International Journal of Physics and Mathematical Sciences ISSN: 2277-2111 (Online)
An Online International Journal Available at http://www.cibtech.org/jpms.htm
2013 Vol. 3 (2) April-June, pp.73-78/Chelimo et al.
Research Article

INCOMMENSURABILITY OF HCP SOLID ^{4}He QUANTUM CRYSTAL

Chelimo L S[1], *Khanna K M[1], Tonui J K[1], Rapando B W[1], Kandie D K[1], Masinde F W[1] and Bitok J K[2]

[1] *Department of Physics and* [2]*Department of Mathematics and Computer Science, University of Eldoret, P.O. Box 1125-30100, Eldoret-Kenya*
**Author for Correspondence*

ABSTRACT

The thermodynamic properties of an incommensurate hcp solid ^{4}he quantum crystal are calculated. The ground state of a quantum crystal is assumed to be incommensurate with point defects; zero-point vacancies and interstitials. We show that vacancies contribution to the specific heat varies as $t^{3/2}$.the vacancy contribution to the specific heat increases at larger temperatures due to thermal excitations. The correction to the specific heat due to both phonon dispersion and vacancies is reminiscent of what has been found experimentally.

Key Words: *Superfluidity, Supersolidity and Incommensurability.*

INTRODUCTION

Experimental findings (Kim & Chan, 2004A; Kim & Chan, 2004B; Rittner & Rappy, 2006; Day & Beamish, 2006) and theoretical studies (Khanna *et al*., 2012), have reported evidence that suggests that, solid ^{4}He becomes a superfluid when cooled below a critical temperature T_c. This has continued to generate a new wave of interest on the possibility of superfluid phase of a solid. Supersolidity of ^{4}He is still controversial, both at the experimental and theoretical levels (Kim *et al*., 2011).

The highly incommensurate quantum crystal referred to as 'supersolid' has been proposed to occur due to the quantum behaviour of point defects namely vacancies and interstitials on a bosonic system. This superfluidity of solid ^{4}He is due to the presence of zero-point vacancies, or interstitial atoms, or both, as an integral part of the ground state (Prokof'ev & Svistunov, 2005). As a consequence, in the absence of symmetry between vacancies and interstitials, superfluidity has a zero probability to occur in commensurate solid which breaks continuous translational symmetry (Prokof'ev & Svistunov, 2005).Over the past few years; experimental findings have shown that supersolidity occurs for the case of incommensurable quantum crystal in which vacancies condense into the ground state. Incommensurability of the ground state of the quantum solid, i.e. non-integer number of atoms per unit cell (Anderson *et al*., 2005; Maris & Balibar, 2007) has been noted to be a density wave that need not exactly match the particle density, so that the ground state may be incommensurate with unequal densities of vacancies and interstitials (Anderson *et al*., 2005).

There have been also other experiments that have been done to measure the temperature dependence of the vacancy density in solid ^{4}He although different experiments lead to considerable differences in the results. The x-ray measurements on solid hcp ^{4}He show that the density of vacancies increases faster than that of interstitials with increasing temperature (Fraass, 1989; Simmons, 1994), indicating that thermal fluctuations favour vacancies more than interstitials.

It has been argued (Anderson *et al*., 2005), based on Jastrow-type wave functions, that it is expected that there will be vacancies in the ground state of a highly quantum fluctuating solid such as ^{4}He, and that such a ground state may be superfluid. These vacancies form the integral feature of the ground state and carry no entropy or energy. However, the vacancies and interstitials are assumed to remain in a strongly-correlated quantum state up to temperatures in the vicinity of 1 K. Thus, they do not make a large contribution to the specific heat other than the incommensurability effect seen at the temperature above 1 K.

