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LETTER TO THE EDITOR

A CALCULATION OF THE GROUND ENERGY OF LIQUID ^{4}He BY THE CELLULAR METHOD

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The ground state energy of liquid ^{4}He has been calculated by several methods. In this paper we apply cellular method, which in the theory of solids is also known as the Wigner-Seitz method[1].

We define a cell by effective free volume per particle. For the sake of simplicity we take as boundary of the cell a sphere. We assume uniform distribution of particles on the sphere and consider motion of a particle inside the sphere with the boundary condition

$$\left(\frac{\partial \psi}{\partial r}\right)_R = 0. \tag{1}$$

Potential in the cell. The interaction between ^{4}He atoms we take to be given by the Yntema-Schneider potential[2]

$$V(r) = \begin{cases} A\,\mathrm{e}^{-\alpha r}, & r < r_a \\ A\,\mathrm{e}^{-\alpha r} - \frac{a}{r^6} - \frac{b}{r^8}, & r > r_a \end{cases}, \tag{2}$$

where r_a is of order of the atomic radius and $A = 1\,200 \cdot 10^{-12}$ ergs, $\alpha = 1/0.212$ Å^{-1}, $a = 1.24 \cdot 10^{-12}$ ergs, $b = 1.89 \cdot 10^{-12}$ ergs; r is in Angstroms. The region $r \leq r_a$, as known, can be left out from the consideration. The choice of the potential is of no importance in the method.

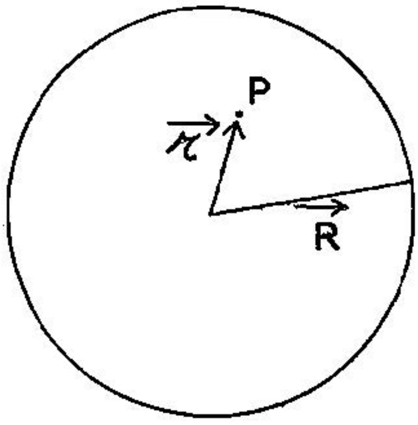

Fig. 1.

Crystal structure of ^{4}He atoms is hexagonal close packed. The number of the first neighbors is then twelve. Thus we take twelve ^{4}He atoms and make uniform distribution of them over a sphere of a radius R (Fig. 1). The potential energy of an atom inside the sphere at the point P due to the presence of twelve uniformly distributed atoms on the sphere is then

$$V(r) = \frac{n_s}{4Rr} \cdot \begin{cases} \frac{2A}{a^2}\left[e^{-a(R-r)} \cdot (aR - ar + 1) - e^{-a(R+r)} \cdot (aR + ar + 1)\right] - \\ - \frac{a}{2}\left(\frac{1}{(R-r)^4} - \frac{1}{(R+r)^4}\right) - \frac{b}{3}\left(\frac{1}{(R-r)^6} - \frac{1}{(R+r)^6}\right), \\ \qquad R - r \geq 1\ (\text{Å}), \\ \frac{2A}{a^2}\left[e^{-a(R-r)} \cdot (aR - ar + 1) - e^{-a(R+r)}(aR + ar + 1)\right), \\ \qquad R - r < 1\ (\text{Å}), \end{cases} \tag{3}$$

where $n_s = 12$.

Ground state energy. Since we are interested in the ground state energy we look for the radial solution of the equation only

$$\left(-\frac{\hbar^2}{2m}\Delta + V\right)\psi = E\psi, \tag{4}$$

that means of the equation

$$\left[-\frac{\hbar^2}{2m}\left(\frac{d^2}{dr^2} + \frac{2}{r}\frac{d}{dr}\right) + \frac{1}{2}V(r)\right]\varphi(r) = E\,\varphi(r), \tag{5}$$

with boundary condition (1) and the potential (3).

We apply the variational procedure

$$\varphi(r) = \varphi_1(r) \cdot \varphi_2(r), \tag{6}$$

where $\varphi_1(r)$ is the asymptotic wave function near the boundary and $\varphi_2(r)$ a variational wave function inside the sphere.

