

## Pair distribution function for interacting bosons and the ground-state energy of solid helium-4

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The pair distribution function  $g(r)$  for a system of bosons interacting through a two-body potential composed of a hard core followed by a square well has been obtained using the reaction matrix formalism for the energy excitation spectrum  $E_k$  and the fundamental definition relating the structure factor  $S(k)$  and  $g(r)$ . This has been used in obtaining the ground state energy of solid  $^4\text{He}$  using the kinetic energy and potential energy expressions of Hansen and Levesque. The most stable ground state of solid  $^4\text{He}$  corresponds to a potential width of  $b=3.8\text{\AA}$ , but the corresponding  $\langle E \rangle/N$  for the density,  $\rho$ , of solid  $^4\text{He}$  is very large compared with the experimental value. However, for  $b=4.81\text{\AA}$  and  $\rho=2.8 \times 10^{22}$  particles/cm<sup>3</sup>,  $\langle E \rangle/N = -11.24$  K =  $-93.4$  Joule/mol. and for  $b=4.82\text{\AA}$  and  $\rho=2.5 \times 10^{22}$  particles/cm<sup>3</sup>,  $\langle E \rangle/N = -6.84$  K =  $-56.8$  Joule/mol. The experimental value for the ground state energy of solid  $^4\text{He}$  =  $-59.5$  J/mol.

**Keywords:** Bosons, Solid helium-4, Ground-state energy

### 1 Introduction

Various attempts<sup>1-3</sup> have been made to determine the pair distribution function (pdf) for bosons interacting through different two-body interactions or potentials. The pdf determined under different conditions shows a different behaviour. For an ideal Bose gas, London<sup>4</sup> showed that at long distances, the pdf denoted by say  $g(r_1 - r_2 = r)$ , behaves like  $r^{-1}$ ,  $r^{-2}$

and  $r^{-2} \exp\left(\frac{-4r(-\beta\mu\pi)^{\frac{1}{2}}}{\lambda_T}\right)$  respectively, according to

whether the temperature  $T$  is below, at and above the  $\lambda$  temperature. Here  $\mu$  is the chemical potential and

$\lambda_T = \left(\frac{2\pi\hbar^2}{mk}\right)^{\frac{1}{2}}$  is the thermal wavelength.

In general, the calculations of the pdf of an interacting Bose gas at very low temperatures have been made using the cluster expansion formalism. In the analysis of an interacting system, the necessary condition is that the Fourier transform of the interaction potential must exist. When the interaction potential is hard core or hard core followed by square well, ordinary Fourier transform calculations cannot be done. For the dilute hard sphere Bose gas, the Fourier transform of the interaction potential is

replaced by a constant  $\frac{8\pi a\hbar^2}{2m}$ . This result is obtained

indirectly and not by direct substitution. For such systems, the reaction –matrix formalism has been successful. In this paper, pdf is calculated by a completely different approach. The formalism is general and is applicable to all kinds of realistic potentials. The starting point is that the Fourier transform of the pdf gives the structure factor  $s(k)$ . The inverse transform will give  $g(r)$  in terms of  $s(k)$ . The structure factor<sup>5</sup>  $s(k)$  is given by

$s(k) = \frac{\hbar^2 k^2}{2m^* E_k}$ , where  $E_k$  is the energy of excitation

spectrum for interacting bosons. We have already determined<sup>6,7</sup>  $E_k$  using the reaction matrix formalism for bosons interacting through different types of two-body interaction potentials. Substituting for  $E_k$  in the expression for  $s(k)$ , and that for  $s(k)$  in the expression for  $g(r)$ , the required expression for  $g(r)$  is obtained. The pdf determined  $b$  here has features which are very similar to those known so far.

