Title
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Publication Date
1966-09-28

UCRL-17159

University of California

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AEC Contract No. W-7405-eng-48

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Victor Kenneth Wong
(Ph. D. Thesis)

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Contents

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ABSTRACT

A study of the equilibrium properties of boson systems at low temperatures with particular emphasis on the Bose-Einstein transition and restricted geometry is undertaken both from the microscopic and the macroscopic viewpoints.

Use of the Green's function formulation enables the systematic study of essentially all microscopic models in the literature. In particular the zeroth-order approximation is the Ideal Bose gas, which is applied to the problem of restricted geometry. The first-order approximations include the Bogoliubov/Ideal, Hartree, Bogoliubov/Hartree, Hartree-Fock, and Bogoliubov/Hartree-Fock approximations. With the sole exception of the Hartree, the first-order approximations display a double-valued behavior in the number density and other thermodynamic functions. Application to restricted geometry results in the same problem as with the Ideal Bose gas, namely that the macroscopic occupation, i.e. the Bose-Einstein condensation, does not strictly appear in restricted geometry. The second-order approximations include the Beliaev/Hartree-Fock, Born-Collision, Bogoliubov/Born-Collision, Beliaev/Born-Collision approximations. We concentrate on the Born-Collision approximation and show that it gives a logarithmic singularity to the specific heat in the Very Dense State limit. The Born-Collision approximation is applied to restricted geometries by a variational technique.

From the macroscopic viewpoint, we show that the Ginzburg-Pitaevskii theory can yield only second-order transitions in film geometries as well as in bulk systems. Based on symmetry considerations, we propose a new, modified theory in which the order function is identified with the "anomalous" self-energy, which we motivate by a microscopic argument. The new theory is shown to agree with the experimental behavior of the superfluid mass density and the jump in the specific heat, to satisfy the exponent scaling laws, to give a third-order transition in film while giving a second-order in bulk, and to yield shifts in the transition temperature in agreement with experimental observations.

I. INTRODUCTION

It is well-known that the ideal Bose gas at rest undergoes a Bose-Einstein condensation into the zero momentum state at a temperature which is dependent on the mass and density of the gas. In 1938, London[1,2] advanced the hypothesis that the Bose-Einstein condensation is the cause of the λ-transition[3] of liquid helium-4, with due allowance for the presence of interaction and the liquid state.

The London hypothesis is made plausible by the experimental fact that helium-4 displays the λ-transition while helium-3 does not. Apart from a difference in mass, the difference between these two substances is that helium-4 atoms are bosons, whereas helium-3 atoms are fermions. Furthermore, estimates[4] show that there is a Bose-Einstein condensation in liquid helium-4. Finally the ideal Bose gas with the same mass and density of liquid helium-4 undergoes a Bose-Einstein condensation at $T_0 = 3.14°K$, which is the same order of magnitude as the λ-transition, $T_\lambda = 2.17°K$.

To include the interactions of liquid helium-4 into a suitable model, there are two general approaches. One approach is to treat liquid helium-4 as a broken-down solid in which the binding forces are too weak to localize the atoms near the lattice points.[5] It is important that the solid is broken-down; for otherwise the wave functions of the individual atoms would not overlap, the symmetry of the total wave function would not have any important consequences, and the Bose-Einstein condensation would be completely irrelevant.

The other approach is to treat liquid helium-4 as a very nonideal Bose gas in which the interatomic forces play an important role. The justification for treating liquid helium like a gas is that the zero point motion[2] has an unusually large effect on the structure, inflating the volume of the liquid to a value almost three times as large as would correspond to the "classical" van der Waals volume. In this dissertation, we follow this latter approach.

After a short introduction to some properties of liquid helium-4 and the macroscopic thermodynamics, we consider the microscopic theory in the equilibrium Green's function formulation (Chap. II). Above the λ-transition (no Bose-Einstein condensation), we discuss the conserving self-energy approximations expanded in terms of the interparticle potential V, and a variational technique for calculating the self-energy. Below the λ-transition (with Bose-Einstein condensation), we consider only uniform condensates, resulting in the Bogoliubov replacement of annihilation and creation operators for the zero momentum state by c-numbers. The structure of conserving and gapless self-energy approximations is reviewed, and a simple manner to classify approximations above and below the λ-transition is proposed.

The general formulation is followed by three successive approximations of the self-energy in terms of the interparticle potential: the zeroth-order (Chap. III), first-order (Chap. IV), and second-order (Chap. V) approximations. In these approximations, we find the formulation quite amenable to a compact discussion of other works and approximations. In particular, we find that all approximations used thus far in the literature are essentially contained in the first two orders of the self-energy approximation. We consider these approximations and restricted geometry in an attempt to understand the behavior of the equilibrium properties of the Helium film.

Finally we consider the macroscopic theory of Ginzburg-Pitaevskii (Chap. VI) and a suitably modified theory. These are applied to several cases of restricted geometries.

A. Liquid Helium-4

The discovery of the anomaly which gave the λ-transition its name was by Keesom and Clusius[7,8] in 1932, who measured a singularity of the specific heat curve at saturated pressure whose profile resembled the shape of the letter λ. Recent measurements by Fairbank, Buckingham, and Kellers[9] of the specific heat at saturated pressure C_{sat} has shown that as the temperature $T \rightarrow T_\lambda$ (T_λ is the temperature of the transition), $C_{sat} \rightarrow \infty$ as the logarithm of the temperature interval $|\Delta T| \equiv |T - T_\lambda|$ to within $10^{-6}\,{}^\circ K$ of T_λ. From $10^{-6}\,{}^\circ K \leq |\Delta T| \leq 10^{-2}\,{}^\circ K$, the specific heat satisfies the empirical equation

$$C_{sat} = 4.55 - 3.00 \log_{10}|\Delta T| - 5.20\,\delta \qquad \left(\frac{\text{joule}}{\text{gm }{}^\circ K}\right) \tag{1.1}$$

where $\delta = 0$ for $T < T_\lambda$, and $\delta = 1$ for $T > T_\lambda$. We note that there is a jump in the specific heat

$$\Delta C_{sat} \equiv C_{sat}(T > T_\lambda) - C_{sat}(T > T_\lambda) = -5.20\,\frac{\text{joule}}{\text{gm }{}^\circ K}\,. \tag{1.2}$$

The saturated pressure specific heat is related to the specific heat at constant pressure C_p by

$$c_p = c_{sat} + T v \alpha_p \left(\frac{\partial P}{\partial T}\right)_{sat}$$

where v is the volume, α_p is the isobaric coefficient of expansion, and $(\partial p/\partial T)_{sat}$ is the slope of the saturated vapor pressure curve. Below $2.5^{\circ}K$, the difference between C_{sat} and C_p is less than one per cent; therefore within experimental error, the two quantities, C_{sat} and C_p, can be used interchangeably. Other measurements along the saturated pressure curve include a measurement of α_p by Atkins and Edwards[10] who show that $\alpha_p \rightarrow \infty$ logarithmically for $10^{-3}\,{}^{\circ}K \leq |\Delta T| \leq 10^{-1}\,{}^{\circ}K$. Recently the superfluid density ρ_s has been measured[11,12] near the λ-transition and within experimental error was found to be $\rho_s \sim (-\Delta T)^{2/3}$. We note in passing that the temperature of the onset of superfluidity coincides with the specific heat anomaly T_λ.

Before measuring the specific heat, Keesom and Clusius[13] also determined the way in which the transition temperature changes with increasing pressure and found an almost vertical λ- curve connecting the melting curve with the saturated vapor curve. The p-T diagram is qualitatively shown in Fig. 1. Recently Lounasmaa,[14] working at elevated pressure near the λ- curve in the vicinity of the point $p=13.04$ atm, $v=24.20$ cm^3/mole, $T=2.023^{\circ}K$, measured the isochoric pressure coefficient $\beta_v \equiv (\partial p/\partial T)_v$ and the isothermal compressibility κ_T. He found that $\beta_v \longrightarrow \infty$ logarithmically for

$10^{-5}\,{}^{\circ}K \leq |\Delta T| \leq 2\times10^{-2}\,{}^{\circ}K$ with a jump and $\kappa_T \sim \Delta p$ with no singularity for $10^{-3}atm \leq |\Delta p| \leq 10^{-2}atm$ with a small jump. Other thermodynamic behavior of liquid Helium-4 near the λ-curve has been discussed by Lounasmaa.[15]

The above experiments were done with rather large samples of helium at pressures equal or greater than the saturated pressure. We now turn to small or thin samples of helium at pressures less than the saturated pressure.[16]

Frederikse[17] measured the specific heat along a given unsaturated pressure curve for an unsaturated film adsorbed onto a jeweler's rouge. He found that the specific heat singularity at saturated pressure has been smoothed over and its maximum shifted to lower temperatures from T_λ as the pressure is decreased. Mastrangelo and Aston[18] re-examined the problem using TiO_2 and found similar behavior in the specific heat. Recently Brewer, Symonds, and Thomson[19] reported that the specific heat maximum for helium in partially-filled vycor pores agrees with those of Frederikse.

Other works concern the measurement of the onset of superfluidity,[20-24] which indicate that the superfluid temperature decreases from T_λ as the pressure is decreased below saturated pressure. However there is a systematic difference between the superfluid temperatures for an unsaturated film[19-22] and the superfluid temperatures for an unsaturated pore.[23,24]

In both film and pores, the superfluid temperature is generally lower than the temperature of the specific heat maximum. It has been suggested that additional surface excitations[19] may be the cause of this disparity. To further complicate the situation, a phase transition which coincides with the λ -transition at saturated pressure has been found[25] in an unsaturated film at temperatures above T_λ , increasing as the pressure is decreased below saturated pressure.

B. Thermodynamics[26]

The thermodynamic potential which arises naturally in using the grand canonical ensemble of statistical mechanics is what we call the Massieu potential[26] $W(\beta, \mathcal{V}, \alpha)$, where $\beta \equiv (k_B T)^{-1}$, $\alpha \equiv -\beta\mu$ with T denoting the temperature, $\mathcal{V}$ the volume, μ the chemical potential, and k_B Boltzmann's constant. The Massieu potential $W(\beta, \mathcal{V}, \alpha)$ is the double Legendre transform[26] in $[U, \beta]$ and $[N, \alpha]$ of the (dimensionless) entropy $S(U, \mathcal{V}, N)$, i.e.

$$W(\beta,\mathcal{V},\alpha) = S - \beta U - \alpha N = \mathcal{V}\beta p(\beta,\alpha) \tag{1.3}$$

where we have used the Euler equation in the entropy representation

$$S = \beta U + \beta p \mathcal{V} + \alpha N \ .$$

The entropic fundamental relation is

$$dS = \beta dU + \beta p d\mathcal{V} + \alpha dN \ .$$

Therefore

$$dW = -U d\beta + \beta p d\mathcal{V} - N d\alpha \ . \tag{1.4}$$

Equation (1.4) leads to the following relations

$$\begin{cases} U = -\left(\dfrac{\partial W}{\partial \beta}\right)_{\mathcal{V},\alpha} & \text{(1.5a)} \\ \beta p = \left(\dfrac{\partial W}{\partial \mathcal{V}}\right)_{\beta,\alpha} & \text{(1.5b)} \\ N = -\left(\dfrac{\partial W}{\partial \alpha}\right)_{\beta,\mathcal{V}} & \text{(1.5c)} \end{cases}$$

and the entropy is calculated from eq. (1.3)

$$S = W + \beta\left(\frac{\partial W}{\partial \beta}\right)_{\mathcal{V},\alpha} + \alpha\left(\frac{\partial W}{\partial \alpha}\right)_{\beta,\mathcal{V}} \quad . \tag{1.6}$$

We can consider W as a function of $(\beta, \mathcal{V}, \mu)$ instead of $(\beta, \mathcal{V}, \alpha)$. Then

$$dW(\beta,\mathcal{V},\mu) = -(U-\mu N)\,d\beta + \beta p\,d\mathcal{V} + \beta N\,d\mu \tag{1.7}$$

and

$$S = W + \beta\left(\frac{\partial W}{\partial \beta}\right)_{\mathcal{V},\mu} \tag{1.8}$$

It is customary, however, to work in the energy representation; and the thermodynamic potential relevant is the grand potential $\Omega(T, \mathcal{V}, \mu)$, which is the double Legendre transform of the energy, i.e.

$$\Omega(T,\mathcal{V},\mu) = U - k_B TS - \mu N = -\mathcal{V}p(T,\mu) \quad . \tag{1.9}$$

Hence the connection between the Massieu potential and the grand potential is

$$W(\beta,\mathcal{V},\mu) = -\beta\,\Omega(T,\mathcal{V},\mu) \quad . \tag{1.10}$$

The Ehrenfest classification of phase transitions is based on the Gibbs potential.

$$G(T,P) = U - k_B TS + p\mathcal{V} = N\mu(T,p) \quad , \tag{1.11}$$

namely that a phase transition shall be called n^{th} order if the n^{th} partial derivative of $G(T,p)$ is discontinuous at the transition, whereas all lower derivatives are equal. The first derivatives of $G(T,p)$ yield the volume and the entropy:

$$\begin{cases} \mathcal{V} = \left(\frac{\partial G}{\partial P}\right)_T & \text{(1.12a)} \\ k_B S = -\left(\frac{\partial G}{\partial T}\right)_{\mathcal{V}} \quad . & \text{(1.12b)} \end{cases}$$

The second derivatives are the isobaric coefficient of thermal expansion

$$\alpha_p \equiv \frac{1}{\mathcal{V}}\left(\frac{\partial \mathcal{V}}{\partial T}\right)_p = \frac{1}{\mathcal{V}}\frac{\partial^2 G}{\partial T \partial p} \quad , \tag{1.13a}$$

the isobaric heat capacity

$$c_p \equiv k_B T\left(\frac{\partial S}{\partial T}\right)_p = -T\frac{\partial^2 G}{\partial T^2} \quad , \tag{1.13b}$$

and the isothermal compressibility

$$\kappa_T \equiv -\frac{1}{\mathcal{V}}\left(\frac{\partial \mathcal{V}}{\partial p}\right)_T = -\frac{1}{\mathcal{V}}\frac{\partial^2 G}{\partial p^2} \quad . \tag{1.13c}$$

II. MICROSCOPIC THEORIES -- GREEN'S FUNCTION FORMULATION

The Green's function formulation[27-30] of quantum statistical physics has enabled the unification of several diverse approaches[31] and approximations to the many-body problem. In the case of interacting bosons, this formulation can be adapted to include the macroscopic occupation of a single state[32,33] and used to discuss the various approximations[34] and liquid helium[35] below the λ-transition.

We limit ourselves to equilibrium systems and, below the λ-transition, to systems with a uniform condensate. We begin with some basic definitions for the normal system above the λ-transition, and we review the formal procedures of conserving approximations and variational calculations of the self-energy. We next consider the anomalous system below the λ-transition, and we review the formal structure of the gapless approximations and the conserving approximations. We end this section with some terminology for approximations above and below the λ-transition, and a treatment of the Bose-Einstein condensation and the Very Dense State limit.

A. Above The λ-Transition (Normal Systems)

1. Basic Definitions

We wish to examine the low-temperature equilibrium properties of a many-particle system of spinless bosons of mass m with a two-body interaction, whose Hamiltonian in second quantized form is given by

(setting $\hbar = 1$)

$$H(t_1) = -\frac{1}{2m}\int_{\mathcal{V}} d^3r_1\, \psi^+(1)\, \nabla_1^2\, \psi(1) \; - \tag{2.1}$$

$$-\frac{1}{2}\int_{\mathcal{V}} d^3r_1 \int_0^{-i\beta} d2\, \psi^+(1)\,\psi^+(2)\, V(12)\, \psi(2)\, \psi(1)$$

where $\psi(1) \equiv \psi(r_1, t_1)$, $\psi^+(1) \equiv \psi^+(r_1, t_1)$ are respectively the annihilation and creation operators in the Heisenberg picture for a boson at position r_1 and time t_1 obeying the usual commutation relations, and

$$V(12) \equiv V(r_1 - r_2)\, \delta(t_1 - t_2) \tag{2.2}$$

is the two-body potential such that $\delta(t)$ satisfies

$$\int_0^{-i\beta} dt\, \delta(t) = 1 \tag{2.3}$$

along the imaginary time axis, and the notation

$$\int_0^{-i\beta} d2\, X(2) = \int_{\mathcal{V}} d^3r_2 \int_0^{-i\beta} dt_2\, X(r_2, t_2) \tag{2.4}$$

with $\mathcal{V}$ being the volume of the system.

As the Hamiltonian does not change the number of particles, $N(t)$, i.e.

$$\left[H(t),\, N(t) \right] = 0$$

where

$$N(t_1) \equiv \int_{\mathcal{V}} d^3r_1\, \psi^+(1)\, \psi(1) \quad , \tag{2.5}$$

it is convenient to work with a modified Hamiltonian

$$\mathcal{H}(t) \equiv H(t) - \mu N(t) \tag{2.6}$$

where μ , a c-number, is to be identified as the chemical potential. The corresponding Heisenberg picture is modified so that for any operator Y(t)

$$i \frac{\partial}{\partial t} Y(t) = \left[Y(t), \mathcal{H}(t) \right] \tag{2.7}$$

or

$$Y(t) = e^{i\mathcal{H}t}\, Y(0)\, e^{-i\mathcal{H}t}$$

For a system in thermodynamic equilibrium at temperature T, the expectation value for any operator may be computed using the grand canonical ensemble of statistical mechanics, viz. for any operator Y(t), the expectation value $\langle$ Y(t) $\rangle$ is

$$\langle Y(t) \rangle \equiv \frac{Sp\left[e^{-\beta\mathcal{H}}\, Y(t) \right]}{Sp\left[e^{-\beta\mathcal{H}} \right]} \tag{2.8}$$

where $\beta \equiv (k_B T)^{-1}$, k_B denotes the Boltzmann constant and Sp denotes the spur operation which is to sum the diagonal elements of the operators in the bracket, summing over all possible states of the system with a given number of particles and over all possible number of particles.

The thermodynamic, causal, imaginary time n-particle Green's function can be defined as

$$G_n(12\cdots 2n) \equiv (-i)^n \left\langle T_t \{\psi(1)\psi(2)\cdots\psi(n) \times \right. \\ \left. \times\, \psi^+(2n)\cdots\psi^+(n+2)\,\psi^+(n+1)\} \right\rangle \tag{2.9}$$

where T_t denotes the Wick time-ordering operation, which is to arrange the ensuing operators in chronological order along the imaginary time axis from 0 to $-i\beta$ with the earlier (closer to the origin) time on the right and the later (farther from the origin) time on the left.

These Green's functions obey the time boundary condition

$$G_n(t_j = -i\beta) = G_n(t_j = 0) \tag{2.10}$$

with the other times fixed in the time interval $[0, -i\beta]$. This quasi-periodic boundary condition permits the introduction of a Fourier series expansion for G_n. For the one-particle Green's function, the Fourier series is

$$G_1(t) = \frac{1}{-i\beta}\sum_{\nu} e^{-\zeta_\nu t}\, G_1(\zeta_\nu) \tag{2.11a}$$

$$\zeta_\nu \equiv \frac{2\pi\nu}{-i\beta}, \qquad \nu = 0, \pm 1, \pm 2, \cdots . \tag{2.11b}$$

The momentum Fourier series is introduced in the usual way

$$G_1(r) = \frac{1}{\mathcal{V}}\sum_{p} e^{ip\cdot r}\, G_1(p) \quad , \tag{2.12}$$

so that the complete Fourier series is

$$G(r,t) = \frac{1}{-i\beta}\sum_{\nu}\frac{1}{V}\sum_{p} e^{i(p\cdot r - z_\nu t)} G(p, z_\nu) \tag{2.13a}$$

with the inversion

$$G(p, z_\nu) = \int_0^{-i\beta} dt \int_V d^3r \, e^{-i(p\cdot r - z_\nu t)} G(r,t) \quad . \tag{2.13b}$$

The spectral function $A(p,\omega)$ may be introduced for imaginary z_ν by the Cauchy integral

$$G(p, z_\nu) = \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} \, \frac{A(p,\omega)}{z_\nu - \omega} \tag{2.14}$$

which implies that the analytic continued[36] $G(p, z)$ is analytic in the whole z-plane minus the support, i.e. nonzero values, of $A(p,\omega)$ for a given momentum, and that $A(p,\omega)$ is given by the discontinuity across the real axis[37] ($\delta \rightarrow 0+$)

$$A(p,\omega) = i\left[G(p, z=\omega+i\delta) - G(p, z=\omega-i\delta)\right] \quad . \tag{2.15}$$

Because of the analyticity of $G(p, z)$, it is sometimes called the analytic propagator.[38] For bosons, the spectral function must in general satisfy

$$A(p,\omega) \quad \begin{matrix} \geq 0 & \omega > 0 \\ = 0 & \omega = 0 \\ \leq 0 & \omega < 0 \end{matrix} \tag{2.16}$$

for a given momentum. Therefore $G(p, z)$ must be continuous across the z real axis at the origin, and $G(p,0)$ may be represented by

$$G(p,0) = -\int_{-\infty}^{\infty} \frac{d\omega}{2\pi} \frac{A(p,\omega)}{\omega} \tag{2.17}$$

where the Cauchy principal value operation is understood.[39]

The Green's function are determined by their equation of motion together with the aforementioned boundary conditions. The equation of motion for G_1 can be written as

$$\begin{aligned} \int_0^{-i\beta} d2\, G_0^{-1}(12)\, G(21') = {} & \delta(11') + \\ & + i \int_0^{-i\beta} d2\, V(12)\, G_2(121'2+) \end{aligned} \tag{2.18}$$

where the operator $G_0^{-1}(12)$ is defined as

$$G_0^{-1}(12) = \left(i \frac{\partial}{\partial t_1} + \frac{1}{2m} \nabla_1^2 + \mu \right) \delta(12) \tag{2.19}$$

If we define an inverse Green's function by

$$\begin{aligned} \delta(11') &= \int_0^{-i\beta} d2\, G^{-1}(12)\, G(21') \\ &= \int_0^{-i\beta} d2\, G(12)\, G^{-1}(21') \end{aligned} \tag{2.20}$$

and the total self-energy as

$$\Sigma^{tot}(11') \equiv G_0^{-1}(11') - G^{-1}(11') \quad , \tag{2.21}$$

then the equation of motion (2.18) reads

$$\int_0^{-i\beta} dz\, \Sigma^{tot}(12)G(21') = i\int_0^{-i\beta} dz\, V(12)\, G_2(121'2^+) \quad . \tag{2.22}$$

Hence we have formally reduced the problem of calculating G_1 to that of calculating the total self-energy Σ^{tot} through the equation of motion (2.22).

The total self-energy can be separated into two parts:

$$\Sigma^{tot}(11') = \Sigma^{o}(11') + \Sigma(11') \tag{2.23}$$

where $\Sigma^{o}(r,t)$ is defined as the sum of all self-energy contributions which are proportional to $\delta(t)$, which gives a constant term in the conjugate variable. Therefore Σ^{o} is the subtraction term, and Σ satisfies the same boundary conditions as for the Green's functions, eq. (2.10). Hence we may introduce the analogous Fourier series, eq. (2.13). Also a spectral function $\Gamma(p,\omega)$ can be introduced such that for imaginary z_ν

$$\Sigma(p,z_\nu) = \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} \frac{\Gamma(p,\omega)}{z_\nu - \omega} \tag{2.24}$$

and

$$\Sigma^{tot}(p,z_\nu) = \Sigma^{o}(p) + \Sigma(p,z_\nu) \quad . \tag{2.25}$$

Hence Σ is sometimes called the analytic self-energy.[38] The same comments which apply to G and A apply to Σ and Γ . $\Gamma(p,\omega)$ is also called the imaginary part of the self-energy since $\Sigma(p, z = \omega \pm i\delta) = \Delta(p,\omega) \mp i\frac{1}{2}\Gamma(p,\omega)$ where the real part $\Delta(p,\omega)$ is related to the imaginary part by

$$\Delta(p,\omega) = \int_{-\infty}^{\infty} \frac{d\omega'}{2\pi} \, \frac{\Gamma(p,\omega')}{\omega-\omega'} \quad . \tag{2.26}$$

Now we express G in terms of Σ . If we Fourier analyze eqs. (2.19)(2.21) and use (2.25), we can write

$$G(p,z_\nu) = \frac{1}{z_\nu - \epsilon(p) - \Sigma(p,z_\nu) + \mu} \tag{2.27}$$

where $\epsilon(p)$ is the single-particle energy

$$\epsilon(p) \equiv \epsilon_p^0 + \Sigma^0(p) \tag{2.28a}$$

$$\epsilon_p^0 \equiv \frac{p^2}{2m} \quad . \tag{2.28b}$$

Hence when the analytic self-energy vanishes, $G(p,z)$ is analytic in the whole z -plane except for a pole at $z = \epsilon(p)-\mu$, which follows from the fact that $A(p,\omega)$ is a delta function with point support at $z = \epsilon(p)-\mu$. In general, $A(p,\omega)$ is given by, using eqs. (2.15)(2.24)(2.25)(2.26)(2.27),

$$A(p,\omega) = \frac{\Gamma(p,\omega)}{[\omega-\epsilon(p)+\Delta(p,\omega)+\mu]^2 + \frac{1}{4}[\Gamma(p,\omega)]^2} \tag{2.29}$$

Hence a suitable approximation for Σ^{tot} or $A(p,\omega)$ will determine the Green's function.

The chemical potential μ is determined by the equation for the particle density

$$n = i\,G(11^+) \tag{2.30a}$$

which reduces to, using eqs. (2.13a)(2.14),

$$n = -\frac{1}{\beta V}\sum_p\sum_\nu G(p,z_\nu) = \frac{1}{V}\sum_p\int_{-\infty}^{\infty}\frac{d\omega}{2\pi}A(p,\omega)f(\omega) \tag{2.30b}$$

where we use the convenient rule for any function $g(z_\nu)$

$$\frac{1}{-i\beta}\sum_\nu g(z_\nu) = -i\oint_C\frac{dz}{2\pi i}f(z)\,g(z) \tag{2.31a}$$

$$f(z) = \frac{1}{e^{\beta z}-1} \tag{2.31b}$$

where C is the contour that encircles the poles of $g(z)$ in the positive direction, which holds only if the poles of $g(z)$ do not coincide with those of $f(z)$ and $z\,f(z)g(z) \rightarrow 0$ as $|z| \rightarrow \infty$.

2. Conserving Self-Energy Approximations

We now consider the problem of ascertaining a suitable approximation for Σ^{tot}. We use as our guideline to a suitable approximation the fact that the approximation must be conserving[40] so as to yield consistent thermodynamics.[41]

It is convenient to introduce an external scalar disturbance[41] coupled to the "density", so as to add to the Hamiltonian (2.1) the term

$$H^{ext}(t_1) = \int_V d^3r_1 \int_0^{-i\beta} d2\, \psi^+(1)\, U^{ext}(12)\, \psi(2) \tag{2.32}$$

where $U^{ext}(12)$ is the arbitrary external disturbance nonlocal in time and space. We can define a functional, W, of U^{ext} by

$$W[U^{ext}] \equiv \ln Sp\{e^{-\beta H}\, T_t(S)\} \tag{2.33a}$$

where S is the imaginary time S-matrix in the interaction picture for a potential U^{ext},

$$S \equiv \exp\left\{-i\int_0^{-i\beta} d1\, d2\, \psi^+(1)\, U^{ext}(12)\, \psi(2)\right\} . \tag{2.33b}$$

The one-particle Green's function can be defined as the functional derivative of W with respect to U^{ext}, i.e.

$$G(11';U^{ext}) = \frac{\delta W[U^{ext}]}{\delta U^{ext}(1'1)} = -i\,\frac{\langle T_t\{S\,\psi(1)\,\psi^+(1')\}\rangle}{\langle T_t\{S\}\rangle} . \tag{2.34}$$

The n-particle Green's function is defined by n functional derivatives, or

$$G_n(12\ldots 2n; U^{ext}) = \frac{(-i)^n}{\langle T_t(S)\rangle} \langle T_t\{S\psi(1)\psi(2)\ldots\psi(n) \cdot \psi^+(2n)\cdots\psi^+(n+2)\psi^+(n+1)\}\rangle . \tag{2.35}$$

The introduction of U^{ext} is a formal device, and we set $U^{ext} = 0$ at the end of all calculations. If we set $U^{ext} = 0$ above, we recover the Green's functions defined previously. However, note the necessity of using an external potential nonlocal in space and time. The cyclic invariance of the trace that defines the expectation values in $G_n(U^{ext})$ implies that the same quasi-periodic boundary conditions, eq. (2.10), holds for $G_n(U^{ext})$. Hence the Fourier series, eq. (2.13), also apply to $G_n(U^{ext})$.