Again on vacancy concentration in solid ^{4}He, the most accurate data comes from the x-ray measurements of the lattice parameter of solid helium as a function of temperature for samples maintained under conditions of nearly constant volume. The lattice parameter is found to decrease as the temperature is raised and it is assumed that this decrease occurs because vacancies are thermally excited. The predicted value of vacancy specific heat appears to be too large to be consistent with the measured specific heat (Fraass, 1989; Simmons, 1994). One possible explanation (9) for this discrepancy is the fact that vacancies are delocalized and form a band of energies (Sample & Swenson, 1965; Ahlers, 1970; Minkiewicz *et al*., 1968) in terms of a classical theory of vacancies involving activation energy and a configuration entropy for their creation (Anderson *et al*., 2005). It is then possible that phonon contribution could be less than what has been believed due to thermal excitation, and that the specific heat experimentally measured arises from vacancies near 1K. Such a classical vacancy contribution to the specific heat has not been seen clearly, instead, the specific heat is well explained almost entirely by T^3 term for a dielectric solid and the leading correction to this fits well to a T^7 term due to anharmonicity of the phonons or the deviation of the phonon dispersion relation from linearity (Khanna *et al*., 2012; Anderson *et al*., 2005, Maris & Balibar, 2007). For long, there have been several attempts to explain these discrepancies but none have been satisfactory and the problem has remained open (Burns & Goodkind, 1994).

In this paper, a statistical thermodynamic theory of low temperature behaviour of an incommensurate quantum solid has been developed. When the ground state of the crystal is incommensurate, the number of atoms N is not equal to the number of sites N_S, i.e. $N \neq N_S$. The two numbers could differ by up to 1% (Anderson *et al*., 2005) such that $N_S > N$. Such a small difference between the number of atoms and the number of lattice sites may have escaped detection in simulations (Ceperly & Bernu, 2004) of the ground state of solid ^{4}He. Direct comparisons of experimental measurements of the density of ^{4}He atoms to the x-rays measurements of the density of sites have not been published for the low pressure hcp phase where the apparent supersolidity has been observed. The lattice constant and incommensurability have been assumed to have constant values to obtain the expressions for entropy and the specific heat of solid ^{4}He.

Theory

In the case of incommensurate system the number of particles is less than the number of sites. Let the number of particles be N and the number of sites be N_S such that $N < N_S$. The incommensurability, ε, is written as,

$$\varepsilon = \frac{N_S - N}{N_S} \qquad 1$$

By definition $\varepsilon \neq 1$ at any time and that we assume there is no disorder and intersite interaction; such that the particles and the sites can be freely permuted. For the case of a bosonic system, the number of ways we can permute sites and particles will be $(N+N_S)!$. Since the particles are identical, permutations among them must be excluded by dividing by $N!$. Similarly, permutation among identical sites be excluded by dividing by $N_S!$. Thus the number of ways in which the particles can be distributed among the sites is given by,

$$P = \frac{(N + N_S)!}{N!N_S!} \qquad 2$$

Hence the statistical count, C, for incommensurability is given as,

$$C = \prod_S P = \prod_S \frac{(N + N_S)!}{N!N_S!} \qquad 3$$

Now we can write,

$$\ell og C = \ell og \prod_S \frac{(N+N_S)!}{N!N_S!} \qquad 4$$

or

$$\ell og C = \sum_S \left[\ell og(N+N_S)! - \ell og N! - \ell og N_S!\right] \qquad 5$$

For a large number x, Sterling theorem gives $log\ x! = x\ log\ x - x$. Using Sterling theorem in Eqn (5) gives,

$$\ell og C = \sum_S \left[(N+N_S)\ell og(N+N_S) - N\ell og N - N_S \ell og N_S\right] \qquad 6$$

Eqn (1) can be used to eliminate N_S in Eqn (6). Such that,

$$\ell og C = \sum_S \left[N\left(\frac{2-\varepsilon}{1-\varepsilon}\right)\ell og N\left(\frac{2-\varepsilon}{1-\varepsilon}\right) - N\ell og N - \left(\frac{N}{1-\varepsilon}\right)\ell og\left(\frac{N}{1-\varepsilon}\right)\right] \qquad 7$$