The properties of  $^4\text{He}$  are dominated by the quantum mechanical effect called the zero point motion owing to their low atomic mass and weak interatomic forces, its atoms do not freeze even in the limit of zero temperature. In fact liquid  $^4\text{He}$  can be solidified only on the application of external pressure of about 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<sup>8-11</sup>. Even when it becomes

solid, not much is understood about the liquid-solid transition. Research is still being done on whether the transition could lead to super-solid  $^4\text{He}$ .

Macmillan<sup>12</sup> calculated the ground-state energy of liquid  $^4\text{He}$  using the Jastrow-type trial wave functions, but Levesque *et al*<sup>13</sup> did calculations for solid  $^4\text{He}$  using localized trial wavefunctions, i.e, the product of Jastrow function and Gaussians centred around the lattice sites. It was shown that such localized wavefunction gives lower ground-state energies at higher densities, whereas at low densities the non-localized wavefunction gives better results. Nosanow and co-workers<sup>14,15</sup> calculated the energy of solid  $^4\text{He}$  using an approximate expression for the energy expectation value obtained by a cluster expansion. The study of the ground state energy of solid  $^4\text{He}$  has benefited from the theory of classical liquids and amorphous solids<sup>16</sup>. Also pair distribution functions of the interacting bosons can be used in the quantum regime<sup>17-19</sup> and under proper circumstances has the capacity to illuminate non-obvious aspects of quantum solid state.

In this paper, the ground state energy of solid  $^4\text{He}$  has been calculated using the expressions for the potential and kinetic energy per particle due to Hansen and Levesque<sup>20</sup>. These expressions are in terms of the *pdf* which is derived in this manuscript in terms of the reaction matrix  $t_{00,00}$ . The use of trial wave function on which the calculations by earlier researchers are based, has been eliminated. However, the choice of the trial wave function is significant in the sense that the results may or may not be reliable.

The interaction potential<sup>6</sup> used by us is assumed to be valid in the solid phase. The calculations have brought out that for  $b=3.8\text{\AA}$ , all the other parameters of the potential remaining the same. The value of  $\langle E \rangle / N$  is more negative, whatever the value of the density  $\rho$  may be. If this is taken as the criterion for liquid-solid transition, then for  $b=3.8\text{\AA}$ ,  $\rho=2.5 \times 10^{22}$  particles  $\text{cm}^{-3}$  or  $\rho=2.8 \times 10^{22}$  particles  $\text{cm}^{-3}$  are the likely particle number density for solid  $^4\text{He}$ . Some values of  $\langle E \rangle / N$  are high in magnitude when compared with experimental values, and some are quite comparable to the experimental values. For instance, for  $b=4.81\text{\AA}$  and  $\rho=2.8 \times 10^{22}$  particles  $\text{cm}^{-3}$ ,  $\langle E \rangle / N = -11.24\text{K} = -91.5\text{Joule/mol.}$ , whereas for  $b=4.82\text{\AA}$  and  $\rho=2.5 \times 10^{22}$  particles  $\text{cm}^{-3}$ ,  $\langle E \rangle / N = -6.84\text{K} = 56.8\text{Joule/mol.}$  which is very close to the experimental value of  $59.5\text{Joule/mol.}$

## 2 Theoretical Derivations for pdf

The Fourier transform of the pair-distribution function  $g(r)$  gives the structure factor of the liquid, i.e,

$$s(k) = \int g(r) \exp(ik.r) d^3r \quad \dots(1)$$

where  $g(r)$  denotes the probability density for finding an atom in the neighbourhood of the point  $r_2$  if another is known to be at the point  $r_1$ . From Eq. (1):

$$g(r) = \frac{1}{(2\pi)^3} \int s(k) \exp(-k.r) d^3k \quad \dots(2)$$

The structure factor  $s(k)$  is related to the excitation energy  $E_k$  by the relation:

$$s(k) = \frac{\hbar^2 k^2}{2m^* E_k} \quad \dots(3)$$

If the expression for  $E_k$  is known for a given system of interacting bosons, it is then substituted in Eq. (3), and the expression for  $s(k)$  is substituted from Eq. (3) in Eq. (2). The pair distribution function  $g(r)$  can be obtained in terms of the parameters of the interaction potential and the relative distance  $r$  between the two interacting particles. The expression for  $E_k$  has been derived<sup>6,7</sup> for bosons interacting with different types of interaction potentials. One of these expressions<sup>6</sup> is:

$$E_k = \left( \frac{\hbar^2 k^2}{2m^*} \right) \left[ 1 + \frac{4m^*}{\hbar^2 k^2} N_0 t_{00,00} \frac{\sin ka}{ka} \right]^{\frac{1}{2}} \quad \dots(4)$$