The equation of motion for $G_1(U^{ext})$ is different from eq. (2.18), viz.

$$\int_0^{-i\beta} d2\, G_0^{-1}(12)\, G(21') = \int_0^{-i\beta} d2\, U^{ext}(12)\, G(21') + \delta(11') + i\int_0^{-i\beta} d2\, V(12)\, G_2(121'2^+) , \tag{2.36}$$

where the Green's functions are all understood to be functionals of U^{ext}. If we insert the functional derivative,

$$\frac{\delta G(11')}{\delta U^{ext}(2'2)} = G_2(121'2') - G(11')\,G(22') , \tag{2.37}$$

into the equation of motion, and define the total self-energy as

$$\Sigma^{tot}(11') = G_0^{-1}(11') - G^{-1}(11') - U^{ext}(11'), \tag{2.38}$$

then eq. (2.36) becomes

$$\begin{aligned}\Sigma^{tot}(11') = {} & i\int_0^{-i\beta} d2\, V(12)\, G(22^+)\cdot\delta(11') + \\ & + \int_0^{-i\beta} d2d3\, V(12)\, \frac{\delta G(13)}{\delta U^{ext}(2^+2)}\, G^{-1}(31') \;.\end{aligned} \tag{2.39}$$

Using $\delta G \cdot G^{-1} + G \cdot \delta G^{-1} = 0$, we find the identity

$$\begin{aligned}\int_0^{-i\beta} d3\, \frac{\delta G(13)}{\delta U^{ext}(2^+2)}\, G^{-1}(31') = {} & \int_0^{-i\beta} d3\, G(13)\, \frac{\delta \Sigma^{tot}(31')}{\delta U^{ext}(2^+2)} + \\ & + G(11')\,\delta(21') \;.\end{aligned} \tag{2.40}$$

Hence the equation of motion takes the form

$$\begin{aligned}\Sigma^{tot}(11') = {} & i\delta(11')\int_0^{-i\beta} d2\, V(12)\, G(22^+) + iV(11')\, G(11') + \\ & + i\int_0^{-i\beta} d2d3\, V(12)\, G(13)\, \frac{\delta \Sigma^{tot}(31')}{\delta U^{ext}(2^+2)} \;.\end{aligned} \tag{2.41}$$

Thus far, we have considered W and Σ as functionals of U^{ext}. However, the natural variable is not U^{ext} but its conjugate G_1 . We may then change to G_1 as our independent functional variable, which is equivalent to making a Legendre transformation from

$W[U^{ext}]$ to $W[G_1]$. The functional derivative in eq. (2.41) becomes

$$\frac{\delta\Sigma^{tot}(31')}{\delta U^{ext}(2^+2)} = \int_0^{-i\beta} d4\, d4'\ \frac{\delta\Sigma^{tot}(31')}{\delta G(44)}\ \frac{\delta G(4'4)}{\delta U^{ext}(2^+2)}$$

$$= \int_0^{-i\beta} d4\, d4'\ \Xi(341'4)\, L(4'242^+) \tag{2.42}$$

where we define the two-particle effective interaction

$$\Xi(1234) \equiv \frac{\delta\Sigma^{tot}(13)}{\delta G(42)}\ , \tag{2.43}$$

and

$$L(1234) \equiv \frac{\delta G(13)}{\delta U^{ext}(42)} \tag{2.44}$$

which is the density correlation function when we take $3=1^+$ and $4=2^+$. By functional differentiating eq. (2.38) with respect to U^{ext}, we find that L satisfies the equation

$$L(121'2') = G(12')G(21') +$$

$$+\int_0^{-i\beta} d3\, d4\, d5\, d6\ \ G(13)G(41')\times \tag{2.45a}$$

$$\times\ \Xi(3546)\, L(6252')$$

or

$$\int_0^{-i\beta} d2\, d2' \left[G^{-1}(12')G^{-1}(21') - \Xi(121'2')\right] L(2'323') = \tag{2.45b}$$

$$\delta(13')\,\delta(31')\ .$$

For later reference, we define the inverse function L^{-1} by

$$\int_0^{-i\beta} d2\,d2'\, L^{-1}(121'2')\, L(2'3'23) = \delta(13)\,\delta(31') \tag{2.46a}$$

so that

$$L^{-1}(121'2') = G^{-1}(12')\,G^{-1}(21') - \Xi(121'2') \;. \tag{2.46b}$$

Substituting eq. (2.42) into eq. (2.41), we finally have the equation of motion in the desired form:

$$\begin{aligned}\Sigma^{tot}(11') = {} & i\delta(11')\int_0^{-i\beta} d2\, V(12)\,G(22^+) + iV(11')\,G(11') + \\ & + i\int_0^{-i\beta} d2\,d3\,d4\,d5\; V(12)\,G(13)\,\Xi(341'5)\,L(5242^+) \;.\end{aligned} \tag{2.47}$$

We note that Σ^{tot} in eq. (2.47) is a functional of G_1. By iterating eq. (2.47) with eqs. (2.43)(2.45a), we obtain an expansion of Σ^{tot} in successive powers of V as a functional of G_1. This is done by taking the lowest order in V in eq. (2.45a) for L, so that

$$\begin{aligned}\Sigma^{tot}(11') = {} & i\delta(11')\int_0^{-i\beta} d2\, V(12)\,G(22^+) + iV(11')\,G(11') + \\ & + i\int_0^{-i\beta} d2\,d3\,d4\,d5\; V(12)\,G(13)\,\Xi(341'5)\,G(24)\,G(52)\end{aligned} \tag{2.48}$$

and treat Ξ as the small term. This iterative procedure leads to the Hartree-Fock approximation to first-order in V :

$$\Sigma_{HF}(11') = i\delta(11')\int_0^{-i\beta} d2\, V(12)\,G(22^+) + i\,V(11')\,G(11') \quad . \tag{2.49}$$

The second-order term in V comes from approximating

$$\begin{aligned} \Xi(121'3) &\simeq \Xi_{HF}(121'3) \\ &= i\delta(11')\delta(23)V(12) + i\delta(13)\delta(21')V(12) \end{aligned}$$

which yields the Born-Collision approximation:

$$\begin{aligned} \Sigma_{BC}(11') = i^2\int_0^{-i\beta} d2d3\, V(12)\,V(31') \times \\ \times\left[G(11')G(32)G(23) + G(13)G(32)G(21')\right] \quad . \end{aligned} \tag{2.50}$$

The third-order term is obtained by taking $\Xi \simeq \Xi_{BC}$ which has six terms; and so on. The nth order term is

$$\begin{aligned} \Sigma^{(n)}(11') = i\int_0^{-i\beta} d2d3d4d5\, V(12)\,G(13)G(24)G(52) \times \\ \times\, \Xi^{(n-1)}(341'5) \quad . \end{aligned} \tag{2.51}$$

These terms correspond to the irreducible diagrams for Σ^{tot} and are shown in Fig. 2. From the topological nature of these diagrams, we note that the Hartree-Fock terms are the entire subtraction term Σ^{0}.

We now show that each order approximation in the expansion of $\Sigma^{tot}[G_1]$ in powers of V is a conserving[40] approximation, so that we are guaranteed consistent thermodynamics.[41] All that needs to be demonstrated is the existence of a functional $\Phi[G_1]$ such that the self-energy is given by

$$\Sigma^{tot}(11') = \frac{\delta\Phi[G_1]}{\delta G(1'1)} \tag{2.52}$$

We prove the existence of $\Phi[G_1]$ by explicitly exhibiting it. Consider the obvious candidate[42] for the n^{th} order approximation

$$\begin{aligned}\Phi^{(n)}[G_1] = \frac{1}{2n}\int_0^{-i\beta} d1d2d3d4\,d5d1'\; V(12)\,\times \\ \times\, G(13)G(24)\,\Xi^{(n-1)}(341'5)\,G(52)\,G(11')\,.\end{aligned} \tag{2.53}$$

We need to show that

$$\Sigma^{(n)}(rs) = \frac{\delta\Phi^{(n)}[G_1]}{\delta G(sr)} \tag{2.54}$$

for an arbitrary G(sr) in $\Phi^{(n)}[G_1]$. This is obviously true, if we assume that the $(n-1)^{th}$ order is conserving so that

$$\Xi^{(n-1)}(141'5) = \Xi^{(n-1)}(4151')\,. \tag{2.55}$$

However, it is well-known[40,41] that the first-order approximation, the Hartree-Fock, is conserving. Hence by induction, we have proven eq. (2.54) for all n's and the proposition that each order approximation is conserving. The n^{th} order self-energy diagram and Φ -diagram are shown in Fig. 3.

3. Variational Calculations of the Self-Energy

A useful calculational procedure is to utilize the stationary property of the grand partition function of the system under variations of some one-body function[31] as the density. This variational property was first established by Lee and Yang,[43] who constructed a stationary functional of the average occupation number multiplied by the fugacity. Stationary functional forms of the same general character have been established in other cases, as a functional of the average occupation number in a form which tends to the virial expansion in the classical limit,[44] and as a functional of distribution functions for "quasi-particles".[45] Luttinger and Ward[46] established a stationary functional form of the self-energy in the Green's function formulation.[41]

We shall follow the Green's function formulation of the variational functional in terms of the self-energy, which, in the light of a more general variational formulation in terms of one-body and two-body functions, can be viewed as a singly stationary[47] or a partially reciprocal[48] formulation.

For formal manipulations, it is convenient to introduce the notation

$$\mathrm{tr}\, X \equiv \mathrm{tr}\, X(11') = \int_0^{-i\beta} d1\; X(11^+) \tag{2.56a}$$

$$tr\, XY \equiv tr\left[X(12)Y(21')\right] = \int_0^{-i\beta} d1\, d2\, X(12)\, Y(21^+) \tag{2.56b}$$

where X and Y are arbitrary one-particle functions. In this notation, we can express the variation of the functional $W\left[U^{ext}\right]$ as

$$\delta W\left[U^{ext}\right] = tr\left(G_1 \delta U^{ext}\right) \tag{2.57}$$

and the variation of the functional $\Phi[G_1]$ as

$$\delta \Phi[G_1] = tr\left(\Sigma^{tot} \delta G_1\right) \quad . \tag{2.58}$$

Now we want to change from U^{ext} to its conjugate G_1 as the independent functional variable of W. This is accomplished by the Legendre transformation

$$W[G_1] = W\left[U^{ext}\right] - tr\left(G_1 U^{ext}\right) \quad . \tag{2.59}$$

Using eqs. (2.57)(2.58) and the definition of $\Sigma^{tot}\left[U^{ext}\right]$, eq. (2.38), we obtain the variation of $W[G_1]$ as

$$\begin{aligned} \delta W[G_1] = {} & \delta \Phi[G_1] - \delta\, tr\left(\Sigma^{tot} G_1\right) + \\ & + \delta\, tr \ln(-G_1) - \delta\, tr\left(G_1 U^{ext}\right) \quad . \end{aligned} \tag{2.60}$$

Apart from a term independent of G_1, we see that $W[G_1]$ is given by, in the limit of $U^{ext} \to 0$,

$$W[G_1] = \Phi[G_1] + tr(\Sigma^{tot}[G_1]G_1] + tr\ ln(-G_1) . \qquad (2.61)$$

It is straightforward to show that eq. (2.61) for $W[G_1]$ is the logarithm of the grand partition function,[41,46] i.e. $W[G_1]$ is equal to the Massieu potential $W(\beta, v, \alpha)$.

Because of the identity of $W[G_1]$ with a thermodynamic potential, we expect that $W[G_1]$ will display variational properties. However, in that we would like to vary $W[G_1]$ with respect to the self-energy Σ^{tot} which is neither a thermodynamic quantity or even real, the variational properties are not so obvious. In fact, we will show that in general we cannot say anything about the sign of the second variation to determine a maximal or minimal property.

Because Σ^{tot} is defined by eq. (2.38), we can consider the change in $W[G_1]$ due to a small change in Σ^{tot}. $W[G_1]$ depends on Σ^{tot} in two ways: first, through its explicit dependence on Σ^{tot}, and second through its dependence through G_1. Therefore the first variation may be written

$$\delta W[G_1] = \delta\Phi[G_1] - tr(\Sigma^{tot}[G_1]\,G_1) . \qquad (2.62)$$

The vanishing of the first variation yields the Euler functional equation

$$\Sigma^{tot}[G_1] = \frac{\delta\Phi}{\delta G_1} \qquad (2.63)$$

which is just the condition for a conserving approximation. Since the approximation is conserving, eq. (2.58), we may calculate $W[G_1]$ in any method desirable. But eq. (2.63) tells us that not only must the approximation be conserving, but also the variations in must preserve the conserving condition in order that W is stationary under variations in Σ^{tot}.

The second variation of $W[G_1]$ is

$$\delta^2 W[G_1] = tr\left(\frac{\delta^2\Phi}{\delta G_1^2}\,\delta G_1 - \delta\Sigma^{tot}\right)\delta G_1 + \\ + tr\left(\frac{\delta\Phi}{\delta G_1} - \Sigma^{tot}\right)\delta^2 G_1 \quad , \tag{2.64}$$

which when evaluated at the point $\Sigma^{tot} = (\delta\Phi/\delta G_1)$ is

$$\begin{aligned}\delta^2 W[G_1] &= tr\left(\frac{\delta^2\Phi}{\delta G_1^2}\,\delta G_1 - \delta\Sigma^{tot}\right)\delta G_1 \\ &= \int_0^{-i\beta} d1\,d1'\,d2\,d2'\;\delta G(1'1)\,\delta G(2'2)\,\times \\ &\qquad \times\left(\frac{\delta^2\Phi[G_1]}{\delta G(1'1)\,\delta G(2'2)} - G^{-1}(12')\,G^{-1}(21')\right)\end{aligned} \tag{2.65}$$

From eqs. (2.43)(2.46b)(2.52), we note that $\delta^2 W$ can be written as

$$\delta^2 W[G_1] = \int_0^{-i\beta} d1\,d1'\,d2\,d2'\;\delta G(1'1)\,L^{-1}(121'2')\,\delta G(2'2) \; . \tag{2.66}$$

Eq. (2.66) gives the general connection of linear response to disturbances and thermodynamic stability.[49] In general, we cannot say anything about the sign of $\delta^2 W$. Hence $W[G_1]$ is stationary with respect to variations in Σ^{tot}. We also note that the indeterminacy of the sign of $\delta^2 W$ follows from our use of a nonlocal in time external potential U^{ext}, which is needed to define time-dependent Green's functions. Thus other formulations, namely time-independent ones,[43-45] will not share this feature, and W would have a maximal property. Hence for "time-independent" approximations, i.e. $G^{-1} \sim \delta(t)$, or $A(\omega) \sim \delta$-fn, or $G(p,\zeta)$ is analytic everywhere in ζ-plane except for a simple pole on the real axis (no cuts), we might expect the maximal property of W to hold.

B. Below the λ-transition (Anomalous System)

1. Basic Definitions

Below the λ-transition, the condensate must be taken into account. To do so, it is convenient to use a matrix representation[50] for the quantized fields ψ and ψ^+. We define the spinor

$$\Psi(r_1,t_1) \equiv \Psi(1) = \begin{pmatrix} \psi(1) \\ \psi^+(1) \end{pmatrix} \tag{2.67}$$

and its adjoint

$$\Psi^+(r_1,t_1) \equiv \Psi^+(1) = \begin{pmatrix} \psi^+(1) \\ \psi(1) \end{pmatrix} \tag{2.68}$$

to contain both the annihilation and creation operators. We shall follow the convention that when two operators are multiplied together at equal times, the ψ^+'s are always to the left of the ψ's regardless of their order in the matrix product. Also we follow the convention of summing over repeated indices (the index 1 is construed to include r_1, t_1, and the matrix index). Thus the number operator is given by

$$N(t_1) = \frac{1}{2} \int_{v} d^3r_1 \; \Psi^{+}(1)\; \Psi(1) \tag{2.69}$$

The modified Hamiltonian, eqs. (2.6)(2.1), can be written in the form

$$\begin{aligned} \mathcal{H}(t_1) = & -\frac{1}{2}\int_{v} d^3r_1 \; \Psi^{+}(1)\left(\frac{\nabla^2}{2m}+\mu\right)\Psi(1) + \\ & + \frac{1}{8}\int_{v} d^3r_1 \int_{0}^{-i\beta} d2 \; \Psi^{+}(1)\Psi^{+}(2)\,V(12)\,\Psi(2)\Psi(1) \end{aligned} \tag{2.70}$$

where V(12) is defined as in eq. (2.2) and is not a matrix.

To include the condensate, we introduce not only an external disturbance U^{ext} coupled to the "density" but also an external source η^{ext} coupled to the quantum field, so as to add to the Hamiltonian, eq. (2.70), the terms

$$\begin{aligned} H^{ext}(t_1) = & \; \frac{1}{2}\int_{v} d^3r_1 \int_{0}^{-i\beta} d2 \; \Psi^{+}(1)\, U^{ext}(12)\, \Psi(2) + \\ & + \int_{v} d^3r_1 \; \Psi^{+}(1)\, \eta^{ext}(1) \end{aligned} \tag{2.71}$$

where $U^{ext}(12)$ is an external 2x2 matrix potential, nonlocal in space and time, coupled to the "density" and the pair operators $\psi(1)\cdot\psi(2)$ and $\psi^{+}(1)\cdot\psi^{+}(2)$, and where $\eta^{ext}(1)$ is an external spinor source

$$\eta^{ext}(1) \equiv \begin{pmatrix} \eta^{ext}(r_1 t_1) \\ \eta^{ext*}(r_1 t_1) \end{pmatrix}$$

coupled to the spinor $\Psi^{+}(1)$.

We introduce the functional $W\left[U^{\text{ext}}, \eta^{\text{ext}}\right]$, analogous to eq. (2.33), by

$$W[U^{ext}, \eta^{ext}] \equiv \ln Sp\left\{ e^{-\beta\mathcal{H}} T_t\left(S[U^{ext}, \eta^{ext}]\right)\right\} \qquad (2.72a)$$

where S is the imaginary time S-matrix in the interaction picture for a potential U^{ext} and a source η^{ext}:

$$S[U^{ext}, \eta^{ext}] = \exp\left\{-i\left[\int_0^{-i\beta} d1d2\, \tfrac{1}{2}\Psi^+(1)\, U^{ext}(12)\, \Psi(2) + \right.\right. \qquad (2.72b)$$

$$\left.\left. + \int_0^{-i\beta} d1\, \Psi^+(1)\,\eta^{ext}(1)\right]\right\} .$$

Then we can define the following Green's functions

$$G_{1/2}(1) \equiv \frac{1}{\sqrt{-i}}\left(\frac{\delta W[U^{ext}, \eta^{ext}]}{\delta\eta^{ext*}(1)}\right)_{U^{ext}} = \sqrt{-i}\;\frac{\langle T_t\{S\,\Psi(1)\}\rangle}{\langle T_t(S)\rangle} \qquad (2.73a)$$

$$G_1(11') \equiv 2\left(\frac{\delta W[U^{ext}, \eta^{ext}]}{\delta U^{ext}(1'1)}\right)_{\eta^{ext}} = -i\;\frac{\langle T_t\{S\,\Psi(1)\Psi^+(1')\}\rangle}{\langle T_t(S)\rangle} \qquad (2.73b)$$

and the cumulant

$$\tilde{G}_1(11') \equiv G_1(11') - G_{1/2}(1)\, G^+_{1/2}(1')$$

$$= \frac{1}{-i}\left(\frac{\delta^2 W[U^{ext}, \eta^{ext}]}{\delta\eta^{ext}(1')\,\delta\eta^{ext*}(1)}\right)_{U^{ext}} . \qquad (2.73c)$$

We note that the separation of the one-particle Green's function G_1 into $G_{\frac{1}{2}}G_{\frac{1}{2}}^{+}$ and $\widetilde{G}_1$ is the time-dependent generalization of the splitting of the one-particle density matrix into an off-diagonal long-range order (ODLRO) part and a regular part, as introduced by Penrose and Onsager[51] and generalized by Yang.[52] We shall refer to $G_{\frac{1}{2}}$ as the condensate wave function and $\widetilde{G}_1$ as the propagator.

The equation of motion for the quantum field and its adjoint may be written

$$\int_0^{-i\beta} d2\, G_0^{-1}(12)\, G_{1/2}(2) = \sqrt{-i}\,\eta^{ext}(1) + \int_0^{-i\beta} d2\, \bar{U}(12)\, G_{1/2}(2) + \\ + \sqrt{-i}\,\frac{1}{2}\int_0^{-i\beta} d2\, v(12)\, \frac{\langle T_t\{S\,\Psi(1)\,\Psi^{+}(2)\,\Psi(2)\}\rangle}{\langle T_t(S)\rangle} \qquad (2.74)$$

where the operator G_0^{-1} is defined

$$G_0^{-1}(12) = \left[\tau^{(3)}\, i\hbar\frac{\partial}{\partial t_1} + \tau^{(0)}\left(\frac{\nabla_1^2}{2m} + \mu\right)\right]\delta(12) \qquad (2.75)$$

where $\delta(12) = \delta(r_1 - r_2)\,\delta(t_1 - t_2)\,\tau^{(0)}$, and the τ's are the Pauli matrices

$$\tau^{(1)} = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}; \quad \tau^{(2)} = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}; \quad \tau^{(3)} = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}; \qquad (2.76)$$

$$\tau^{(0)} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} .$$

The matrix $\overline{U}$ is given in terms of U^{ext} and its transpose $(U^{ext})^T$

$$\overline{U} \equiv \frac{1}{2}\left[U^{ext} + \gamma^{(1)}(U^{ext})^T\gamma^{(1)}\right] .$$

We now introduce the notation

$$\Sigma_{1/2}(1) \equiv \frac{1}{2}\int_0^{-i\beta} d2\, V(12)\, \frac{\langle T_t\{S\,\Psi(1)\Psi^+(2)\Psi(2)\}\rangle}{\langle T_t(S)\rangle} , \tag{2.77}$$

and the equation of motion reads

$$\int_0^{-i\beta} d2\, G_0^{-1}(12)\, G_{1/2}(2) = \sqrt{-i}\,\Sigma_{1/2}(1) + \sqrt{-i}\,\eta^{ext}(1) + + \int_0^{-i\beta} d2\, \overline{U}(12)\, G_{1/2}(2) . \tag{2.78}$$

Note that if $\Sigma_{1/2}(1)$ is approximated by

$$\sqrt{-i}\,\Sigma_{1/2}(1) = \frac{i}{2}\int_0^{-i\beta} d2\, V(12)\, G_{1/2}(1)\, G_{1/2}^+(2)\, G_{1/2}(2) , \tag{2.79}$$

eq. (2.78) is identical to the equation investigated by Gross,[53-55] Pitaevskii,[56] and Fetter[57] for nonuniform condensate wave functions.

We consider only uniform condensates at equilibrium in which

$$G_{1/2}(1) = \sqrt{-in_0}\begin{pmatrix}1\\1\end{pmatrix} = G_{1/2}^+(1) \tag{2.80a}$$

and

$$\Sigma_{1/2}(1) = \begin{pmatrix}\Sigma_{1/2}^{(1)}\\ \Sigma_{1/2}^{(2)}\end{pmatrix} = constant \tag{2.80b}$$

where n_o is the number density of the condensate. Note that eq. (2.80) is just the Bogoliubov replacement, in which the quantum fields are replaced by a c-number proportion to $\sqrt{n_o}$. The equation of motion for $G_{\frac{1}{2}}$, eq. (2.78), then becomes a relation between the chemical potential μ and the number density of the condensate n_o , viz.

$$\mu = \frac{1}{2\sqrt{n_0}}\left[\Sigma^{(1)}_{1/2} + \Sigma^{(2)}_{1/2}\right] \tag{2.81a}$$

or

$$\mu = \frac{(-i)^{-3/2}}{2n_0\beta v}\int_0^{-i\beta} d1\, \Sigma_{1/2}(1)\, G^{+}_{1/2}(1) \quad . \tag{2.81b}$$

In the above approximation, eq. (2.79), we have

$$\mu = n_0 V_0$$

where

$$V_0 \equiv \int_0^{-i\beta} d2\, V(12) \quad .$$

The other equation relating μ and n_o is the equation for the number density

$$n = \frac{i}{2} G(11^{+}) = n_0 + \frac{i}{2}\tilde{G}(11^{+}) \quad . \tag{2.82}$$

2. Self-Energy and Gapless Approximations

The equation of motion for G_1 can be obtained from the equation of motion for $G_{\frac{1}{2}}$, eq. (2.78), by functional differentiating (2.78) with respect to η^{ext} at constant U^{ext}. We get

$$\int_0^{-i\beta} d2\, G_0^{-1}(12)\,\tilde{G}_1(21') = \int_0^{-i\beta} d2\, \bar{U}(12)\,\tilde{G}(21') + \delta(11') + \left(\frac{\delta \Sigma_{1/2}(1)}{\delta \eta^{ext}(1')}\right)_{U^{ext}} . \tag{2.83}$$

We define the total self-energy Σ_1^{tot} by the usual Dyson equation (matrix version)

$$\Sigma^{tot}(11') \equiv G_0^{-1}(11') - \tilde{G}^{-1}(11') - \bar{U}(11') \tag{2.84}$$

and the inverse propagator $\tilde{G}^{-1}$ by

$$\begin{aligned} \delta(11') &= \int_0^{-i\beta} d2\, \tilde{G}^{-1}(12)\,\tilde{G}(21') \\ &= \int_0^{-i\beta} d2\, \tilde{G}(12)\,\tilde{G}^{-1}(21') \quad . \end{aligned} \tag{2.85}$$

Then the equation of motion (2.83) reads

$$\Sigma^{tot}(11') = \int_0^{-i\beta} d2 \left(\frac{\delta \Sigma_{1/2}(1)}{\delta \eta^{ext}(2)}\right)_{U^{ext}} \tilde{G}^{-1}(21') \quad . \tag{2.86}$$

We have been considering $\Sigma_{1/2}$ as a functional of $[\,U^{ext}, \eta^{ext}\,]$. The natural variables are their conjugates $[\,G_1\,, G_{\frac{1}{2}}^{+}\,]$. We now change from η^{ext} to its conjugate $G_{\frac{1}{2}}^{+}$

as the independent functional variable. This is equivalent to a Legendre-transformation of $W\left[U^{ext}, \eta^{ext}\right]$ to $W\left[U^{ext}, G_{\frac{1}{2}}^{+}\right]$ which is physically equivalent to the renormalization of the condensate wave function.[58] Then the functional derivative becomes

$$\left(\frac{\delta \Sigma_{1/2}(1)}{\delta \eta^{ext}(2)}\right)_{U^{ext}} = \int_{0}^{-i\beta} d3\, \sqrt{-i}\left(\frac{\delta \Sigma_{1/2}(1)}{\delta G_{1/2}(3)}\right)_{U^{ext}} \tilde{G}(32) \tag{2.87}$$

where we used eq. (2.73). Hence the equation of motion (2.86) becomes

$$\Sigma^{tot}(12) = \sqrt{-i}\left(\frac{\delta \Sigma_{1/2}(1)}{\delta G_{1/2}(2)}\right)_{U^{ext}} . \tag{2.88}$$

Hence, given an approximation for $\Sigma_{1/2}$, eq. (2.88) gives us the corresponding approximation for Σ_{1}^{tot}. We shall show later that such approximations are gapless.

