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Final Report

Some Aspects of Correlation in Many-Particle Systems

Principal Investigator: Dr. Allen Miller

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Author of Report: Dr. Allen Miller

Personnel Supported by Report: Dr. Allen Miller (in part)

Mr. Harvey Scher (in part)

Mr. Bruce Friedman (in part)

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Abstract

An expansion is given for the ground-state energy of a system of interacting Bose particles, using Rayleigh-Schrodinger perturbation theory with the scattering part of the interaction as the perturbation. The result in second order reproduces the energy shift found by various authors. The energy spectrum of the zero-order Hamiltonian contains a gap of magnitude $\int_0^\infty V_k$ where V_k is the Fourier transform of the two-particle interaction. This gap removes the third-order divergence resulting when the entire interaction is used as the perturbation. The structure factor, computed to first order, is in qualitative agreement with experiment for large momentum values. For non-zero temperature, expressions are obtained for the depletion of the zero-momentum mode and the specific heat, using the zero-order Hamiltonian. The specific heat exhibits a discontinuity at the critical point. Quantitative estimates for the magnitude of the specific heat at the critical point yield results which are in fair agreement with empirical values for liquid helium.

Introduction

As is well known, liquid helium II can be idealized as a system of interacting Bose particles. The non-interacting system was studied by London¹ who showed that below a "critical" temperature, a condensation phenomenon occurs. The average number of particles in the zero momentum mode is of the same order of magnitude as the total particle number. In contrast, the average number of particles in any other state is of the order of unity. The term "Bose-Einstein condensation" is used to denote the special role of the zero-momentum mode.

For the interacting system, it will not suffice to use simple perturbation theory. Brueckner and Sawada² and also Huang and Yang³ have shown that the ground state energy per particle is not independent of the total particle number N in third order and beyond; instead, it becomes infinite in the limit of large N .

The first microscopic theory of the interacting system is due to Bogoliubov⁴. Assuming sufficiently weak interatomic forces, he showed that the Hamiltonian could be diagonalized by a canonical transformation. The transformed Hamiltonian represents a set of non-interacting quasi-particles which obey Bose statistics. For large momenta, the energy spectrum of the quasi-particles is quadratic and is identical to that of the ideal system. But for low momenta, the spectrum is linear (phonons) a radical departure from the free particle results. The spectrum found is similar to that proposed earlier by Landau⁵, based on thermodynamic data.

Two approximations are necessary in the Bogolinbov theory. First, it is assumed that condensation is still present when the interactions are taken into account. Thus, for sufficiently low temperatures, the average value of $N_0 = a_0^\dagger a_0$ will be large, compared to unity. (We denote the number operator for the zero momentum mode by N_0 ; a_0^\dagger and a_0 are the creation and destruction

operators for the zero momentum mode, respectively.) The commutator $[a_0, a_0^+]$, (which is exactly unity for Bose statistics) is small compared to $\langle N_0 \rangle$. Hence, a_0 approximately commutes with a_0^+ . Both these operators can therefore be replaced by the constant $\langle N_0 \rangle^{1/2}$; the value of $\langle N_0 \rangle^{1/2}$ can be determined later by the requirements of self-consistency, when the ground state has been determined. This approximation is called the c-number approximation. It is worthwhile to remark that the c-number approximation ignores the fluctuation in $N_0 = a_0^+ a_0$; this is justified because the theory yields a fluctuation in N_0 which is of the order of magnitude of $\langle N_0 \rangle^{1/2}$, much smaller than $\langle N_0 \rangle$.

The second approximation is to omit the terms in the Hamiltonian H which contain less than two factors of a_0 or a_0^+ . A straightforward analysis shows that this approximation is valid only for weak interactions. That this is to be expected can be seen from the following argument: Due to the interaction, states other than the zero-momentum mode are occupied. It is said that the zero-momentum mode is "depleted". For sufficiently weak interactions, the depletion is small. Then the terms of H containing less than two factors of a_0 or a_0^+ will be unimportant since $\langle N_0 \rangle \gg \langle N \rangle - \langle N_0 \rangle$.

Lee, Huang and Yang⁶ have investigated the hard sphere Bose gas, using a pseudopotential for the two-particle interaction. Their method can be shown to be equivalent to that of Bogolinbov; their results for the ground state energy and the excitation spectrum are similar to the Bogolinbov results. Lee and Yang⁷ have extended the study to non-zero temperature and have computed the specific heat. The specific heat is found to exhibit a discontinuity at the critical temperature; the magnitude of the discontinuity is proportional to the hard sphere diameter.

Extensive studies have been completed on the interaction between the quasi-particles. (The quasi-particle interaction is contained in the terms dropped by the Bogoliubov truncation of the Hamiltonian.) The ground state

energy has been examined by Wu⁸ for the hard sphere gas. Applying perturbation theory to the quasi-particle interaction, Wu obtained the next order term beyond that calculated by Lee, Huang and Yang.

By employing the Green function method of quantum field theory, Beliaev⁹ and later Hugenholtz and Pines¹⁰ have confirmed the results of Wu. Hohenberg has reformulated the Green function method using variational derivative techniques. His work enables the computation of the density correlation function to one order beyond the Bogoliubov approximation.

Several workers have studied the properties of truncated Hamiltonians which are more complete than that of Bogoliubov. Girardeau and Arnowitt¹² have added all pair scattering terms to the Bogoliubov Hamiltonian and diagonalized the resulting Hamiltonian by a canonical transformation. The energy spectrum that is obtained contains a gap in the limit of long wavelength and thus shows that the success of Bogoliubov in obtaining a phonon spectrum was fortuitous.

Takano¹³ has considered correlations beyond simple pair scattering. He shows the existence of a collective mode which removes the gap. However, it is not easy to obtain the corrections to the equation-of-motion used by Takano.

Luban¹⁴ has considered the thermodynamics of the Girardeau-Arnouitt model. The phase transition at the critical temperature is found to be of first order.

Lieb and Leninger¹⁵ have shown that in one dimension a system of bosons interacting pairwise via delta-function potentials can be solved exactly. Lieb¹⁶ has investigated the excitation spectrum and has shown that in this model there is a double spectrum. The two dispersion curves possess a common slope in the limit of low momentum.

The work described in this report has been motivated by the desire to obtain a systematic perturbation theory to compute basic properties of the

Bose system in a region of temperature above as well as below the critical temperature. For this purpose, we develop a method which avoids the use of the Bogolinbov d -number approximation.