For the values of  $k$  for which  $\frac{4m^*}{\hbar^2 k^2} N_0 t_{00,00} \frac{\sin ka}{ka} < 1$ , Eq. (3) becomes approximately:

$$s(k) = 1 - \frac{2m^*}{\hbar^2 k^2} N_0 t_{00,00} \frac{\sin ka}{ka} \quad \dots(5a)$$

There could be some misgivings about the use of Eqs (3 and 5a), but the following may be noted: Eq. (3) was obtained by Feynmann<sup>21</sup> and according to Feynmann with rising  $k$ ,  $s(k)$  starts off linearly as

$\frac{\hbar k}{2mc}$ , rises then to a maximum near  $k = \frac{2\pi}{a}$  (where  $a$  is the atomic spacing) and falls again to approach with possible minor oscillations, the limit unity.

Consequently, the quantity  $E_k = \frac{\hbar^2 k^2}{2m^* s(k)}$  should start linearly as  $\hbar kc$ , but should then show a dip with a minimum at  $k = k_0$ , say near  $\frac{2\pi}{a}$ , and finally rising eventually as  $\frac{\hbar^2 k^2}{2m^*}$ . The energy curve is reasonably valid for all  $k$  from zero up to and slightly beyond the minimum. The excitations behave much like interacting Bose particles which may be created and destroyed and whose energy as a function of momentum is given by  $E_k = \frac{\hbar^2 k^2}{2m^* s(k)}$ .

Very large  $k$  values corresponding to high excitations are not of concern since for temperatures of a few Kelvin, such high states would not be appreciably excited. Thus, Eq. (3) is sufficiently valid in the region in which  $s(k)$  first rises to a maximum and then oscillates to a limiting value of unity. Eq. 5(a) is based on the requirement that:

$$\frac{4m^*}{\hbar^2 k^2} N_0 t_{00,00} \frac{\sin ka}{ka} < 1 \quad \dots(5b)$$

It can be shown that this condition given in Eq. (5b) for our parameters of the potential is satisfied for  $k$  values  $\geq 1.3\text{\AA}^{-1}$ . The structure factor  $s(k)$  reaches its maximum height around  $k=1.3\text{\AA}^{-1}$ , then oscillates and reaches a limiting value unity<sup>22</sup> around  $k = 9\text{\AA}^{-1}$ . The Feynmann relation given in Eq. (3), is valid at least within the range of  $k$  values. If the  $k$  values for which Eq. 5(b) is valid would have fallen outside this range, then the calculations would be considered as untenable. Since Eq. (3) is valid at least for  $1.3\text{\AA}^{-1} < k < 9\text{\AA}^{-1}$ , in which  $s(k)$  contributes to the physics of the problem in a meaningful manner, the calculations cannot be considered as meaningless or wrong. Moreover, the value of the ground state energy for solid <sup>4</sup>He that we obtain agrees very well with the experimentally measured value, then it is taken as a strong support for the validity of our assumptions and the consequent calculations.

