

## Many – Body Theory of Solid ${}^4_2\text{He}$

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### Abstract

The t – matrix formalism of many – body theory has been used to calculate the total energy  $E$  of helium,  ${}^4_2\text{He}$  in its solid state or crystalline state. The interaction potential between the two helium atoms is assumed to be a two – body interaction potential composed of a hard – core followed by a square well. Zero – point energy (ZPE),  $\epsilon_0$ , in the crystalline state has been calculated using the Heisenberg's uncertainty principle. The energy,  $V$ , due to the inter – particle interaction has also been calculated. When the width,  $b$ , of the square well potential is  $5.1 \text{ \AA}$ , the ratio,  $\frac{\epsilon_0}{E}$  is 94 per cent, and when the value of  $b = 4.9 \text{ \AA}$ , the ratio is approximately 98 per cent.

**Keywords:** *t – matrix formalism, zero point energy, hexagonal close - packing, anharmonicity, phonons.*

### 1. Introduction

Helium was first solidified<sup>1</sup> by W.H. Keesom in Leiden in 1926. Experiments conducted by Sir Francis Simon and Keesom concentrated on the study of melting curve, the specific heat, and the thermal conductivity of solid  ${}^4_2\text{He}$ . Their measurements showed that the Lindemann criteria by Lindemann ratio of  $\delta = \frac{a^2}{\sigma}$  (where  $a$  is the mean square vibrational amplitude, and  $\sigma$  is hard – sphere diameter) does not hold in solid helium at melting.

Cooling of liquid  ${}^4_2\text{He}$  towards absolute zero temperature does not result in the solidification of  ${}^4_2\text{He}$  liquid. However,  ${}^4_2\text{He}$  becomes solid<sup>2</sup> under large external pressure of the order of 25 atmospheres or more in the limit  $T \rightarrow 0$ . At very high pressure, the liquid helium can become a high density liquid resulting in solidification, or crystallization, and can go to close packing that could be either face centred cubic (FCC) or hexagonal close-packing (HCP)<sup>3</sup>. At very high pressure,  $P = 4.9 \text{ kbar}$ ,  ${}^4_2\text{He}$  can be compressed<sup>4,5,6</sup> into close – packed (FCC and HCP) with volume  $V = 9.03 \text{ cm}^3 / \text{mole}$ , and interaction space of the linear lattice  $R = 2.11 \text{ \AA}$ .

In the solid phase,  ${}^4_2\text{He}$  in the crystalline state behaves like a quantum solid. Now in physics, a quantum solid (like crystalline  ${}^4_2\text{He}$ ) is the type of solid that is intrinsically restless in the sense that atoms continuously vibrate about their position and exchange places even at absolute zero of temperature. The typical quantum solid, both in low density and high density, is the solid  ${}^4_2\text{He}$  which is crystalline and is hexagonal close packed (HCP) system. The atoms in a quantum crystalline solid core arranged in a regular array that may be characterized by a lattice of points. The atoms are held in the array by the interatomic bonds, meaning thereby that the atoms interact with each other, and there may be some specific form of interaction potential between the atoms.

The vibrations of the atoms about their position when quantized are called phonons. Phonons in solid helium are most directly observed by inelastic neutron scattering. Measurements on all phases show that, although solid helium is highly anharmonic, most phonons are well defined and have long lifetimes<sup>7</sup>. The expanded BCC  ${}^4_2\text{He}$  phase is so anharmonic that phonon energies can be determined at low wave vector  $Q$  only. At higher  $Q$ , the scattering intensity contains fascinating interference effects between one phonon and multiphonon scattering contributions. The more compressed FCC phase of helium is sufficiently less anharmonic and can be well described without short – range corrections. Thus, the intrinsic restlessness of a quantum solid, like crystalline  ${}^4_2\text{He}$ , is manifested in terms of finite zero – point- energy (ZPE) due to Heisenberg's uncertainty principle. Another part of energy could be a consequence of the anharmonic behaviour of the atoms in the crystalline state. Therefore, we have added anharmonic terms to the harmonic terms and have calculated the energy of the solid  ${}^4_2\text{He}$  (crystalline helium). We have also calculated the zero point energy (ZPE) and the relative magnitudes of the two energies are compared.

### 2. Theoretical Derivations

In the crystalline state at  $T \rightarrow 0$ , the kinetic energy tends to zero or is negligible. The important parts of the energy will be the zero point energy (ZPE), and the energy due to the anharmonic behaviour of the atoms. The ZPE will be calculated using the uncertainty

principle, and the energy due to anharmonicity is calculated by introducing anharmonic term given by

$$\epsilon_a = \gamma x^4 + \alpha x^6 \quad (1)$$

where  $x$  is the displacement of the atom from its equilibrium position and each term in Eq. (1) must have units of energy. Quantities  $\gamma$  and  $\alpha$  are parameters of anharmonicity or perturbation .