Section I begins with a discussion of Rayleigh-Schrodinger perturbation theory (R-S) applied to the Bose gas. We show how the straight-forward use of R-S perturbation theory in a calculation of the ground state energy leads to divergent results in third and higher orders. A simple modification of the R-S method is given which avoids these divergent terms. The structure factor is computed to second order in the modified perturbation scheme. The calculation reveals the expansion parameter, which is a function of the Fourier transform of the potential. The parameter is small at large momentum values but approaches one half in the limit of vanishing momentum. The structure factor is in qualitative agreement with experiment in the region of large momentum. In the low momentum region, the perturbation series for the structure factor converges slowly so that the first few terms do not provide a good representation.

In Section II, we present a mathematical introduction to the methods used in our calculation of the statistical mechanics of the lowest order Hamiltonian. The ideal gas is used as an illustration.

Section III contains the calculation of the statistical mechanics of the Bose gas interacting through the Hartree-Fock potential. A discontinuity in the specific heat is obtained. The magnitude of the discontinuity is proportional to the rate of depletion of the zero-momentum mode with increasing temperature. By using the Yntema-Schneider¹⁷ potential, qualitative agreement with the experimental specific heat is obtained. The range of validity of the calculation is examined and is found to exclude only the case of a weak repulsive interaction near the transition temperature.

Section I

Modified Perturbation Theory and Structure

Factor of a Many - Boson System

We first wish to study the properties of a system of N interacting Bose particles with the use of Rayleigh - Schrodinger (R-S) perturbation theory.

The Hamiltonian we shall consider is¹⁸

$$\begin{aligned}
 H &= H_0 + H_1, \\
 H_0 &= \sum_{\mathbf{k}} T_{\mathbf{k}} a_{\mathbf{k}}^{\dagger} a_{\mathbf{k}}, \\
 H_1 &= \frac{1}{2\Omega} \sum_{\mathbf{g}, \mathbf{g}', \mathbf{k}} V_{\mathbf{g}} a_{\mathbf{k}'-\mathbf{g}}^{\dagger} a_{\mathbf{k}+\mathbf{g}}^{\dagger} a_{\mathbf{k}} a_{\mathbf{k}'}.
 \end{aligned} \tag{1.1}$$

In Eq. (1.1), $T_{\mathbf{k}} = \hbar^2 \mathbf{k}^2 / 2m$ is the kinetic energy of particles of momentum $\hbar \mathbf{k}$ and mass m . The operators $a_{\mathbf{k}}^{\dagger}$ and $a_{\mathbf{k}}$ are creation and annihilation operators for these particles and satisfy the commutation relations:

$$\begin{aligned}
 [a_{\mathbf{k}'}, a_{\mathbf{k}}] &= 0; \quad [a_{\mathbf{k}'}^{\dagger}, a_{\mathbf{k}}^{\dagger}] = 0; \\
 [a_{\mathbf{k}'}, a_{\mathbf{k}}^{\dagger}] &= \delta_{\mathbf{k}\mathbf{k}'}.
 \end{aligned} \tag{1.2}$$

$V_{\mathbf{g}}$ is the Fourier transform of the two-body potential $V(\vec{r})$:

$$V_{\mathbf{g}} = \int d^3r e^{-i\vec{g}\cdot\vec{r}} V(\vec{r}).$$

The allowed values of the wave vector in the sums are determined by imposing periodic boundary conditions in a cube of length L and volume

$$\Omega = L^3. \text{ Hence, } k_x = 2\pi m_x / L, \quad k_y = 2\pi m_y / L, \\ k_z = 2\pi m_z / L, \quad m_x, m_y, m_z = 0, \pm 1, \pm 2, \dots$$

In calculating the ground state energy of the Hamiltonian H , a difficulty integral appears in the third order of the perturbation expansion. In section 1.A we show how this difficulty can be circumvented by a modification of the R-S expansion, and we give results for the ground state energy up to third order. In section 1.B, the structure factor of the Bose system is computed in the modified perturbation scheme.

A. Modification of the R-S Perturbation Expansion

The interaction H_1 (Eq. 1.1) contains two types of terms. First, we have terms that are called forward and exchange scattering terms. They correspond to $\mathbf{q} = 0$ and $\mathbf{q} = \mathbf{k}' - \mathbf{k}$. These terms do not result in any net exchange of momentum between the Bose particles. Hence, the plane wave eigenstates of H_0 are also eigenstates of the forward and exchange terms. We are thus led to separate out these terms from the interaction H_1 and include them in the unperturbed Hamiltonian.

The second type of term in H_1 is composed of that part of the interaction which remains, after the forward and exchange terms are removed. These terms allow the Bose particles to exchange momentum. These terms will be the perturbation and are denoted by H_1' .

Thus,

$$H = H_0' + H_1', \\ H_0' = \sum_{\mathbf{k}} T_{\mathbf{k}} n_{\mathbf{k}}^{op} + \frac{N(N-1)}{2\Omega} V_0 + \frac{1}{2\Omega} \sum_{\mathbf{k} \neq \mathbf{k}'} V_{\mathbf{k}-\mathbf{k}'} n_{\mathbf{k}}^{op} n_{\mathbf{k}'}^{op} \quad (1.3)$$

$$H'_1 = \frac{1}{\Omega} \sum_{\substack{\vec{g}, \vec{k}, \vec{k}' \\ \vec{g} \neq 0, \vec{g} \neq \vec{k}' - \vec{k}}} \frac{V_{\vec{g}}}{2} a_{\vec{k}' - \vec{g}}^{\dagger} a_{\vec{k} + \vec{g}}^{\dagger} a_{\vec{k}} a_{\vec{k}'}$$

where

$$n_{\vec{k}}^{\text{or}} = a_{\vec{k}}^{\dagger} a_{\vec{k}}$$

Examining the modified free Hamiltonian H'_0 we find that the ground state energy is not zero, but is given by

$$E'_0 = \frac{N(N-1)}{2\Omega} V_0. \quad (1.4)$$

Eq. (1.4) is easily obtained by simply setting $n_0 = N$ and $n_{\vec{k}} = 1$ for $\vec{k} \neq 0$. The next excited state of the Hamiltonian H'_0 with total momentum zero is the state of a single excited pair with momentum $(\vec{q}, -\vec{q})$.