Substituting for  $s(k)$  from Eq. 5(a) into Eq. (2) gives:

$$g(r) = \frac{1}{(2\pi)^3} \int_0^\infty \exp(-ik.r) d^3k, \\ - \frac{2m^* N_0 t_{00,00}}{(2\pi)^3 \hbar^2} \int_0^\infty \frac{\exp(-ik.r)}{k^2} \frac{\sin ka}{ka} d^3k$$

Integrals from 0 to  $k'=1.3\text{\AA}^{-1}$

or

$$g(r) = \delta(r) - \frac{2m^* N_0 t_{00,00}}{(2\pi)^3 \hbar^2} \left[ \frac{4\pi}{ar} \left\{ \frac{\pi r}{2}, 0 < r \leq a \right\} \right] \quad \dots(6)$$

where the contribution from the integrals from 0 to  $k'$  has been dropped since it does not affect the physics of the problem.

For a high density gas of bosons interacting through a potential composed of a hard core followed by a square well<sup>6</sup>,  $N_0 t_{00,00}$  is given by :

$$N_0 t_{00,00} = \frac{\hbar^2 \lambda^2}{2m^* a^2} - \frac{4\pi \rho V_0 (b-a)^3}{3} \quad \dots(7)$$

For a low-density gas of bosons, the corresponding expression<sup>20</sup> is given by :

$$N_0 t_{00,00} = \rho \left[ \frac{4\pi \hbar^2 a}{m^*} \left\{ 1 + (8\pi \rho a^3)^{\frac{1}{2}} + \frac{16\pi \rho a^3}{3} \right\} - \frac{4\pi V_0 (b-a)^3}{3} \right] \quad \dots(8)$$

Substituting for  $N_0 t_{00,00}$  from Eq. (7) in Eq. (6),  $g(r)$  is obtained for a high-density gas of bosons interacting through a potential composed of a hard core followed by a square well, i.e.,

$$g(r) = \delta(r) - \frac{\lambda^2}{(2\pi)^3 a^2} \left[ \frac{4\pi}{ar} \left\{ \frac{\pi r}{2}, 0 < r \leq a \right\} \right] \\ + \frac{2m^*}{(2\pi)^3 \hbar^2} \frac{4\pi \rho V_0 (b-a)^3}{3} \left[ \frac{4\pi}{ar} \left\{ \frac{\pi r}{2}, 0 < r \leq a \right\} \right] \quad \dots(9)$$

The corresponding expression for the low-density Bose (dilute Bose gas) is obtained between Eqs (6 and 8) as:

$$g(r) = \delta(r) - \frac{2m^* \rho}{(2\pi)^3 \hbar^2} \left[ \frac{4\pi \hbar^2 a}{m^*} \left\{ 1 + (8\pi \rho a^3)^{\frac{1}{2}} + \frac{16\pi \rho a^3}{3} \right\} - \frac{4\pi V_0 (b-a)^3}{3} \right] \left[ \frac{4\pi}{ar} \left\{ \frac{\pi r}{2}, 0 < r \leq a \right\} \right] \quad \dots(10)$$

If the substitution  $V_0=0$  is made in Eq. (9),  $g(r)$  is obtained for a high-density hard-sphere Bose gas and, by substituting  $V_0=0$  in Eq. (10);  $g(r)$  is obtained for a dilute hard-sphere Bose gas.

For values of  $k$  for which  $\frac{\sin ka}{ka} \rightarrow 1$ , the value of  $g(r)$  for a system of bosons interacting through a two-body potential composed of a hard-core followed by a square well becomes:

$$g(r) = \delta(r) - \frac{2m^* N_0 t_{00,00}}{(2\pi)^3 \hbar^2} \left[ \frac{4\pi}{r} \left\{ \begin{array}{l} \frac{\pi}{2}, r > 0 \\ 0, r = 0 \\ -\frac{\pi}{2}, r < 0 \end{array} \right\} \right] \dots(11)$$

### 3 Discussion of the pdf

The following are the well-known features of the pdf:

- (i) It should not have a singularity at  $r = 0$ .
- (ii) It should have the limiting value unity as  $r \rightarrow 0$ , since as  $r_2 \rightarrow r_1$ , one is sure to find a particle there or pdf should have a delta function.
- (iii) For a hard-sphere Bose gas, it should not vanish inside the hard sphere<sup>2</sup>. According to earlier calculations, it varies as  $(\rho a^3)^{1/2}$  for a dilute hard-sphere Bose gas.
- (iv) For temperatures less than  $T_\lambda$ , it should behave like  $1/r$ . Earlier calculations show that the leading term in the pdf of a dilute hard-sphere Bose gas is  $\frac{-2a}{r} \rho_0^2$ , where  $a$  is the hard-sphere radius and  $\rho_0$  is the occupation number density of the ground state.  $\rho_0$  is small compared with the total particle number  $N_0$  if the temperature  $T$  is around  $T_\lambda$ .

We shall now discuss how far the expressions derived by us for the pdf have the features mentioned above, and what new results have been obtained by us.

Eqs (9-11) clearly show that the pdf has no singularity at  $r=0$  and it tends to unity for  $r \rightarrow 0$ . For a high-density hard sphere Bose gas, Eq. (9) shows that the pdf does not vanish inside the hard-sphere. Its value is  $g(r) = \frac{-\lambda^2}{4\pi a^3}$ . For a dilute hard-sphere Bose gas, Eq. (10) shows that the pdf does not vanish inside the hard sphere and in our case it varies linearly with  $\rho a$  rather than  $(\rho a^3)^{1/2}$ .

Also in this work, the pdf varies as  $1/r$ . The leading term for the pdf for the high-density hard-sphere Bose gas is  $\frac{-\lambda^2}{4\pi a^2 r}$ . Similarly, an expression for the low-

density hard-sphere Bose gas can be obtained. The coefficient of  $\frac{1}{r}$  in our case is  $\frac{-\lambda^2}{4\pi a^2}$ , and in the earlier calculations it is  $-2a\rho_0^2$ . These relative magnitudes are the same when it is realized that  $\rho_0$  is small compared with  $N_0$  for temperatures  $T$  around  $T_\lambda$ .

The effect of the attractive well after the hard core is to increase the value of  $g(r)$ , which means that the probability density for finding an atom in the neighbourhood of the point  $r_2$ , if another is known to be at the point  $r_1$ , has increased. This is equivalent to localization, which is a precondition for condensation and solidification. This also explains that for liquid <sup>4</sup>He to condense, it is necessary that the two-body interaction potential must have some attractive part after the hard core.

When the temperatures are very low, such that  $\frac{\sin ka}{ka} \rightarrow 1$ , Eq. (11) shows that both the terms that constitute  $g(r)$  are defined at  $r = 0$ . This is not so in the case of Eqs (9 and 10). In Eq. (11) at  $r=0$ ,  $g(r) = 1$ , and therefore, as  $r_2 \rightarrow r_1$ , one is sure to find a particle there and hence, the system has condensed. This shows that the condition for the system to condense is that  $\frac{\sin ka}{ka} \rightarrow 1$ .

### 4 Ground State Energy of Solid <sup>4</sup>He

We shall now use the value of  $g(r)$  derived for the high density Bose gas to calculate the ground state energy of solid <sup>4</sup>He. Precisely, we shall use Eq. (9) for  $g(r)$ .

The Hamiltonian for a system of  $N$  helium atoms, each of mass  $m$  and interacting through a two-body potential  $V(r_{ij})$ , is written as:

$$H = \frac{-\hbar^2}{2m} \sum_{i=1}^N \nabla_i^2 + \sum_{\substack{1 \leq i < j \leq N \\ i \neq j}} V(r_{ij}) \dots(12)$$

where  $r_{ij} = |r_i - r_j|$ .