If N_S is uniquely determined, then it may have only one value for a given crystalline system. We could denote this value as $n_0 = N_S > N$. Hence the summation over S in Eqn (7) will have only one term on its right- hand- side. Consequently, we can write,

$$\ell og C = N\left(\frac{2-\varepsilon}{1-\varepsilon}\right)\ell og N\left(\frac{2-\varepsilon}{1-\varepsilon}\right) - N\ell og N - \left(\frac{N}{1-\varepsilon}\right)\ell og\left(\frac{N}{1-\varepsilon}\right) \qquad 8$$

According to the theory of Bose- Einstein condensation (BEC), the following well known relations are used (Khanna, 1986),

$$\frac{Nh^3}{Vg(2\pi mkT)^{\frac{3}{2}}} = 2.612 \qquad 9$$

For spinless bosons $g = 1$, V = volume of the container and k is the Boltzmann's constant. Thus we can write,

$$N = AT^{\frac{3}{2}} \qquad 10$$

Where,

$$A = 2.612V\frac{(2\pi mk)^{\frac{3}{2}}}{h^3} \qquad 11$$

The Gibb's free energy is expressed as,

$$G = -\int k\ell og C dT \qquad 12$$

Substituting for $logC$ from Eqn (8) using Eqn (10) and integrating Eqn (12) gives,

$$G = -\frac{2}{5}kAT^{\frac{5}{2}}\left[\left(\frac{2-\varepsilon}{1-\varepsilon}\right)\ell og\left(\frac{2-\varepsilon}{1-\varepsilon}\right) - \left(\frac{1}{1-\varepsilon}\right)\ell og\left(\frac{1}{1-\varepsilon}\right)\right] \qquad 13$$

The Entropy S

The entropy of the system is given by,

$$S = -\left(\frac{\partial G}{\partial T}\right)_p \qquad 14$$

Substituting Eqn (13) in Eqn (14) gives,

$$S = kAT^{\frac{3}{2}}\left[\left(\frac{2-\varepsilon}{1-\varepsilon}\right)\ell og\left(\frac{2-\varepsilon}{1-\varepsilon}\right) - \left(\frac{1}{1-\varepsilon}\right)\ell og\left(\frac{1}{1-\varepsilon}\right)\right] \qquad 15$$

The Specific Heat C_V

The specific heat can be expressed as (19),

$$C_V = T\left(\frac{\partial S}{\partial T}\right)_V \qquad 16$$

$$C_V = \frac{3}{2}kAT^{\frac{3}{2}}\left[\left(\frac{2-\varepsilon}{1-\varepsilon}\right)\ell og\left(\frac{2-\varepsilon}{1-\varepsilon}\right) - \left(\frac{1}{1-\varepsilon}\right)\ell og\left(\frac{1}{1-\varepsilon}\right)\right] \qquad 17$$

RESULTS AND DISCUSSION

The entropy and the specific heat dependence on the temperature of the incommensurate crystalline quantum solid ^{4}He have been calculated using the various parameters given in Table 3.1.

Table 3.1: Parameters description and their corresponding values

Parameter description	**Value**	
Boltzmann's constant, *k*	1.38×10^{-16} erg K^{-1}	
Volume of container, *V*	3.358×10^{-23} cm^3	(Grigor'ev *et al*., 2007)
Planck's constant, *h*	6.623×10^{-27} erg-sec	
Particle mass of ^{4}He, *m*	6.646×10^{-24} gm	
Incommensurability, ε	0.01	Ref. (8)
Constant, *A*	0.132 gm $cm^3 sec^{-3} erg^{-3/2} K^{-3/2}$	Ref. (18)