The energy of this state is obtained by setting $n_0 = N-2$,

$$n_{\vec{q}} = 1, \quad n_{-\vec{q}} = 1, \quad n_{\vec{k}} = 0 \quad \text{for } \vec{k} \neq 0, \vec{q}, -\vec{q}.$$

Thus,

$$(E'_0)_{\vec{q}} = \frac{2q^2}{2m} + \frac{N(N-1)}{2\Omega} V_0 + \frac{2(N-2)}{\Omega} V_{\vec{q}} + \frac{V_{2\vec{q}}}{\Omega}.$$

(1.5)

If we take the difference between (1.5) and (1.4), we have

$$(E'_0)_{\vec{q}} - E'_0 = \frac{2q^2}{2m} + \frac{2(N-2)}{\Omega} V_{\vec{q}}. \quad (1.6)$$

In the limit $q \rightarrow 0$, there is a gap of magnitude $2(N-2)V_0/\Omega$ between the ground state and the first excited state of the Hamiltonian H'_0 . It is the presence of this gap in the energy for an excited pair that prevents the

divergence of the third order perturbation term, as we shall soon see.

Using H_0' as the unperturbed Hamiltonian and H_1' as the interaction, the energy corrections to the ground state are as follows:

$$E_0' = \frac{N(N-1)}{2\Omega} V_0,$$

$$E_1' = 0,$$

$$E_2' = \frac{N(N-1)}{\Omega (2\pi)^2} \int_0^\infty q^2 \frac{V_q^2 dq}{\frac{q^2}{2m} + \frac{2(N-2)V_q}{\Omega}} \quad (1.7)$$

$$E_3' = \frac{N(N-1)}{4\Omega (2\pi)^6} \iint \frac{d^3q d^3q' V_q V_{q'} (V_{q-q'} + V_{q+q'})}{\left[\frac{q^2}{2m} + \frac{2(N-2)V_q}{\Omega} \right] \left[\frac{q'^2}{2m} + \frac{2(N-2)V_{q'}}{\Omega} \right]}$$

Note that the denominations in the integrands are of the form

$$\frac{2q^2}{2m} + \frac{2(N-2)V_q}{\Omega}. \quad \text{The second term precludes the}$$

possibility of a low momentum divergence.

B. Structure Factor of Interacting Bose Gas

It has been shown by Van Hove²⁵ and also by Cohen and Feynman²⁶ that in an inelastic neutron scattering experiment one can measure the probability per unit time that a slow neutron transfer energy $\hbar\omega$ and momentum $\hbar\vec{k}$ to the Boson system. For the ground state, the probability is

$$W(\vec{k}, \omega) = A S(\vec{k}, \omega) \quad (1.8)$$

in the Born approximation. Here, A is a constant which characterizes the neutron - Boson interaction, while $S(\vec{k}, \omega)$ is called the dynamic structure factor and depends only on the properties of the Boson system. It is defined

by

$$S(\vec{k}, \omega) = \sum_n (\rho_{\vec{k}}^{\dagger})_{n0} \delta(\omega - \omega_{n0}). \quad (1.9)$$

In Eq. (1.9), $\rho_{\vec{k}}^{\dagger}$ is the density fluctuation of momentum \vec{k} , defined by

$$\begin{aligned} \rho_{\vec{k}}^{\dagger} &= \int d^3r \rho(\vec{r}) e^{i\vec{k} \cdot \vec{r}} = \sum_{\vec{f}} e^{i\vec{k} \cdot \vec{r}_{\vec{f}}} \\ &= \sum_{\vec{f}} a_{\vec{f} + \vec{k}}^{\dagger} a_{\vec{f}}. \end{aligned} \quad (1.10)$$

The subscript n and 0 in $(\rho_{\vec{k}}^{\dagger})_{n0}$ denote matrix elements between the exact boson state n and the ground state. Also, $\hbar \omega_{n0}$ is the excitation energy of the state n above the ground state.

The differential cross section for inelastic neutron scattering can be obtained from Eq. (1.8) by integrating over the energy $\hbar\omega$. Thus, the differential cross section is proportional to

$$S(\vec{k}) = \frac{1}{N} \int_0^{\infty} d\omega S(\vec{k}, \omega). \quad (1.11)$$

$S(\vec{k})$ is called the liquid structure factor. It is the Fourier transform of the pair correlation function $\rho(\vec{r})$. Thus,

$$\begin{aligned} S(\vec{k}) &= \frac{1}{N} \langle 0 | \rho_{\vec{k}} \rho_{\vec{k}}^{\dagger} | 0 \rangle_H = \int d^3r \rho(\vec{r}) e^{-i\vec{k} \cdot \vec{r}}, \\ \rho(\vec{r}) &= \frac{1}{N} \langle 0 | \rho^{\dagger}(0) \rho(\vec{r}) | 0 \rangle_H \end{aligned} \quad (1.12)$$

The state $|0\rangle_H$ refers to the exact ground state.

To obtain $S(R)$, we use the perturbation expansion of the ground state for the matrix element of the density fluctuations in Eq. (1.12).

From R-S perturbation theory, the ground state can be expanded to second order.

The result is

$$|0\rangle^{(2)} = a|0\rangle + \sum_n' \frac{|n\rangle \langle n|H_1|0\rangle}{E_0' - E_n'} + \sum_{n,m} \frac{|n\rangle \langle n|H_1|m\rangle \langle m|H_1|0\rangle}{(E_0' - E_n')(E_0' - E_m')}. \quad (1.14)$$

The coefficient a of the unperturbed state $|0\rangle$ in Eq. (1.14) is a normalization factor which must be chosen such that ${}^{(2)}\langle 0|0\rangle = 1$.

This calculation yields

$$a = 1 - \frac{1}{2} \sum_n \frac{|(H_1)_{n0}|^2}{(E_0' - E_n')^2}$$

Eq. (1.14) can be applied specifically to our Hamiltonian, Eq. (1.3).

