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Solid $_2^4He$ and zero–point energy

Abstract

At very low temperatures, becomes crystalline under high pressure of order of 65 Atmospheres or more. The solid structure is hexagonal close packed (HCP) and the size of the crystal increases. , being a quantum solid, is intrinsically restless with a large zero–point energy , which is of the order of 98 percent of the total energy, in the crystalline state. The balance two percent will be the energy due to interparticle interaction. The total energy in the crystalline state can be calculated using the Gaussian form of the Lennard–Jones potential and the t–matrix formalism. The zero–point energy is calculated using Heisenberg's uncertainty principle. If is to be of the order of 98 percent of , the interparticle distance X turns out to be of the order of 1.5 Å, which is less than the hard sphere radius.

Keywords: zero–point energy, –transition, hexagonal close pack, bose condensate

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Introduction

It is found that cooling $_2^4He$ liquid from T_λ towards absolute zero temperature does not result in the solidification of $_2^4He$ liquid. However, $_2^4He$ becomes solid under large external pressure of the order of 25 Atmospheres or more. Helium was first solidified in Leiden by Keesom WH[1] on June 25, 1926. Measurements on specific heat and thermal conductivity of solid Helium are given by Glyde HR.[2] To study the properties of any interacting system, such as solid $_2^4He$, the pair potential between the atoms has to be precisely known. Between the Helium atoms, the pair potential,[3,4] V(r), is weakly attractive at large separation, $r \geq 3$ Å, with a minimum well depth $\in = 10.95K$. At close approach, $r \leq \sigma = 2.63$ Å, where hard–core radius is σ. For $V(\sigma) = 0$, $V(r)$ becomes steeply repulsive. The volume of solid $_2^4He$ is 21.1 cm³/mole. Since Helium is light, its thermal wavelength λ_T, is long. At T=1.0 K, $\lambda_T \cong 10$ Å for $_2^4He$. Helium is thus difficult to localize. Attempts to localize it lead to a high kinetic or zero–point energy. Since V(r) is weak, Helium does not solidify under attraction via V(r). Rather, it solidifies only under large external pressure as a consequence of the existence of the hard core of V(r), much as billiard balls form a lattice under pressure. At higher pressure, $_2^4He$ gets compressed into close-packed (FCC and HCP) phases. At 4.9 kbars, FCC $_2^4He$ has a volume of 9.03 cm³/mole and $\sigma = 2.11$ Å.

The degree of the quantumness in a solid is sometimes characterized by

$$\Lambda = \frac{1}{2\pi}\frac{\lambda}{\sigma} = \frac{h}{\sigma\left(2m\in\right)^{\frac{1}{2}}} \quad (1)$$

Where Λ, is the de Boer parameter, which is the ratio of the de Broglie wavelength, $\lambda = \frac{h}{p} = \frac{h}{\sqrt{2m\in}}$ to the minimum separation of the atoms in the crystal which is σ. If λ is comparable to σ, the solid is highly quantum. Moreover, the de Boer parameter, Λ and the Lindmann ratio, δ are practically identical, and thus a large Λ means quantum and very anharmonic vibration. In physics, a quantum solid 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 temperature. The typical quantum solid, both in low density and high density, is the solid $_2^4He$ which is crystalline and is hexagonal–close–packed system. The atoms in a quantum crystalline solid are arranged in a regular array that may be characterized by a lattice of points. The atoms are held in the lattice by the inter–atomic bonds, meaning thereby that the atoms interact with each other, and there may be some specific form of interaction potential between the atoms.

We now turn to the basic ideas and information that lead us to write the present manuscript. The properties of $_2^4He$ are dominated by the quantum–mechanical effect called zero–point motion which is the dynamical property of $_2^4He$. Due to the low atomic mass and weak inter–atomic forces, $_2^4He$ atoms do not freeze even in the limit of zero temperature. Liquid $_2^4He$ can be solidified only on the application of external pressure of 25 bars or more, in addition to cooling. The effect allows the presence of delocalized vacancies in the crystalline solid that can condense into a coherent state at low temperatures.[5] Even when it becomes solid, the liquid–solid transition is not well understood.

In this manuscript, we have concentrated on the physical characteristics of solid $_2^4He$, one is that $_2^4He$ crystals will be treated as quantum crystals, and the second is the calculation of the interaction energy between the $_2^4He$ atoms. Since a quantum solid is intrinsically restless, the uncertainties in the values of position r and the momentum p should be finite, and they are large in $_2^4He$ because of its low mass. Hence, Δr and Δp should be large. At absolute zero temperature,[6,7] the

zero–point fluctuations of atoms in solid $^4_2 He$ are about 30 percent of the inter–atomic spacing, and as a consequence the zero–point energy represents roughly 98 percent of the total energy of the crystal. This means that in the crystalline state $\left(T \rightarrow 0 \right)$, the interaction energy between the helium atoms will be roughly 2 percent of the total energy of the system. Thus, if E_o is the total energy and ϵ_1 is interaction energy, and $\in_o$ is the zero–point energy, then,

$$\in_1 = \frac{2}{100} E_O \qquad (2)$$

$$\in_o = \frac{98}{100} E_O \qquad (3)$$

Zero–Point Energy (ZPE)

If X is the average inter–particle distance or inter-atomic spacing of the linear lattice, then the zero–point fluctuation ΔX_o of the atoms in solid helium is about 30 percent of X. Hence,

$$\Delta X_0 = \frac{30}{100} X \qquad (4)$$

In the literature,[7] X has two values, one is when X = 2.11 Å, and second when X = 3.67 Å. Both of these values will be used to get the numerical value for the zero–point–energy $\in_o$. Now, if ΔX_o is the uncertainty in the value of the position, and Δp_0 is the uncertainty in the value of the momentum, then according to Heisenberg's uncertainty principle,

$$\Delta p_o = \frac{\hbar}{\Delta X_O} \qquad (5)$$

The zero-point-energy is then given by

$$\in_0 = \frac{\left(\Delta p_o \right)^2}{2m} = \frac{\hbar^2}{2m(\Delta X_O)} \qquad (6)$$

Where m=6.46x10⁻²⁴g is the mass of the $^4_2 He$ atom. Equation (6) shows that the value of zero–point-energy $\in_o$ changes as ΔX_o varies and the value of ΔX_o depend on the value of X as shown in Equation (4).

Here we have quoted two extreme values for X (X = 2.11Å and X =3.67Å). It is simple to calculate the value of X that will lead to the value of $\in_o$ that will be 98 percent of the total energy E_o. Again there are two values for E_o in the literature;[7] E_o = 25K and E_o =14K. In order that $\in_o$ be 98 percent of E_o, the value of X will be the order of 1.7 Å which means that in the crystalline state the inter- particle distance between the atoms should be of the order of 1.7Å. However, this needs to be verified experimentally, may be by using the neutron scattering method.[8]

Conclusion

Our calculations bring out that if the zero-point-energy ($\in_o$), is to be 98 percent of the total energy (E_o), then the inter-particle distance between $^4_2 He$ atoms should be of the order of 1.5 Å which is less than the hard- core radius. More experimental and theoretical work needs to be done to determine the exact value of the fluctuation in position (ΔX_o) since this will determine ϵ_o, and we then calculate whether ϵ_o is really 98 percent of E_o. In our next attempt, many-body theory will be used to calculate $\in_o$.

Acknowledgments

Conflicts of interest

Authors declare there is no conflict of interest.

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