Because the Green's functions $G_{\frac{1}{2}}$, G_1, $\tilde{G}_1$ satisfy the same boundary condition as the normal Green's function, eq. (2.10), we may introduce the Fourier series (2.13). The Fourier analysis of eqs. (2.84)(2.75) are

$$\Sigma^{tot}(p, z_\nu) = G_0^{-1}(p, z_\nu) - \tilde{G}^{-1}(p, z_\nu) \tag{2.84'}$$

and

$$G_0^{-1}(p, z_\nu) = \begin{pmatrix} z_\nu - \epsilon_p^0 + \mu & 0 \\ 0 & -z_\nu - \epsilon_p^0 + \mu \end{pmatrix} \tag{2.75'}$$

where we have taken the limit $U^{ext} \longrightarrow 0$. We separate the total self-energy into the subtraction term plus the analytic self-energy

$$\Sigma^{tot}(p,\zeta_\nu) = \Sigma^0(p) + \Sigma(p,\zeta_\nu) \qquad (2.89a)$$

with

$$\Sigma^0(p) = \Sigma^0(-p) = \begin{pmatrix} E^0(p) & F^0(p) \\ F^0(p) & E^0(p) \end{pmatrix} \qquad (2.89b)$$

and

$$\Sigma(p,\zeta_\nu) = \begin{pmatrix} \Sigma_{11}(p,\zeta_\nu) & \Sigma_{12}(p,\zeta_\nu) \\ \Sigma_{21}(p,\zeta_\nu) & \Sigma_{22}(p,\zeta_\nu) \end{pmatrix} \qquad (2.89c)$$

such that

$$\Sigma_{12}(p,\zeta_\nu) = \Sigma_{21}(p,\zeta_\nu) = \Sigma_{21}(p,-\zeta_\nu) \qquad (2.89d)$$

$$\Sigma_{11}(p,-\zeta_\nu) = \Sigma_{22}(p,\zeta_\nu) \quad , \qquad (2.89e)$$

since the Hamiltonian is symmetric in ψ and ψ^+ operators and hence invariant under time reversal. Because of space invariance, all quantities depend on the magnitude of the momentum. Therefore we have, after inverting the matrix $\tilde{G}^{-1}$,

$$\tilde{G}(p,\zeta_\nu) = \frac{1}{D}\begin{pmatrix} -\zeta_\nu - \tilde{E}(p) - \Sigma_{11}(-p,-\zeta_\nu) & F(p) + \Sigma_{12}(p,\zeta_\nu) \\ F(p) + \Sigma_{12}(p,\zeta_\nu) & \zeta_\nu - \tilde{E}(p) - \Sigma_{11}(p,\zeta_\nu) \end{pmatrix} \tag{2.90a}$$

where $D = \det(\tilde{G}^{-1})$ or

$$D = -\Big\{\big[\zeta_\nu + \tilde{E}(p) + \Sigma_{11}(-p,-\zeta_\nu)\big]\big[\zeta_\nu - \tilde{E}(p) - \Sigma_{11}(p,\zeta_\nu)\big] + \\ + \big[F(p) + \Sigma_{12}(p,\zeta_\nu)\big]^2\Big\} \tag{2.90b}$$

with

$$\tilde{E}(p) \equiv E(p) - \mu \tag{2.91a}$$

$$E(p) \equiv \epsilon_p^\circ + E^\circ(p) , \tag{2.91b}$$

and we drop the superscript o on F(p). We can introduce a spectral function $\tilde{A}(p,\omega)$ for the propagator $\tilde{G}(p,\zeta_\nu)$ such that for imaginary ζ_ν

$$\tilde{G}(p,\zeta_\nu) = \int_{-\infty}^{\infty}\frac{d\omega}{2\pi}\,\frac{\tilde{A}(p,\omega)}{\zeta_\nu - \omega} , \tag{2.92}$$

which satisfies the sum rule, for a given momentum,

$$\int_{-\infty}^{\infty} \frac{d\omega}{2\pi} \tilde{A}(p,\omega) = \tau^{(3)} \quad . \tag{2.93}$$

We now show that eq. (2.88) leads to gapless approximations. We follow Hohenberg and Martin[35] and apply a gauge transformation onto the source η^{ext}, i.e. $\eta^{\text{ext}}(1) \rightarrow exp[i\tau^{(3)}\alpha] \cdot \eta^{\text{ext}}(1)$ where α is a constant. For an infinitesimal $\delta\alpha$, we have

$$\delta\eta^{ext}(1) = i\,\tau^{(3)}\,\delta\alpha \cdot \eta^{ext}(1) \quad . \tag{2.94}$$

The corresponding changes in $G_{\frac{1}{2}}$ and $\Sigma_{\frac{1}{2}}$ are

$$\delta G_{1/2}(1) = i\,\tau^{(3)}\,G_{1/2}(1)\,\delta\alpha \tag{2.95a}$$

$$\delta \Sigma_{1/2}(1) = i\,\tau^{(3)}\,\Sigma_{1/2}(1)\,\delta\alpha \quad . \tag{2.95b}$$

The crux of the matter is that U^{ext} does not change for a constant α . Therefore we can write

$$\delta\Sigma_{1/2}(1) = \int_0^{-i\beta} dz \left(\frac{\delta \Sigma_{1/2}(1)}{\delta G_{1/2}(2)} \right)_{U^{ext}} \delta G_{1/2}(2) \quad ,$$

which becomes, using eqs. (2.95)(2.88),

$$i\,\tau^{(3)}\,\Sigma_{1/2}(1)\,\delta\alpha = \frac{1}{\sqrt{-i}} \int_0^{-i\beta} dz\, \Sigma_1^{tot}(12)\; i\,\tau^{(3)}\,G_{1/2}(2)\,\delta\alpha \quad .$$

As $\delta\alpha \rightarrow 0$

$$\Sigma_{1/2}(1) = \frac{1}{\sqrt{-i}} \int_0^{-i\beta} d2 \left[\tau^{(3)} \Sigma^{tot}(12)\, \tau^{(3)}\right] G_{1/2}(2) \quad (2.96)$$

Recalling eq. (2.81) for the chemical potential, we have

$$\mu = -\frac{1}{2n_0\beta V} \int_0^{-i\beta} d1\, d2\; G^{+}_{1/2}(1) \left[\tau^{(3)} \Sigma^{tot}(12)\, \tau^{(3)}\right] G_{1/2}(2) \quad (2.97)$$

As $G_{\frac{1}{2}}^{+} = G_{\frac{1}{2}}$ are constants for a uniform system, the integration picks out the $p = 0$, $\zeta_\nu = 0$ component of Σ^{tot} . Therefore eq. (2.97) reduces to the Hugenholtz-Pines[33] form

$$\begin{aligned} \mu &= \Sigma^{tot}_{11}(0,0) - \Sigma^{tot}_{12}(0,0) \\ &= \left[E^0(0) - F^0(0)\right] + \left[\Sigma_{11}(0,0) - \Sigma_{12}(0,0)\right] \end{aligned} \quad (2.98)$$

If we assume that Σ^{tot} is well-behaved near $p = 0$, $\zeta_\nu = 0$, we have from eq. (2.90b)

$$D = \left[\mu - E^0(p) - \Sigma_{11}(0,0)\right]^2 - \left[F^0(0) + \Sigma_{12}(0,0)\right]^2 , \quad (2.99)$$

which vanishes with the insertion of eq. (2.98), indicating the presence of excitations for arbitrary small p and ζ_ν , or no energy gap.

The sufficient (but perhaps not necessary) condition that an approximation be gapless is that the self-energy be derivable from the functional $\Sigma_{1/2}[U^{ext}, G_{\frac{1}{2}}]$ by eq. (2.88). The sufficiency of (2.88) is guaranteed by the constancy of U^{ext} under a gauge transformation of the first kind on the source η^{ext}.

3. Self-Energy and Conserving Approximations

In the normal system, we found a conserving expansion of $\Sigma^{tot}[U^{ext}]$ in terms of V and G_1 by utilizing the properties of the U^{ext} dependence and then considering Σ^{tot} not as a functional of U^{ext} but its conjugate G_1, i.e. $\Sigma^{tot}[G_1]$. This procedure is equivalent mathematically to a Legendre transformation of $W[U^{ext}]$ to $W[G_1]$ or, more picturesquely, to a propagator renormalization.

In the anomalous case, we can do the same. In the previous section, we have already Legendre transformed $W[U^{ext}, \eta^{ext}]$ to $W[U^{ext}, G_{\frac{1}{2}}^{+}]$. We can now complete the transformation to $W[G_1, G_{\frac{1}{2}}^{+}]$. This has been done in a more general context, and we shall not repeat it here. The generalized expressions for $\Sigma_{\frac{1}{2}}[G_1, G_{\frac{1}{2}}^{+}]$ and $\Sigma_1^{tot}[G_1, G_{\frac{1}{2}}^{+}]$ are found in eqs. (I.45)(I.46) respectively of reference 58. Furthermore, a functional $\Phi[G_1, G_{\frac{1}{2}}^{+}]$ can be constructed such that

$$\Sigma^{tot}(11') = \left(\frac{\delta\Phi[G_1, G_{1/2}^{+}]}{\delta G_1(1'1)}\right)_{G_{1/2}^{+}} \qquad (2.100)$$

$$\Sigma_{1/2}(1) = \frac{1}{2\sqrt{-i}} \left(\frac{\delta \Phi[G_1, G^+_{1/2}]}{\delta G^+_{1/2}(1)} \right)_{\tilde{G}_1} \tag{2.101}$$

as demonstrated by eqs. (II.25)(II.30) respectively of reference 58. Existence of such a functional $\Phi[G_1, G_{\frac{1}{2}}^+]$, as in the normal case, guarantees the conservation laws and consistent thermodynamics.

Φ depends on $G_{\frac{1}{2}}^+$ in two ways: first, through the explicit dependence and second through the $G_{\frac{1}{2}}^+$ dependence of G_1. Therefore

$$\Sigma_{1/2}(1) = \frac{1}{2\sqrt{-i}} \left\{ \left(\frac{\delta \Phi[G_1, G^+_{1/2}]}{\delta G^+_{1/2}(1)} \right)_{G_1} + \right.$$

$$\left. + \int_0^{-i\beta} d2\, d3 \left(\frac{\delta \Phi[G_1, G^+_{1/2}]}{\delta G_1(32)} \right)_{G^+_{1/2}} \left(\frac{\delta G_1(32)}{\delta G^+_{1/2}(1)} \right)_{\tilde{G}_1} \right\}$$

and

$$2 \int_0^{-i\beta} \Sigma^{tot}(31)\, G_{1/2}(3)\, d3 =$$

$$\int_0^{-i\beta} d2\, d3 \left(\frac{\delta \Phi[G_1, G^+_{1/2}]}{\delta G_1(32)} \right)_{G^+_{1/2}} \left(\frac{\delta G_1(32)}{\delta G^+_{1/2}(1)} \right)_{\tilde{G}_1}$$

so that

$$\Sigma_{1/2}(1) = \frac{1}{\sqrt{-i}} \int_0^{-i\beta} d3\, \Sigma^{tot}(31)\, G_{1/2}(3) + \frac{1}{2\sqrt{-i}}\, S_{1/2}(1) \tag{2.102a}$$

where

$$S_{1/2}(1) \equiv \left(\frac{\delta \Phi[G_1, G_{1/2}^{+}]}{\delta G_{1/2}^{+}(1)} \right)_{G_1} \quad . \tag{2.102b}$$

From the equation for the chemical potential (2.81), we see that

$$\mu = -\frac{1}{2n_0 \beta V} \int_0^{-i\beta} d1\, d2\, G_{1/2}(2)\, \Sigma^{tot}(21)\, G_{1/2}^{+}(1) - \mu_g \quad , \tag{2.103a}$$

where

$$\mu_g = \frac{1}{4n_0 \beta V} \int_0^{-i\beta} d1\; S_{1/2}(1)\, G_{1/2}^{+}(1) \quad . \tag{2.103b}$$

But for a uniform system, $G_{\frac{1}{2}}$ and $G_{\frac{1}{2}}^{+}$ are constants from eq. (2.80); and the integration in eq. (2.103a) evaluates Σ^{tot} at the values $p = z_\nu = 0$, while the matrix summation adds up the 11 and 12 components of Σ^{tot} to give

$$\mu = E^0(0) + F^0(0) + \Sigma_{11}(0,0) + \Sigma_{12}(0,0) - \mu_g \quad . \tag{2.104}$$

To interpret this equation, we consider the poles of $\mathcal{G}_1$ for small p and z_ν assuming the good behavior of $\Sigma^{tot}(p, z_\nu)$. Then D , eq. (2.90b), becomes

$$D = -\left\{ \zeta_\nu^2 - \left[E^\circ(0) + \Sigma_{11}(0,0) - \mu \right]^2 + \right. \qquad (2.105)$$

$$\left. + \left[F^\circ(0) + \Sigma_{12}(0,0) \right]^2 \right\} \quad ,$$

and the vanishing of D gives the limit as p → o of the energy spectrum. From eq. (2.105), we find that D vanishes with $\zeta_\nu^2 = \mathcal{E}_p^2$ where

$$\lim_{p \to 0} \mathcal{E}_p = 2\mu_g \left[F^\circ(0) + \Sigma_{12}(0,0) \right] + \mu_g^2 \quad . \qquad (2.106)$$

This shows that, in general, a conserving approximation leads to an energy gap in the spectrum of $\tilde{G}_1$. The source of the energy gap lies in the fact that the condensate, by its very nature, does not have any exchange properties; therefore diagrams with $\tilde{G}_1$ overcount, necessitating subtracting diagrams explicitly with $G_{\frac{1}{2}}$'s. The no-exchange property of the condensate is a reflection of the long-range order present in the condensate, which in turn is a consequence of a broken symmetry. The symmetry group in this case is the gauge group -- a group of gauge transformations of the first kind -- which is broken by the presence of $G_{\frac{1}{2}}^+$, $\tilde{G}_1$'s , etc. In a conserving approximation, we consider the Green's function G_1 which is invariant under the gauge group, which is no longer the proper symmetry group in our formulation. This disparity makes it increasingly difficult for excitations to "propagate" as G_1 , leading to the energy gap. The proper symmetry in our formulation is attained by considering $\tilde{G}_1$ as the propagator, which leads to the closing of the energy gap and the gapless approximations. We also note that the energy gap to each order approximation in V progresses as the number density of the condensate raised to the order considered. To first-order, we have $\mu_g^{(1)} \sim 0(n_o)$; second order, $\mu_g^{(2)} \sim 0(n_o^2)$; $n^{\underline{th}}$ order, $\mu_g^{(n)} \sim 0(n_o^n)$. Therefore the energy gap is $\sim 0(n_o^n)$ in the $n^{\underline{th}}$ order in V. Hence as we approach the λ -transition, the energy gap in the conserving approximation vanishes as expected. At the λ -transition, we have a gapless spectrum and in general two solutions to $D = 0$, viz.

$$\begin{aligned} \mu &= \Sigma_{11}^{tot}(0,0) \pm \Sigma_{12}^{tot}(0,0) \\ &= \left[E^0(0) \pm F^0(0)\right] + \left[\Sigma_{11}(0,0) \pm \Sigma_{12}(0,0)\right] \end{aligned} \qquad (2.107)$$

We see that the + sign corresponds to the conserving approximation and the - sign to the gapless approximations.

C. Approximations Below and Above the λ -transition

1. Nomenclature

We have seen that there is one physically interesting approximation above the λ -transition, and that is a conserving approximation. Below the λ -transition, we have two choices, either a conserving approximation or a gapless approximation. Hence there are two combinations which may be suitable on both sides of the λ -transition:

a wholly conserving approximation below and above, or a gapless/conserving approximation -- conserving above and analytic continued below to be combined with a gapless approximation. Note that while the order of the conserving approximation above and below must be the same, it need not be so for the gapless/conserving approximations since the gapless approximations singles out the role of the condensate from the rest of the system and hence can assume a different order.

A word should be said concerning the manner in which we name the approximations. For the conserving approximations, we use only generic names (e.g. Hartree-Fock) without any reference to the particular originator of the approximation as applied to the boson system. However since the gapless approximations are characteristic to the boson system, we shall name them after the originator of the approximation regardless of the temperature at which the approximation was first used. Finally we classify an approximation as $n^{\underline{th}}$ order where n is the higher of the order below and above.

2. Bose-Einstein Condensation and the Very Dense State Limit

Consider the system above the λ -transition and approaching the transition from above. We wish to give a criteria for the Bose-Einstein transition. Consider a quantum state characterized by momentum p . Let us define N_p as the number of particles in state p and $n_p \equiv N_p/\mathcal{V}$ as the number density of state p . Now when we take our $N/\mathcal{V}$ limit (i.e. $N \rightarrow \infty$, $\mathcal{V} \rightarrow \infty$, $n = N/\mathcal{V} < \infty$), we characterize a sparse state, dense state, very dense state, and a macroscopic state by the various inequalities and limits:

sparse	$0 \leq N_p \leq 1$	$n_p \longrightarrow 0$
dense	$1 < N_p$	$n_p \longrightarrow 0$
very dense	$1 \ll N_p$	$n_p \longrightarrow 0$
macroscopic	$N_p \longrightarrow \infty$	$n \geq n_p > 0$.

The Bose-Einstein transition is characterized by the appearance of a macroscopic state. For a system at rest, which is the only system we consider, the macroscopic state has $p = 0$.

In our formulation, the number of particles in the p state is

$$N_p = \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} A(p,\omega) f(\omega) \quad , \tag{2.108}$$

and $A(p,\omega)$ can be written from eq. (2.28)

$$A(p,\omega) = \frac{\Gamma(p,\omega)}{[\omega - \epsilon'(p) - \Delta'(p,\omega) - \eta]^2 + \frac{1}{4}[\Gamma(p,\omega)]^2} \quad , \tag{2.109}$$

where

$$\eta = -\mu + \epsilon(0) + \Delta(0,0) \tag{2.110}$$

and

$$\epsilon'(p) = \epsilon(p) - \epsilon(0) \tag{2.111a}$$

$$\Delta'(p,\omega) = \Delta(p,\omega) - \Delta(0,0) \quad . \tag{2.111b}$$

It is easy to see that eq. (2.108) is well-behaved for large ω's, so that any divergence in N_o must come from small ω's. Recalling the general property of A, eq. (2.16), we shall assume that $A(p,\omega)$ is suitably smooth near $\omega = 0$, such that the divergence in N_o will have its origin in the pole of the statistical factor $f(\omega)$. This is a physically reasonable assumption as the sin qua non of the Bose-Einstein transition is the Bose statistics. Even when the spectral function is as singular as a δ-function

$$A(p,\omega) = \begin{cases} 2\pi\,\delta(\omega - \epsilon_p + \mu) & \epsilon_0 - \mu > 0 \\ 0 & \text{otherwise} \end{cases}$$

so that eq. (2.108) reads

$$N_p = f(\epsilon_p - \mu) = \frac{1}{e^{\beta(\epsilon_p-\mu)}-1} \quad , \qquad \epsilon_p - \mu > 0 \, ,$$

N_o has a divergence at $\mu = \epsilon_0$ which is a reflection of the pole in $f(\omega)$. Therefore, for very dense states, we can approximate N_p by expanding $f(\omega)$ about $\omega = 0$, i.e.

$$N_p \simeq \frac{1}{\beta}\int_{-\infty}^{\infty}\frac{d\omega}{2\pi}\,\frac{A(p,\omega)}{\omega} \; ; \qquad N_p \gg 1 \, . \tag{2.112}$$

This approximation is called the Very Dense State limit. Using eqs. (2.14)(2.26), we rewrite eq. (2.112) as

$$N_p \simeq \frac{1}{\beta\left[\epsilon'(p) + \Delta'(p,0) + \eta\right]} \; ; \quad N_p \gg 1 \, . \tag{2.113}$$

Hence the Bose-Einstein transition ($N_0 \longrightarrow \infty$) occurs at

$$\eta = -\mu + \epsilon(0;\mu\beta) - \Delta(0,0;\mu\beta) = 0 \quad . \tag{2.114}$$

This equation relating μ and β along with the equation for the pressure will determine a transition line on the (pT) plane.

In order that eq. (2.112) is valid, the main contribution to the integral must come from ω's such that $\beta\omega << 1$. Hence the width of the spectral function must be contained in the small ω interval, i.e. for ω's satisfying $\beta\omega << 1$, $\beta\Gamma(p,\omega) << 1$. Furthermore, the peak of the spectral function must be in this range, i.e. for $\beta\omega << 1$, $\beta[\epsilon'(p) + \Delta'(p,\omega) + \eta] << 1$. From these two conditions, we see that our initial assumption of a suitably smooth $A(p,\omega)$ about $\omega = 0$ is transferred to an assumption on the continuity of the self-energy $\Sigma^{tot}(p,\zeta_\nu)$ about the point $\zeta = 0$. We know that $\Sigma^{tot}(p,\zeta)$ is continuous across the origin along the imaginary axis, and the added assumption concerns the entire neighborhood of the origin excluding the cuts on the real axis. In a sense, this assumption is analogous to the assumption of continuity of $\Sigma^{tot}(p,\zeta)$ about the Fermi surface in order that the Landau fermi-liquid theory is valid. Indeed, one can interpret the above assumption as defining the normal boson system.

We note that the Very Dense State limit, eq. (2.112), can be rewritten as

$$-\beta N_p \equiv \sum_\nu G(p,\zeta_\nu) \simeq G(p,0) \quad . \tag{2.115}$$

This limit should not be confused with the quasi-particle approximation, viz.

$$\sum_{\nu} G(p,z_\nu) \simeq \sum_{\nu} \frac{1}{z_\nu - \tilde{\epsilon}_p} = -\beta f(\tilde{\epsilon}_p) \quad . \tag{2.116}$$

If however we apply the Very Dense State limit to the final expression in eq. (2.116), we do get eq. (2.115). This merely asserts the commutivity of the two limiting cases, not their equality, and the fact that the Very Dense State limit is trivial if the quasi-particle approximation is valid. Hence the main utility of the Very Dense State limit is in dispersive systems, i.e. the second and higher-order approximations.

Let us rewrite eq. (2.110) in terms of the analytic self-energy

$$\eta = -\mu + \Sigma^{tot}(p=z=0) \quad . \tag{2.117}$$

We note that $\eta > 0$ above the transition and vanishes on the transition. It would be convenient then to analytic continue eq. (2.117) below the transition, i.e.

$$\eta = -\mu + \tilde{\Sigma}^{tot}_{11}(p=z=0) \tag{2.118}$$

where $\tilde{\Sigma}^{tot}_{11}$, the 11 element of the matrix $\tilde{\Sigma}^{tot}$, is the analytic continuation of Σ^{tot} defined above. By analytic continuation, we mean continuing the propagator G_1 above to the propagator $\tilde{G}_{11}$ below. Since Σ^{tot} above is a functional of G_1, this operation defines $\tilde{\Sigma}^{tot}_{11}$. In general, $\eta < 0$ below the transition.

III. ZEROTH-ORDER APPROXIMATION

The zeroth-order approximation is merely our classification of the ideal Bose gas, which was first studied for a non-massive system.[59] For the massive system, we note that the approximation is trivially conserving -- since the interaction V is zero, the function Φ is independent of G_1 and $G_{\frac{1}{2}}^{+}$, and $\Sigma_{\frac{1}{2}}$, Σ^{tot} both vanish.

We consider first the bulk limit for the ideal Bose gas and show that the transition is first-order. We apply the ideal Bose gas to restricted geometry, first writing down the thermodynamics for an ideal Bose gas in an arbitrary rectangular box. For concreteness, we specialize to a film geometry and study first the zero temperature limit. We find that the ground state is not macroscopically occupied until $T = 0$ and that c_p diverges as $T \rightarrow 0$ indicating a film analogue of the first-order transition at $T_o > 0$ in the bulk limit occuring at $T = 0$. At arbitrary nonzero temperatures, we reduce the thermodynamic quantities to expressions involving six functions of ξ and α, which are tabulated. We then discuss the equation for density holding ground state occupancy constant and varying L, and the equation for energy holding L fixed and varying T. In each case we find three distinct regions. For the constant ground state occupancy case, we find classical, quantum diffraction, and quantum statistical effects easily discernable. In the constant film thickness case, we find regions of two-dimensional Bose gas, three-dimensional Bose gas, and three-dimensional Boltzmann gas behavior. Finally because of the reduction to functions of ξ and α, we write down scaling laws enabling easy calculation of thermodynamic quantities of any film system once one film system has been solved completely.

A. The Bulk Limit

Above the critical temperature T_0, the equation of motion (2.26) (2.27) yields the usual $\epsilon_p^0 = p^2/2m$ spectrum for G_1. The chemical potential μ is determined by eq. (2.30)

$$n = i\, G(11^+) = \frac{1}{\mathcal{V}} \sum_p f(\epsilon_p^0 - \mu) \, . \qquad (3.1)$$

We now take the bulk limit, letting the volume $\mathcal{V}$ and the total number get arbitrarily large keeping the number density, $n = N/\mathcal{V}$, at a given finite value. Then the sum over momentum is converted to an integral by the usual prescription

$$\frac{1}{\mathcal{V}} \sum_p \Rightarrow \int \frac{d^3p}{(2\pi\hbar)^3}$$

where we have inserted the $\hbar$'s in explicitly. Eq. (3.1) becomes

$$n \lambda_T^3 = F_{3/2}(\alpha) \qquad (3.2)$$

where $\alpha = -\beta\mu$ and λ_T is the thermal wavelength at temperature T

$$\lambda_T^2 \equiv \frac{2\pi\hbar^2\beta}{m} = \frac{h^2}{2\pi m k_B T} \qquad (3.3)$$

and $F_\sigma(\alpha)$ is the σ-th order Bose-Einstein Functions[60]

$$F_\sigma(\alpha) \equiv \frac{1}{\Gamma(\sigma)} \int_0^\infty \frac{x^{\sigma-1}dx}{e^{x+\alpha}-1} = \sum_{n=1}^\infty \frac{e^{-n\alpha}}{n^\sigma} \quad . \tag{3.4}$$

The critical temperature T_o is given by

$$n\lambda_{T_o}^3 = F_{3/2}(0) = \zeta(\tfrac{3}{2}) = 2.612 \tag{3.5}$$

and is a function of density n and mass m . For values suitable for helium-4, we find that $T_o \simeq 3.14^\circ K$, which is to be compared with the λ -transition temperature, $T_\lambda \simeq 2.17^\circ K$.