A straight forward calculation yields the result

$$|0\rangle^{(2)} = a|0\rangle - \frac{\sqrt{N(N-1)}}{2\Omega} \sum_{\mathcal{E}}' \frac{V_{\mathcal{E}} a_{\mathcal{E}}^+ a_{-\mathcal{E}}^+ |0\rangle_{N-2}}{\mathcal{E}^2/m + 2\rho V_{\mathcal{E}}} + \frac{\sqrt{N(N-1)(N-2)(N-3)}}{4\Omega^2} \sum_{\mathcal{E}, \mathcal{E}'}' \frac{V_{\mathcal{E}} V_{\mathcal{E}'} a_{\mathcal{E}}^+ a_{-\mathcal{E}}^+ a_{\mathcal{E}'}^+ a_{-\mathcal{E}'}^+ |0\rangle_{N-4}}{\mathcal{E}, \mathcal{E}' [\mathcal{E}^2/m + \mathcal{E}'^2/m + 2\rho(V_{\mathcal{E}} + V_{\mathcal{E}'})] [\frac{\mathcal{E}^2}{m} + 2\rho V_{\mathcal{E}}]}$$

(The notation $|0\rangle_{N-2}$ refers to the ground state of the non-interacting system of $N-2$ particles, etc.)

To evaluate
$$S(\vec{k}) = \frac{1}{N} \langle 0 | \rho_{\vec{k}} \rho_{\vec{k}}^\dagger | 0 \rangle_H,$$

we use the identity
$$\rho_{\vec{k}} \rho_{\vec{k}}^\dagger = N \bar{v} + \sum_{l, l'} a_{l'-\vec{k}}^\dagger a_{l+\vec{k}}^\dagger a_{l'} a_l,$$

an immediate consequence of the commutation relations Eq. (1.2).

Thus
$$S(\vec{k}) = 1 + \frac{1}{N} \langle 0 | \sum_{l, l'} a_{l'-\vec{k}}^\dagger a_{l+\vec{k}}^\dagger a_{l'} a_l | 0 \rangle_H.$$

Inserting our result for $|0\rangle^{(2)}$ in the above expression for $S(\vec{k})$ yields our result for the structure factor:

$$S^{(2)}(\vec{k}) = 1 - \frac{1}{2} \rho \bar{V}_{\vec{k}} \left(\frac{k^2}{m} + \rho \bar{V}_{\vec{k}} \right) + \frac{1}{8} \left[\frac{\rho \bar{V}_{\vec{k}}}{\frac{k^2}{2m} + \rho \bar{V}_{\vec{k}}} \right]^2$$

$$+ \frac{1}{16} \frac{1}{(2\pi)^3} \int d^3 q \frac{\rho \bar{V}_{\vec{q}}}{\frac{q^2}{2m} + \rho \bar{V}_{\vec{q}}} \left[\frac{\bar{V}_{\vec{q}-\vec{k}}}{\frac{(q-k)^2}{2m} + \rho \bar{V}_{\vec{q}-\vec{k}}} + \frac{\bar{V}_{\vec{q}+\vec{k}}}{\frac{(q+k)^2}{2m} + \rho \bar{V}_{\vec{q}+\vec{k}}} \right]$$

The notation $S^{(2)}(\vec{k})$ signifies the structure factor with terms up to second order in H_1' included.

Examining Eq. (1.15), it is seen that the expansion parameter for can be roughly designated by $\frac{1}{2} \rho \bar{V}_{\vec{k}} / \frac{k^2}{2m} + \rho \bar{V}_{\vec{k}}$. Hence, at high k , a rapid convergence of the series can be expected. However, at small k , the series converges slowly, since each term in the series is roughly one half the preceding term in the limit $k \rightarrow 0$.

Suppose we retain only the first order correction to $S(\vec{k})$ in Eq. (1.15) and compare the qualitative form of the results with experiment. The experimental values for $S(\vec{k})$ are characterized by damped oscillations about unity for high values of k . Experimental curves for $S(\vec{k})$ are contained in the work performed by Henshaw²⁷. -13-

To compare with Eq. (1.5), suppose we employ the soft core potential

$$\bar{V}_k = \frac{3V_0}{(ka)^2} \left[\frac{\sin ka}{ka} - \cos ka \right]$$

where a is the radius of the soft core and where $V_0 = 4\pi C a^3 / 3$.

(Here, C is the magnitude of the potential barrier.) Then, for large k ,

Eq. (1.15) becomes

$$S^{(2)}(k) \approx 1 - \frac{3mV_0}{k^2(ka)^2} \left[\frac{\sin ka}{ka} - \cos ka \right] \quad (1.16)$$

Note that the general form of Eq. (1.16) is in accord with the empirical results.

In conclusion, we might add that we expect the series expansion for the ground state energy, Eq. (1.7) to be rapidly converging. For the phase space factors in the integrals over the momentum q in the expressions for the corrections to the ground state energy are such as to deemphasize the low momentum region.

So the slow convergence of the series for $S(k)$, in the region of small k , has no counterpart in the series for the ground state energy because in the latter series, the sum over all momentum levels contributes a density of states factor that diminishes the importance of the low momentum states. Hence, we believe that the expressions Eq. (1.7) for the ground state energy up to second order is a good approximation to the exact perturbed ground state energy.

In the next section, we shall pursue an investigation of the thermodynamic properties of a Bose system using the lowest order Hamiltonian H_0' , with the view of obtaining reasonable quantitative agreements with experiment for quantities such as the specific heat.

Section II

Base Gas with Hartree-Fock Interaction

A. The Transition Temperature and Zero-Momentum Mode Occupation

According to statistical mechanics, all thermodynamic properties can be obtained from the canonical partition function Q_N , defined by

$$Q_N(\Omega, T) = \sum_n e^{-\beta E_n}, \quad \beta = \frac{1}{kT}. \quad (2.1)$$

Here, E_n is the n th energy level of the N -body system, T is the absolute temperature and k is Boltzmann's constant.