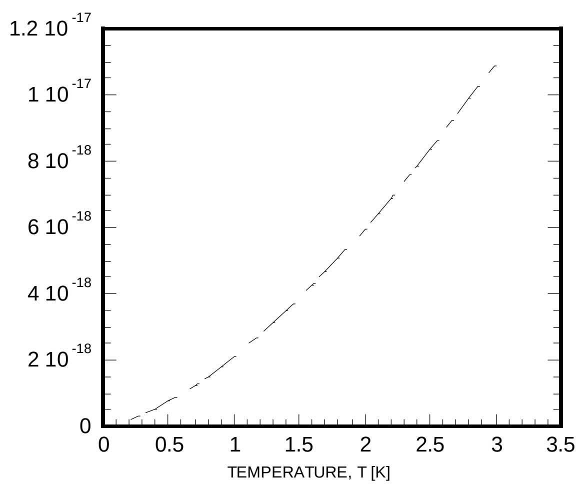

Figure 3.1: Entropy variation with Temperature for ε = 0.01

The variation of S with T is described by Eqn (15), and Eqn (17) describes the variation of C_v with T. Both the variations are proportional to $T^{3/2}$. According to Debye theory of specific heat (Fetter & Walecka, 2003), C_v varies as T^3 as $T \to 0$. The specific heat for ^{4}He below 0.6 K varies as $C_v = (0.0204 \pm 0.0004)T^3$ J/gm-deg (Morse, 1964). Whereas according to Bose-Einstein condensation theory of ideal Bose gas (Morse, 1964; Fetter & Walecka, 2003), the specific heat of helium for $T<T_c$ is given by $C_v = 1.926R\left(T/T_c\right)^{3/2}$.

In our calculation the specific heat C_v varies as $T^{3/2}$ indicating that the incommensurate hcp solid ^{4}He quantum crystal assembly may behave as an assembly of free bosons at very low temperatures.

Anderson *et al*. (2005) obtained an expression for free energy, G, phenomenologically. Using that value of G to obtain expressions for S and C_v leads to T^3 dependence of S and C_v. This shows that the contribution to S and C_v is due to the acoustic superfluid mode. Figure 3.1 shows that the vacancy entropy increases non-linearly with increase in temperature. The $T^{3/2}$ term vacancy contribution to the entropy of solid ^{4}He is less than the T^3 term due to the phonons at low temperature (Khanna *et al*., 2012). These results suggest that thermal excitations favour both disorder of vacancies and phonon dispersion in the quantum crystal at temperatures above 0.2 K.

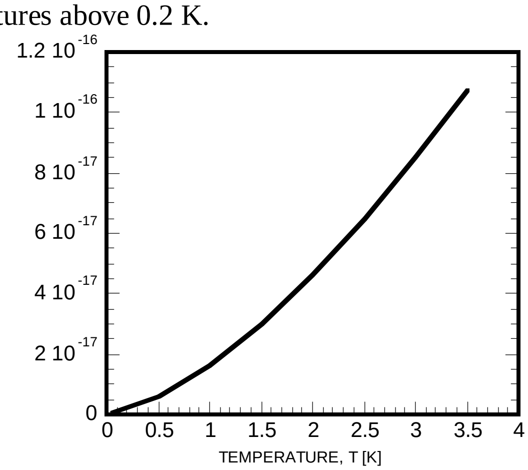

Figure 3.2: Specific Heat variation with Temperature for ε = 0.01

Figure 3.2 shows the variation of specific heat with temperature. The $T^{3/2}$ temperature dependence of the specific heat is lower than the well known T^3 dependence for the case of a dielectric solid (Fetter & Walecka, 2003). The vacancy contribution to the specific heat appears to be higher than the contribution due to phonon dispersion above 1 K (Khanna *et al*., 2012).At low temperature, vacancies and interstitials are strongly correlated up to the vicinity of 1 K (Anderson *et al*., 2005). This down plays the role of these point defects contribution to the phonon specific heat below 0.2 K and this is as seen in Fig. 3.2, but they can possibly enhance Bose-Einstein condensation that results in supersolid state of ^{4}He. These findings of vacancy contribution to the specific heat at low temperature, below 1 K, may now confirm that the excess specific heat observed (Simmons, 1994; Sample & Swenson, 1965; Ahlers, 1970) that leads to T^7 term could now be confirmed as due to phonon dispersion (Khanna *et al*., 2012; Anderson *et al*., 2005; Maris & Balibar, 2007) and not due to vacancies in an incommensurate quantum solid. The large vacancy contribution to the specific heat at higher temperatures above 1 K could be strongly linked to thermal excitations as seen in the x-ray studies (Anderson *et al*., 2005) as well as their delocalization.