The two-body interaction potential between the helium atoms is a hard core followed by a square well, i.e,

$$V(r_{ij}) = \begin{cases} +\infty, & 0 < r < a \\ -V_0, & a < r < b \\ 0, & r > b \end{cases} \dots(13)$$

where

$$a = 2.1 \text{ \AA}$$

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

$b = \text{variable}$

...(14)

Following Hansen and Levesque<sup>20</sup>, the potential energy and kinetic energy per particle in terms of  $g(r)$  can be written as:

$$\frac{\langle V \rangle}{N} = \frac{1}{2} \rho \int g(r) V(r) d^3 r \quad \dots(15)$$

$$\frac{\langle T \rangle}{N} = \frac{1}{2} \rho \int g(r) T(r) d^3 r + \frac{3\hbar^2}{4m} A \quad \dots(16)$$

where

$$T(r) = \frac{\hbar^2}{4m} \left[ \frac{d^2 u(r)}{dr^2} + \frac{2}{r} \frac{du(r)}{dr} \right] \frac{1}{\rho} \quad \dots(17)$$

Knowing  $\langle V \rangle/N$  and  $\langle T \rangle/N$  in the ground state will give the total ground state energy per particle since:

$$\frac{\langle E \rangle}{N} = \frac{\langle T \rangle}{N} + \frac{\langle V \rangle}{N} \quad \dots(18)$$

To calculate  $\langle V \rangle/N$ , we replace<sup>23</sup>  $V(r)$  by  $t_{00,00}$  in Eq. (15) to obtain the ground-state energy of solid <sup>4</sup>He. Eq. (15) now becomes:

$$\begin{aligned} \frac{\langle V \rangle}{N} &= \frac{1}{2} \rho \int g(r) t_{00,00} d^3 r \\ &= -\frac{1}{2} \rho \left\{ \begin{array}{l} \frac{1}{G_0(a,a)} \\ -4\pi \int_a^\infty r^2 V(r) dr \left[ 1 - \frac{G_0(a,r)}{G_0(a,a)} \right]^2 \end{array} \right\} g(r) d^3 r \\ &= -\rho \left[ \frac{1}{G_0(a,a)} + \frac{2\pi V_0 (b-a)^3}{3} \right] \int_0^\infty g(r) d^3 r \\ &= -\rho \left[ \frac{2\pi V_0 (b-a)^3}{3} - \frac{2\pi a \hbar^2}{m} \right] \left[ 1 - \frac{\lambda^2}{6a^2} (3b^2 - a^2) \right] \\ &\quad + \frac{4\pi \rho V_0 m^* (b-a)^3 (3b^2 - a^2)}{9\hbar^2} \end{aligned}$$

To calculate  $\langle T \rangle/N$ , we have to first know  $T(r)$ . Eq. (17) gives Eq. (20)  $T(r)$  for  $n=5$ ,

$$T(r) = \frac{5\hbar^2 B^5}{m \rho r^7} \quad \dots(20)$$

Eq. (16) now becomes:

$$\frac{\langle T \rangle}{N} = \frac{3\hbar^2 A}{4m} + \frac{5\hbar^2 B^5}{2m} \int \frac{1}{r^7} g(r) d^3 r \quad \dots(21)$$

For the kinetic energy term,  $g(r)$  can be approximated within the region  $a < r < b$  as:

$$g(r) = \frac{-m^*}{2\pi\hbar^2} \left[ \frac{\hbar^2 \lambda^2}{2m^* a^2} - \frac{4\pi\rho V_0 (b-a)^3}{3} \right] \frac{1}{r} \quad \dots(22)$$

Substituting for  $g(r)$  from Eq. (22) in Eq. (21) results in

$$\begin{aligned} \frac{\langle T \rangle}{N} &= \frac{3\hbar^2 A}{4m} - \frac{5m^* B^5}{m} \left( \frac{1}{a^5} - \frac{1}{b^5} \right) \\ &\quad \times \left[ \frac{\hbar^2 \lambda^2}{2m^* a^2} - \frac{4\pi\rho V_0 (b-a)^3}{3} \right] \quad \dots(23) \end{aligned}$$

For numerical calculations, the following values for the various quantities will be used:

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

$$B = 1.11 \times 10^{-8} \text{ cm}$$

$$A = 2.1 \text{ \AA}$$

$$A = \frac{5.3}{a^2}$$

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

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

## 5 Calculations

Eq. (19) is used to calculate  $\langle V \rangle/N$ ; Eq. (23) to calculate  $\langle T \rangle/N$ , and the value of  $\langle E \rangle/N$  is then obtained from Eq. (18). All the values are presented in Tables 1-3.