A partial list of thermodynamic quantities of interest, derivable from Q_N , are given below:

$$A = -\frac{1}{\beta} \log Q_N, \quad (\text{Helmholtz Free Energy})$$

$$U = \frac{\partial}{\partial \beta} \log Q_N, \quad (\text{Internal Energy})$$

$$C_V = \left. \frac{\partial U}{\partial T} \right|_{\Omega}, \quad (\text{Heat Capacity at Constant Volume})$$

To begin the task of evaluating the partition function, we insert the eigenvalues of H'_0 , given in Eq. (1.3), for the values of E_n in Eq. (2.1). Thus,

$$Q_N = \sum_{\sum n_R = N} \exp \left\{ -\beta \left[\sum_R T n_R + \frac{N(N-1)}{2\Omega} V_0 + \frac{1}{2\Omega} \sum_{R \neq S} V_{R-S} n_R n_S \right] \right\}$$

Each state in the canonical ensemble has a fixed total particle number N . Hence the second term in the exponent can be removed outside the sum. The partition function can now be written

$$Q_N = e^{-\beta \frac{N(N-1)}{2R} V_0} \tilde{Q}_N \quad (2.3)$$

where \tilde{Q}_N is defined by

$$\tilde{Q}_N = \sum_{\sum n_R = N} \exp\left\{-\beta \left[\sum_{i,j} \frac{1}{R} T_{ij} n_i n_j + \frac{1}{2R} \sum_{j \neq k} V_{j-k} n_j n_k \right]\right\}. \quad (2.4)$$

To compute \tilde{Q}_N , we define $\tilde{Q}(N, m_0)$ by

$$\tilde{Q}(N, m_0) = \sum_{\substack{\sum n_R = N \\ k \neq 0}} \exp\left\{-\beta \left[\sum_{i,j} \frac{1}{R} T_{ij} n_i n_j + \zeta \rho \sum_{k \neq 0} V_{k-k} n_k + \frac{1}{2R} \sum_{\substack{j \neq 0 \\ k \neq 0 \\ j \neq k}} V_{j-k} n_j n_k \right]\right\} \quad (2.5)$$

where $\zeta = \frac{m_0}{N}$

Hence,
$$\tilde{Q}_N = \sum_{m_0=0}^N \tilde{Q}(N-m_0, m_0). \quad (2.6)$$

Note that $\tilde{Q}(N, m_0)$ can be thought of simply as the partition function of a system of N particles, whose single particle levels do not include the zero momentum level.

Let $\tilde{Q}(N-m_0, n_0)_{MAX}$ denote the maximum term in the sum on n_0 in Eq. (2.6). Then, in the limit of large N ,

$$\log \tilde{Q}_N = \log \tilde{Q}(N-m_0, n_0)_{MAX} \quad (2.7)$$

The verification of Eq. (2.7) is simple:

Write

$$Q_{MAX} \leq Q_N \leq N Q_{MAX}$$

Thus,

$$\frac{\log Q_{MAX}}{N} \leq \frac{\log Q_N}{N} \leq \frac{\log Q_{MAX}}{N} + \frac{\log N}{N}$$

Now

$$\frac{\log Q_{MAX}}{N}$$

is not zero in the limit $N \rightarrow \infty$, but

$$\frac{\log N}{N} \rightarrow 0. \quad \text{Thus, } \frac{\log Q_N}{N} = \frac{\log Q_{MAX}}{N},$$

which verifies Eq. (2.7).

The generating function for $\tilde{Q}(N, m_0)$ is defined by

$$\mathcal{Q}(z, \xi) = \sum_{N=0}^{\infty} z^N \tilde{Q}(N, m_0) \quad (2.8)$$

$$\mathcal{Q}(z, \xi) = \sum_{\{n_A\}}' z^{\sum n_A} \exp \left\{ -\beta \left[\sum_A (T_A + \xi p_A) + \sum_{\substack{A, B=1 \\ A \neq B}}^R \frac{V_{AB} n_A n_B}{2N} \right] \right\}. \quad (2.9)$$

The prime on the summation signs indicates the deletion of the zero momentum state from the sum. The symbol $\{n_A\}$ denotes the fact that we sum over the entire set of occupation numbers (except n_0), each occupation number assumes the values: $1, 2, 3, \dots, \infty$.

To evaluate Eq. (2.9), we replace n_g by $\langle n_g \rangle$, where the average is performed in the ideal gas ensemble, and will be computed later. This replacement enables the calculation of the sums in Eq. (2.9) since the summands are now separable. We obtain

$$\frac{\log \mathcal{Q}(z, \xi)}{\Omega} = -\frac{1}{2\pi^2} \int_0^\infty dk k^2 \log \left(1 - z \exp \left\{ -\beta \left[T_R + \xi \rho V_R + \frac{1}{2\Omega} \sum_{g \neq h} \frac{V_{gh}}{R} \langle n_g \rangle \langle n_h \rangle \right] \right\} \right) \quad (2.10)$$

Now Q_N can be obtained from $\mathcal{Q}(z)$ by means of the identity

$$Q_N = \frac{1}{2\pi i} \oint \frac{dz}{z^{N+1}} \mathcal{Q}(z), \quad (2.11)$$

an immediate consequence of Eq. (2.8). The contour is any closed curve containing the pole $z = 0$ and lying within the radius of convergence of $\mathcal{Q}(z)$.

In the limit $N \rightarrow \infty$, $\Omega \rightarrow \infty$, $\frac{N}{\Omega} \rightarrow \rho$, Eq. (2.7) can be written in the form

$$Q_N = \frac{1}{2\pi i} \oint dz e^{\Omega F(\rho, z)} \quad (2.12)$$

where $F(\rho, z) = f(\rho, z) - \rho \log z$

$$f(\rho, z) = \lim_{N \rightarrow \infty} \frac{\log \mathcal{Q}(z)}{\Omega}$$

The integral (2.12) is in a form in which it can be evaluated by the method of saddle-point integration. (Details can be found in reference 28, particularly pages 461-463. See also reference 29, Chapter 4, for an outline of the general method).

The result is that Q_N is given by

$$\frac{\log Q_N}{\Omega} = \frac{\log \lambda(z)}{\Omega} - \rho \log z \quad (2.13)$$

where z is the solution of the equation

$$z \frac{\partial}{\partial z} \frac{\log \lambda(z)}{\Omega} = \rho \quad (2.14)$$

Substituting Eq. (2.10) in Eqs. (2.13) and (2.14) gives the result

$$\frac{\log \tilde{Q}(N-n_0, n_0)}{\Omega} = \frac{\log \lambda(z, \xi)}{\Omega} - \rho(1-\xi) \log z, \quad (2.14)$$

where z is determined from the solution of the equation

$$\rho(1-\xi) = \frac{z}{2\pi^2} \int \frac{dk k^2}{\exp\{\beta[T_R + \xi \rho V_R + \sum_{q \neq R} \frac{V_{q-R}}{2n} \langle n_q \rangle]\} - 1} \quad (2.15)$$

We now wish to maximize $\tilde{Q}(N-n_0, n_0)$ to obtain \tilde{Q}_N from Eq. (2.7). The maximal condition, using Eqs. (2.14) and (2.15) is

$$\log z = \frac{\beta z}{2\pi^2} \int \frac{dk k^2 V_R}{\exp\{\beta[T_R + \xi \rho V_R + \frac{1}{2n} \sum_{q \neq R} V_{q-R} \langle n_q \rangle]\} - 1} \quad (2.16)$$

The two simultaneous equations (2.16) and (2.15) determine z and ξ .