These parameters can be either,

- i) Independent of temperature T,
- ii) May depend linearly on temperature,
- iii) May have quadratic dependence on temperature.

In general,

$$\gamma = \frac{\eta\omega_0}{a_0^4} \text{ and } \alpha = \frac{\eta\omega_0}{a_0^6} \quad (2)$$

where  $\omega_0$  is the natural frequency of vibration of atom( also called the Debye frequency), and  $a_0$  is the lattice constant. The Debye temperature  $\theta_D$  for  ${}^4\text{He}$  compressed into close – pack is 25 K and this corresponds to  $\omega_0 = 34.5 \times 10^{11} \text{ s}^{-1}$ . The value of  $a_0$  (lattice constant or inter - atomic spacing) is  $2.11 \text{ \AA}$  for HCP and FCC.

Substituting from eq. (2) in eq.(1) gives,

$$\epsilon_a = \frac{\eta\omega_0}{a_0^4} x^4 + \frac{\eta\omega_0}{a_0^6} x^6 \quad (3)$$

According to the theory of second quantization,  $x$  can be written in terms of annihilation operator ( $a$ ) and creation operator ( $a^+$ ), i.e.

$$x = \left( \frac{\eta}{2m\omega} \right)^{\frac{1}{2}} (a^+ + a) \quad (4)$$

Consequently the energy shift due to first term on the right hand side of Eq. (3) will be (after lengthily calculations).

$$\Delta E_n^1 = \left( \frac{\eta\omega_0}{a_0^4} \right) \left( \frac{\eta}{2m\omega_0} \right)^2 (6n^2 + 6n + 3) \quad (5)$$

Similarly the energy shift due to the second term on the right hand side of Eq. (3), after length the calculations, will be,

$$\Delta E_n^1 = \left( \frac{\eta\omega_0}{a_0^6} \right) \left( \frac{\eta}{2m\omega_0} \right)^3 (20n^3 + 32n^2 + 39n + 3) \quad (6)$$

The energy of the harmonic oscillator is, say,  $E_h$ , such that,

$$E_h = \eta\omega_0 \left( n + \frac{1}{2} \right) \quad (7)$$

Now the total energy  $E_A$ , of the anharmonic system will be the sum of the Eq. (5), (6) and (7), i.e

$$E_A = \eta\omega_0 \left( n + \frac{1}{2} \right) + \left( \frac{\eta\omega_0}{a_0^4} \right) \left( \frac{\eta}{2m\omega_0} \right)^2 (6n^2 + 6n + 3) + \left( \frac{\eta\omega_0}{a_0^6} \right) \left( \frac{\eta}{2m\omega_0} \right)^3 (20n^3 + 32n^2 + 39n + 3) \quad (8)$$

Eq. (8) gives the energy of the  ${}^4\text{He}$  quantum crystalline system due to the anharmonicity of the system.

Now the total energy  $E$  of the frozen (solid or crystalline) system will be composed of,

- i) Kinetic energy (that may be very small in the limit of  $T \rightarrow 0$ , which could be negligible).
- ii) Zero – point – energy ( ZPE) due to intrinsic restlessness since  ${}^4\text{He}$  is a quantum solid.
- iii) Energy due to anharmonicity
- iv) Energy due to inter - particle interaction between the atoms lying frozen at their lattice sites. Eq. (8) gives the energy due to kinetic energy and the energy due to anharmonicity. We have now to calculate the energy due to zero –point energy ( ZPE) and the energy due to interparticle interaction when the system is in the crystalline state.

### 3. Zero – point energy (ZPE)

If  $\Delta x_0$  is the zero – point fluctuation in the inter-particle distance of atoms in solid helium, then the ZPE is given by

$$\epsilon_0 = \frac{(\Delta p_0)^2}{2m} = \frac{\eta^2}{2m(\Delta x_0)^2} \quad (9)$$

It is observed that  $\Delta x_0$  is 30 percent of  $x_0$ , which is the inter – particle distance in the solid  ${}^4\text{He}$ , then

$$\Delta x_0 = \frac{30}{100} x_0 \quad (10)$$

Thus we can write  $\epsilon_0$  as

$$\epsilon_0 = \frac{50\eta^2}{9mx_0^2} \quad (11)$$

#### 4. Energy Due to Interparticle Interactions

The energy due to interparticle interaction can be calculated in two ways. Either one assumes the existence of pair interaction only, or one assumes the existence of many – body interaction in which case we have to use the t- matrix formalism<sup>8,9,10,11,12</sup>. In either case, one has to choose a suitable two – body interaction potential.