Below T_o , the Bose-Einstein condensation sets in, and the chemical potential, eq. (2.81), vanishes and the equation of motion (2.90) yields the ϵ_p^o spectrum for $\tilde{G}_1$. $G_{\frac{1}{2}}$ or n_o is determined by eq. (2.82)

$$n = \frac{i}{2} G_1(11^+) = n_o + \frac{1}{V} \sum_p \frac{1}{e^{\beta\epsilon_p^o}-1} \quad . \tag{3.6}$$

In the bulk limit, we get

$$(n-n_o)\lambda_T^3 = 2.612 \ ; \qquad T \leq T_o \ . \tag{3.7}$$

The thermodynamic quantities can be easily calculated in the bulk limit.[2] The specific heat at constant volume is continuous with a discontinuous slope at T_o . This has led some to denote the transition as a third-order transition. But if we follow Ehrenfest's lead in classifying transitions, we should determine the order from the Gibbs potential in pT plane. Hence we calculate the Massieu potential W , which is related to the pressure by eq. (1.3) and is given microscopically by eq. (2.61). For the ideal gas, we have above T_0

$$\begin{aligned} W &= -\mathrm{tr}\,\ln(-G_1^{-1}) \\ &= \sum_p \ln(1+f(\tilde{\varepsilon}_p^0)) \\ &= v\lambda_T^{-3}F_{5/2}(\alpha) \end{aligned} \tag{3.8}$$

where the bulk limit is taken and the integral was integrated by parts. The pressure p as a function of (β, α) is given by

$$\beta\lambda_T^3 P = F_{5/2}(\alpha) \quad . \tag{3.9}$$

For small α's, we can invert eq. (3.9) by the expansion[61]

$$F_{5/2}(\alpha) = \zeta(\tfrac{5}{2}) - \zeta(\tfrac{3}{2})\alpha + \Gamma(-\tfrac{3}{2})\alpha^{3/2} + O(\alpha^2) \tag{3.10}$$

to obtain an explicit form for the chemical potential μ as a function of (T, p), which is just the Gibbs potential per particle, eq. (1.11). Holding the pressure fixed at P , we find

$$\mu(T>T_0) = -c_1 k_B T_0\left(\frac{\Delta T}{T_0}\right) - c_2 k_B T_0\left(\frac{\Delta T}{T_0}\right)^{3/2} + O(\Delta T^2) \tag{3.11}$$

where $T_0(P)$ is defined by

$$P = k_B T_0 \lambda_{T_0}^{-3} \zeta(\tfrac{5}{2}) \tag{3.12}$$

and

$$\Delta T \equiv T - T_0 \tag{3.13}$$

$$c_1 \equiv \frac{5}{2} \frac{\zeta(5/2)}{\zeta(3/2)} \tag{3.14a}$$

$$c_2 \equiv \frac{\Gamma(-3/2)}{\zeta(3/2)} \; c_1^{3/2} \quad . \tag{3.14b}$$

Below the transition, we have

$$\mu(T < T_0) = 0 \quad . \tag{3.15}$$

Hence the transition is first-order, with the Clausius-Clapeyron equation

$$\frac{dP}{dT} = c_1 n k_B = \frac{5}{2} \lambda_T^{-3} \zeta(\tfrac{5}{2}) k_B \quad . \tag{3.16}$$

Note that from the $(\Delta T)^{3/2}$ term in eq. (3.11), the specific heat at constant pressure diverges as $\Delta T \rightarrow 0+$ as

$$c_P = \frac{3}{4} c_2 n k_B \left(\frac{\Delta T}{T_0}\right)^{-1/2} \quad . \tag{3.17}$$

Below T_o , the pressure is fixed by the temperature alone, and c_p is not defined. The divergence of c_p is a reflection of the thermodynamic instability that sets in at the transition.

B. Restricted Geometry

The ideal Bose gas confined to a finite (in any dimensions) geometry has been of considerable interest. The geometries investigated has been the film geometry[62-66] and narrow channels.[67,68] Moreover the geometry may have infinite extent in some dimensions[64,65] or be strictly finite.[63,66-68]

We first write down the general thermodynamic expressions for the ideal Bose gas confined to any rectangular box. We next specialized the geometry to the film geometry as defined below and investigate the $T \rightarrow 0$ limit. The general equations are written down and discussed. Finally, we derive some general scaling laws.

1. General Thermodynamics

Let us first consider the ideal Bose gas confined to a rectangular box of dimensions (L_1,L_2,L_3), where we impose the boundary condition that the wave function vanishes on the box. Thus the energy levels are given by

$$E(\ell_1 \ell_2 \ell_3) = \frac{\pi}{4}\frac{\lambda_T^2}{\beta}\sum_{i=1}^{3}\left(\frac{\ell_i}{L_i}\right)^2 ; \quad \ell_i = 1,2,3\ldots \qquad (3.18)$$

where ℓ_i is the quantum number associated with the dimensions L_i . The Massieu potential W is given by

$$W(\beta,V,\alpha) = -\sum_{\substack{l_1 l_2 l_3\\=1}}^{\infty} \ln\left[1-\exp\left(-\beta E(l_1 l_2 l_3)-\alpha\right)\right] . \qquad (3.19)$$

Therefore, from eqs. (1.5), we find

$$N(\beta,V,\alpha) = \sum_{\substack{l_1 l_2 l_3\\=1}}^{\infty} N_{l_1 l_2 l_3} \qquad (3.20a)$$

$$U(\beta,V,\alpha) = \sum_{\substack{l_1 l_2 l_3\\=1}}^{\infty} N_{l_1 l_2 l_3} \; E(l_1 l_2 l_3) \qquad (3.20b)$$

$$P(\beta,V,\alpha) = \sum_{\substack{l_1 l_2 l_3\\=1}}^{\infty} N_{l_1 l_2 l_3} \left[-\frac{\partial}{\partial V} E(l_1 l_2 l_3)\right] \qquad (3.20c)$$

where $N_{l_1 l_2 l_3}$ is the mean number of particles in state (l_1 , l_2, l_3)

$$N_{l_1 l_2 l_3} = \left[\exp\left(\beta E(l_1 l_2 l_3)+\alpha\right)-1\right]^{-1} . \qquad (3.21)$$

The pressure is dependent upon the geometry of the system. We shall consider three geometries below. The first geometry of interest is the bulk geometry where all three dimensions can be varied. We set $L_1 = L_2 = L_3 = \mathcal{V}^{1/3}$ and obtain

$$-\frac{\partial}{\partial \mathcal{V}} E(\ell_1 \ell_2 \ell_3) = \frac{2}{3\mathcal{V}} E(\ell_1 \ell_2 \ell_3) \tag{3.22a}$$

and

$$\mathcal{P}(\beta, \mathcal{V}, \alpha) = \frac{2}{3} u(\beta, \mathcal{V}, \alpha) \tag{3.22b}$$

where $u = U/\mathcal{V}$ is the energy density. The second case of interest is that of a film geometry in which one dimensions, say L_3, is considered rigidly fixed. Then

$$-\frac{\partial}{\partial \mathcal{V}} \left[E(\ell_1 \ell_2 \ell_3) \right] = \frac{1}{\mathcal{V}} \left[E(\ell_1 \ell_2 \ell_3) - \frac{\pi}{4\beta} \left(\frac{\lambda_T}{L_3} \right)^2 \ell_3^2 \right] \tag{3.23a}$$

and

$$\mathcal{P}(\beta, \mathcal{V}, \alpha) = u(\beta, \mathcal{V}, \alpha) - \frac{\pi}{4\beta \mathcal{V}} \left(\frac{\lambda_T}{L_3} \right)^2 \sum_{\ell_1 \ell_2 \ell_3 = 1}^{\infty} \ell_3^2 N_{\ell_1 \ell_2 \ell_3} \; . \tag{3.23b}$$

The third case of interest is the pore geometry in which two dimensions, say L_2 and L_3, are considered rigidly fixed. Then

$$-\frac{\partial}{\partial V} E(l_1 l_2 l_3) = \frac{2}{V}\left[E(l_1 l_2 l_3) - \frac{\pi}{4\beta}\lambda_T^2\left(\frac{l_2^2}{L_2^2} + \frac{l_3^2}{L_3^2}\right)\right] \tag{3.24a}$$

and

$$P(\beta,V,\alpha) = 2u(\beta,V,\alpha) - \\ - \frac{\pi}{2\beta V}\lambda_T^2 \sum_{\substack{l_1 l_2 l_3 \\ =1}}^{\infty}\left(\frac{l_2^2}{L_2^2} + \frac{l_3^2}{L_3^2}\right) N_{l_1 l_2 l_3} \quad . \tag{3.24b}$$

Finally, the total (mean) entropy of the system is given by the Legendre transformation back to the extensive parameters, eq. (1.6). Using eqs. (3.20ab), we find the usual expression

$$S = \sum_{\substack{l_1 l_2 l_3 \\ =1}}^{\infty}\left[(1 + N_{l_1 l_2 l_3})\ln(1 + N_{l_1 l_2 l_3}) - \\ - N_{l_1 l_2 l_3}\ln N_{l_1 l_2 l_3}\right] \quad . \tag{3.25}$$

2. Film Geometry

Now we consider the film geometry in more detail. Let us define the dimensionless parameters

$$\xi_1 = \frac{\lambda_T}{L_1} \quad , \quad \xi_2 = \frac{\lambda_T}{L_2} \quad , \quad \xi_3 = \frac{\lambda_T}{L_3} \quad .$$

No physical system is infinite in extent, but the temperature needed for size effects for a typical length of one millmeter is of the order of $10^{-12}\,{}^{\circ}K$ for helium, which is clearly too low for our present technology. Therefore we can take some of the lengths to be effectively infinite in extent. For the film geometry, we take the limit $\xi_1 \longrightarrow 0$, $\xi_2 \longrightarrow 0$ as we apply the summation formulas in Appendix A to eqs. (3.20ab)(3.23b) to obtain the equations, valid for nonzero temperatures,

$$n\lambda_T^3 = \phi_{10}(\xi,\alpha) \tag{3.26a}$$

$$\beta u\lambda_T^3 = \phi_{20}(\xi,\alpha) + \frac{\pi}{4}\phi_{11}(\xi,\alpha) \tag{3.26b}$$

$$\beta P\lambda_T^3 = \phi_{20}(\xi,\alpha) \tag{3.26c}$$

where

$$\phi_{jk}(\xi,\alpha) = \xi^{2k+1}\sum_{n=1}^{\infty} F_j\left(\frac{\pi}{4}\xi^2 n^2 + \alpha\right) n^{2k} \tag{3.27a}$$

or

$$\phi_{jk}(\xi,\alpha) = \xi^{2k+1}\sum_{n=1}^{\infty} F_j\left(\frac{\pi}{4}\xi^2(n^2-1) + \alpha'\right) n^{2k} \tag{3.27b}$$

where we used

$$\alpha' = \alpha + \frac{\pi}{4}\xi^2 \tag{3.28}$$

and

$$\xi = \xi_3 \quad , \quad L = L_3 . \tag{3.29}$$

In Appendix A, we prove the following asymptotic limits for ϕ_{jk} :

$$\phi_{jk}(\xi,\alpha) \xrightarrow[\xi\to 0]{} \left(\frac{2}{\pi}\right)^k (2k-1)!!\, F_{j+k+1/2}(\alpha) - \\ - \delta_{k0}\frac{1}{2}\xi F_j(\alpha) \tag{3.30}$$

$$\phi_{jk}(\xi,\alpha) \xrightarrow[\xi\to\infty]{} \xi^{2k+1} F_j(\alpha') \quad . \tag{3.31}$$

Therefore as the bulk limit is approached, $\xi \longrightarrow 0$, eqs.(3.26) becomes

$$n\lambda_T^3 = F_{3/2}(\alpha) - \frac{1}{2}\xi F_1(\alpha) \tag{3.32a}$$

$$\beta u \lambda_T^3 = \frac{3}{2}F_{5/2}(\alpha) - \frac{1}{2}\xi F_2(\alpha) \tag{3.32b}$$

$$\beta P \lambda_T^3 = F_{5/2}(\alpha) - \frac{1}{2}\xi F_2(\alpha) \tag{3.32c}$$

and the other thermodynamic quantities are easily derived from these equations.

The opposite limit, $\xi \to \infty$, is the zero-temperature limit for a fixed film thickness L, in which the temperature is so low that $\xi \to \infty$ but yet high enough so that $\xi_1 \to 0$, $\xi_2 \to 0$. Using the asymptotic limit of $\bar{\Phi}_{jk}$, eq. (3.31), we obtain

$$n\lambda_T^3 = \xi F_1(\alpha') \tag{3.33a}$$

$$\beta u\lambda_T^3 = \xi F_2(\alpha') + \frac{\pi}{4}\xi^3 F_1(\alpha') \tag{3.33b}$$

$$\beta p\lambda_T^3 = \xi F_2(\alpha') \quad . \tag{3.33c}$$

Let us consider this limit in more detail.

a. Zero-Temperature Limit ($\xi \to \infty$)

To interpret eqs. (3.33), we consider the following thermodynamic quantities due to the ℓ th band

$$n_\ell \equiv \frac{N_\ell}{L_1L_2L} = \frac{1}{L_1L_2L}\sum_{\ell_2\ell_3=1}^{\infty} N_{\ell_1\ell_2\ell} \tag{3.34a}$$

$$u_\ell \equiv \frac{U_\ell}{L_1L_2L} = \frac{1}{L_1L_2L}\sum_{\ell_1\ell_2=1}^{\infty} N_{\ell_1\ell_2\ell}\, E(\ell_1\ell_2\ell) \tag{3.34b}$$

$$p_\ell \equiv u_\ell - n_\ell E_\ell \tag{3.34c}$$

where

$$E_\ell = \frac{\pi}{4}\xi^2\ell^2 \quad . \tag{3.35}$$

We get in the limit of $\xi \longrightarrow \infty$ the following expressions

$$n_\ell \lambda_T^3 = \xi F_1\left(\alpha' + \frac{\pi}{4}\xi^2(\ell^2-1)\right) \tag{3.36a}$$

$$\beta u_\ell \lambda_T^3 = \xi F_2\left(\alpha' + \frac{\pi}{4}\xi^2(\ell^2-1)\right) + n_\ell E_\ell \tag{3.36b}$$

$$\beta p_\ell \lambda_T^3 = \xi F_2\left(\alpha' + \frac{\pi}{4}\xi^2(\ell^2-1)\right) \quad . \tag{3.36c}$$

We see that the terms from the excited bands, i.e. n_ℓ, u_ℓ, p_ℓ for $\ell > 1$, all vanish exponentially as T ⟶ 0. Hence as T ⟶ 0 , all the particles squeeze into the first band, and we find a strictly two-dimensional behavior. Therefore eqs. (3.33) are just equal to the first-band contributions from eq. (3.36). We call this limit the first-band approximation.

The ground state occupancy $N_{111} \equiv [e^{\alpha'} - 1]^{-1}$ can be obtained in this limit by studying the behavior of α' as T ⟶ 0 . From eq. (3.33a) we see that

$$n\lambda_T^3 = -\xi \ln \alpha'$$

where we have expanded, for small α'

$$F_1(\alpha') = -\ln(1 - e^{-\alpha'}) \simeq \ln \alpha' .$$

Therefore as T ⟶ 0 , we have

$$\alpha' = e^{-n\lambda_T^2 L} \sim e^{-\frac{1}{T}} \tag{3.37}$$

and the ground state occupancy is

$$N_{111} \simeq \frac{1}{\alpha'} = e^{n\lambda_T^2 L} \sim e^{\frac{1}{T}} , \tag{3.38}$$

so that macroscopic occupation does not strictly appear until T = 0 , which is well-known.

In order to discuss the specific heat, the energy density may be written

$$u(T,v,N) = n k_B T \frac{F_2(\alpha')}{F_1(\alpha')} + n E_1 \tag{3.39a}$$

and the enthalpy density is

$$h(T,v,N) = 2n k_B T \frac{F_2(\alpha')}{F_1(\alpha')} + n E_1 . \tag{3.39b}$$

The specific heats are found by differentiating eqs. (3.39) to get

$$c_v(T) = nk_B\left[\frac{F_2(\alpha')}{F_1(\alpha')} + \right.$$
$$\left. + T\left(\frac{\partial\alpha'}{\partial T}\right)_v \left(\frac{F_2(\alpha')F_0(\alpha')}{F_1^2(\alpha')} - 1\right)\right] \tag{3.40a}$$

$$c_p(T) = 2nk_B\left[\frac{F_2(\alpha')}{F_1(\alpha')} + \right.$$
$$\left. + T\left(\frac{\partial\alpha'}{\partial T}\right)_p \left(\frac{F_2(\alpha')F_0(\alpha')}{F_1^2(\alpha')} - 1\right)\right] . \tag{3.40b}$$

From eq. (3.33a) we find

$$T\left(\frac{\partial\alpha'}{\partial T}\right)_v = \frac{F_1(\alpha')}{F_0(\alpha')} . \tag{3.41a}$$

From eq. (3.33c) we find

$$T\left(\frac{\partial\alpha'}{\partial T}\right)_p = 2\,\frac{F_2(\alpha')}{F_1(\alpha')} . \tag{3.41b}$$

Inserting eqs. (3.41) into (3.40), we have

$$c_v(T) = nk_B\left[2\,\frac{F_2(\alpha')}{F_1(\alpha')} - \frac{F_1(\alpha')}{F_0(\alpha')}\right] \tag{3.42a}$$

$$c_p(T) = 2nk_B\left[2\,\frac{F_2^2(\alpha')\,F_0(\alpha')}{F_1^3(\alpha')} - \frac{F_2(\alpha')}{F_1(\alpha')}\right] \tag{3.42b}$$

which has the limits, as T ⟶ 0 ,

$$c_v(T) = \frac{2k_B\,\zeta(2)}{L}\,\frac{1}{\lambda_T^2} \sim T \tag{3.43a}$$

$$c_p(T) = \frac{4k_B\,\zeta^2(2)}{L}\,\frac{1}{\lambda_T^2}\,e^{n\lambda_T^2 L} \sim T e^{\frac{1}{T}} \tag{3.43b}$$

The diverges of c_p does not violate Nernst's postulate as the entropy density is

$$s = \xi\,\lambda_T^{-3}\,F_2(\alpha') \xrightarrow[T\to 0]{} \frac{\zeta(2)}{L}\,\frac{1}{\lambda_T^2} \sim T \tag{3.44}$$

and vanishes at zero temperature. We note that there is a thermodynamic instability at $T = 0$, as

$$\left(\frac{\partial \mathcal{P}}{\partial v}\right)_T = -\,\frac{nk_B T}{v}\;\frac{F_1(\alpha')}{F_0(\alpha')}$$

vanishes exponentially as T ⟶ 0 , and the usual consequences of Nernst's postulate does not all hold, namely for c_p . This curious situation occurs because the analogue of the first-order transition at

T_0 for the bulk limit takes place at $T = 0$ in the film geometry.

In the pore geometry,[67] it has been shown that a finite system can behave as a one-dimensional system. In our infinite system, just as we have demonstrated the strict two-dimensional behavior of a film geometry, we can likewise do the same for the pore geometry. The equations analogous to eqs. (3.33) are

$$n \lambda_T^3 = \xi^2 F_{1/2}(\alpha')$$

$$\beta u \lambda_T^3 = \frac{1}{2} \xi^2 F_{3/2}(\alpha') + \frac{\pi}{4} \xi^4 F_{1/2}(\alpha')$$

$$\beta P \lambda_T^3 = \xi^2 F_{3/2}(\alpha')$$

where we have taken the system with

$$\xi = \xi_2 = \xi_3 \quad , \quad L = L_2 = L_3$$

and

$$\alpha' = \alpha + \frac{\pi}{2} \xi^2 \quad .$$

b. Nonzero Temperatures

Now we return to the general equations (3.26) and calculate the thermodynamics for arbitrary temperatures.

In order to calculate the specific heat, we write the energy density as

$$u(\xi,\alpha) = n k_B T \left[\frac{\phi_{20}(\xi,\alpha) + \frac{\pi}{4}\phi_{11}(\xi,\alpha)}{\phi_{10}(\xi,\alpha)} \right] \tag{3.45a}$$

and the enthalpy density as

$$h(\xi,\alpha) = n k_B T \left[\frac{2\phi_{20}(\xi,\alpha) + \frac{\pi}{4}\phi_{11}(\xi,\alpha)}{\phi_{10}(\xi,\alpha)} \right] \tag{3.45b}$$

We need the various derivatives of ϕ_{jk} , viz.

$$\frac{\partial}{\partial\xi}\phi_{jk}(\xi,\alpha) = \frac{2k+1}{\xi}\phi_{jk}(\xi,\alpha) - \\ - \frac{\pi}{2\xi}\phi_{j-1,\,k+1}(\xi,\alpha) \tag{3.46a}$$

$$\frac{\partial}{\partial\alpha}\phi_{jk}(\xi,\alpha) = -\phi_{j-1,\,k}(\xi,\alpha) \quad ; \tag{3.46b}$$

and from eqs. (3.26a)(3.26c), we obtain respectively

$$T\left(\frac{\partial\alpha}{\partial T}\right)_v = \frac{\phi_{10}(\xi,\alpha) + \frac{\pi}{4}\phi_{01}(\xi,\alpha)}{\phi_{00}(\xi,\alpha)} \tag{3.47a}$$

$$T\left(\frac{\partial\alpha}{\partial T}\right)_p = \frac{2\phi_{20}(\xi,\alpha) + \frac{\pi}{4}\phi_{11}(\xi,\alpha)}{\phi_{10}(\xi,\alpha)} \tag{3.47b}$$

The specific heats are then calculated by the equations

$$c_v(T) \equiv \left(\frac{\partial u}{\partial T}\right)_v$$

$$= \left(\frac{\partial u}{\partial T}\right)_{expl.} + \left(\frac{\partial u}{\partial \alpha}\right)_\xi \left(\frac{\partial \alpha}{\partial T}\right)_v - \frac{\xi}{2T}\left(\frac{\partial u}{\partial \xi}\right)_\alpha \tag{3.48a}$$

$$c_p(T) \equiv \left(\frac{\partial h}{\partial T}\right)_p$$

$$= \left(\frac{\partial h}{\partial T}\right)_{expl.} + \left(\frac{\partial h}{\partial \alpha}\right)_\xi \left(\frac{\partial \alpha}{\partial T}\right)_p - \frac{\xi}{2T}\left(\frac{\partial h}{\partial \xi}\right)_\alpha \tag{3.48b}$$

which result in, using eqs. (3.45)(3.46)(3.47)

$$c_v(T) = n k_B \left[\frac{1}{\phi_{10}}\left(2\phi_{20} + \frac{\pi}{4}\phi_{11} + \frac{\pi^2}{16}\phi_{02}\right) - \right.$$

$$\left. - \frac{1}{\phi_{00}\phi_{10}}\left(\phi_{10}^2 + \frac{\pi}{4}\phi_{10}\phi_{01} + \frac{\pi^2}{16}\phi_{01}^2\right)\right] \tag{3.49a}$$

and

$$c_p(T) = n k_B \left[\frac{\phi_{00}}{\phi_{10}^3}\left(4\phi_{20}^2 + \frac{3\pi}{4}\phi_{11}\phi_{20} + \frac{\pi^2}{16}\phi_{11}^2\right) - \right.$$

$$\left. - \frac{1}{\phi_{10}^2}\left(2\phi_{10}\phi_{20} - \frac{\pi^2}{16}\phi_{10}\phi_{02} + \pi\phi_{01}\phi_{20} + \frac{\pi^2}{8}\phi_{01}\phi_{11}\right)\right] \tag{3.49b}$$

By the use of eqs. (3.30)(3.31), one can easily verify that eqs. (3.49) reduce to the first-band approximation, eqs. (3.40), as T ⟶ 0 and to the usual expressions in the bulk limit.

Equations (3.26)(3.49) contains much of the thermodynamic properties of the film geometry at arbitrary temperature. Note that the thermodynamics are dependent on 6 functions $\phi_{00}, \phi_{10}, \phi_{20}, \phi_{01}, \phi_{11}, \phi_{02}$. These functions have been computed and are tabulated in Tables 1-6. Also $\phi_{10}, \phi_{20}, \phi_{11}$ are plotted in Figs. 4, 5, 6.

Figure 4 and the equation for n , eq. (3.26a), give us directly a relation for the density n(T) for a given occupation of the ground state, N_1

$$N_1 = \frac{1}{e^{\alpha'}-1}$$

and a given film thickness L . However it is more interesting to hold the density fixed and to compare the temperature of the film with the corresponding bulk system for a given occupation of the ground state. Mathematically, we need the inverse ratio of eq. (3.26a) with the corresponding equation for the bulk system, i.e.

$$\frac{T}{T_b} = \left(\frac{\lambda_{T_b}}{\lambda_T}\right)^2 = \left[\frac{F_{3/2}(\alpha_b)}{\phi_{10}(\xi,\alpha)}\right]^{2/3} \tag{3.50a}$$

with

$$\alpha' = \alpha + \frac{\pi}{4}\xi^2 = \alpha_b \tag{3.50b}$$

where T_b is the bulk temperature for a given ground state occupancy $N_0 = [e^{\alpha_b}-1]^{-1}$, as defined by

$$n\lambda_{T_b}^3 = F_{3/2}(\alpha_b) \quad .$$

Eq. (3.50) is plotted in Fig. 7, where instead of T/T_b versus , we have defined

$$\xi_b \equiv \xi \frac{\lambda_{T_b}}{\lambda_T} = \frac{\lambda_{T_b}}{L} . \tag{3.51}$$

The interesting feature of Fig. 7 is that $T > T_b$ for a region of small ξ_b ; i.e. as we "slice" the bulk system, decreasing L and keeping n fixed, we find that the temperature must first increase and then decrease in order to maintain the same occupation of the ground state. The $T > T_b$ region can be viewed as a region in which "classical" effects dominate. To see this, let us consider the point where $T = T_b$, i.e. we look for solutions to the equation

$$F_{3/2}(\alpha_b) = \phi_{10}\left(\bar{\xi}_b , \alpha_b - \frac{\pi}{4}\bar{\xi}_b^2\right) \tag{3.52}$$

for a given α_b . One solution is $\bar{\xi}_b = 0$, which is trivial and corresponds to the bulk system itself. A nontrivial solution does exist in general as evidenced by Figs. 4 and 7. As we increase α_b , $\bar{\xi}_b$ becomes larger and larger. Finally in the classical limit of large α_b's, $\bar{\xi}_b \longrightarrow \infty$; and there is no finite nontrivial solution to eq. (3.52) as shown in Appendix B. Hence the region $\xi_b < \bar{\xi}_b$ is a classical region. The physical effect is that as we "slice" the system decreasing L and keeping n constant, we drastically reduce the number of available energy levels including the ground state. Therefore to maintain the same ground state occupation, we must increase the temperature. However, as we continue to "slice" the system, the ground state energy increases making it increasingly difficult to occupy the ground state, and the temperature must be decreased to maintain constant occupation of the ground state. This latter effect is clearly a quantum diffraction effect which takes hold when the deBroglie wave length is comparable to the film thickness ($\xi \gtrsim 1$), generating the first-band approximation.

In addition to the "classical" effect for small ξ and the quantum diffraction effect for large ξ, there is a quantum statistical effect in the region of very small α_b or large occupation of the ground state. If $\alpha_b <<< 1$, say $\lesssim 10^{-8}$, then

$$F_1(\alpha_b) >> F_1\left(\frac{\pi}{4}\xi_b^2(n^2-1)+\alpha_b\right) \qquad n \geq 2$$

and

$$\Phi_{10}\left(\xi_b, \alpha_b - \frac{\pi}{4}\xi_b^2\right) \simeq \xi_b F_1(\alpha_b) . \tag{3.53}$$

Using eq. (3.53), we can explicitly solve eq. (3.52) to get

$$\xi_b = \frac{F_{3/2}(\alpha_b)}{F_1(\alpha_b)} = -\frac{2.612}{\ln\alpha_b} = -\frac{1.14}{\log_{10}\alpha_b} . \tag{3.54}$$

Note that the approximation which led to eq. (3.53) is not the same as the first-band approximation which is valid for large ξ for all

ϕ_{jk}'s, while the above approximation is valid for small ξ and is dependent on the divergences of $F_1(\alpha_b)$ as $\alpha_b \rightarrow 0$. The physical interpretation of this approximation is that the ground state is so densely occupied due to the quantum statistics that it dominates all the other states in the system. Because of statistical correlation, the effective length for quantum effects may be much larger than the deBroglie wave length, the measure of quantum diffraction effects. This effective length due to statistical correlation is obviously dependent on the range of α_b in which we are interested. If, for instance, we were interested in comparing some macroscopic behavior of a bulk system and a film within ½°K of the bulk critical temperature, T_o, which corresponds to a maximum α_b of 10^{-2}, the effective length according to eq. (3.54) is of the order of 15 Å. However $\alpha_b \sim 10^{-2}$ is stretching the validity of eq. (3.54); and if we solve eq. (3.52) by Fig. 4, we find an effective length of the order of 35 Å. Hence we can define a "small" system as one with $L \lesssim 35$ Å in which the ground state is densely occupied and dominates the system, and a "large" system as one with $L \gtrsim 35$ Å in which "classical" effects are prevalent so that all states need to be summed. According to this estimate, the diffraction effects which begins at $L \sim 10$ Å is completely pre-empted by the statistical effects which begins at a much larger $L \sim 35$ Å. This estimate gives a microscopic understanding to the "large" and "small" systems introduced by Goble and Trainor[66] on the basis of the specific heat behavior within ½°K of T_o. They also suggested a correlation length of the order of 40 Å.