Eq. (2.14) then gives \tilde{Q}_N .

We must now evaluate the integrals. First, consider the sum

$\frac{1}{2n} \sum_{q \neq R} V_{q-R} \langle n_q \rangle$ which appears in the exponent of the integrals in Eq. (2.15) and (2.16). The region in which q is large contributes

negligibly, due to the exponential factor. We therefore replace V_{g-2} by \bar{V} .

Changing the sum to an integral yields the result

$$\frac{1}{2n} \sum_{g \neq k} V_{g-2} \langle n_g \rangle = \frac{\bar{V} \sigma \tilde{F}_3(1)}{2} \quad (2.17)$$

$$\sigma \equiv \left(\frac{2m}{4\pi \hbar^2} \right)^{3/2}, \quad \tilde{F}_n(z) = \frac{1}{\Gamma(n)} \int_0^\infty \frac{dx x^{n-1}}{\frac{1}{z} e^x - 1}$$

The numerical value of $\tilde{F}_{3/2}(1) = 2.612$.

Defining α by $z = e^{-\alpha}$, we can now rewrite Eq. (2.15) and Eq. (2.16) as follows:

$$\rho(1-\xi) = \sigma \int_0^\infty \frac{y^{1/2} dy}{e^{y + \beta \xi \rho V_0 + 1.3 \beta \sigma V_0 + \alpha} - 1} \quad (2.18)$$

$$-\alpha = \beta \sigma V_0 \int_0^\infty \frac{y^{1/2} dy}{e^{y + \beta \xi \rho V_0 + 1.3 \beta \sigma V_0 + \alpha} - 1} \quad (2.19)$$

The chemical potential μ is defined by $\mu = -\alpha/\beta$.

To proceed further, we define the temperature T^0 by $T^0 = \frac{4\pi \hbar^2}{2mk} \rho^{2/3}$.

We also define the dimensionless parameter x by $x \equiv \rho V_0 / kT^0$

and the parameter $\gamma = \frac{-\alpha}{x (T/T^0)^{1/2}}$.

The magnitude of T^0 for helium is 5.97°K .

We also define $F_n(s) = \frac{1}{\Gamma(n)} \int_0^\infty y^{n-1} dy / (e^{y+s} - 1)$.

With this notation, Eqs. (2.18) and (2.19) become

$$\left(\frac{T^0}{T} \right)^{3/2} (1-\xi) = \gamma, \quad (2.20)$$

and
$$\gamma = F_{3/2} \left(\xi x \frac{T^0}{T} + x \left(\frac{T}{T^0} \right)^{1/2} (1 - \xi) \right). \quad (2.21)$$

γ can be eliminated from the pair of equations, Eq. (2.20) and (2.21).

The result is

$$\left(\frac{T^0}{T} \right)^{3/2} (1 - \xi) = F_{3/2} \left(2\xi x \frac{T^0}{T} + x \left(\frac{T}{T^0} \right)^{1/2} - x \frac{T^0}{T} \right). \quad (2.22)$$

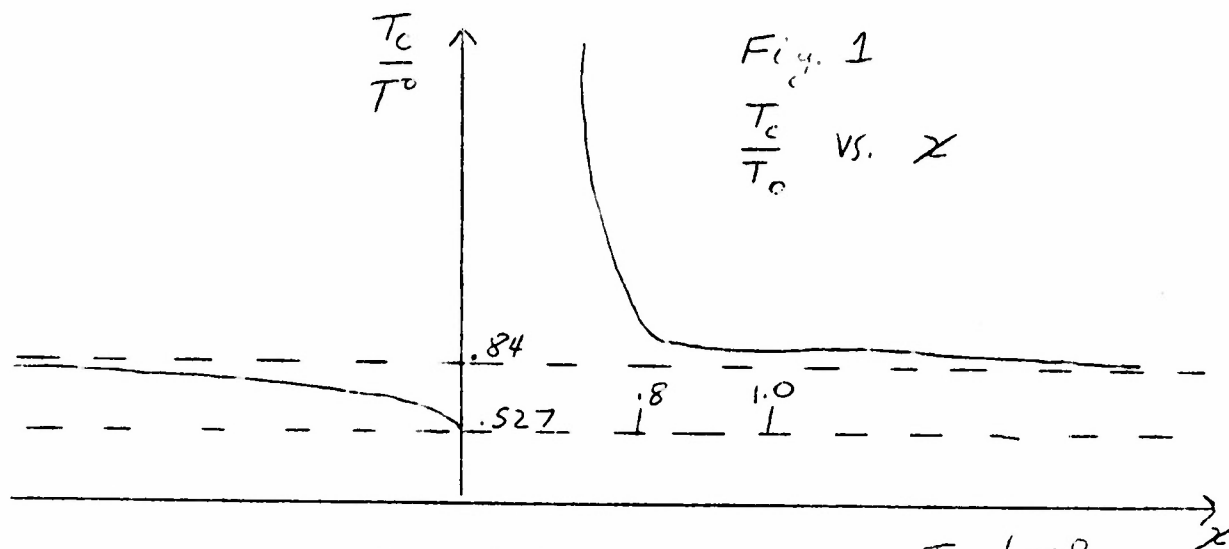
Eq. (2.22) is a transcendental equation for ξ , the fractional occupation of the zero momentum state. For each value of x , there will be a solution for ξ . Of course, $x \equiv \frac{\rho \bar{V}_0}{\kappa T^0}$ is a measure of the strength of the interaction.

The transition temperature T_c is defined to be the value of T for which $\xi = 0$. Hence, from Eq. (2.22), we have

$$\frac{T^0}{T_c} = F_{3/2} \left(x \left(\frac{T_c}{T^0} \right)^{1/2} - x \frac{T^0}{T_c} \right), \quad (2.23)$$

as the equation giving T_c .

We solve Eq. (2.23) graphically for T_c/T^0 as a function of x , by imparting values to T^0/T_c and determining the corresponding value of x . (Numerical values of $F_{3/2}$ were obtained from reference 1, page 44.) The result is a single-valued function of x , which we illustrate in Fig. 3.1.