The function $\varphi_1(r)$ is determined by the equation

$$\left[-\frac{\hbar^2}{2m}\left(\frac{d^2}{dr^2}+\frac{2}{r}\frac{d}{dr}\right)+\frac{1}{2}V_{r\to R}(r)\right]\varphi_1(r)=0, \quad r \to R. \tag{7}$$

The solution of this equation is[3]

$$\varphi_1(r) = e^{-C\cdot e^{-\beta(R-r)}}, \tag{8}$$

where $C = 441.44/R\beta$.

We determine the function $\varphi_2(r)$ by its behaviour near the point $r = 0$ and a factor $e^{-\gamma(r-r_0)^2}$ which has to take care of the motion in the rest of the region.

The variational function is therefore

$$\varphi(r) = \frac{\sin \delta r}{r} e^{-\gamma(r-r_0)^2} e^{-Ce^{-\beta(R-r)}}, \tag{9}$$

where δ, γ, and β are variation parameters and r_0 is the point of minimum of the potential.

The expectation value of the energy for the wave function (9) is

$$\frac{E}{N} = \Bigg\{-8.3678 \cdot 10^{-16} \int_0^R \sin^2 \delta r \, e^{-2\gamma(r-r_0)^2} e^{-\frac{882,88}{\beta R} e^{-(R-r)}}$$

$$\cdot \left[-\delta^2 - 2\gamma + 4\gamma^2 (r-r_0)^2 + \frac{441,44}{R}(4\gamma r - 4\gamma r_0 - \beta) e^{-\beta(R-r)} + \right.$$

$$\left. + \frac{441.44}{R^2} e^{-2\beta(R-r)} - \operatorname{ctg} \delta r \cdot \left(4\gamma\delta r - 4\gamma\delta r_0 + \frac{882,88}{R} \cdot \delta \cdot e^{-\beta(R-r)}\right)\right] dr +$$

$$+ 1.5 \cdot 10^{-12} \int_0^{R-1} \sin^2 \delta r \, e^{-2\gamma(r-r_0)^2} e^{-\frac{882,88}{\beta R} e^{-\beta(R-r)}} \cdot \frac{1}{R \cdot r} \cdot$$

$$\cdot \Big[107{,}8656\,(e^{-a(R-r)}(aR - ar + 1) - e^{-a(R+r)}(aR + ar + 1)) -$$

$$- 0{,}62\left(\frac{1}{(R-r)^4} - \frac{1}{(R+r)^4}\right) - 0.63\left(\frac{1}{(R-r)^6} - \frac{1}{(R+r)^6}\right)\Big]\, dr +$$

$$+ 161.798 \cdot 10^{-12} \int\limits_{R-1}^{R} \sin^2 \delta r\, e^{-2\gamma(r-r_0)^2}\, e^{-\frac{882{,}88}{\beta R}\cdot e^{-\beta(R-r)}} \cdot$$

$$\cdot \frac{1}{Rr}\left[e^{-a(R-r)}(aR - ar + 1) - e^{-a(R+r)}(aR + ar + 1)\right] dr\Big\} :$$

$$: \int\limits_{0}^{R} \sin^2 \delta\, r\, e^{-2\gamma(r-r_0)^2} \cdot e^{-\frac{882{,}88}{\beta R}\cdot e^{-\beta(R-r)}}\, dr. \tag{10}$$

Varying the parameters and performing calculations of the right side we obtain the energy minimum

$$E/N = -\,2.73 \cdot 10^{-16} \text{ ergs}$$

for the values of parameters

$$\beta = 1.62, \qquad \gamma = 0.06, \qquad \delta = 0.52,$$

and $R = 4.01$ Å (R is determined from the experimental density). The experimental value of $E/N = -\,9.73 \cdot 10^{-16}$ ergs is more than three times smaller. This result is reasonable because in the cell method the short range correlation motion is not properly taken into account due to the uniform distribution of atoms on the sphere. But still the result shows that the method can be used in the theory of ^{4}He liquid particularly where quantitative values are not of first importance. We do not discuss here other results reported for example in Refs. [3,4,5,6] as procedures are basically different.

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