Let us now consider the energy of the system as a function of temperature, which can be determined directly from eqs. (3.26) and Figs. 4, 5, and 6. Eqs. (3.26b)(3.26a) can be written as, respectively,

$$e(t) = t\left[\frac{\phi_{20}(\xi,\alpha) + \frac{\pi}{4}\phi_{11}(\xi,\alpha)}{\phi_{10}(\xi,\alpha)}\right] \tag{3.55a}$$

$$\zeta(\tfrac{3}{2})\, t^{-3/2} = \phi_{10}(\xi,\alpha) \tag{3.55b}$$

where $t = T/T_o$, $\xi_o = \lambda_{T_o}/L$, and $e = u/(nk_B T_o)$ are all dimensionless. Let us fix L and vary T . We find that eq. (3.55) reduces to

$$e(t) = \frac{\zeta(2)}{\zeta(3/2)}\xi_o t^2 + \frac{\pi}{4}\xi_o^2 \qquad t \ll 1 \tag{3.56}$$

$$e(t) = \frac{3}{2}t + \frac{1}{4}\xi_o\sqrt{t} \qquad t \gg 1 \, . \tag{3.57}$$

It turns out for L = 100 Å that the function $\phi_{20} + \frac{\pi}{4}\phi_{11}$ is almost constant in (ξ , α), so that eq. (3.55) becomes

$$e(t) = \left[\frac{\phi_{20} + \frac{\pi}{4}\phi_{11}}{\zeta(3/2)}\right] t^{5/2} \sim t^{5/2} \, . \tag{3.58}$$

Hence we can identify three regions:

(a) for $T \gg T_0$, $\alpha \gtrsim 1$, we have a three-dimensional Boltzmann gas, so that $e \sim T$;

(b) for $T \sim T_0$, $\alpha << 1$, we have a three-dimensional Bose gas with $e \sim T^{5/2}$;

(c) for $T << T_0$, $\alpha <<< 1$, we have a two-dimensional Bose gas with $e \sim T^2$.

In Fig. 8, we plot $e(t)$ for $L = 10$ Å and $L = 100$ Å.

We note from eqs. (3.56)(3.57)(3.58) that the specific heat at constant volume, $C_v \sim (\partial e/\partial T)$, starts off near $T = 0$ proportional to (T/L), then goes over to a $T^{3/2}$ dependence, reaches a maximum, and descends at large T to the classical value. From eq. (3.57), we see that the rate of descent to the classical value at large T becomes larger and larger as the film thickness decreases. This implies that the specific heat maximum has increased or shifted to higher temperatures or both. Goble and Trainor has plotted the specific heat at constant volume showing that the maximum moves to higher temperatures and is broadened as the film thickness is decreased.

3. Scaling Laws

We now turn to some general scaling laws. The basis for these laws is in the reduction of thermodynamic quantities to expressions involving the $\Phi_{jk}(\xi, \alpha)$ functions. Hence if we transform (or scale) the system keeping ξ and α invariant, then we have laws relating the thermodynamic quantities for the two systems. Let the systems be primed and unprimed. If ξ is to be invariant, the lengths are related by

$$\frac{L}{L'} = \frac{\lambda_T}{\lambda_{T'}} = \left(\frac{T'}{T}\right)^{1/2} . \qquad (3.59)$$

If α is to be invariant, the densities[69] are related by

$$\frac{n}{n'} = \left(\frac{\lambda_{T'}}{\lambda_T}\right)^3 = \left(\frac{L'}{L}\right)^3 . \qquad (3.60)$$

Then the thermodynamic quantities in the unprimed system with density n and film thickness L at temperature T are related to the primed system with density n' and film thickness L' at temperature T' by

$$\frac{P}{P'} = \frac{u}{u'} = \frac{k}{k'} = \left(\frac{L'}{L}\right)^5 \qquad (3.61)$$

$$\frac{c_v}{c_{v'}} = \frac{c_p}{c_{p'}} = \left(\frac{L'}{L}\right)^3 . \qquad (3.62)$$

The utility of these scaling laws in principle is that it permits the calculation of any film system once one film system, i.e. one fixed value of L, has been solved for all densities and temperatures.

IV. FIRST-ORDER APPROXIMATIONS

Almost all interacting boson systems studied in the literature fall into this group of approximations. The reasons for this proclivity can be said to be twofold. First, the first-order approximation is clearly the simplest way to include interactions into the system. Second, the first-order approximation has no dispersive character for the self-energy; and hence all first-order theories may be characterized by a gas of suitably defined quasi-particles.

We begin by constructing the general microscopic theory for any first-order approximation. In doing so, we also derived the total energy of the system good for any orders. We then consider in succession the following approximations: Bogoliubov/Ideal, Hartree, Bogoliubov/Hartree, Hartree-Fock, and Bogoliubov/Hartree-Fock approximations. Finally the application of these theories to the restricted geometry is considered.

A. General Theory

The general theory of the first-order approximation above the λ -transition is straightforward and will not be presented here. We consider the general theory below the λ -transition. The general first-order total self-energy is

$$\Sigma^{tot} = \Sigma^{o}(p) = \begin{pmatrix} E^{o}(p) & F^{o}(p) \\ F^{o}(p) & E^{o}(p) \end{pmatrix} \qquad (4.1)$$

where all frequency dependence is absent. The propagator, eq. (2.90), becomes

$$\tilde{G}(p,z_\nu) = \frac{1}{D}\begin{pmatrix} -z_\nu - \tilde{E}(p) & F(p) \\ F(p) & z_\nu - \tilde{E}(p) \end{pmatrix} \qquad (4.2a)$$

with

$$D = -\left\{ z_\nu^2 - \tilde{E}^2(p) + F^2(p) \right\} \qquad (4.2b)$$

where

$$\tilde{E}(p) = \epsilon_p^0 + E_p^0 - \mu \qquad (4.3a)$$

and

$$F(p) = F_p^0 \quad . \qquad (4.3b)$$

The excitation spectrum of G_1 is given by $D = 0$, or

$$z_\nu = \pm \mathcal{E}(p) \qquad (4.4a)$$

where

$$\mathcal{E}(p) = \sqrt{\tilde{E}^2(p) - F^2(p)} \quad . \qquad (4.4b)$$

We can interpret these poles of G_1 as a double spectrum, which to this order agrees with the double spectrum of Mohling.[70] The two poles may be displayed explicitly by writing eq. (4.2a) as

$$\tilde{G}(p,\zeta_\nu) = \frac{1}{\zeta_\nu - \mathcal{E}(p)} \begin{pmatrix} u_p^2 & -u_p v_p \\ -u_p v_p & v_p^2 \end{pmatrix} - \frac{1}{\zeta_\nu + \mathcal{E}(p)} \begin{pmatrix} v_p^2 & -u_p v_p \\ -u_p v_p & u_p^2 \end{pmatrix} \tag{4.5}$$

where

$$u_p^2 = \frac{1}{2}\left[\frac{\tilde{E}(p)}{\mathcal{E}(p)} + 1\right] \tag{4.6a}$$

$$v_p^2 = \frac{1}{2}\left[\frac{\tilde{E}(p)}{\mathcal{E}(p)} - 1\right] \tag{4.6b}$$

$$u_p v_p = \frac{1}{2}\,\frac{F(p)}{\mathcal{E}(p)} \quad ; \tag{4.6c}$$

and the spectral function for G_1 is

$$\tilde{A}(p,\omega) = 2\pi\,\delta(\omega - \mathcal{E}(p)) \begin{pmatrix} u_p^2 & -u_p v_p \\ -u_p v_p & v_p^2 \end{pmatrix} - 2\pi\,\delta(\omega + \mathcal{E}(p)) \begin{pmatrix} v_p^2 & -u_p v_p \\ -u_p v_p & u_p^2 \end{pmatrix} . \tag{4.7}$$

We note that the u_p and v_p are just the coherence coefficients usually introduced by a canonical transformation, in which u_p measures the admixture of the new creation operator in the old creation operator and v_p measures the admixture of the new annihilation operator in the old creation operator. Also note that this $\tilde{A}(p,\omega)$ satisfies the sum rule, eq. (2.93).

The first-order theory predicts in general a depletion of the ground state. At temperature T , the number density is given by

$$\begin{aligned} n-n_0 &= \frac{1}{v}\sum_{p}\int_{-\infty}^{\infty}\frac{d\omega}{2\pi}\,\tilde{A}_{11}(p,\omega)\,f(\omega) \\ &= \frac{1}{v}\sum_{p}\left[u_p^2 f(\varepsilon_p) + v_p^2\left(1+f(\varepsilon_p)\right)\right] \end{aligned} \tag{4.8}$$

where

$$f(\omega) = \frac{1}{e^{\beta\omega}-1} \tag{4.9}$$

and we have written ε_p for $\varepsilon(p)$. As T → 0 , we have the depletion

$$n_0 = n - \frac{1}{v}\sum_{p} v_p^2 \quad . \tag{4.10}$$

1. The Total Energy

Now we write down some general expressions for the energy that is not restricted to first-order theory. The general expressions are then specialized to the general first-order theory by the use of the spectral function eq. (4.7).

The total energy of the system is just the expectation value of the Hamiltonian. Below the λ -transition, we can take the expectation value of the modified Hamiltonian, eq. (2.6), and put it into the form

$$\begin{aligned} \langle \mathcal{H}(t_1) \rangle &\equiv U - \mu N \\ &= \frac{i}{4} \int_{\mathcal{V}} d^3 r_1 \left[\tau^{(3)} i \frac{\partial}{\partial t_1} - \frac{\nabla_1^2}{2m} - \mu \right] G(11') \Big|_{\substack{r_1' \to r_1 \\ t_1' \to t_1}} . \end{aligned} \tag{4.11}$$

Recalling the definition of $\tilde{G}_1$, eq. (2.73c) and its Fourier series eq. (2.13), we reduce the matrix eq. (4.11) to an ordinary equation

$$\begin{aligned} u - \mu n = {} & -\tfrac{1}{2} n \mu - \\ & - \frac{1}{\beta \mathcal{V}} \sum_{p} \sum_{\nu} \tfrac{1}{2} (z_\nu + \epsilon_p^{\circ}) \, \tilde{G}_{11}(p, z_\nu) \end{aligned} \tag{4.12}$$

where we wrote

$$\tilde{G}(p, z_\nu) = \begin{pmatrix} \tilde{G}_{11}(p, z_\nu) & \tilde{G}_{12}(p, z_\nu) \\ \tilde{G}_{12}(p, z_\nu) & \tilde{G}_{11}(p, -z_\nu) \end{pmatrix}$$

and $u = U/\mathcal{V}$ is the energy density. Introducting the spectral function, we write eq. (4.12) as

$$\begin{aligned} u - \mu n = {} & \frac{1}{\mathcal{V}} \sum_{p} \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} \, \tfrac{1}{2} (\omega + \epsilon_p^{\circ}) \, \tilde{A}_{11}(p, \omega) \, f(\omega) - \\ & - \tfrac{1}{2} n \mu \end{aligned} \tag{4.13}$$

If we divide the Hamiltonian into two parts

$$\mathcal{H}(t) = \left[H_0(t) - \mu N(t)\right] + H_{int}(t)$$

where $H_o(t)$ is just the kinetic energy, we can define an interaction energy as

$$\langle H_{int}(t)\rangle \equiv U_{int}$$

$$= \frac{i}{4}\int_{v} d^3r_1 \left[\tau^{(3)} i\frac{\partial}{\partial t_1} + \frac{\nabla_1^2}{2m} + \mu\right] G(11')\Big|_{\substack{r_1' \to r_1 \\ t_1' \to t_1}} \quad (4.14)$$

Going through the identical steps which led from eq. (4.11) to (4.13), we find

$$u_{int} = \frac{1}{v}\sum_{p}\int_{-\infty}^{\infty}\frac{d\omega}{2\pi}\,\frac{1}{2}(\omega - \epsilon_p^0)\,\tilde{A}_{11}(p,\omega)\,f(\omega) + \\ + \frac{1}{2}n\mu \quad (4.15)$$

Finally eq. (4.13) can be written as

$$u - \mu n = \frac{1}{v}\sum_{p}\int_{-\infty}^{\infty}\frac{d\omega}{2\pi}\,\omega\tilde{A}_{11}(p,\omega)\,f(\omega) - u_{int} \quad (4.16)$$

Above the λ -transition, the procedure is the same. We have

$$\begin{aligned} U - \mu N &\equiv \langle \mathcal{H}(t_1) \rangle \\ &= \frac{i}{2} \int_V d^3 r_1 \left[i \frac{\partial}{\partial t_1} - \frac{\nabla_1^2}{2m} - \mu \right] G(11') \Bigg|_{\substack{r_1' \to r_1 \\ t_1' \to t_1}} \end{aligned} \tag{4.17}$$

$$\begin{aligned} U_{int} &\equiv \langle H_{int}(t_1) \rangle \\ &= \frac{i}{2} \int_V d^3 r_1 \left[i \frac{\partial}{\partial t_1} + \frac{\nabla_1^2}{2m} + \mu \right] G(11') \Bigg|_{\substack{r_1' \to r_1 \\ t_1' \to t_1}} \end{aligned} \tag{4.18}$$

and

$$u - \mu n = -\frac{1}{\beta V} \sum_p \sum_\nu \frac{1}{2} (\zeta_\nu + \epsilon_p^0) G(p, \zeta_\nu) - \frac{1}{2} n\mu \tag{4.19a}$$

$$= \frac{1}{V} \sum_p \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} \frac{1}{2} (\omega + \epsilon_p^0) A(p, \omega) f(\omega) - \frac{1}{2} n\mu \tag{4.19b}$$

$$= \frac{1}{V} \sum_p \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} \omega A(p, \omega) f(\omega) - u_{int} \tag{4.19c}$$

where

$$u_{int} = \frac{1}{V}\sum_{p}\int_{-\infty}^{\infty}\frac{d\omega}{2\pi}\,\frac{1}{2}(\omega-\epsilon_p^o)\,A(p,\omega)\,f(\omega) + + \frac{1}{2}n\mu \qquad (4.20)$$

We note the formal similarity between these equations for the energy above with those below. However the similarity disappears once we introduce explicit spectral functions since $\widetilde{A}$ has two poles. Note also that eqs. (4.16)(4.19c) are generalizations of the Koopman's theorem in solid state physics. Now we insert the explicit first-order spectral functions to demonstrate these remarks.

The first-order spectral function above is

$$A(p,\omega) = 2\pi\,\delta(\omega - \tilde{\epsilon}_p) \qquad (4.21a)$$

where

$$\tilde{\epsilon}_p \equiv \epsilon_p - \mu = \epsilon_p^o + \Sigma^o(p) - \mu \quad , \qquad (4.21b)$$

and the first-order spectral function below is from eq. (4.7)

$$\widetilde{A}_{11}(p,\omega) = 2\pi\, u_p^2\,\delta(\omega - E_p) - 2\pi\, v_p^2\,\delta(\omega + E_p) \qquad (4.22)$$

The energy above is, inserting eq. (4.21) into (4.19)(4.20),

$$u-\mu n = \frac{1}{v}\sum_{p} \tilde{\epsilon}_p f(\tilde{\epsilon}_p) - u_{int} \tag{4.23a}$$

$$u_{int} = \frac{1}{v}\sum_{p} \frac{1}{2}\Sigma^{0}(p) f(\tilde{\epsilon}_p) \quad . \tag{4.23b}$$

The energy below is, inserting eq. (4.22) into (4.15)(4.16),

$$u-\mu n = \frac{1}{v}\sum_{p} \mathcal{E}_p f(\mathcal{E}_p) - \frac{1}{v}\sum_{p} \mathcal{E}_p v_p^2 - \\ - u_{int} \tag{4.24a}$$

$$u_{int} = \frac{1}{2v}\sum_{p}\left[\mathcal{E}_p - \epsilon_p^{0}(u_p^2 + v_p^2)\right] f(\mathcal{E}_p) - \\ - \frac{1}{2v}\sum_{p} v_p^2(\mathcal{E}_p + \epsilon_p^{0}) + \frac{1}{2}n\mu \quad . \tag{4.24b}$$

2. The Massieu Potential

From eq. (1.3), we see that the Massieu potential is given by

$$W/v = s - \beta(u-\mu n) = \beta p \tag{4.25}$$

Because of the δ -function in A(p, ω), eq. (4.21), the entropy of the normal system above is

$$S = \sum_p \left[(1+f(\tilde{\varepsilon}_p)) \ln (1+f(\tilde{\varepsilon}_p)) - f(\tilde{\varepsilon}_p) \ln f(\tilde{\varepsilon}_p) \right]$$
$$= \sum_p \left[\beta \tilde{\varepsilon}_p f(\tilde{\varepsilon}_p) + \ln (1+f(\tilde{\varepsilon}_p)) \right] \quad . \tag{4.26a}$$

Below the transition, we note that superfluid component do not contribute to the entropy.[71] The normal (quasi-particle) component has a spectral function like eq. (4.21) except $\tilde{\varepsilon}_p \longrightarrow \varepsilon_p$. Therefore the entropy is below

$$S = \sum_p \left[(1+f(\varepsilon_p)) \ln (1+f(\varepsilon_p)) - f(\varepsilon_p) \ln f(\varepsilon_p) \right]$$
$$= \sum_p \left[\beta \varepsilon_p f(\varepsilon_p) + \ln (1+f(\varepsilon_p)) \right] \quad . \tag{4.26b}$$

Combining eqs. (4.26) with those for the energy, eqs. (4.23)(4.24), we get the Massieu potential above

$$\frac{W}{V} = \frac{1}{V} \sum_p \ln (1+f(\tilde{\varepsilon}_p)) +$$
$$+ \frac{\beta}{V} \sum_p \frac{1}{2} \Sigma^0(p) f(\tilde{\varepsilon}_p) \tag{4.27a}$$

and below

$$\frac{W}{V} = \frac{1}{V}\sum_p \ln(1+f(\varepsilon_p)) + \frac{\beta}{2V}\sum_p v_p^2(\varepsilon_p - \epsilon_p^0) + \\ + \frac{\beta}{2V}\sum_p \left[\varepsilon_p - \tilde{\epsilon}_p^0(u_p^2 + v_p^2)\right] f(\varepsilon_p) + \\ + \frac{1}{2} n_0 \mu \tag{4.27b}$$

where we write

$$\tilde{\epsilon}_p^0 = \epsilon_p^0 - \mu \tag{4.27c}$$

Then by eq. (4.25), we immediately have the pressure for first-order approximations.

Summarizing the thermodynamics above, we write

$$n = \frac{1}{V}\sum_p f(\tilde{\epsilon}_p) \tag{4.28a}$$

$$u = \frac{1}{V}\sum_p \tilde{\epsilon}_p f(\tilde{\epsilon}_p) - u_{int} + \mu n \tag{4.28b}$$

$$s = \frac{1}{V}\sum_p \ln(1+f(\tilde{\epsilon}_p)) + \frac{\beta}{V}\sum_p \tilde{\epsilon}_p f(\tilde{\epsilon}_p) \tag{4.28c}$$

$$f = -\frac{1}{\beta V}\sum_{p} \ln\left(1+f(\tilde{\epsilon}_p)\right) - u_{int} + \mu n \qquad (4.28d)$$

$$p = \frac{1}{\beta V}\sum_{p} \ln\left(1+f(\tilde{\epsilon}_p)\right) + u_{int} \qquad (4.28e)$$

$$\begin{aligned} h = {} & \frac{1}{\beta V}\sum_{p} \ln\left(1+f(\tilde{\epsilon}_p)\right) + \\ & + \frac{1}{V}\sum_{p} \tilde{\epsilon}_p f(\tilde{\epsilon}_p) + \mu n \end{aligned} \qquad (4.28f)$$

$$g = n\mu \qquad (4.28g)$$

where

$$u_{int} = \frac{1}{V}\sum_{p}\left[\frac{1}{2}\Sigma^{0}(p)\, f(\tilde{\epsilon}_p)\right] \qquad (4.28h)$$

and

$$f \equiv u - k_B T s$$

$$h \equiv u + P$$

$$g \equiv u - k_B T s + P$$

Summarizing the thermodynamics below, we write

$$n = n_0 + \frac{1}{V}\sum_p \left[(u_p^2 + v_p^2) f(\varepsilon_p) + v_p^2\right] \tag{4.29a}$$

$$\begin{aligned} u = \frac{1}{V}\sum_p \varepsilon_p f(\varepsilon_p) - \frac{1}{V}\sum_p \varepsilon_p v_p^2 - \\ - u_{int} + \mu n \end{aligned} \tag{4.29b}$$

$$s = \frac{1}{\beta}\sum_p \ln(1 + f(\varepsilon_p)) + \frac{\beta}{V}\sum_p \varepsilon_p f(\varepsilon_p) \tag{4.29c}$$

$$\begin{aligned} f = -\frac{1}{\beta V}\sum_p \ln(1 + f(\varepsilon_p)) - \frac{1}{V}\sum_p \varepsilon_p v_p^2 - \\ - u_{int} + \mu n \end{aligned} \tag{4.29d}$$

$$p = \frac{1}{\beta V}\sum_p \ln(1 + f(\varepsilon_p)) + \frac{1}{V}\sum_p \varepsilon_p v_p^2 + u_{int} \tag{4.29e}$$

$$h = \frac{1}{\beta V}\sum_p \ln(1 + f(\varepsilon_p)) + \frac{1}{V}\sum_p \varepsilon_p f(\varepsilon_p) + \mu n \tag{4.29f}$$

$$g = n\mu \tag{4.29g}$$

where

$$u_{int} = \frac{1}{2V}\sum_{p}\left[\mathcal{E}_p - \epsilon_p^0\left(u_p^2 + v_p^2\right)\right] f(\mathcal{E}_p) - \\ - \frac{1}{2V}\sum_{p} v_p^2\left(\mathcal{E}_p + \epsilon_p^0\right) + \frac{1}{2} n\mu \tag{4.29h}$$

which can be written

$$u_{int} = \frac{1}{2V}\sum_{p}\left[\mathcal{E}_p - \tilde{\epsilon}_p^0\left(u_p^2 + v_p^2\right)\right] f(\mathcal{E}_p) - \\ - \frac{1}{2V}\sum_{p} v_p^2\left(\mathcal{E}_p + \tilde{\epsilon}_p^0\right) + \frac{1}{2} n_0\mu \quad . \tag{4.29i}$$

Thus to be able to do thermodynamics, we need the energy spectrum ϵ_p and the chemical potential μ above, the energy spectrum $\mathcal{E}_p$ with the energy parameters E(p), F(p) and the chemical potential μ below. These quantities are all specified once the self-energy is known.

B. Bogoliubov/Ideal Approximation

The Bogoliubov/Ideal approximation is the natural extension to nonzero temperatures above and below the transition of the system first studied by Bogoliubov[72] at zero temperatures. We emphasize that the extension is natural because, unlike other gapless/conserving approximations, the Bogoliubov/Ideal involves no analytic continuation. The Bogoliubov approximation at T = 0 has been extended to strong potentials in a dilute gas by the use of a pseudopotential[73] and a simultaneous expansion of the potential in powers of the two-body scattering amplitude.[74] Furthermore, the Bogoliubov approximation has been extended to nonzero temperatures below the transition using an extended grand canonical formulation[75] and Green's function.[76]

The approximation is defined below by the functional $\Sigma_{\frac{1}{2}}\left[U^{ext}, G_{\frac{1}{2}}^{+}\right]$ in the form eq. (2.79) which leads to the chemical potential

$$\mu = n_0 V_0 = -\eta \qquad (4.30)$$

and the self-energy by eq. (2.88)

$$\Sigma^{tot}(11') = \frac{i}{2}\delta(11')\int_0^{-i\beta} d2\, V(12)\, G_{1/2}^{+}(2)\, G_{1/2}(2) + \\ + i\, V(11')\, G_{1/2}(1)\, G_{1/2}^{+}(1') \quad , \qquad (4.31a)$$

which reduces to, for a uniform condensate

$$\Sigma^{tot}(11') = n_0 V_0\, \delta(11') + n_0 V(11')\left[\tau^{(0)} + \tau^{(1)}\right] . \qquad (4.31b)$$

In momentum space, we can write the self-energy as

$$\Sigma^{tot} = \Sigma^{0}(p) = \begin{pmatrix} n_0(V_0 + V_p) & n_0 V_p \\ n_0 V_p & n_0(V_0 + V_p) \end{pmatrix} \qquad (4.32)$$

where

$$V_p \equiv \int_v d^3r \; V(r) \, e^{ipr} \qquad ;$$

and we can easily see that the Hugenholtz-Pines form is explicitly satisfied by eqs. (4.29)(4.32). From eq. (4.4), we see that the spectrum is the usual Bogoliubov one:

$$\mathcal{E}(p) = \sqrt{\epsilon_p^o \left(\epsilon_p^o + 2n_o V_p\right)} \tag{4.33}$$

with

$$\tilde{\mathcal{E}}(p) = \epsilon_p^o + n_o V_p \tag{4.34a}$$

$$F(p) = n_o V_p \tag{4.34b}$$

$$\tilde{\mathcal{E}}^o(p) = \epsilon_p^o - n_o V_o \tag{4.34c}$$

With the energy spectrum eqs. (4.33)(4.34) and the chemical potential eq. (4.30), we can insert them into eqs. (4.29) to obtain the thermodynamics. The integrals involving the Bogoliubov energy spectrum needed for thermodynamics are summarized in Appendix C for small values of $(\beta n_o V_o)$. We note that among the seven thermodynamic functions summarized in eqs. (4.29), only two of them, the number density and the entropy density, are not dependent upon the chemical potential μ explicitly. The import of this observation is that conclusions reached concerning n and s at constant volume are valid for all approximations with the same spectrum.

In particular, let us consider the number density,[77]

$$n = n_0 + \lambda_T^{-3} B_3(\beta n_0 V_0) + \frac{1}{\mathcal{V}} \sum_p v_p^2 \tag{4.35a}$$

which can be written as, up to order n_0 ,

$$n = n_0 + \lambda_T^{-3}\left[\zeta(\tfrac{3}{2}) - \sqrt{2\pi}\,\alpha^{1/2} + \zeta(\tfrac{1}{2})\,\alpha + O(\alpha^2)\right] \tag{4.35b}$$

where

$$\alpha \equiv -\beta\eta = \beta n_0 V_0 \geqslant 0 \quad . \tag{4.35c}$$

Holding the number N and the volume $\mathcal{V}$ of the system fixed, we defined the transition temperature $T_0(n)$ by setting $\eta = 0$ in eq. (4.35a)

$$n = \lambda_{T_0}^{-3}\, \zeta(\tfrac{3}{2}) \quad . \tag{4.36}$$

We note that for very small α , there is no solution to eq. (4.35a) if $\Delta T \equiv (T - T_0) < 0$. However a solution does exist if we allow $\Delta T > 0$. The positive α term in (4.35a) would then turn the solution back into the $\Delta T < 0$ region. To see this, we rewrite eq. (4.35a) as

$$a^2 y^2 + y\left[2(x^{3/2}-1)\,a - c\,V_{T_0}\,x^2\right] + (x^{3/2}-1)^2 = 0 \qquad (4.37)$$

where

$$a \equiv 1 + \zeta(\tfrac{1}{2})\,V_{T_0}\,x^{1/2} \qquad (4.38a)$$

$$c \equiv 2\pi / \zeta(\tfrac{3}{2}) \qquad (4.38b)$$

$$V_{T_0} \equiv \beta V_0\,\lambda_{T_0}^{-3} \qquad (4.38c)$$

and $y \equiv n_0/n$, $x \equiv T/T_0$ are dimensionless parameters. The solutions to eq. (4.37) are

$$y = \frac{1}{2a^2}\left[c\,V_{T_0}\,x^2 - 2(x^{3/2}-1)\,a\right] \pm \\ \pm \frac{1}{2a^2}\left[(c\,V_{T_0}\,x^2)^2 - 4ac\,V_{T_0}\,x^2\,(x^{3/2}-1)\right]^{1/2} . \qquad (4.39)$$

For small ΔT, we take the minus sign to obtain

$$\frac{n_0}{n} \sim \left(\frac{\Delta T}{T_0}\right)^2 . \qquad (4.40)$$

The solution begins to turn back when the discriminant of (4.39) vanishes, defining $\chi_c \equiv T_c/T_o$

$$c V_{T_0} \chi_c^2 = 4a\left(\chi_c^{3/2}-1\right) \quad , \tag{4.41}$$

which yields for small V_{T_0}

$$\frac{T_c-T_0}{T_0} \simeq \frac{\pi}{3\zeta(3/2)} V_{T_0} \quad . \tag{4.42}$$

For small values of $\delta T = (T - T_c) < 0$, we find from eq. (4.39) using the positive sign

$$\frac{n_0 - n_0(T_c)}{n} \sim \left(-\frac{\delta T}{T_c}\right)^{1/2} \tag{4.43}$$

where

$$\frac{n_0(T_c)}{n} = \frac{1}{4a^2} c V_{T_0} \chi_c^2 \tag{4.44}$$

which has the limit $(\pi/2)(\zeta(3/2))^{-1} V_{T_0}$ for small V_{T_0} . Such behavior of n_o/n was pointed out recently by Luban and Grobman [78] for two specific models, but we see its generality, occuring whenever a Bogoliubov energy spectrum exists. To complete the analysis, we note that

$$\frac{n_0(T_0)}{n} = \frac{1}{a^2} c V_{T_0} \tag{4.45}$$

and

$$\frac{n_0 - n_0(T_0)}{n} \sim \left(-\frac{\Delta T}{T_0}\right) \quad . \tag{4.46}$$

This behavior of $n_0(T)$ is summarized in Fig. 9.