As x approaches infinity in the positive direction, T_c/T_0 approaches the value 0.84 from above. As x approaches infinity in the negative direction, T_c/T_0 approaches the value 0.84 from below. As x approaches zero from negative values, $T_c/T_0 \rightarrow 0.527$ so that in this case, T_c approaches the ideal gas transition temperature, $0.527 T_0$. Note that the effect of the interaction is always to raise the critical temperature.

For $0 < x < 0.86$, T_c/T_0 is greater than two and rapidly increases with an almost vertical slope. We shall show presently that the values $T_c/T_0 > 2$, (corresponding to $0 < x < 0.86$) are not bonafide critical temperatures and will also discuss the criteria for an acceptable critical temperature.

The density ρ of liquid helium in the λ -region is of the order of 10^{21} cm.⁻³, and for this density $\kappa T_0 \cong 10^{-16}$ ergs. Inserting these values of ρ and κT_0 into the definition of x gives $x \cong 10^3$. (In the calculation, we have used $V_0 \cong 10^{-34}$ erg cm.³, a result obtained from numerical estimates based on the Yntema-Schneider potential¹⁷).

We now examine temperatures below T_c . In Eq. (2.22), we can expand the function $F_{3/2}$ for small values of the argument. The expansion is¹

$$F_{3/2}(\alpha) = \Gamma(-\frac{1}{2}) \alpha^{-\frac{1}{2}} + \sum_{m=0}^{\infty} \frac{(-1)^m}{m!} \zeta(\frac{3}{2}-m) \alpha^m$$

where ζ is the Riemann zeta-function.

Employing this expansion (which converges rapidly for small ξ), we obtain

$$\xi = \frac{2.612 + 1.46 \left[x \left(\frac{T}{T_0} \right)^{1/2} - x \frac{T^0}{T} \right] - \left(\frac{T^0}{T} \right)^{3/2} - 3.54 \gamma}{\left(3.54 x T^0 / T \right)^{1/2} - 2.92 x \frac{T^0}{T} + \left(\frac{T^0}{T} \right)^{3/2}} \quad (2.24)$$

where
$$\gamma = \left[x \left(\frac{T}{T_0} \right)^{1/2} 1.3 - x \frac{T^0}{T} \right]^{1/2} .$$

In obtaining Eq. (2.24), we have also expanded in powers of ξ .

For $x \leq 0.85$, the large argument expansion of $F_{3/2}(\alpha)$ can be used¹.

Then Eq. (2.22) becomes

$$\left(\frac{T^0}{T} \right)^{3/2} (1-\xi) = e^{-2\xi x \frac{T^0}{T} - x \left(\frac{T}{T_0} \right)^{1/2} 1.3 + x \frac{T^0}{T}} \quad (2.25)$$

Before turning to the calculation of thermodynamic quantities, we examine the range of validity of our results for T_c . We must require that $\left(T \frac{\partial \xi}{\partial T} \right)_c$ be negative for a true transition. (That is, ξ must be a decreasing function of T as $T \rightarrow T_c$.) If we compute $\left(T \frac{\partial \xi}{\partial T} \right)_c$ we find that this requirement does hold except for $x \leq .85$. Thus, the results are valid for all x except near the transition temperature. Near the transition temperature, the results are valid for negative x and for $x \geq .85$ but not for $x < .85$.

B. Thermodynamic Functions

We are now in a position to calculate the energy and specific heat of the system of Bose particles interacting with the Hartree-Fock part of the interaction

The internal energy of the system is defined by

$$U = \frac{\sum_n E_n e^{-\beta E_n}}{\sum_n e^{-\beta E_n}} \quad (2.26)$$

Using Eqs. (2.3), (2.10) and (2.14), we have

$$\frac{\log Q_N}{N} = -\frac{\beta p V_0}{2} - \frac{1}{2\pi^2 f} \int_0^{\infty} dk k^2 \log \left\{ 1 - \exp \left(-\beta \left[T_0 + \xi p \frac{V_0}{T_0} + \frac{1}{2\Omega} \sum_{q \neq k} \frac{V_q \langle n_q \rangle}{\delta - k} \right] - \alpha \right) + (1-\xi) \alpha \right\}.$$

(2.27)

Combining Eqs. (2.26), (2.27) and using Eqs. (2.15), (2.18) and (2.19) gives the result

$$\frac{U}{N} = \frac{p V_0}{2} + \frac{3}{2} \left(\frac{T}{T_0} \right)^{3/2} (kT) F_{5/2} \left(\beta \left[\xi p \frac{V_0}{T_0} + \frac{1}{2\Omega} \sum_q V_q \langle n_q \rangle \right] + \alpha \right) + \left\{ \xi p \frac{V_0}{T_0} + \frac{1}{2\Omega} \sum_q V_q \langle n_q \rangle \right\} (1-\xi).$$

(2.28)

To obtain the specific heat, we differentiate Eq. (2.28) with respect to the temperature, make use of Eq. (3.11), the fact that $\frac{\partial F_n(\alpha)}{\partial \alpha} = -F_{n-1}(\alpha)$

and Eqs. (2.20) and (2.17). The result is

$$\begin{aligned} \frac{C_V}{Nk} &= \frac{15}{4} \left(\frac{T}{T_0} \right)^{3/2} F_{5/2} \left(2\xi x \frac{T_0}{T} + x \left(\frac{T}{T_0} \right)^{1/2} - x \frac{T_0}{T} \right) \\ &+ 2(1-\xi) \left(-T \frac{\partial \xi}{\partial T} \right) x \frac{T_0}{T} + \left[\xi x \frac{T_0}{T} + x \left(\frac{T}{T_0} \right)^{1/2} \right] \left(-T \frac{\partial \xi}{\partial T} \right) (2.29) \\ &+ 3(1-\xi) \left\{ x \frac{T_0}{T} + \frac{3}{2} (1-\xi) \left[x \left(\frac{T}{T_0} \right)^{1/2} - x \frac{T_0}{T} \right] \right\}. \end{aligned}$$

Since $T \frac{\partial \xi}{\partial T}$ is discontinuous at the λ -point, we see from Eq. (2.29) that the specific heat is discontinuous at this temperature.