## 6 Discussion of the Ground-State Energy of Solid <sup>4</sup>He

We have calculated the ground-state energy of solid <sup>4</sup>He assuming that the two-body interaction potential which is valid in the gas phase or liquid phase is also valid in the solid phase. Similar assumptions have been made by other researchers<sup>20</sup>.

Table 1 — Variation of  $\langle V \rangle/N$ ,  $\langle T \rangle/N$  and  $\langle E \rangle/N$  with  $b$  for  $\rho=2.0 \times 10^{22}$  particles/cm<sup>3</sup>

$b$ in Å	$\langle V \rangle/N$ $\times 10^{-16}$ in erg	$\langle T \rangle/N$ $\times 10^{-16}$ in erg	$\langle T \rangle/N$ $\times 10^{-16}$ in erg	$\langle E \rangle/N$ in °K
3.10	-118.69	19.78	-98.91	-71.32
3.20	-190.37	7.85	-182.52	-132.25
3.50	-192.97	8.73	-184.14	-133.41
3.80	-225.73	8.89	-216.84	-152.11
4.10	-210.77	9.70	-201.07	-145.72
4.50	-135.46	8.42	-127.04	-98.40
4.60	-104.37	8.58	-95.79	-71.02
4.70	-64.42	8.21	-56.20	-40.73
4.80	-26.91	9.00	-14.91	-10.80
4.81	-18.02	8.99	-9.03	-6.34
4.82	-18.10	8.75	-9.35	-7.26
4.83	-13.05	8.78	-4.26	-3.09
4.85	-4.06	9.25	5.22	3.79
4.90	21.79	8.68	30.47	22.08
5.10	101.02	10.66	111.68	88.93

Table 2 — Variation of  $\langle V \rangle/N$ ,  $\langle T \rangle/N$  and  $\langle E \rangle/N$  with  $b$  for  $\rho=2.06 \times 10^{22}$  particles/cm<sup>3</sup>

$b$ in Å	$\langle V \rangle/N$ $\times 10^{-16}$ in erg	$\langle T \rangle/N$ $\times 10^{-16}$ in erg	$\langle T \rangle/N$ $\times 10^{-16}$ in erg	$\langle E \rangle/N$ in °K
3.10	-126.7	13.89	-112.81	-81.74
3.40	-147.1	3.55	-143.55	-104.00
3.60	-156.0	3.38	-152.62	-110.6
3.80	-159.2	3.33	-155.87	-112.90
4.10	-148.6	3.45	-145.15	-105.20
4.40	-114.1	3.76	-110.34	-79.93
4.60	-75.59	4.06	-70.53	-51.11
4.70	-48.89	4.24	-44.65	-32.35
4.75	-35.84	4.34	-31.50	-22.82
4.80	-20.41	4.44	-15.97	-11.57
4.81	-17.32	4.46	-12.86	-9.32
4.82	-13.46	4.49	-8.98	-6.50
4.85	-4.39	4.55	0.16	-0.12
4.90	12.84	4.67	17.51	12.69
5.10	90.95	5.17	95.72	69.36

From Tables 1 and 2, it is clear that the value of  $\langle E \rangle/N$  is more negative for  $b=3.8$  Å, keeping all the other parameters of the two-body interaction potential the same. If the criterion for liquid-solid phase transition is that  $\langle E \rangle/N$  should be more negative, then the two-body interaction potential with  $b=3.8$  Å along with the other parameters of the interaction potential given in Tables 1 and 2 will be the most appropriate interaction parameters in the solid phase. The density of solid <sup>4</sup>He is  $2.5 \times 10^{22}$  particles cm<sup>-3</sup> or  $2.8 \times 10^{22}$  particles cm<sup>-3</sup>,  $\langle E \rangle/N = -307.32 \times 10^{-16}$  erg = -222.9 K. These values are very high in magnitude