In literature there are a number of two – body potentials that can be used for calculations. Two important such potentials are, the Gaussian equivalent of the Lennard – Jones potential<sup>13</sup> and the square well potential. Lennard – Jones potential in its original form cannot be used since its integration is impossible. However, in this manuscript, we consider a two – body interaction potential between  ${}^4\text{He}$  atoms that is composed of a hard – core followed by a square well given by

$$V(r_{ij}) = \begin{cases} +\infty & 0 < r < a \\ -V_0 & a < r < b \\ 0, & r > b \end{cases} \quad (12)$$

Following Hansen and Levesque<sup>14</sup>, the potential energy per particle in terms of the pair – distribution function (PDF),  $g(r)$  is written as,

$$\frac{V}{N} = \frac{\rho}{2} \int g(r)V(r)d^3r \quad (13)$$

where  $\rho = \frac{N}{V}$ , is the particle number density and  $V(r)$

is the interaction potential. To calculate  $\frac{V}{N}$ , we

replace<sup>15</sup>  $V(r)$  by the reaction matrix  $t_{00,00}$  in Eq. (13)

to obtain the ground state energy<sup>13</sup> of solid  ${}^4\text{He}$ . The value of  $\frac{V}{N}$  then becomes,

$$\frac{V}{N} = -\rho \left[ \frac{2\pi V_0 (b-a)^3}{3} - \frac{2\pi a \eta^2}{m} \right] \left[ 1 - \frac{\lambda^2 (3b^2 - a^2)}{6a^2} \right] \quad (14)$$

The values of various quantities in Eq. (14) are

$$\frac{m^*}{m} = 1.2$$

$$m = 6.64 \times 10^{-24} \text{ g}$$

$$V_0 = 5.0 \times 10^{-16} \text{ erg}$$

$$\eta = 1.1 \times 10^{-27} \text{ erg sec}$$

$$a = 2.1 \times 10^{-8} \text{ cm}$$

$$b = 3.1 \text{ \AA} \text{ to } 5.1 \text{ \AA}$$

$$\rho = 2.0 \times 10^{22} \text{ Particles per cm}^{-3} \text{ to } 2.8 \times 10^{22} \text{ Particles per cm}^{-3}$$

#### 5. Calculations and Results

Calculations show that for  $\rho = 2.0 \times 10^{22}$  particles  $\text{cm}^{-3}$

and  $b = 4.9 \text{ \AA}$ , energy per particle  $\frac{\epsilon_0}{N} = 22.08 \text{ K}$

which is very close to the value of 25K quoted any Glyde<sup>16</sup>. For  $\rho = 2.06 \times 10^{22}$  particles  $\text{cm}^{-3}$  and  $b =$

$4.9 \text{ \AA}$ ,  $\frac{\epsilon_0}{N} = 12.69 \text{ K}$ , which is close to another value

of 14 K quoted by Glyde<sup>16</sup>. Depending upon the value

of  $\rho$ , another experimental<sup>17</sup> value for  $\frac{\epsilon_0}{N} = 6.0 \text{ K}$ ,

and it is found experimentally that  $\frac{\epsilon_0}{N}$  varies with  $\rho$ .

The three significant energies are the ones given by Eq. (8), Eq. (11) and Eq. (14). The sum of these three energies gives the total energy E. Table 1 below gives a summary of the results.

**Table 1: Values of  $\frac{V}{N}$ , E and  $\frac{\epsilon_0}{N}$  for  $b = 5.1 \text{ \AA}$  and  $4.9 \text{ \AA}$  respectively.**

b (Å)	$\frac{V}{N}$ ( $10^{-16}$ erg)	E ( $10^{-16}$ erg)	$\frac{\epsilon_0}{E}$ (%)
5.1	101.02	2220	95.45
4.9	21.79	2140	98.00

#### 6. Discussions

The calculations presented in table 1 show that as the width of the square – well potential increases, total energy of the helium atoms in the crystalline state

increases,  $\frac{V}{N}$  also increases and the ratio  $\frac{\epsilon_0}{E}$  is less

than the anticipated value of 98 %. This means that increase in width of the square – well potential lead to decrease in the quantum fluctuation. When the ZPE is 98% of the total energy E,  $x_0 \approx 1.7 \text{ \AA}$ , and this is less

than the hard – core radius  $a \cong 2.1 \text{ \AA}$ , and this should be acceptable since under high pressure, which is necessary to obtain the crystalline state, the inter-particle distance  $x_0$ , may decrease. More experimental work needs to be done to determine the exact value of the fluctuation,  $\Delta x_0$ , in the position of  ${}^4\text{He}$  atoms.

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