To examine the result, Eq. (2.29), first consider the limit of low temperature. As $T \rightarrow 0$, $\xi \rightarrow 1$. A lengthy, but straight-forward calculation yields the result

$$\left(\frac{C_V}{Nk}\right)_{T \rightarrow 0} = \left(\frac{\rho V_0}{k T_0}\right)^2 \left(\frac{T_0}{T}\right)^{1/2} e^{-\rho V_0 / kT} \quad (2.30)$$

The exponential result is expected since there is an energy gap in the energy spectrum.

Next, consider the case in which the temperature is in the neighborhood of the critical temperature. For temperatures above T_c , $\xi = 0$, $T \frac{\partial \xi}{\partial T} = 0$ and $T \frac{\partial f}{\partial T} = 0$

so that

$$\left(\frac{C_V}{Nk}\right)_+ = \frac{15}{4} \left(\frac{T}{T_0}\right)^{3/2} F_{5/2} \left(x \left(\frac{T}{T_0}\right)^{1/2} - \frac{x T_0}{T}\right) + \frac{3}{2} \left[x \left(\frac{T}{T_0}\right)^{1/2} - \frac{x T_0}{T} \right] \quad (2.31)$$

At the critical temperature, C_V is essentially a constant, independent of x . $(C_V)_+ / Nk$ at T_c varies from a value of 3.5 at $x = 1$ to a value of 3.2 at $x = \infty$.

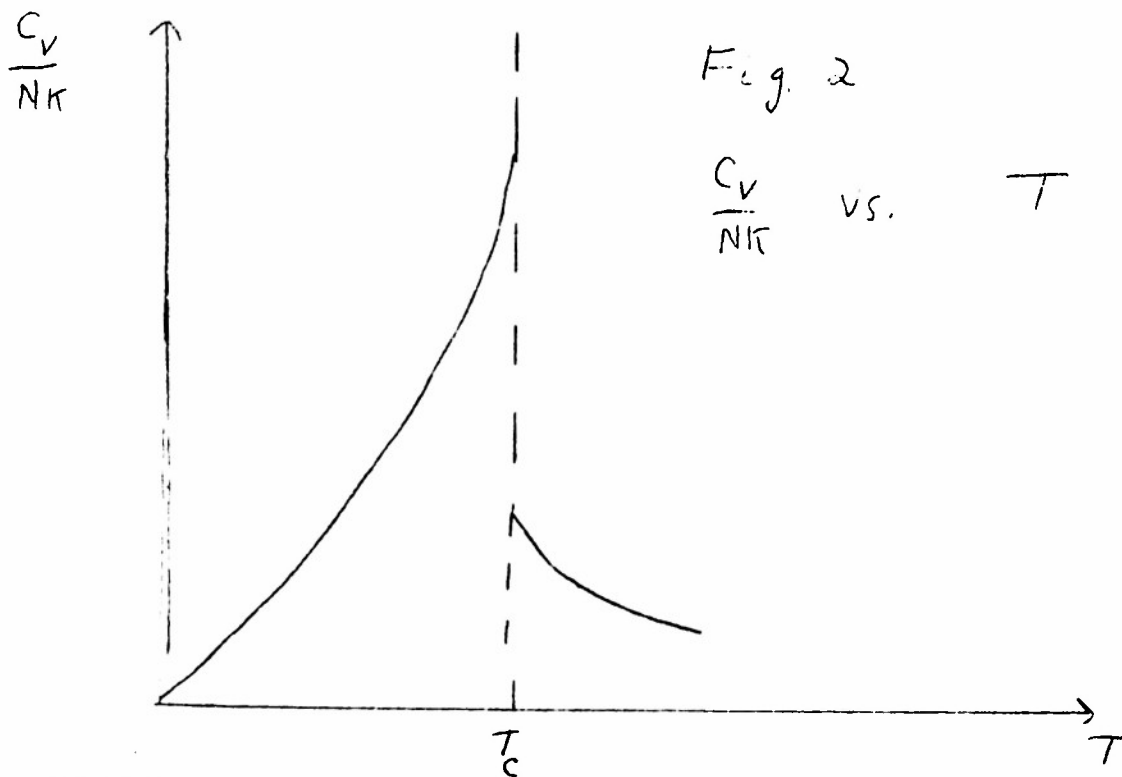
For temperatures just below T_c , Eq. (2.29) yields

$$\begin{aligned} \left(\frac{C_V}{Nk}\right)_{T \sim T_c} &= \frac{15}{4} \left(\frac{T}{T_0}\right)^{3/2} F_{3/2} \left(x \left(\frac{T}{T_0}\right)^{1/2} - \frac{x T_0}{T}\right) \\ &+ \left[2x \frac{T_0}{T} + x \left(\frac{T}{T_0}\right)^{1/2} - 1.3 \right] \left(-T \frac{\partial f}{\partial T}\right)_c \\ &+ \frac{3}{2} \left[x \left(\frac{T}{T_0}\right)^{1/2} - \frac{x T_0}{T} \right]. \end{aligned} \quad (2.32)$$

We can now compute the magnitude of the discontinuity of the specific heat at the transition:

$$\frac{\Delta c_v}{kT} = \left(c_{v-} - c_{v+} \right) = \left[2x \frac{T^0}{T} + x \left(\frac{T_c}{T^0} \right)^{1.3} \right] \left(-T \frac{\partial \xi}{\partial T} \right)_c \quad (2.33)$$

The discontinuity, Eq. (2.33) is proportional both to x and to $\left(T \frac{\partial \xi}{\partial T} \right)_c$. We sketch c_v / kT in Fig. 2 for large x .



C. Conclusion

The experimental values for c_v at the λ -point have been determined by Fairbank, Buckingham and Kellers³¹ (to within 10^{-6} degree of the λ -point). Their results indicate that c_v is finite and continuous at T_λ and that c_p has a logarithmic singularity at T_λ .

The theoretical result for $\left(c_{v-} / kT \right)_{T \sim T_c}$ given by Eq. (2.32) is in order of magnitude agreement with the observed value of

(for pressure of 0.05 atmosphere), as given in reference 31. However, Eq. (2.33) predicts a discontinuity in $(c_v/NK)_c$, disagreeing with the results contained in reference 31. But the discontinuous behavior of c_v/NK at the critical point is in qualitative agreement with experimental data on c_v/NK reported in Atkins³². The experimental values of c_v noted by Atkins³² are derived from work performed prior to the work of Fairbank, Buckingham and Kellers. The theoretical expression for $(c_v)_+$ in Eq. (2.31) evaluated at T_c is in order-of-magnitude agreement with the data reported by Atkins³².

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