We see from the above analysis that there are two temperatures in the system, T_0 and T_c. In order to determine where the transition occurs, we must calculate the thermodynamics. Luban and Grobman[78] went ahead and calculated the specific heat at constant volume, assuming that T_c is the transition temperature. From eq. (4.43), they found $c_v \sim (-\delta T)^{-1/2}$. We shall show that this is not the case when the interaction is more general than V_0. When $V_p \simeq V_0$, the thermodynamics appear to be ill-defined. Finally, we note that our equation for the energy, eqs. (4.29b)(4.29h), reduces to the form used by GKW[75] if we set $u_{\text{int}} = \frac{1}{2} n_0 \mu$. The other terms of u_{int} do not appear in GKW as they ignored the interaction term in the Hamiltonian. These interaction terms are very important near the transition.

The thermodynamics can be obtained from the Massieu potential or the pressure, from which the Gibbs potential at constant pressure may be calculated. We shall be contented with the first two terms of the expansion of V_p about $p = 0$, i.e.

$$V_p \simeq V_0 + V_1 \frac{\lambda_T^2}{h^2} p^2 + \cdots \quad . \tag{4.47}$$

The crucial terms are the interaction terms

$$u_{int} \simeq k_B T \lambda_T^{-3}\left[\left(\zeta(\tfrac{3}{2}) + \frac{3}{4\pi}\frac{V_1}{V_0}\zeta(\tfrac{5}{2})\right)\alpha + O(\alpha^2)\right] \quad (4.48)$$

where the $O(\alpha)$ terms come from the first term of eq. (4.29i). If we ignore these terms as in GKW, we get

$$P = \frac{k_B T}{\lambda_T^3}\left[\zeta(\tfrac{5}{2}) - \zeta(\tfrac{3}{2})\alpha + \tfrac{4}{3}\sqrt{2\pi}\,\alpha^{3/2} + O(\alpha^2)\right] . \quad (4.49)$$

Holding the pressure fixed and expanding the temperature about $T_o(P)$ defined by setting $\eta = 0$ in eq. (4.49), we see that there is no solution to eq. (4.49) for $\Delta T < 0$ and $\eta < 0$ for small values of $|\Delta T|$, $|\eta|$. If we allow $\Delta T > 0$, we find a Gibbs potential per particle which is double-valued as a function of temperature, which is certainly difficult to interpret. If we include u_{int}, the term linear in α cancels out, and we find $\mu \sim (-\Delta T)^{2/3}$ which leads to a divergent entropy. However if we keep the V_1 term in the expansion (4.47), we find to first-order in V_1,

$$P = \frac{k_B T}{\lambda_T^3}\left[\zeta(\tfrac{5}{2}) + \frac{3}{4\pi}\frac{V_1}{V_0}\zeta(\tfrac{5}{2})\alpha + O(\alpha^{3/2})\right] \quad (4.50)$$

which yield the Gibbs potential per particle at constant pressure $P = k_B T_0 \lambda_{T_0}^{-3} \zeta(5/2)$

$$\mu(T<T_0) = -\frac{10\pi}{3} \frac{V_1}{V_0} k_B T_0 \left(\frac{\Delta T}{T_0}\right) + O(\Delta T^{3/2}) . \tag{4.51}$$

The analogous equation above is that for the ideal gas, eq. (3.11)

$$\begin{aligned} \mu(T>T_0) &= -\frac{5}{2} \frac{\zeta(5/2)}{\zeta(3/2)} k_B T_0 \left(\frac{\Delta T}{T_0}\right) - \\ &\quad - c_2 k_B T_0 \left(\frac{\Delta T}{T_0}\right)^{3/2} + O(\Delta T^2) . \end{aligned} \tag{4.52}$$

Hence the transition occurs at T_0 and appears to be first-order with a change in entropy per particle

$$\begin{aligned} \Delta\left(\frac{s}{n}\right) &\equiv \frac{s}{n}(T>T_0) - \frac{s}{n}(T<T_0) \\ &= \frac{5}{2} \frac{\zeta(5/2)}{\zeta(3/2)} - \frac{10\pi}{3} \frac{V_0}{V_1} . \end{aligned} \tag{4.53}$$

From the $(\Delta T)^{3/2}$ terms in eqs. (4.52)(4.53), we see that c_p diverges on both sides of the transition as $|\Delta T|^{-\frac{1}{2}}$. Since the change in entropy per particle must satisfy

$$0 \leq \Delta\left(\frac{a}{n}\right) \leq \frac{5}{2}\,\frac{\zeta(5/2)}{\zeta(3/2)} \quad ,$$

we see from eq. (4.53) that $V_1 > 0$ and that

$$\frac{V_0}{V_1} \leq \frac{3}{4\pi}\,\frac{\zeta(5/2)}{\zeta(3/2)} \simeq 0.12 \tag{4.54}$$

Hence the Bogoliubov/Ideal approximation is strictly a weak potential system. If the potential is too strong, the system finds it more favorable to remain in the ideal phase, as we can see from the free energy below the transition

$$\begin{aligned} f &= -\frac{k_B T}{\lambda_T^3}\left[\zeta\left(\tfrac{5}{2}\right) + \left(\frac{3}{4\pi}\frac{V_1}{V_0}\zeta\left(\tfrac{5}{2}\right) - \zeta\left(\tfrac{3}{2}\right)\right)\alpha + O\left(\alpha^{3/2}\right)\right] \\ &= f_{ideal} - \frac{k_B T}{\lambda_T^3}\left[\frac{3}{4\pi}\frac{V_1}{V_0}\zeta\left(\tfrac{5}{2}\right) - \zeta\left(\tfrac{3}{2}\right)\right]\alpha + O\left(\alpha^{3/2}\right) \end{aligned} \tag{4.55}$$

The specific at constant volume may be obtained from the free energy, or more easily from the energy

$$u = \frac{k_B T}{\lambda_T^3}\left[\frac{3}{2}\zeta(\tfrac{5}{2}) + \left(\frac{3}{4\pi}\frac{V_1}{V_0}\zeta(\tfrac{5}{2}) - \zeta(\tfrac{3}{2})\right)\alpha + O(\alpha^{3/2})\right] + \tag{4.56}$$
$$+ \frac{1}{2} n\mu$$

From eq. (4.35), we see that α satisfy the equation

$$A\alpha - B\sqrt{\alpha} + C = 0 \tag{4.57}$$

where

$$\begin{cases} A = [\zeta(\tfrac{1}{2}) - V_T^{-1}]/\zeta(\tfrac{3}{2}) \\ B = \sqrt{2\pi}/\zeta(\tfrac{3}{2}) \\ C = 1 - (T_0/T)^{3/2} \end{cases} \tag{4.58}$$

with solutions

$$\alpha = \frac{1}{2A}\left[B \pm \sqrt{B^2 - 4AC}\right] \simeq \begin{cases} B/A - C/B \\ C/B \end{cases} \tag{4.59}$$

for $C \ll 1$

Therefore, taking the plus sign

$$\alpha(T) \simeq \frac{\sqrt{2\pi}}{\zeta(\frac{1}{2}) + V_T^{-1}} - \frac{3}{2\sqrt{2\pi}}\zeta(\tfrac{3}{2})\frac{\Delta T}{T_0} \tag{4.60}$$

and

$$\lim_{T \to T_0^-} T\left(\frac{\partial \alpha}{\partial T}\right)_v = \frac{\sqrt{2\pi}\, V_{T_0}}{2\left[\zeta(1/2) + V_{T_0}^{-1}\right]^2} - \frac{3}{2\sqrt{2\pi}}\, \zeta\left(\tfrac{3}{2}\right) . \tag{4.61}$$

The specific heat at constant volume is from eq. (4.56)

$$\begin{aligned} c_v &= \left(\frac{\partial u}{\partial T}\right)_{vN} \\ &= \frac{k_B}{\lambda_T^3}\left[\frac{15}{4}\zeta\left(\tfrac{5}{2}\right) + \left(\frac{3}{4\pi}\frac{V_1}{V_0}\zeta\left(\tfrac{5}{2}\right) - \zeta\left(\tfrac{3}{2}\right)\right) T\left(\frac{\partial \alpha'}{\partial T}\right)_v\right] . \end{aligned} \tag{4.62}$$

Therefore c_v is finite at T_0 and has a finite discontinuity across the transition.

Finally we note that the isotherms in the $\mathcal{P}v$ plane do not have a finite interval with zero slope, but rather an instability at the transition, i.e. $(\partial \mathcal{P}/\partial v) \to 0$ as $\eta \to 0$. Despite the fact that $\Delta s > 0$, we have $\Delta v = 0$; therefore we cannot write down a Clausius-Claperyon equation for the transition. Hence we conclude that the phase transition is a vertical line in the PT plane and of zero extent in the $\mathcal{P}v$ plane. Furthermore we interpret the transition as a first-order one, despite the above characteristics, because of the presence of the latent heat.

C. Hartree Approximation

The Hartree approximation is the simplest conserving approximation, in which only the direct first-order term is included in the self-energy. For bosons, one usually includes the exchange term, as the exchange term is of the same order as the direct term for short-range potentials. However this model has some desirable features: it is soluble and it is uniquely gapless as well as conserving.

Let us consider the Hartree approximation above. We have

$$\begin{aligned} \Phi[G_1] &= \frac{i}{2}\int_0^{-i\beta} d1\, d2\; G(11)\, V(12)\, G(22) \\ &= -\frac{1}{2} n^2 V_0 \beta \mathcal{V} \quad , \end{aligned} \tag{4.63}$$

$$\begin{aligned} \Sigma^{tot}(11') &= i\,\delta(11') \int_0^{-i\beta} d2\; V(12)\, G(22) \\ &= \delta(11')\, n V_0 \quad . \end{aligned} \tag{4.64}$$

Therefore

$$\Sigma^0(p) = n V_0 \tag{4.65}$$

$$W = \frac{1}{2} n^2 V_0 \beta \mathcal{V} - \sum_p \ln\left(1 - e^{-\beta(\epsilon_p^0 + \eta)}\right) \tag{4.66}$$

$$u_{int} = \frac{1}{2} n^2 V_0 \tag{4.67}$$

$$\eta = -\mu + n V_0 \quad . \tag{4.68}$$

Taking the $N/\mathcal{V}$ limit, we have the following thermodynamic expressions

$$n = \lambda_T^{-3} F_{3/2}(\alpha') \tag{4.69a}$$

$$u = \frac{3}{2} k_B T \lambda_T^{-3} F_{5/2}(\alpha') + \frac{1}{2} n^2 V_0 \tag{4.69b}$$

$$P = k_B T \lambda_T^{-3} F_{5/2}(\alpha') + \frac{1}{2} n^2 V_0 \quad , \tag{4.69c}$$

where

$$\alpha' = \beta\eta \geqslant 0 \quad . \tag{4.70}$$

We note the importance of the interaction term (4.67), for the entire effect of the interaction is wrapped up here.

Now we go below. We have

$$\Phi[G_1, G_{1/2}^{+}] = \frac{i}{4}\int_0^{-i\beta} d1\, d2\, G(11)\, V(12)\, G(22) \tag{4.71}$$

$$\Sigma^{tot}(11') = \frac{i}{2}\,\delta(11')\int_0^{-i\beta} d2\; V(12)\,G(22)$$

$$= \delta(11')\, n V_0 \qquad (4.72)$$

$$\Sigma_{1/2}(1) = \frac{1}{\sqrt{-i}}\,\frac{i}{2}\,G_{1/2}(1)\int_0^{-i\beta} d2\; V(12)\,G(22)$$

$$= \sqrt{n_0}\;\; n V_0 \begin{pmatrix} 1 \\ 1 \end{pmatrix} \qquad (4.73)$$

$$S_{1/2}(1) = 0 \quad . \qquad (4.74)$$

Eq. (4.74) tells us that the spectrum is gapless. In fact, from eq. (4.72) we have

$$\Sigma^0(p) = \begin{pmatrix} nV_0 & 0 \\ 0 & nV_0 \end{pmatrix} \qquad (4.75)$$

and eq. (4.73) gives

$$\mu = nV_0 \qquad (4.76a)$$

$$\eta = -\mu + n'V_0 = -n_0V_0 \quad ; \qquad (4.76b)$$

so that

$$\mathcal{E}_p = \epsilon_p^0 \quad . \tag{4.77}$$

The Massieu potential is

$$W = \frac{1}{2} n^2 V_0 \beta \mathcal{V} - \sum_p \ln\left(1 - e^{-\beta \epsilon_p^0}\right) . \tag{4.78}$$

Taking the $N/\mathcal{V}$ limit, we have the thermodynamic expressions

$$n = n_0 + \lambda_T^{-3} \zeta(\tfrac{3}{2}) \tag{4.79a}$$

$$u = \frac{3}{2} k_B T \lambda_T^{-3} \zeta(\tfrac{5}{2}) + \frac{1}{2} n^2 V_0 \tag{4.79b}$$

$$P = k_B T \lambda_T^{-3} \zeta(\tfrac{5}{2}) + \frac{1}{2} n^2 V_0 \quad . \tag{4.79c}$$

If we calculate the chemical potential $\mu(T,P)$ at constant P for linear deviations, $\Delta T = T - T_0$, from $T_0(P)$ defined by setting $\eta = 0$ in eq. (4.69c) or (4.79c), i.e.

$$P = k_B T \lambda_{T_0}^{-3} \zeta(\tfrac{5}{2}) + \frac{1}{2} V_0 \lambda_{T_0}^{-6} \zeta^2(\tfrac{3}{2}) \quad , \tag{4.80}$$

we find that the first-order transition of the ideal gas is absent.

To demonstrate this assertion, we note that above the transition we have

$$\mu = V_0 \lambda_T^{-3} \zeta\left(\tfrac{3}{2}\right) + V_0 \Gamma\left(-\tfrac{1}{2}\right) \lambda_T^{-3} \sqrt{\beta\eta} + \cdots \tag{4.81a}$$

$$\begin{aligned} P = {} & k_B T \lambda_T^{-3} \zeta\left(\tfrac{5}{2}\right) + \tfrac{1}{2} V_0 \lambda_T^{-6} \zeta^2\left(\tfrac{3}{2}\right) + \\ & + V_0 \zeta\left(\tfrac{3}{2}\right) \Gamma\left(-\tfrac{1}{2}\right) \lambda_T^{-6} \sqrt{\beta\eta} + \cdots \quad , \end{aligned} \tag{4.81b}$$

which yields upon the elimination of η for P fixed by eq. (4.80)

$$\mu(T>T_0) = V_0 \lambda_{T_0}^{-3} \zeta\left(\tfrac{3}{2}\right) - \frac{5}{2} \frac{\zeta(5/2)}{\zeta(3/2)} k_B T_0 \left(\frac{\Delta T}{T_0}\right) + \cdots \quad . \tag{4.82}$$

Below the transition, we have

$$\mu = V_0 \lambda_T^{-3} \zeta\left(\tfrac{3}{2}\right) - \eta \tag{4.83a}$$

$$\begin{aligned} P = {} & k_B T \lambda_T^{-3} \zeta\left(\tfrac{5}{2}\right) + \tfrac{1}{2} V_0 \lambda_T^{-6} \zeta^2\left(\tfrac{3}{2}\right) - \\ & - \eta \lambda_T^{-3} \zeta\left(\tfrac{3}{2}\right) + \tfrac{1}{2} \eta^2 V_0 \quad , \end{aligned} \tag{4.83b}$$

which gives

$$\mu(T<T_0) = V_0 \lambda_{T_0}^{-3} \zeta\left(\tfrac{3}{2}\right) - \frac{5}{2} \frac{\zeta(5/2)}{\zeta(3/2)} k_B T_0 \left(\frac{\Delta T}{T_0}\right) + \cdots \qquad (4.84)$$

Eqs. (4.83)(4.84) demonstrate that the first-order transition is absent. In its place, we have a third-order transition.

To demonstrate the third-order transition, we calculate the specific heats explicitly. The enthalpy per particle above is

$$\frac{h}{n} = V_0 \lambda_T^{-3} F_{3/2}(\alpha') + \frac{5}{2} k_B T \frac{F_{5/2}(\alpha')}{F_{3/2}(\alpha')} , \qquad (4.85)$$

and

$$\begin{aligned} \frac{c_p}{n k_B} &= \frac{1}{k_B} \left(\frac{\partial}{\partial T} \frac{h}{n}\right)_p \\ &= \frac{3}{2} V_T F_{3/2} + \frac{5}{2} \frac{F_{5/2}}{F_{3/2}} + \\ &\quad + T\left(\frac{\partial \alpha'}{\partial T}\right)_p \left[\frac{5}{2}\left(\frac{F_{5/2} F_{1/2}}{F_{3/2}^2} - 1\right) - V_T F_{1/2}\right] \end{aligned} \qquad (4.86)$$

with

$$T\left(\frac{\partial \alpha'}{\partial T}\right)_p = \frac{\frac{5}{2} F_{5/2} + \frac{3}{2} V_T F_{3/2}^2}{F_{3/2} + V_T F_{3/2} F_{1/2}} \qquad (4.87)$$

where

$$V_T \equiv \frac{V_0}{\lambda_T^3 k_B T} . \tag{4.88}$$

Therefore, substituting eq. (4.87) into (4.86), we get

$$\frac{c_p(T>T_0)}{n k_B} = \frac{1}{1+V_T F_{1/2}} \left[\frac{25}{4} \frac{F_{5/2}^2 F_{1/2}}{F_{3/2}^3} - \frac{15}{4} \frac{F_{5/2}}{F_{3/2}} + \right.$$

$$\left. + \frac{15}{4} V_T \frac{F_{5/2} F_{1/2}}{F_{3/2}} - \frac{9}{4} V_T F_{3/2} \right] . \tag{4.89}$$

Below we have

$$\frac{h}{n} = n V_0 + \frac{5}{2} \frac{k_B T}{n \lambda_T^3} \zeta\left(\frac{5}{2}\right) \tag{4.90}$$

and

$$\frac{c_p(T<T_0)}{n k_B} = \frac{15}{4} \frac{\zeta(5/2)}{n \lambda_T^3} + \frac{25}{4} \frac{\zeta^2(5/2)}{V_T (n \lambda_T^3)^3} . \tag{4.91}$$

From eqs. (4.89)(4.91), we see that as $\eta \to 0$ we have

$$c_p(T_0+) = c_p(T_0-)$$

$$= n k_B \left[\frac{25}{4} \frac{\zeta^2(5/2)}{V_T \zeta^3(3/2)} + \frac{15}{4} \frac{\zeta(5/2)}{\zeta(3/2)} \right] . \tag{4.92}$$

Note that c_p is defined on both sides of $T_o(P)$ and is finite at T_o. If we substitute into eq. (4.92) $V_{T_o} = 0.73$ (the appropriate number for helium at T_λ), we get

$$c_p(T_0) = 3.1\ nk_B$$

which is comparable to the classical limit of $2.5\ nk_B$. In mass units, we have

$$c_p(T_0) = 1.5\ \frac{\text{cal}}{\text{gm}\ {}^\circ\text{K}} = 6.4\ \frac{\text{joule}}{\text{gm}\ {}^\circ\text{K}} ,$$

which is the value of $c_{sat}(T)$ for helium at about $|T - T_\lambda| = 0.1^\circ K$.

To finish our demonstration that Hartree gives a third-order transition, we need to show that the slope of $c_p(T)$ is discontinuous at T_o. This can be done explicitly by differentiating eqs. (4.89) (4.91). Instead, we note that c_p satisfies the following relation

$$c_p = c_v - \frac{T}{v} \frac{(\partial P/\partial T)_v^2}{(\partial P/\partial v)_T} . \tag{4.93}$$

From the form of the energy equations (4.49b)(4.59b), we see that

$$c_v = c_{v,\text{ideal}}$$

and from eqs. (4.69c)(4.79c), we can write eq. (4.93) as

$$\begin{aligned} c_p = {} & c_{v,\text{ideal}} - \\ & - \frac{T}{v}\left[\left(\frac{\partial P}{\partial v}\right)_{T,\text{ideal}} - n^2 V_0 v^{-1}\right]^{-1} \left(\frac{\partial P}{\partial T}\right)^2_{v,\text{ideal}} \end{aligned} \tag{4.94}$$

Since $c_{\upsilon,\text{ideal}}$ has a discontinuity in slope and $(\partial P/\partial T)^2_{\upsilon,\text{ideal}}$ and $(\partial P/\partial \upsilon)_{T,\text{ideal}}$ do not, we conclude that c_p has a discontinuity in its slope. Also eq. (4.74) shows how the interaction term quenches the divergence in the ideal Bose gas at T_0.

London[2] in his smooth potential model for a Bose-Einstein liquid arrived at a Hartree approximation by an intuitive approach attempting to take into account the volume characteristics of a liquid. The mathematics of his model is identical to the Hartree approximation, thus leading to the same results.

D. Bogoliubov/Hartree Approximation

Below the transition, we consider the following self-energy matrix

$$\Sigma^0(p) = \begin{pmatrix} nV_0 + n_0V_p & n_0V_p \\ n_0V_p & nV_0 + n_0V_p \end{pmatrix} \tag{4.95}$$

which is just the Bogoliubov self-energy, eq. (4.32), plus the analytic continuation of the Hartree self-energy. The chemical potential is

$$\mu = \mu_B + \mu_H = n_0V_0 + n'V_0 = nV_0 \tag{4.96}$$

$$\eta = -\mu + n'V_0 = -n_0V_0 \quad . \tag{4.97}$$

We see that μ satisfies the Hugenholtz-Pines form so that the energy spectrum is gapless. In fact

$$\varepsilon_p = \sqrt{\epsilon_p^0(\epsilon_p^0 + 2n_0V_p)} \tag{4.98}$$

with

$$\tilde{\varepsilon}(p) = \epsilon_p^0 + n_0 V_p \tag{4.99a}$$

$$F(p) = n_0 V_p \tag{4.99b}$$

$$\tilde{\varepsilon}^0(p) = \epsilon_p^0 - n V_0 \quad . \tag{4.99c}$$

Note that the energy spectrum remains that of Bogoliubov and hence leads to the double-value behavior of $n_0(T)$. The basic difference between Bogoliubov/Ideal and Bogoliubov/Hartree is in the chemical potential, eqs. (4.96)(4.97), which affects the thermodynamics through the interaction term $\frac{1}{2}n^2 V_0$.

The effect of the interaction term $\frac{1}{2}n^2 V_0$ is not trivial near the transition. We note that

$$n^2 = \lambda_T^{-6}\,\zeta^2\!\left(\tfrac{3}{2}\right)\left[1 - \frac{2\sqrt{2\pi}}{\zeta(3/2)}\sqrt{\alpha} + O(\alpha)\right] \tag{4.100a}$$

where

$$\alpha \equiv -\beta\eta = \beta n_0 V_0 \geq 0 \qquad ; \tag{4.100b}$$

and the thermodynamic quantities, eq. (4.29), are ill-defined for small values of $\alpha > 0$ and $\Delta T \equiv T - T_0 < 0$. This demonstrates the subtle nature of the transition and the need for careful analysis in creating approximations for the transition.

Above the transition, of course, everything is well-defined as we have just the Hartree approximation.

One can generalize the above equations to include the Hartree-Fock term above the transition but only as an additive constant term to the Hartree one, i.e., we take $V_p \simeq V_0$ and write

$$\Sigma^0(p) = \begin{pmatrix} 2nV_0 & n_0V_0 \\ n_0V_0 & 2nV_0 \end{pmatrix} \tag{4.101}$$

$$\begin{cases} \mu = n_0V_0 + 2n'V_0 = 2nV_0 - n_0V_0 \\ \eta = -\mu + 2n'V_0 = -n_0V_0 \end{cases} \tag{4.102}$$

$$\begin{cases} \mathcal{E}(p) = \sqrt{\epsilon_p^0(\epsilon_p^0 + 2n_0V_0)} \\ \tilde{\mathcal{E}}(p) = \epsilon_p^0 + n_0V_0 \\ F(p) = n_0V_0 \end{cases} \tag{4.103}$$

The system defined by eqs. (4.101-103) is just the system studied perturbatively by Lee and Yang[79,80] who replaced V_0 by the Fermi pseudopotential, and more recently by Popov[81] who replaced V_0 by the t-matrix. Because the analysis was perturbative, neither Lee and Yang nor Popov had problems with double-valued functions near the transition. One should note that the effect of the interaction term above the transition was ignored by Popov, who found that the thermodynamics above was exactly that of the ideal gas, not like the Hartree with a third-order transition and specifically a finite c_p.

As a crude approximation to eq. (4.101), one can neglect the off-diagonal terms as they are small near the transition. This leads to the theory of Huang, Yang, and Luttinger[82]

$$\Sigma^{o}(p) = \begin{pmatrix} 2nV_0 & 0 \\ 0 & 2nV_0 \end{pmatrix} \qquad (4.104)$$

$$\begin{cases} \mu = 2nV_0 - n_0 V_0 \\ \eta = -n_0 V_0 \end{cases} \qquad (4.105)$$

$$\begin{cases} \mathcal{E}(p) = \tilde{\mathcal{E}}(p) = \epsilon_p^{o} + n_0 V_0 \\ F(p) = 0 \end{cases} , \qquad (4.106)$$

which is not the Hartree approximation, eqs. (4.75-77), off by a factor of 2 because of the fundamental difference in the chemical potential. Recently Luban and Grobman[78] arrived at the same theory although starting from the Hartree-Fock approximation. Eq. (4.106) leads to the following equation for the number density

$$n - n_0 = \lambda_T^{-3} F_{3/2}(\beta n_0 V_0) \qquad (4.107)$$

which leads to the same double-value behavior as from the Bogoliubov case, eq. (4.35). The pressure is given by eq. (4.29d)

$$P = k_B T \lambda_T^{-3} F_{3/2}(\beta n_0 V_0) + n^2 V_0 - \tfrac{1}{2} n_0^2 V_0 . \qquad (4.108)$$

Eqs. (4.107)(4.108) duplicate eqs. (39) of HYL.[82] Working at constant temperature, HYL argue that the double-valued functions (actually triple-valued including the function above T_0) should be regularized by the Maxwell construction, yielding a "first-order transition." One can apply the same treatment to the more general Bogoliubov/Hartree approximation.

