



LOW TEMPERATURE THERMODYNAMIC BEHAVIOUR IN A SYSTEM OF INTERACTING BOSONS

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Abstract: The radial distribution function, second virial Coefficient and specific heat are calculated for a system of interacting bosons using the methods of statistical mechanics. The results show that the values of the second virial co-efficient and specific heat fluctuate around 0.6 °K, agreeing with the experimentally observed abrupt changes in the thermodynamic properties of liquid ^4He around 0.6 K.

Introduction:

In our present; work, we consider a system of bosons interacting via a two body potential composed of a hard core followed by a square well and calculate the radial distribution function $g(r)$ using the fundamental relation between $g(r)$ and the structure factor $S(q)$. Also, we use the Feynman relation between the excitation energy $E(q)$ and the structure factor $S(q)$. From such knowledge of $g(r)$ we proceed to calculate the second virial coefficient $B_2(T)$ with the usual statistical mechanical relation and then proceed to calculate the specific heat C_v of these interacting bosons.

Theoretical formulations:

We assume the bosons to be interacting via a two-body potential composed of a hard repulsive core followed by an attractive square well by

$$U(r) = \begin{cases} \alpha & r < a \\ -V_0 & a < r < b \\ 0 & r > a \end{cases} \quad (1)$$

Where, a is the hard-core diameter which, in our present case, is the diameter of a ^4He atom. For such a system of interacting bosons, the r.d.f. can be calculated by using the equation:

$$g(r) = 1 + \frac{1}{2\pi^2 \rho r} \int_0^\infty [S(q) - 1] q \sin qr dq \quad (2)$$

Where, $S(q)$ is the structure factor given by

$$S(q) = \frac{h^2 q^2}{2m^* E(q)} \quad (3)$$

In equation (3), m^* is the effective mass and $E(q)$ is the excitation energy.

For the inter particle potential given by equation (1), $E(q)$ is given by (Ref. Khanna, K.M. & Phukan, A.N. Physica 60, 1972):

$$E(q) = \left[\frac{\hbar^4 q^4}{4m^* a^2} + \left\{ \frac{\hbar^4 x^2}{2m^* a^3} - \frac{4\pi\rho V_0 \hbar^2 (b-a)^3}{3m^* a} \right\} q \sin qa \right]^{\frac{1}{2}} \quad (4)$$

With $E(q)$ given by equation (4), equation (3) & (2) after detailed integrating give

$$g(r) = 1 + \frac{Y}{r} \quad (5)$$

Where,

$$Y = -\frac{m^* a}{2\pi\rho\hbar^4} \left\{ \frac{\hbar^4 x^2}{2m^* a^3} - \frac{4\pi\rho V_0 \hbar^2 (b-a)^3}{3m^* a} \right\} \quad (6)$$

Y is a constant in our case.

The second virial co-efficient is given by the r.d.f. $g(r)$ through the well-known relation:

$$B_2(T) = -\frac{2\pi}{3K_B T} \int_0^\infty r^3 g(r) \frac{\partial U(r)}{\partial r} dr \quad (7)$$

In equation (7) the term $r \frac{\partial U(r)}{\partial r}$ has the dimension of energy. One can write,

$$r \frac{\partial U(r)}{\partial r} = AK_B T f(r) \quad (8)$$

Where, A is a constant which, due to three degrees of freedom for each particle, is equal to 3.

In equation (8), $f(r)$ has been identified with the Mayer function defined by

$$f(r) = \exp\{-\beta U(r)\} - 1 \quad (9)$$

Where, $U(r)$ is the inter-particle potential.

With this approach and using equation (5) & (7) we finally obtain

$$B_2(T) = 2\pi \{ \exp(\beta V_0) - 1 \} \left\{ \frac{(b^3 - a^3)}{3} + Y \frac{(b^2 - a^2)}{2} \right\} \quad (10)$$

With $E_2(T)$ given by equation (10), the specific heat C_V is obtainable from the equation,

$$C_V = 2\rho K_B T \frac{\partial}{\partial T} B_2(T) + \rho K_B T^2 \frac{\partial^2}{\partial T^2} B_2(T) \quad (11)$$

Using equation (10), this gives

$$C_V = -2\pi \left\{ \frac{(b^3 - a^3)}{3} + Y \left(\frac{b^2 - a^2}{2} \right) \frac{\rho V_0^2}{K_B T^2} \exp\left(\frac{V_0}{K_B T} \right) \right\} \quad (12)$$

Numerical calculations:

We have used the following set of values for the different parameters appearing in equations (10) and (12) to calculate $B_2(T)$ and C_V .

$$\rho = 2 \times 10^{22} \text{ particles / cm}^3$$

$$V_0 = 16.11 \times 10^{-16} \text{ erges}$$

$$K_B = 16.11 \times 10^{-16} \text{ ergs}$$

$$b = 6.0 \text{ \AA}$$

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

$$\frac{m^*}{m} = 1.6$$

$$m = 6.646 \times 10^{-24} \text{ gm} = \text{Mass of a } ^4\text{He atom.}$$

The results of these calculations are recorded in Table -1.

| T in $^{\circ}\text{K}$ | $B_2(T)$ in $\text{cm}^3 / \text{particle}$ | C_V in $\text{ergs}/^{\circ}\text{K}$ |
|---------------------------|---|---|
| 0.2 | 78.7036×10^3 | 74.00×10^{13} |
| 0.4 | 16.8050×10^9 | 39.50×10^9 |
| 0.6 | 10.0446×10^{13} | 10.49×10^4 |
| 0.8 | 7.7655×10^{16} | 4.56×10^6 |
| 1.0 | 4.1985×10^{16} | 15.791×10^8 |
| 1.2 | 0.6003×10^{16} | 1.568×10^8 |
| 1.4 | 0.1496×10^{16} | 0.287×10^8 |
| 1.6 | 0.0527×10^{16} | 0.078×10^8 |
| 1.8 | 0.0234×10^{16} | 0.027×10^8 |
| 2.0 | 0.0122×10^{16} | 0.012×10^8 |
| 2.22 | 0.0096×10^{16} | 0.000×10^8 |

Discussions:

1. The values for the second virial co-efficient and specific heat show abrupt, changes around $T = 0.6^{\circ}\text{K}$. This seems to agree with the experimentally observed abrupt changes in the thermodynamic properties of liquid ^4He around $T = 0.6^{\circ}\text{K}$.
2. Both $B_2(T)$ and C_V decrease with increase of temperature in the range $0.2^{\circ}\text{K} < T < 2.2^{\circ}\text{K}$.
3. The change in the values becomes very high in the region $T < 1.0^{\circ}\text{K}$.
4. Since we are dealing with a quantum degenerate assembly of interacting bosons, the quantum effects are pronounced at low temperatures. The attractive forces between the molecules being strong enough, discrete quantum states of the relative motion of two molecules exist, and loosely bound polarization molecule is formed. This has an effect, on the second virial coefficient at low temperatures and this effect is determined by the strength of the attractive molecular forces. Further, when the temperature is sufficiently low, the energy of the system is mainly potential and the most operative part of the potential is the "attractive part," which naturally reduces the pressure and thereby makes the second virial coefficient, more negative.
5. Calculations with another type of potential, namely the hard core followed by a combination of repulsive and attractive components (Ref. Khanna K.M. & Das B.N.,

Physica 76 (1974) 137) which could satisfactorily explain the energy excitation spectrum in liquid ^4He , is in progress and will be reported elsewhere.

References:

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