Table 3 — Variation of  $\langle V \rangle/N$ ,  $\langle T \rangle/N$  and  $\langle E \rangle/N$  with  $b$  and particle density  $\rho$ 

$b$ in Å	$\rho \times 10^{22}$ particles/ cm <sup>3</sup>	$\langle V \rangle/N$ $\times 10^{-16}$ in erg	$\langle T \rangle/N$ $\times 10^{-16}$ in erg	$\langle T \rangle/N$ $\times 10^{-16}$ in erg	$\langle E \rangle/N$ in °K
3.80	2.8	-135.42	8.086	-307.32	-222.69
3.80	2.5	-280.29	7.573	-272.72	-196.60
4.81	2.8	-25.404	9.893	-15.511	-11.238
4.82	2.5	-19.196	9.658	-9.438	-6.839

compared with the experimental value for  $\langle E \rangle/N$  which is around -6.0K.

However, we note from Table 1 that everything else remaining the same, for  $b=4.81$  Å,  $\langle E \rangle/N = -6.34$  K which is very close to the experimental value of around -6.0 K. Whereas in Table 2, good agreement is obtained for  $b=4.82$  Å which gives  $\langle E \rangle/N = -6.5$  K. But when we use the solid <sup>4</sup>He density =  $2.8 \times 10^{22}$  particles/cm<sup>3</sup> and  $b=4.81$  Å,  $\langle E \rangle/N = -11.238$  K, and for  $b=4.82$  Å,  $\rho=2.5 \times 10^{22}$  particles/cm<sup>3</sup>,  $\langle E \rangle/N = -6.839$  K; and these values compare favourably with the experimental values, keeping in mind the complexities involved in making measurements at very low temperatures.

Tables 1 and 2 show that the values of  $\langle E \rangle/N$  for  $b$  between 3.2 Å and 4.1 Å are exceptionally more negative and exhibit a bump around  $b=3.8$  Å. These could be considered as meta-stable states of the system around which the liquid-solid phase transition is more probable. But all these calculations, incidentally and so many other straightforward calculations (which have not been reported here) have not given us sufficient insight as to what the exact criterion for the liquid-solid phase transition for <sup>4</sup>He is. If it is taken for granted that  $\langle E \rangle/N$  is the most reliable value for the ground state of solid <sup>4</sup>He, then for  $\rho = 2.0 \times 10^{22}$  or  $2.06 \times 10^{22}$  particles/cm<sup>3</sup> and  $b=4.81$  Å or 4.82 Å, the ground state energy in the solid phase is more negative.

If, however, the most reliable parameter is the particle number density  $\rho$ , then for  $\rho = 2.8 \times 10^{22}$  particles/cm<sup>3</sup> and  $b=4.81$  Å, the liquid solid phase transition occurs for  $\langle E \rangle/N = -11.239$  K. Whereas for  $b=4.82$  Å and  $\rho=2.5 \times 10^{22}$  particles/cm<sup>3</sup>,  $\langle E \rangle/N = -6.839$  K, which compares favourably with experimental value.

## 7 Conclusion

We thus come to the conclusion that a system of bosons, interacting through a two-body potential composed of a hard core followed by a square well

such that  $a=2.1\text{\AA}$ ,  $V_0=5.0\times 10^{-16}$  erg,  $b=4.18\text{\AA}$  or  $4.82\text{\AA}$  and  $\rho=2.8\times 10^{22}$  particles/cm<sup>3</sup> or  $2.5\times 10^{22}$  particles/cm<sup>3</sup>, can undergo liquid-solid phase transition such that  $\langle E \rangle/N$  compares very favourably with the experimental value for the ground-state energy of solid <sup>4</sup>He.

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