E. Hartree-Fock Approximation

The Hartree-Fock approximation is the first-order conserving approximation in which the exchange term as well as the direct term have been taken into account. The Hartree-Fock approximation was first studied at $T = 0$ by Girardeau and Arnowitt,[83] who found an energy gap in the energy spectrum. Prior to this calculation, the Hartree-Fock at nonzero temperatures was studied by several others,[84,85] but no energy gap was found because of the several approximations used. Tolmachev[86] examined the Hartree-Fock equations at nonzero temperatures in greater detail and reported an energy gap. The Hartree-Fock equations were solved iteratively by Luban[87] who found an energy gap in the second iteration.

We first consider the Hartree-Fock above the transition and investigate the question of a shift in the transition temperature. We next go below the transition and show that there is an energy gap when the Hartree-Fock equation is solved self-consistently, thus justifying the iterative solution.

As Hohenberg[34] has emphasized, the existence of the energy gap in itself is not an unphysical result, since there is no a priori reason that the excitations of $\tilde{G}_1$ should be of the sound-wave type. However the thermodynamics, for the iterative solution, does exhibit near the transition the double-value behavior of the other approximations.

1. Above the Transition

Let us begin with a brief resume of the microscopic theory. We have

$$\Phi[G_1] = \frac{i}{2}\int_0^{-i\beta} d1\,d2\,V(12)\left[G(11)\,G(22) + G(12)\,G(21)\right] \qquad (4.109)$$

$$\Sigma^{tot}(11') = i\,\delta(11')\int_0^{-i\beta} d2\,V(12)\,G(22) + i\,V(11')\,G(11') . \qquad (4.110)$$

Therefore

$$\Sigma^{o}(p) = nV_0 + \frac{1}{\mathcal{V}}\sum_{q} V(p-q)\,f(\tilde{\epsilon}_q) \qquad (4.111)$$

where

$$\tilde{\epsilon}(q) \equiv \epsilon(q) - \mu = \epsilon^{o}_{q} + \Sigma^{o}(q) - \mu \qquad (4.112)$$

satisfies the integral equation

$$\tilde{\epsilon}(p) = \epsilon^{o}_{p} + nV_0 - \mu + \frac{1}{\mathcal{V}}\sum_{q} V(p-q)\,f(\tilde{\epsilon}_q) . \qquad (4.113)$$

The transition is given by the vanishing of

$$\eta \equiv -\mu + \Sigma^{o}(0) = -\mu + nV_0 + \frac{1}{\mathcal{V}}\sum_{q} V(q)\,f(\tilde{\epsilon}_q) \qquad (4.114)$$

and the thermodynamics by the Massieu potential

$$\begin{aligned} W = {} & \sum_{p} \ln\left(1 + f(\tilde{\epsilon}_p)\right) + \frac{1}{2}n^2 V_0 \beta \mathcal{V} + \\ & + \frac{1}{2}\beta\,\frac{1}{\mathcal{V}}\sum_{p,q} V(p-q)\,f(\tilde{\epsilon}_p)\,f(\tilde{\epsilon}_q) . \end{aligned} \qquad (4.115)$$

For a very short-range potential, $V_p = V_o$, we see that we get the Hartree approximation, eqs. (4.63-70), with $V_o \longrightarrow 2V_o$. Hence the specific heats are finite. We also note that in the limit of very short-range potential, the transition temperature T_o is not shifted from that of the ideal Bose gas. GKW[75] (in their Appendix B) found in the short-range limit a temperature shift, which is entirely spurious and is due to their use of free-particle statistical factors rather than self-consistent statistical factors. We present a very pedestrian treatment of the above idea in Appendix D.

To obtain a shift in the transition temperature, one has to include the momentum dependence of V_p. The easiest procedure is to expand V_p

$$V_p = V_0 + V_1 \frac{\lambda_T^2}{\hbar^2} p^2 + \cdots \qquad , \qquad (4.116)$$

so that eq. (4.111) can be written

$$\Sigma^0(p) = \Sigma^0(0) + n V_1 \left(\lambda_T^2 \hbar^{-2} p^2 \right) \qquad (4.117a)$$

where

$$\Sigma^0(0) = 2n V_0 + V_1 \lambda_T^2 \hbar^{-2} \frac{1}{v} \sum_q q^2 f(\tilde{\epsilon}_q) \qquad ; \qquad (4.117b)$$

and eq. (4.112) can be written

$$\tilde{\epsilon}(p) = \frac{p^2}{2m^*} + \eta \qquad (4.118)$$

where the effective mass m^* is defined

$$\frac{1}{m^*} = \frac{1}{m} + 2nV_1 \lambda_T^2 \hbar^{-2} \quad . \tag{4.119}$$

As the spectrum (4.118) is just the free-particle spectrum, we get immediately the shift in the transition temperature from that for the ideal Bose gas

$$\frac{\Delta T_0}{T_0^i} = 4\pi \, \frac{nV_1}{k_B T_0^i} \tag{4.120a}$$

$$= -\frac{8\pi^2}{3} \frac{n}{\lambda_{T_0^i}^2 \, k_B T_0^i} \int_0^\infty V(r) r^4 dr \quad , \tag{4.120b}$$

since from (4.116) and the definition of V_p

$$V_1 = -\frac{2\pi}{3\lambda_T^2} \int_0^\infty V(r) r^4 dr \quad . \tag{4.120c}$$

and we defined $\Delta T_0 \equiv T_0 - T_0^{\,i}$, where $T_0^{\,i}$ is the transition temperature for the ideal Bose gas. Note that the shift depends on the weighted radial integral of the potential. For helium, the cutoff for $V(r)$ at small r is not well-known and plays an important role in ascertaining ΔT_0 .

To develop the theory further, let us take into account the strength of the interaction and replace the potential (direct and exchange) in eq. (4.111) by the two-body scattering matrix $\langle pq | T | pq \rangle$ so that

$$\Sigma^{o}(p) = \frac{1}{v} \sum_{q} \langle pq | T | pq \rangle f(\varepsilon_q) \quad , \tag{4.121}$$

where T satisfies the operator equation T = V + VGGT. We approximate the general T-matrix by the "free" reaction matrix[88] for a nondegenerate Bose gas

$$\langle pq | T | pq \rangle = -\frac{8\pi\hbar^2}{m} \frac{2\hbar}{|p-q|} \times \sum_{\substack{\ell \\ \text{even}}} (2\ell+1)\, \delta_\ell \left(\frac{1}{2\hbar} |p-q| \right) \tag{4.122}$$

where δ_ℓ is the phase shift of a wave of angular momentum ℓ. We define a "total" phase shift $\Delta(k)$ where k is the wave number ($p = \hbar k$)

$$\Delta(k) \equiv \sum_{\substack{\ell \\ \text{even}}} (2\ell+1)\, \delta_\ell(k) \tag{4.123a}$$

and expand it about small k's.

$$\Delta(k) = \sum_{n=0}^{\infty} a_n \lambda_T^n k^n \tag{4.123b}$$

We restrict ourselves to the case where $a_0 = 0$, or $\delta(0) = 0$ which prevents the occurence of a real or virtual bound state. When $\delta(0) \neq 0$, we see that $\Sigma^{o}(p)$ diverges at $p = 0$. There are indications that a virtual bound state exists for two helium atoms,[89] as the $\ell = 0$ phase shift approaches $\pi/2$ as $p \longrightarrow 0$.

However the effect of statistics, which as been neglected except to select even ℓ's between the two particles in evaluating eq. (4.122), would probably remove this virtual bound state. Thus we have, substituting eqs. (4.122)(4.123) into (4.121),

$$\Sigma^0(p) = -\frac{4k_BT\lambda_T^3}{v}\sum_{s=1}^{\infty} a_s\left(\frac{\lambda_T}{2\hbar}\right)^{s-1}\sum_q |p-q|^{s-1} f(\tilde{\epsilon}_q) \quad (4.124)$$

Since $\Sigma^0(p) = +\Sigma^0(-p)$, we expand $\Sigma^0(p)$ about small p

$$\Sigma^0(p) = k_BT\sum_{r=0}^{\infty} c_r\left(\frac{\lambda_T}{\hbar}p\right)^{2r} \quad (4.125a)$$

where

$$c_r = \frac{1}{(2r)!}\left(\frac{\hbar}{\lambda_T}\right)^{2r}\left[\nabla_p^{2r}\Sigma^0(p)\right]_{p=0}\cdot\frac{1}{k_BT} \quad (4.125b)$$

In particular, we see that

$$c_0 = -\frac{4\lambda_T^3}{v}\sum_{s=1}^{\infty} a_s\left(\frac{\lambda_T}{2\hbar}\right)^{s-1}\sum_q q^{s-1} f(\tilde{\epsilon}_q) \quad (4.126)$$

and

$$c_1 = -\frac{\lambda_T^3}{v}\sum_{s=1}^{\infty}\frac{s(s+1)}{2}a_{s+2}\left(\frac{\lambda_T}{2\hbar}\right)^{s-1}\sum_q q^{s-1} f(\tilde{\epsilon}_q) \quad (4.127)$$

Using the same argument that led to eq. (4.120), we see that to first-order

$$\frac{\Delta T_0}{T_0^i} = 4\pi\, c_1(T_0^i) \tag{4.128}$$

and to the same order, $c_1(T)$ is given by in the $N/\mathcal{V}$ limit

$$c_1(T) = -\frac{1}{\pi^2}\sum_{s=1}^{\infty} s(s+1)\, a_{s+2}\left(\frac{\pi m^*}{m}\right)^{\frac{s}{2}+1} \times \Gamma\left(\frac{s}{2}+1\right) F_{\frac{s}{2}+1}(\beta\eta) \tag{4.129}$$

where m^* is given by

$$\frac{m}{m^*} = 1 + 4\pi c_1 \tag{4.130a}$$

and η by

$$\beta\eta = -\beta\mu + c_0 \quad . \tag{4.130b}$$

Eqs. (4.128)(4.129)(4.130) gives in principle the shift in T_0 once the phase shifts for two particles are known. To see how this works, let us consider a weakly interacting gas such that the phase shifts may be calculated by the Born approximation, i.e.

$$\tan\delta_\ell \simeq \delta_\ell(k) = -\frac{\pi m}{2\hbar^2}\int_0^{\infty} V(r)\, J^2_{\ell+1/2}(kr)\, r\,dr \quad , \tag{4.131}$$

where $J_{\ell+\frac{1}{2}}$ is the Bessel function. One can easily show that the "total" phase shift is

$$\Delta(k) = -\frac{m}{2\hbar^2} k \int_0^\infty V(r)\, r^2 dr - \qquad\qquad \\ -\frac{m}{4\hbar^2}\int_0^\infty V(r) \sin(2kr)\, r\, dr \quad . \qquad (4.132)$$

Expanding the sine function, we find the following a_n's upon comparison with eq. (4.123b)

$$\begin{cases} a_1 = -2\pi\beta\lambda_T^{-3}\int_0^\infty V(r)\, r^2 dr \\ a_{2n} = 0 \\ a_{2n+1} = (-1)^{n+1}\beta\lambda_T^{-3-2n}\dfrac{\pi 2^{2n}}{(2n+1)!}\int_0^\infty V(r)\, r^{2+2n} dr \end{cases} \qquad (4.133)$$

where n = 1,2,3, ... Taking just the first term of eq. (4.129), we see that

$$c_1 = -\frac{2\pi}{3}\frac{\beta}{\lambda_T^2} n \int_0^\infty V(r)\, r^4 dr \quad ; \qquad (4.134)$$

and ΔT_0, eq. (4.128), becomes identical to eq. (4.120). Hence in the Born approximation, we recover our previous analysis in terms of the potential directly. Note the feature that all even a_n's vanishes, which in the Born approximation can be traced directly to the fact that the "total" phase shift Δ is just k times the sum of the forward and backward amplitude $f(\theta)$ which are even in k. The utility of this reaction matrix approach is that it allows us to go beyond the Born approximation.

For example, a hard core of radius r_0 has phase shifts which satisfies

$$\tan\delta_\ell(k) = \frac{j_\ell(kr_0)}{n_\ell(kr_0)} , \tag{4.135}$$

where j_ℓ and n_ℓ are spherical Bessel functions with the following expansions

$$j_\ell(\rho) = 2^\ell \rho^\ell \sum_{m=0}^{\infty} \frac{(-1)^m(\ell+m)!}{m!\,(2\ell+2m+1)!}\,\rho^{2m}$$

$$n_\ell(\rho) = -2^{-\ell}\rho^{-(2\ell+1)} \sum_{m=0}^{\infty} \frac{(2\ell-2m)!}{m!\,(\ell-m)!}\,\rho^{2m} .$$

Expanding the phase shifts for small kr_0, we find that the "total" phase shift is given by

$$\Delta(k) = -r_0 k - \frac{1}{9}(r_0 k)^5 - \cdots .$$

Note again that all even a_n's vanishes; moreover $a_3 = 0$. Therefore taking the first nonvanishing term in eq. (4.129), we find that

$$\frac{\Delta T_0}{T_0^i} = 4\pi^2 \frac{\zeta(5/2)}{\zeta(3/2)} \frac{n r_0^5}{\lambda_{T_0^i}^2} . \tag{4.136}$$

We note that the shift is upwards in the case of only hard cores and that the shift appears in the a_5 expansion coefficient of the "total" phase shift.

For our second example, let us consider the case of a hard core potential with an additional weak potential outside of the hard core. We assume that the weak potential's phase shift are well approximated by the Born approximation. The hard core can then be separated out of the problem by including its effect entirely within the boundary conditions for the wavefunction. The resulting problem with the weak potential with hard core boundary conditions, we solve in the Born approximation. We find that the phase shifts are given by

$$\begin{aligned} \sin\left(\delta_\ell - \delta_\ell^{HC}\right) = -\frac{m}{\hbar^2}\left[\cos\left(\arctan \frac{j_\ell(kr_0)}{n_\ell(kr_0)}\right)\right] \times \\ \times \Bigg[\int_{r_0}^{\infty} j_\ell(kr)\, V^{WP}(r)\, u_\ell(kr)\, r\, dr + \\ + \frac{j_\ell(kr_0)}{n_\ell(kr_0)} \int_{r_0}^{\infty} n_\ell(kr)\, V^{WP}(r)\, u_\ell(r)\, r\, dr\Bigg], \end{aligned} \tag{4.137}$$

where r_0 is the radius of the hard core, the superscripts HC and WP refer to the hard core and weak potential respectively, and $u_\ell(r)$ is the exact radial wavefunction. Since $V^{WP}(r)$ is so weak, we approximate $u_\ell(r)$ by

$$u_\ell \approx \bar{u}_\ell(r) = kr\left[j_\ell(kr)\, n_\ell(kr_0) - j_\ell(kr_0)\, n_\ell(kr)\right], \tag{4.138}$$

so that eq. (4.137) can be written

$$\delta_\ell^{WP}(k) \equiv \delta_\ell(k) - \delta_\ell^{HC}(k)$$

$$= -\frac{m}{\hbar^2} k \left[\cos\left(\arctan \frac{j_\ell(kr_0)}{n_\ell(kr_0)} \right) \right]^2 \times$$

$$\times \left[\int_{r_0}^{\infty} j_\ell^2(kr) V^{WP}(r) r^2 dr + 2 \frac{j_\ell(kr_0)}{n_\ell(kr_0)} \int_{r_0}^{\infty} j_\ell(kr) n_\ell(kr) V^{WP}(r) r^2 dr \right. \tag{4.139}$$

$$\left. + \left(\frac{j_\ell(kr_0)}{n_\ell(kr_0)} \right)^2 \int_{r_0}^{\infty} n_\ell^2(kr) V^{WP}(r) r^2 dr \right] .$$

One can verify that as $r_0 \longrightarrow 0$, we recover eq. (4.131), recalling the definition of the spherical Bessel function

$$j_\ell(x) \equiv \sqrt{\frac{\pi}{2x}}\; J_{\ell+1/2}(x) \; .$$

Since the phase shifts separate into $\delta_\ell = \delta_\ell^{HC} + \delta_\ell^{WP}$, we can likewise write $a_3 = a_3^{HC} + a_3^{WP}$. But we know that $a_3^{HC} = 0$. Hence to the first approximation, the effect of the hard core is implicit, acting through δ_ℓ^{WP}. To calculate the "total" phase shift, we expand for small r_0 to get

$$\Delta^{WP}(k) = -2\pi\beta\lambda_T^{-2} \left[\frac{1}{2} k \int_{r_0}^{\infty} V^{WP}(r) r^3 dr + \right.$$

$$+ \frac{1}{4} \int_{r_0}^{\infty} V^{WP}(r) \sin(2kr)\, r\, dr + \tag{4.140}$$

$$+ r_0 \int_{r_0}^{\infty} V^{WP}(r) \sin(2kr)\, dr +$$

$$\left. + k r_0^2 \int_{r_0}^{\infty} V^{WP}(r) \cos(2kr)\, dr \right]$$

and

$$a_3^{WP} = \frac{2\pi}{3}\beta\lambda_T^{-5}\left[\int_{r_0}^{\infty} V^{WP}(r)\, r^4 dr + \right.$$
$$\left. + 4r_0\int_{r_0}^{\infty} V^{WP}(r)\, r^3 dr + 6r_0^2\int_{r_0}^{\infty} V^{WP}(r)\, r^2 dr\right] . \tag{4.141}$$

Combining eqs. (4.128)(4.129)(4.141), we see

$$\frac{\Delta T_0}{T_0^i} = -\frac{8\pi^2}{3} n\, \lambda_{T_0^i}^{-2}\, \frac{1}{k_B T_0^i}\left[\int_{r_0}^{\infty} V^{WP}(r)\, r^4 dr + \right.$$
$$\left. + 4r_0\int_{r_0}^{\infty} V^{WP}(r)\, r^3 dr + 6r_0^2\int_{r_0}^{\infty} V^{WP}(r)\, r^2 dr\right] . \tag{4.142}$$

Therefore if the weak potential is of one sign, the effect of the hard core is to enhance the shift due to the weak potential alone, i.e. eq. (4.120).

For our third and last example, we consider the problem of a soft core, which we approximate by the square repulsive potential. We assume a potential given by

$$U(r) = \frac{m}{\hbar^2} V(r) = \begin{cases} \gamma^2 & r < R \\ 0 & r > R \end{cases} . \tag{4.143}$$

The s-wave phase shift satisfies the equation

$$k\cot\delta_0 = \frac{k\tan(kR)\tanh\left(R\sqrt{\gamma^2-k^2}\right) + \sqrt{\gamma^2-k^2}}{\tanh\left(R\sqrt{\gamma^2-k^2}\right) - \frac{1}{k}\sqrt{\gamma^2-k^2}\,\tan(kR)} , \tag{4.144}$$

which can be expanded for small k's as

$$k\cot\delta_0 = -\frac{1}{a} + \frac{1}{2}r_0 k^2 + O(k^4) \tag{4.145}$$

with

$$a = R\left(1 - \frac{\tanh(\gamma R)}{\gamma R}\right) \equiv R Z \tag{4.146a}$$

and

$$r_0 = R\left(1 + \frac{1}{Z}(\gamma R)^{-2} + \frac{1}{3}\frac{1}{Z^2}\right) . \tag{4.146b}$$

For small k's, i.e. $kR \ll \ell$, we have that the phase shift $\delta_\ell(k) \sim k^{2\ell+1}$. Therefore, for the a_3 expansion coefficient of the "total" phase shift, we need only the s-wave phase shift. Expanding eq. (4.145), we find

$$\begin{aligned} a_3 &= \lambda_T^{-3}\left[\frac{1}{3}a^3 - \frac{1}{2}a^2 r_0\right] \\ &= \frac{1}{6}R\lambda_T^{-3}\left[1 + 2Z^3 - 3Z^2 - 3Z(\gamma R)^{-2}\right] . \end{aligned} \tag{4.147}$$

Combining (4.128)(4.129)(4.147), we see that

$$\frac{\Delta T_0}{T_0^i} = -\frac{2\pi}{3}nR^3\left[1 + 2Z^3 - 3Z^2 - 3Z(\gamma R)^{-2}\right] . \tag{4.148}$$

Finally, we take note of the work of Brout[90] on the nature of the transition based on the Hartree-Fock approximation above the λ-transition. Brout uses the same type of expansion as GKW, viz. in terms of the free statistical factors, to show a change in the order of the transition. We have pointed out that the shift in the transition temperature must be calculated using self-consistent statistical factor, since the *sin qua non* of the transition is the statistics. Likewise, consistent thermodynamics is generated only by conserving approximation which implies self-consistent statistical factors. In particular, for a very short-range potential, Brout's demonstration fails, while the Hartree-Fock exhibits a third-order transition if only diagonal elements of the self-energy are retained below (a Hartree-like approximation). This brings us to the final comment that the nature of the transition is amenable to discussion only as the approximations above and below are well-defined.

2. Below the Transition

The Hartree-Fock approximation may be represented below the transition by the functionals

$$\begin{aligned}\Phi[G_1, G^+_{1/2}] = {} & \frac{i}{4}\int_0^{-i\beta} G(11)V(12)G(22)\,d1\,d2 \; + \\ & + \frac{i}{2}\int_0^{-i\beta} d1\,d2\; G(12)V(12)G(21) \; - \\ & - \frac{i}{2}\int_0^{-i\beta} d1\,d2\; G_{1/2}(1)G^+_{1/2}(2)V(12)G_{1/2}(2)G^+_{1/2}(1)\end{aligned} \qquad (4.149)$$

$$\begin{aligned}\Sigma^{tot}(11') = {} & \frac{i}{2}\delta(11')\int_0^{-i\beta} d2\, V(12)G(22) \; + \\ & + i\,V(11')\,G(11')\end{aligned} \qquad (4.150)$$

$$\begin{aligned} S_{1/2}(1) &= -2i\, G_{1/2}(1) \int_0^{-i\beta} d2\, G_{1/2}^{+}(2)\, V(12)\, G_{1/2}(2) \\ &= -4 n_0 V_0\, G_{1/2}(1) \quad . \end{aligned} \tag{4.151}$$

In momentum space, we write

$$\Sigma^{tot} = \Sigma^{0}(p) = \begin{pmatrix} nV_0 + n_0 V_p + g_{11}(p) & n_0 V_p + g_{12}(p) \\ n_0 V_p + g_{12}(p) & nV_0 + n_0 V_p + g_{11}(p) \end{pmatrix} \tag{4.152}$$

where we defined

$$g_{11}(p) = \frac{1}{\mathcal{V}} \sum_q V(p-q) \int_{-\infty}^{\infty} \frac{d\omega}{2\pi}\, \tilde{A}_{11}(q,\omega)\, f(\omega) \tag{4.153a}$$

$$g_{12}(p) = \frac{1}{\mathcal{V}} \sum_q V(p-q) \int_{-\infty}^{\infty} \frac{d\omega}{2\pi}\, \tilde{A}_{12}(q,\omega)\, f(\omega) \quad . \tag{4.153b}$$

From eqs. (2.103)(2.104), we calculate the chemical potential μ as

$$\mu = nV_0 + g_{11}(0) + g_{12}(0) \tag{4.154a}$$

with

$$\mu_g = -2 n_0 V_0 \quad . \tag{4.154b}$$

The energy parameters are

$$\tilde{\mathcal{E}}(p) = \epsilon_p^0 + n_0 V_p + g_{11}(p) - g_{11}(0) - g_{12}(0) \qquad (4.155a)$$

$$F(p) = n_0 V_p + g_{12}(p) \qquad (4.155b)$$

with an energy spectrum

$$\mathcal{E}(p) = \sqrt{\tilde{\mathcal{E}}(p)^2 - F(p)^2} \qquad (4.156a)$$

which has an energy gap, using eqs. (2.106)(4.154b)(4.155b)

$$\lim_{p\to 0} \mathcal{E}(p) = -4 n_0 V_0\, g_{12}(0)\,. \qquad (4.156b)$$

Using these energy parameters, we rewrite eqs. (4.153) as

$$g_{11}(p) = \frac{1}{\mathcal{V}} \sum_q V(p-q) \left[u_q^2 f(\mathcal{E}_q) + v_q^2 (1 + f(\mathcal{E}_q)) \right] \qquad (4.157a)$$

$$g_{12}(p) = -\frac{1}{\mathcal{V}} \sum_q V(p-q)\, u_q v_q \left[1 + 2 f(\mathcal{E}_q) \right] \qquad (4.157b)$$

where u_p, v_p are defined by (4.6)(4.155). Thus below the transition, we have two integral equations, (4.157ab), for the two parameters g_{11}, g_{12}, instead of the one equation above the transition. This is a reflection of the two external potential introduced below the transition, U^{ext} and η^{ext}, versus U^{ext} above, and the concomitant double and single Legendre transformation, respectively, needed for a conserving approximation.

If we iterate eqs. (4.157) or (4.153) in some fashion rather than solving them consistently, we can reproduce several works in the literature. These iteration schemes will yield a gapless spectrum until the iteration is sufficiently far along to yield a nonzero $g_{12}(0)$ (see eq. (4.126b)).

a. Iteration in V_p

In this scheme, we begin by setting $V_p = 0$ on the right hand side of eqs. (4.153) and iterating. The zeroth iteration yields the ideal gas. The first iteration is obtained by setting the spectral function equal to that of the ideal gas

$$\tilde{A}_{11}^{(1)} = 2\pi\delta(\omega - \epsilon_p^0 + \mu) \quad ; \quad \tilde{A}_{12}^{(1)} = 0$$

to get

$$\begin{cases} g_{11}^{(1)}(p) = \frac{1}{\mathcal{V}} \sum_{q} V(p-q) f(\tilde{\epsilon}_p^0) \\ g_{12}^{(1)}(p) = 0 \end{cases} \tag{4.158}$$

Hence the self-energy matrix is

$$\left[\Sigma^0(p)\right]^{(1)} = \begin{pmatrix} nV_0 + nV_p + g_{11}^{(1)}(p) & n_0 V_p \\ n_0 V_p & nV_0 + nV_p + g_{11}^{(1)}(p) \end{pmatrix} \tag{4.159}$$

with an energy spectrum

$$\mathcal{E}^{(1)}(p) = \sqrt{(\epsilon_p^0 + g_{11}^{(1)}(p) - g_{11}^{(1)}(0) + n_0 V_p)^2 - (n_0 V_p)^2} \tag{4.160}$$

which has no gap. This calculation was first done by Zubarev and Tserkovnikov.[84]

The second iteration is obtained by substituting into eq. (4.153) the spectral function based on $[\Sigma^0(p)]^{(1)}$. Eq. (4.159) yields a nonzero $A_{12}^{(2)}(p,\omega)$; hence $\mathcal{E}^{(2)}(p)$ has an energy gap.

b. Iteration in n_0

In this scheme, we begin by setting $n_0 = 0$ on the right hand side of eqs. (4.157) and iterating. The zeroth iteration, solved self-consistently, yields the analytic continuation below of the Hartree-Fock approximation above the transition:

$$[\Sigma^0(p)]^{(0)} = \begin{pmatrix} nV_0 + g_{11}^{(0)}(p) & 0 \\ 0 & nV_0 + g_{11}^{(0)}(p) \end{pmatrix} \tag{4.161}$$

where

$$g_{11}^{(0)}(p) = \frac{1}{V} \sum_q V(p-q)\, f(\mathcal{E}^{(0)}(q)) \tag{4.162}$$

$$\left\{ \begin{aligned} \mathcal{E}_q^{(0)} &= \tilde{E}^{(0)}(q) = \epsilon_p^0 + nV_0 + g_{11}^{(0)}(p) - \mu^{(0)} \\ F^{(0)}(q) &= 0 \\ \mu^{(0)} &= nV_0 + g_{11}^{(0)}(0) \end{aligned} \right. \tag{4.163}$$

.

