Y2(),HH,J,UFO1,UFO2,N1)
    LET TT=T(J)
    LET V1=Y1(J)
    LET V2=Y2(J)
    LET A1  = F1(V1,V2,TT,N1)*HH
    LET A2  = F2(V1,V2,TT,N1)*HH
    !-----------------------------------------------------
    LET TT= T(J)  + 0.25*HH
    LET V1= Y1(J) + 0.25*A1
    LET V2= Y2(J) + 0.25*A2
    LET B1= F1(V1,V2,TT,N1)*HH
    LET B2= F2(V1,V2,TT,N1)*HH
    !-----------------------------------------------------
    LET TT= T(J)  + 3/8*HH
```

```
    LET V1= Y1(J) +[ 3/32*A1 + 9/32*B1]
    LET V2= Y2(J) +[ 3/32*A2 + 9/32*B2]
    LET C1= F1(V1,V2,TT,N1)*HH
    LET C2= F2(V1,V2,TT,N1)*HH
    !-----------------------------------------------------
    LET TT= T(J)  + 12/13*HH
    LET V1= Y1(J) +[1932/2197*A1 - 7200/2197*B1 + 7296/2197
                    *C1]
    LET V2= Y2(J) +[1932/2197*A2 - 7200/2197*B2 + 7296/2197
                    *C2]
    LET D1= F1(V1,V2,TT,N1)*HH
    LET D2= F2(V1,V2,TT,N1)*HH
    !-----------------------------------------------------
    LET TT= T(J)  + HH
    LET V1= Y1(J) + [439/216*A1 - 8*B1 + 3680/513*C1 -
                     845/4104*D1]
    LET V2= Y2(J) + [439/216*A2 - 8*B2 + 3680/513*C2 -
                     845/4104*D2]
    LET E1= F1(V1,V2,TT,N1)*HH
    LET E2= F2(V1,V2,TT,N1)*HH
    !-----------------------------------------------------
    LET TT= T(J)  + 0.5*HH
    LET V1= Y1(J)+[-8/27*A1+2*B1 - 3544/2565*C1+ 1859/4104
                                  *D1-11/40*E1]
    LET V2= Y2(J)+[-8/27*A2+2*B2 - 3544/2565*C2+ 1859/4104
                                  *D2-11/40*E2]
    LET G1= F1(V1,V2,TT,N1)*HH
    LET G2= F2(V1,V2,TT,N1)*HH
    !-----------------------------------------------------
    LET UFO1=Y1(J)+(25/216*A1+1408/2565*C1+2197/4104*D1-1/5
                    *E1)
    LET UFO2=Y1(J)+(16/135*A1+6656/12825*C1+28561/56430*D1
                    -9/50*E1+2/55*G1)
    LET Y2(J+1)=Y2(J)+(16/135*A2+6656/12825*C2+28561/56430
                    *D2-9/50*E2+2/55*G2)
END SUB
!-------------------------------------------------------------
SUB SOLUTION(A,AE,EIG,Q,K)
    LET E=(Q^2/A)*EIG/[1.602*10^(-12)]
    LET AOO=10^(-8)
    PRINT "  K=  ";K
    PRINT "EIG=  ";
    PRINT USING "+#.########^^^^^":EIG
    PRINT " Ao=  ";
    PRINT USING "+#.########^^^^^":A/AE;
    PRINT " Bohr radius"
    PRINT "  A=  ";
    PRINT USING "+#.########^^^^^":A/AOO;
    PRINT " angstrom"
    PRINT "  E=  ";
    PRINT USING "+#.########^^^^^":E;
    PRINT " eV"
END SUB
```

```
SUB PRINA(T(),Y1(),Y2(),NN,TOLS,TOLR)
    PRINT "NN= ";NN, "H= ";(T(NN)-T(0))/NN
    FOR J=0 TO 2
        IF J=0   THEN SET COLOR 7
        IF J=0   THEN PRINT "T(J)";TAB(16);"Y1";
                           TAB(30);"Y2"
        SET COLOR 18
        PRINT T(J);TAB(14);Y1(J);TAB(28);Y2(J)
    NEXT J
    !-----------------------------
    SET COLOR 4
    FOR J=NN-3 TO NN
        IF J=NN-3 THEN SET COLOR 7
        IF J=NN-3 THEN PRINT "T(J)";TAB(16);"Y1";TAB(30);
                           "Y2";TAB(45);"ASM"
        IF J=NN THEN
           SET COLOR 14
           PRINT T(J);TAB(14);Y1(J);TAB(28);Y2(J);TAB(43);
                           ASM(T(J))
        ELSE
           SET COLOR 4
           PRINT T(J);TAB(14);Y1(J);TAB(28);Y2(J);TAB(43);
                           ASM(T(J))
        END IF
    NEXT J
    PRINT
    SET COLOR 2
    PRINT "Y1(NN)     =";
    SET COLOR 2
    PRINT USING "+#.#########^^^^^":Y1(NN)
    SET COLOR 4
    PRINT "ASM(T(NN))=";
    SET COLOR 2
    PRINT USING "+#.#########^^^^^":ASM(T(NN))
    PRINT
    PRINT "A0         =";
    SET COLOR 2
    PRINT USING "+#.#########^^^^^":ABS(A0)
    SET COLOR 4
    PRINT "Y2(NN)     =";
    SET COLOR 2
    PRINT USING "+#.#########^^^^^":ABS(Y2(NN))
    PRINT
    PRINT "TOL FOR A-RKF= ";TOLR
END SUB
END
```