In conclusion, apart from the approach used here, it may be also possible to use the activation energy E_v (Maris & Balibar, 2007) for vacancy formation to calculate the vacancy contribution to the specific heat. The algebraic sum of phonon dispersion and vacancy contribution could give a closer approximation to the specific heat of the incommensurate quantum hcp solid ^{4}He at the vicinity of 1 K. The effects of other lattice defects that may include interstitials, grain boundaries and dislocations contribution towards the specific heat are yet to be known either experimentally or theoretically.

REFERENCES

Kim E and Chan M H W (2004a). Probable observation of a supersolid helium phase. *Nature* **427** (6971) 225-227.

Kim E and Chan M H W (2004b). Observation of superflow in solid helium. *Science* **305** 1941.

Rittner A S C and Reppy J D (2006). Observation of classical rotational inertia and non-classical supersolid signals in solid helium-4 below 250mK. *Physical Review Lett*ers **97** 115302.

Day J and Beamish J (2006). Pressure-Driven Flow of Solid Helium. *Physical Review Letters* **96** 105304.

Khanna K M, Chelimo L S, Torongey P K and Rotich S K (2012). Superfluidity of Crystalline Supersolid ^{4}He Under High External Pressure. *The African Review of Phys*ics **7** (0012) 107-113.

Kim D Y, West J T, Engstrom T A, Mulders N and Chan M H W (2011). *The 26th International Conference on Low Temperature Physics, Beijing, China.*

Prokof'ev N and Svistunov B (2005). Supersolid state of matter. *Physical Review Lett*ers **94** (15) 155302.

Anderson P W, Brinkman W F and Huse D A (2005). Thermodynamics of an incommensurate quantum solid. *Science* **310** 1164-1166.

Maris H J and Balibar S J (2007). Supersolidity and the thermodynamics of solid helium. *Journal of Low temperature Phys*ics **147** (516) 539.

Fraass B A, Granfors P R and Simmons R O (1989). X-ray measurements of thermal vacancies in solid helium-4. *Physical Re*view **B 39** 124.

Simmons R O (1994). Vital records-travis county, TX-Divorce. *Journal of Physics and Chemistry of Solids* **55** 895.

Sample H H and Swenson C A (1967). Heat Capacity of hcp and bcc Solid Helium 3. *Physical Review.* **158** (1) 188-199.

Ahlers G (1970). Thermal Properties of hcp He^4. *Physical Review* **A 2** 1505.

Minkiewicz V J, Kitchens T A, Lipschultz F P, Nathans R and Shirane G (1968). The phonon spectrum of hcp He^4. *Physical Re*view **174** 267-275.

Burns C A, Goodkind J M (1994). Is a non-equilibrium supersolid possible in solid ^{4}He? *Journal of Low Temperature Phys*ics **95** 695.

Ceperly D M, Bernu B (2004). Ring exchanges and the supersolid phase of helium-4. *Physical Review Lett*ers **93** 155303.

Khanna K M (1986). Statistical Mechanics and Many-Body Problem (To-day and To-morrow Printers and Publishers, New Dehli) 79.

Morse P M (1964). Thermal Physics (W. A. Benjamin, Inc. New York) 103.

Grigor ev V N, Maidanov V A, Rubanskii V Yu, Rubets S P , Rudavskii E Ya , Rybalko A S Syrnikov Ye V and Tikhii V A (2007). Observation of glassy phase of ^{4}He in the region of supersolid effects. *Physical Review* **B 76** (22) 224524.

Fetter A L and Walecka J D (2003). Quantum Theory of Many Particle Systems (Dover Publications, Inc. New York) 395.