The first iteration is obtained by substituting into eqs. (4.153) the spectrum function based on the self-energy (4.161), which yields

$$\left[\Sigma^{0}(p)\right]^{(1)} = \begin{pmatrix} nV_0 + n_0 V_p + g_{11}^{(0)}(p) & n_0 V_p \\ n_0 V_p & nV_0 + n_0 V_p + g_{11}^{(0)}(p) \end{pmatrix} \tag{4.164}$$

and

$$\mathcal{E}^{(1)}(p) = \sqrt{\left[\epsilon_p^0 + g_{11}^{(0)}(p) - g_{11}^{(0)}(0)\right]\left[\epsilon_p^0 + g_{11}^{(0)}(p) - g_{11}^{(0)}(0) + 2n_0 V_p\right]} \tag{4.165}$$

which is gapless.

The second iteration yields

$$\left[\Sigma^{0}(p)\right]^{(2)} = \begin{pmatrix} nV_0 + n_0 V_p + g_{11}^{(1)}(p) & n_0 V_p + g_{12}^{(1)}(p) \\ n_0 V_p + g_{12}^{(1)}(p) & nV_0 + n_0 V_p + g_{11}^{(1)}(p) \end{pmatrix} \tag{4.166}$$

where

$$g_{11}^{(1)}(p) = \frac{1}{2\mathcal{V}} \sum_q V(p-q) \left[\frac{\tilde{E}^{(1)}(q)}{\mathcal{E}^{(1)}(q)} \left[1 + 2f(\mathcal{E}_q^{(1)})\right] - 1 \right] \tag{4.167a}$$

$$g_{12}^{(1)}(p) = -\frac{1}{2\mathcal{V}} \sum_q V(p-q) \frac{F^{(1)}(q)}{\mathcal{E}^{(1)}(q)} \left[1 + 2f(\mathcal{E}_q^{(1)})\right] \tag{4.167b}$$

and the spectrum is

$$\mathcal{E}^{(2)}(p) = \sqrt{[\tilde{E}^{(2)}(p)]^2 - [F^{(2)}(p)]^2} \qquad (4.168a)$$

$$\tilde{E}^{(2)}(p) = \epsilon_p^0 + n_0 V_p + g_{11}^{(1)}(p) - g_{11}^{(1)}(0) - g_{12}^{(1)}(0) \qquad (4.168b)$$

$$F^{2}(p) = n V_p + g_{12}^{(1)}(p) \quad . \qquad (4.168c)$$

This iteration scheme was used by Luban.[87]

Other iteration schemes of the same structure may be concocted as needed. For instance, we can have an iteration in g_{11} and g_{12}, in which we first set $g_{11} = g_{12} = 0$ and obtain the Bogoliubov/Hartree approximation for the zeroth iteration. The first iteration would have an energy gap. Finally if we iterate only in g_{12}, the zeroth iteration is the Bogoliubov/Hartree-Fock approximation which we shall discuss in the next section. The above comments are just concrete examples of the fact that the Hartree-Fock approximation includes all the terms to first order in V, and hence contains all other first-order approximations.

In discussing the thermodynamics of the Hartree-Fock approximation, we follow Luban in his iterated solution for g_{11} and g_{12} and point out a trivial sign difference[91] which leads to double-valued functions. In particular, let us consider the number density, eq. (4.29a), which can be written

$$n = n_0 + \frac{1}{V}\sum_{p} \frac{\tilde{\mathcal{E}}(p)}{\mathcal{E}(p)} f(\varepsilon_p) + \frac{1}{2V}\sum_{p}\left[\frac{\tilde{\mathcal{E}}(p)}{\mathcal{E}(p)} - 1\right] , \qquad (4.169)$$

where the superscript (2) has been deleted (see eq. (4.168)). For very small n_0's, eq. (4.169) may be expanded as, keeping the lowest order term,

$$n = \zeta(\tfrac{3}{2})\lambda_T^{-3} - \sqrt{\pi V_T}\,\lambda_T^{-3}(8\pi)^{1/4}(\beta n_0 V_0)^{1/4} + O(\sqrt{\beta n_0 V_0}) \qquad (4.170)$$

Eq. (4.170) has no solution for small ΔT and $\eta = -n_0 V_0 < 0$ for $\Delta T = T - T_0 < 0$. In fact, the solution of eq. (4.170) for small $\Delta T > 0$ is

$$\frac{n_0}{n} \sim \left(\frac{\Delta T}{T_0}\right)^4 , \qquad (4.171)$$

which is to be compared with eq. (4.40) for the Bogoliubov spectrum. Thus the analogous expression to eq. (4.37) must be a quartic equation.

More important is the fact that eq. (4.170) through the interaction terms u_{int} lead to thermodynamic functions which are double-valued and thus ill-defined. There is, however, an open question on whether the self-consistent Hartree-Fock would display such a behavior or not.

F. Bogoliubov/Hartree-Fock Approximation

The Bogoliubov/Hartree-Fock approximation is the final first-order approximation which we consider. As mentioned before, this approximation, like the others, may be obtained as a special case of the Hartree-Fock approximation. The Bogoliubov/Hartree-Fock approximation was first studied by Shohno[92] who derived it by a normal-mode analysis. We give now the Green's function derivation of it.

Above the transition, we have just the Hartree-Fock approximation, eqs. (4.109-115). It is convenient to define a function

$$g(p) \equiv \frac{1}{\mathcal{V}} \sum_{q} V(p-q)\, f(\tilde{\epsilon}_q) \tag{4.172a}$$

so that $\tilde{\epsilon}_p$ is given by

$$\tilde{\epsilon}_p = \epsilon_p^0 + g(p) - g(0) + \eta \, . \tag{4.172b}$$

Below the transition, we consider the following self-energy matrix

$$\Sigma^0(p) = \begin{pmatrix} nV_0 + n_0V_p + \tilde{g}(p) & n_0V_p \\ n_0V_p & nV_0 + n_0V_p + \tilde{g}(p) \end{pmatrix} \tag{4.173}$$

where $\tilde{g}(p)$ is the analytic continuation of $g(p)$, i.e.

$$\tilde{g}(p) = \frac{1}{\mathcal{V}} \sum_{q} V(p-q) \int_{-\infty}^{\infty} \frac{d\omega}{2\pi}\, \tilde{A}_{11}(q,\omega)\, f(\omega) \, , \tag{4.174}$$

and the chemical potential

$$\mu = \mu_B + \mu_{HF} = nV_0 + \tilde{g}(0) . \tag{4.175}$$

Note that eq. (4.175) satisfies the Hugenholtz-Pines form and hence leads to a gapless energy spectrum, viz.

$$\mathcal{E}(p) = \sqrt{(\epsilon_p^0 + c_p)(\epsilon_p^0 + c_p + 2n_0V_p)} \tag{4.176a}$$

$$\tilde{E}(p) = \epsilon_p^0 + n_0V_p + c_p \tag{4.176b}$$

$$F(p) = n_0 V_p \tag{4.176c}$$

where we defined

$$c_p = \tilde{g}(p) - \tilde{g}(0) \quad . \tag{4.176d}$$

Eqs. (4.176) give the spectrum derived by Shohno. Since Shohno does not include the interaction term, $\mathcal{U}_{\text{int}}$, into the thermodynamics, the double-value behavior of the thermodynamic functions does not appear. Nevertheless the double-value behavior of the number density is implicitly wrapped up in Shohno's eq. (3.31).

G. Restricted Geometry

One of the major objections in using the ideal Bose gas as a model for liquid helium-4 confined to some restricted geometry where a length is definitely finite is that the Bose-Einstein condensation no longer occurs in the strict sense at nonzero temperatures. This feature is general since the Bose-Einstein condensation is a phase-space phenomenon. This feature is explicitly exhibited in the absence of any macroscopic occupation of the ground state in the film geometry until $T \to 0$, as shown in Chapter III.

Unfortunately, the first-order approximations do not help the situation at all. The Bose-Einstein condensation is still largely a phase-space phenomenon, and any change in the phase-space like to a two-dimensional geometry would change the phenomena and obliterate the Bose-Einstein condensation. To demonstrate this assertion, let us consider the number density above the transition and work downwards; from eq. (4.28a), we have

$$N = \frac{1}{v} \sum_{p} f(\tilde{\epsilon}_p) \qquad (4.177)$$

where

$$\tilde{\epsilon}_p = \epsilon_p^0 + \Sigma^0(p) - \mu \, . \qquad (4.178)$$

Since the expansion of $\Sigma^0(p)$ about $p = 0$ is

$$\Sigma^0(p) = \Sigma^0(0) + p^2 \left(\frac{\partial \Sigma^0(p)}{\partial p^2} \right)_{p=0} + \cdots \, ,$$

we see from (4.178) that $\tilde{\epsilon}_p \sim p^2$ for small momenta. Hence proceeding from the above, one finds the identical phase-space effect occuring as in the ideal gas case to force a condensate in the bulk limit and to give no condensate for restricted geometries. In particular in the bulk limit, eq. (4.177) yields at

$$n \sim \int_0 \frac{p^2 dp}{\beta p^2} < \infty$$

and further decrease in the temperature for fixed n yields the condensation. In restricted geometry, say the film geometry,

$$n \sim \sum_{\ell=1}^{\infty} \int_0 \frac{p\,dp}{\beta[p^2 + c\lambda_T^2 L^{-2}(\ell^2-1)]}$$

which at low temperatures $\lambda_T >> L$ becomes the first-band approximation and

$$n \sim \int_0 \frac{p\,dp}{\beta p^2} \longrightarrow \infty .$$

Therefore we have no condensate until $T = 0$.

Therefore we conclude that the first-order approximations do not include enough of the effect of interactions on the Bose-Einstein condensation to change it from being a phase-space phenomenon. In this spirit, we now turn to investigate the next order, namely the second-order approximations.

V. SECOND-ORDER APPROXIMATIONS

To second-order in the potential V, we have the gapless approximation first studied by Beliaev[32] at zero temperature and extended to nonzero temperatures by Hohenberg[34] and by Tserkovnikov,[93] and the conserving approximation known as the Born-Collision approximation. The gapless approximation used by Beliaev when extended above the λ-transition leads naturally to the conserving Hartree-Fock approximation. Hence the gapless/conserving approximation thus generated is the Beliaev/Hartree-Fock approximation. The Beliaev work can be extended further to the Beliaev/Born-Collision approximation so that we have second-order on both sides of the λ-transition. Finally we can have first-order below and second-order above, or the Bogoliubov/Born-Collision approximation.

Of the four possible second-order approximations, we shall pay particular attention to the conserving one, the Born-Collision approximation. We show that the Born-Collision approximation above the λ-transition contains the essential features of the more complex theory of Patashinskii and Pokrovskii.[94]

A. Beliaev/Hartree-Fock Approximation

The Beliaev/Hartree-Fock approximation is given above the transition by the Hartree-Fock equations, eqs. (4.109-115). Below the transition, the equations are quite different.

Recall that the Bogoliubov approximation was obtained from the functional $\Sigma_{\frac{1}{2}}\left[U^{ext}, G_{\frac{1}{2}}^{+}\right]$ in the form, eq. (2.79), which yielded the self-energy via eq. (2.88). For the Beliaev approximation, we consider the functional $\Sigma_{\frac{1}{2}}[U^{ext}, G_{\frac{1}{2}}^{+}]$ which includes all first-order diagrams,[95] i.e.

$$\sqrt{-i}\,\Sigma_{1/2}(1) = \frac{i}{2}\, G_{1/2}(1)\int_0^{-i\beta} d2\, V(12)\left[G_{1/2}(2)\,G_{1/2}^{+}(2) + \tilde{G}(22)\right] + \\ + i\int_0^{-i\beta} d2\, V(12)\, G_{1/2}(2)\, \tilde{G}(12) \tag{5.1}$$

The self-energy is calculated by eq. (2.88) which can be written

$$\Sigma^{tot}(11') = \sqrt{-i}\,\left(\frac{\delta\Sigma_{1/2}(1)}{\delta G_{1/2}(1')}\right)_{\substack{expl.\\ U^{ext}}} + \\ + \sqrt{-i}\int_0^{-i\beta} d2\,d3\, \left(\frac{\delta\Sigma_{1/2}(1)}{\delta\tilde{G}(23)}\right)_{G_{1/2}} \left(\frac{\delta\tilde{G}(23)}{\delta G_{1/2}(1')}\right)_{U^{ext}} . \tag{5.2}$$

Recalling the identity

$$\left(\frac{\delta\tilde{G}(23)}{\delta G_{1/2}(1')}\right)_{U^{ext}} = -\int_0^{-i\beta} d4\,d5\,\tilde{G}(24)\,\frac{\delta\Sigma^{tot}(45)}{\delta G_{1/2}(1')}\,\tilde{G}(53) ,$$

we rewrite eq. (5.2) as

$$\Sigma^{tot}(11') = \sqrt{-i}\,\left(\frac{\delta\Sigma_{1/2}(1)}{\delta G_{1/2}(1')}\right)_{\substack{expl.\\ U^{ext}}} + \\ + \sqrt{-i}\int_0^{-i\beta} d2\,d3\,d4\,d5\,\frac{\delta\Sigma_{1/2}(1)}{\delta\tilde{G}(23)}\,\tilde{G}(24)\,\frac{\delta\Sigma^{tot}(45)}{\delta G_{1/2}(1')}\,\tilde{G}(53) . \tag{5.3}$$

To obtain the desired order of approximation, we iterate eq. (5.3) with respect to $\delta \Sigma^{tot} / \delta G_{\frac{1}{2}}$. Applying eq. (5.3) to the functional (5.1), we see that the first term of (5.3) gives the Hartree-Fock terms and that the second term with the Hartree-Fock terms inserted into $\delta \Sigma^{tot} / \delta G_{\frac{1}{2}}$ gives the Beliaev second-order terms. Thus the total self-energy is

$$
\begin{aligned}
\Sigma^{tot}(11') = {} & \frac{i}{2}\delta(11')\int_0^{-i\beta} d2\, V(12)\left[G_{1/2}(2)\, G^{+}_{1/2}(2) + \tilde{G}(22)\right] + \\
& + i\, V(11')\left[G_{1/2}(1)\, G^{+}_{1/2}(1) + \tilde{G}(11')\right] + \\
& + \frac{i^2}{2}\tilde{G}(11')\int_0^{-i\beta} d2\, d3\; V(12)\, V(31') \times \\
& \qquad \times \left[\tilde{G}(32)\, G_{1/2}(2)\, G^{+}_{1/2}(3) + G_{1/2}(3)\, G^{+}_{1/2}(2)\, \tilde{G}(23)\right] + \\
& + \frac{i^2}{2} G_{1/2}(1)\, G^{+}_{1/2}(1')\int_0^{-i\beta} d2\, d3\; V(12)\, V(31')\, \tilde{G}(23)\, \tilde{G}(32) + \\
& + i^2\int_0^{-i\beta} d2\, d3\; V(12)\, V(31')\, \tilde{G}(13) \times \\
& \qquad \times \left[\tilde{G}(32)\, G_{1/2}(2)\, G^{+}_{1/2}(1') + G_{1/2}(3)\, G^{+}_{1/2}(2)\, \tilde{G}(21')\right] + \\
& + i^2\int_0^{-i\beta} d2\, d3\; V(12)\, V(31')\, G_{1/2}(1)\, G^{+}_{1/2}(3)\, \tilde{G}(32)\, \tilde{G}(21') \; .
\end{aligned}
\tag{5.4}
$$

B. Born-Collision Approximation (Self-Consistent Calculation)

We now consider the Born-Collision approximation, the second-order conserving approximation, above the transition. This approximation can be defined by the functional $\Phi[G_1]$ as

$$\Phi[G_1] = \frac{i}{2}\int_0^{-i\beta} d1\, d2\; V(12)\left[G(11)G(22) + G(12)G(21)\right] + $$
$$+ \frac{i^2}{4}\int_0^{-i\beta} d1 d2 d3 d4\; V(12)\,V(34)\; \times \tag{5.5}$$
$$\times \left[G(13)G(31)G(24)G(42) + G(14)G(42)G(23)G(31)\right].$$

The total self-energy is obtained by eq. (2.52)

$$\Sigma^{tot}(11') = i\,\delta(11')\int_0^{-i\beta} d2\; V(12)G(22) + i\,V(11')\,G(11') + $$
$$+ i^2\int_0^{-i\beta} d2\, d3\; V(12)\,V(31')\; \times \tag{5.6}$$
$$\times \left[G(11')G(32)G(23) + G(13)G(32)G(21')\right].$$

We recognize the first term of eq. (5.6) as the Hartree-Fock terms, which is the entire subtraction term Σ^0. In most of the analysis, we are interested in the dispersive part of the total self-energy

$$\Sigma(11') = i^2\int_0^{-i\beta} d2\, d3\; V(12)\,V(31')\; \times \tag{5.7}$$
$$\times \left[G(11')G(32)G(23) + G(13)G(32)G(21')\right].$$

which we shall refer to simply as the self-energy.

We now Fourier transform eq. (5.7) to obtain the analytic self-energy in the form

$$\begin{aligned}\Sigma(p,z) = {} & \frac{1}{\mathcal{V}^3}\sum_{p'\bar{p}\bar{p}'}{}' (2\pi\hbar)^3\,\delta(p+p'-\bar{p}-\bar{p}')\,\frac{1}{2}\left[V(p-\bar{p})+V(p-\bar{p}')\right]^2 \times \\ & \times \int_{-\infty}^{\infty}\frac{d\omega}{2\pi}\,\frac{1}{z-\omega}\int\frac{d\omega'}{2\pi}\int\frac{d\bar{\omega}}{2\pi}\int\frac{d\bar{\omega}'}{2\pi}\,2\pi\,\delta(\omega+\omega'-\bar{\omega}-\bar{\omega}') \times \\ & \times A(p'\omega')\,A(\bar{p}\,\bar{\omega})\,A(\bar{p}'\,\bar{\omega}') \times \\ & \times \left[f^-(\omega')f^+(\bar{\omega})f^+(\bar{\omega}') - f^+(\omega')f^-(\bar{\omega})f^-(\bar{\omega}')\right],\end{aligned} \qquad (5.8)$$

where the integrals over the ω's go from $-\infty$ to ∞, and $f^-(\omega) = f(\omega)$, $f^+(\omega) = 1 + f(\omega)$. We first note that as $z \longrightarrow 0$ in eq. (5.8), we get the real part of the self-energy $\Delta(p,0)$ since $\Sigma(p,z)$ is continuous across the real axis at the origin. Furthermore the imaginary part can be easily obtained from eqs. (2.24)(5.8), viz.

$$\begin{aligned}\Gamma(p,\omega) = {} & \frac{1}{\mathcal{V}^3}\sum_{p'\bar{p}\bar{p}'}{}' (2\pi\hbar)^3\,\delta(p+p'-\bar{p}-\bar{p}')\,\frac{1}{2}\left[V(p-\bar{p})+V(p-\bar{p}')\right]^2 \times \\ & \times \int\frac{d\omega'}{2\pi}\int\frac{d\bar{\omega}}{2\pi}\int\frac{d\bar{\omega}'}{2\pi}\,2\pi\,\delta(\omega+\omega'-\bar{\omega}-\bar{\omega}') \times \\ & \times A(p'\omega')\,A(\bar{p}\,\bar{\omega})\,A(\bar{p}'\,\bar{\omega}') \times \\ & \times \left[f^-(\omega')f^+(\bar{\omega})f^+(\bar{\omega}') - f^+(\omega')f^-(\bar{\omega})f^-(\bar{\omega}')\right].\end{aligned} \qquad (5.9)$$

Eqs. (5.8)(5.9) are very complicated nonlinear integral equations which are practically intractable as they stand.

One reduction which we can make depends on the fact that we are dealing with a homogeneous system in space. Therefore the spectral function $A(p,\omega)$ and the self-energy $\Sigma(p,\zeta)$ are functions only of the magnitude of the momentum. If we write the momentum δ -function as

$$(2\pi\hbar)^3\delta(p+p'-\bar{p}-\bar{p}') = \int_{\mathcal{V}} d^3r \; e^{ir\cdot(p+p'-\bar{p}-\bar{p}')/\hbar} ,$$

we can do the angular integrations in eq. (5.8) to obtain, in the $N/\mathcal{V}$ limit,

$$\Sigma(p,\zeta) = \frac{\hbar^{-9}}{2\pi^5}\int_0^\infty r^2 dr \int_0^\infty p'^2 dp' \int_0^\infty \bar{p}^2 d\bar{p} \int_0^\infty \bar{p}'^2 d\bar{p}' \times$$

$$\times j_0\left(\frac{rp}{\hbar}\right) j_0\left(\frac{rp'}{\hbar}\right) j_0\left(\frac{r\bar{p}}{\hbar}\right) j_0\left(\frac{r\bar{p}'}{\hbar}\right) \mathcal{F}(pp'\bar{p}\bar{p}';\zeta) \qquad (5.10)$$

where $j_0(x) = x^{-1}\sin x$ and $\mathcal{F}(pp'\bar{p}\bar{p}';\zeta)$ is defined as

$$\mathcal{F} = \frac{1}{2}\left[V(p-\bar{p}) + V(p-\bar{p}')\right]^2 \int\frac{d\omega}{2\pi}\frac{1}{\zeta-\omega}\int\frac{d\omega'}{2\pi}\int\frac{d\varpi}{2\pi}\int\frac{d\varpi'}{2\pi} \times$$

$$\times 2\pi\delta(\omega+\omega'-\varpi-\varpi') A(p'\omega') A(\bar{p}\varpi) A(\bar{p}'\varpi') \times \qquad (5.11)$$

$$\times \left[f^-(\omega')f^+(\varpi)f^+(\varpi') - f^+(\omega')f^-(\varpi)f^-(\varpi')\right] .$$

A similar reduction can be performed on the imaginary part (5.9).

In order to proceed further in the reduction of the self-energy to a more tractable form, we make two approximations. First of all and more significant, we take the Very Dense State limit not only for the initial and final states but for all intermediate states of eq. (5.11). This means mathematically that we expand the statistical factors as

$$f(\omega) \simeq \frac{1}{\beta\omega} \tag{5.12}$$

and apply the eqs. (2.108)(2.113)

$$\int \frac{d\omega}{2\pi} A(p,\omega) f(\omega) \simeq \frac{1}{\beta W_p} \tag{5.13}$$

with

$$W_p = \epsilon'(p) + \Delta'(p,0) + \eta \tag{5.14}$$

to eq. (5.10-11) after taking $z \longrightarrow 0$. Physically, this means that we consider the system to be very close to the transition so that all significant contribution to the self-energy comes from the states which are very densely occupied, viz. the low momentum states. Hence we incorporate into the system explicitly the high degree of correlation among the low momentum states as they "anticipate" the macroscopic occupation of the zero momentum state. Second, we restrict the potential to a very short-ranged potential, so that

$$V_p \simeq V_0 = \int_{v} d^3r \, V(r) \tag{5.15}$$

This assumption reduces the Hartree-Fock terms to a constant

$$\Sigma^0(p) = 2nV_0$$

which changes the transition to a third-order one but in no way affect the energy spectrum which remains a free-particle one. Therefore $\epsilon'(p) = \epsilon_p^0$ and

$$W_p = \epsilon_p^0 + \Delta'(p,0) + \eta \tag{5.16}$$

$$\eta = -\mu + 2nV_0 + \Delta(0,0) \,. \tag{5.17}$$

Applying the approximations (5.12-15) to eqs. (5.10)(5.11), we find that the real part of the self-energy (as $z \to 0$) satisfies the equation

$$\Delta'_p = -\frac{V_0^2}{\pi^5 \hbar^4 \beta_0^2} \int_0^\infty r^2 dr \left[j_0\left(\frac{rp}{\hbar}\right) - 1 \right] D^3(r) \tag{5.18}$$

$$D(r) = \int_0^\infty q^2 dq \, j_0\left(\frac{rq}{\hbar}\right) \frac{1}{W_q} \,, \tag{5.19}$$

where we defined $\Delta'_p = \Delta'(p,0) = \Delta_p - \Delta_0$ and W_q by eqs. (5.16-17). Note that eqs. (5.18-19) is a nonlinear homogeneous integral equation for Δ'_p. Note also that any reference to the imaginary part has been eliminated, eqs. (5.18-19) is independent of $\Gamma(p,\omega)$. Finally we note that if $\operatorname{Im} z > 0$ in $\Sigma(p, z)$, we cannot effect the reduction to an equation similar to eq. (5.18-19).

1. Real Part of Self-Energy at $\zeta = 0$

We now solve the integral equations for Δ'_p , eqs. (5.18)(5.19) for the limiting case $\eta \rightarrow 0$ and the general case of $\eta > 0$. The limit $\eta \rightarrow 0$ leads to the divergence of N_o , the number in the zero momentum state, and corresponds to moving onto the transition from above. On the other hand, when $\eta > 0$, N_o is finite corresponding to the region above the transition.

Because of the Very Dense State limit, the range of momentum in which the integral equation (5.18,19) is valid is restricted. If we define a momentum p_2 by $\beta W_{p_2} = 1$, we can expect the integral equation to be valid only for $p \ll p_2$. This restriction applies also to the dummy variable q in the integral for D(r), since the Very Dense State limit was taken also for intermediate states. Therefore if the integral for D(r) has some nonnegligible contribution from momenta near p_2 , this signals the breakdown of the integral equation. However, when the contributions all come from the low momenta states $p \ll p_2$ and the integral D(r) converges for large q's, the upper limit of D(r) can be effectively extended to infinity.

a. On the Transition

Eq. (5.19) can be written, in the limit $\eta \rightarrow 0$, as

$$D(r) = \int_0^\infty dq \, \frac{q^2}{\Delta'_q + \epsilon^0_q} \, j_0\!\left(\frac{rq}{\hbar}\right) . \qquad (5.20)$$

Let us define a momentum p_o such that $\Delta'_{p_o} = \epsilon^0_{p_o}$. From physical grounds, we expect the self-energy to dominate the kinetic energy at low momenta because of the high correlation. In fact, in the region $p \ll p_o$, ϵ^o_q can be neglected in (5.20). To see this, we consider the case for the slowest convergence of the r-integration of (5.18) which occurs when Δ'_q is neglected in (5.20). The resulting integrand for the r-integration

$$\frac{1}{r}\left[j_0\left(\frac{rp}{\hbar}\right) - 1\right]$$

has a peak at $r \simeq \hbar/p$ but also yields a logarithmically divergent integral. This divergence we ignore as we expect Δ'_q to dominate and as we are merely interested in the peak of the integrand. Now we estimate the contributions to $D(\hbar/p)$:

$$D\left(\frac{\hbar}{p}\right) \simeq \int_0^{p_0} dq \, \frac{q^2}{\Delta'_q} \, j_0(q/p) + \int_{p_0}^{p_2} dq \, \frac{q^2}{\epsilon^0_q} \, j_0(q/p) \, . \qquad (5.21)$$

Note that the second integral is proportional to $\mathrm{Si}(p_2/p) - \mathrm{Si}(p_o/p)$, which vanishes for $p \ll p_o, p_2$. Hence we neglect ϵ^o_q in the integral for $D(r)$.[96] Furthermore if $\Delta'_q = A_o q^{\alpha_o}$ and $\alpha_o > 1$ (so that the integral (5.20) converges as $q \to \infty$) and $\alpha_o < 2$ (so that the integral (5.17) converges as $r \to \infty$), we can extend the integral over q to infinity. Summarizing, we have

$$D(r) = \int_0^\infty j_0\left(\frac{rp}{\hbar}\right) \frac{q^2 \, dq}{\Delta'_q} \qquad (5.22)$$

which is valid for $0 \leq p \ll p_o$ and $1 < \alpha_o < 2$.

The estimation of the two terms for D(r) can be made more precise if we utilize the solution $\Delta'_p = A_o p^{3/2}$ and the asymptotic expansion for Si(x)

$$Si(x) = \frac{\pi}{2} - \frac{\cos x}{x} - \frac{\sin x}{x^2} + \cdots$$

so that[97]

$$I_\Delta(p) \equiv \int_0^{p_0} j_0(q/p)\,\frac{q^2 dq}{\Delta'_q} \simeq 2mp^2\sqrt{\frac{\pi}{2p_0 p}}$$

in the limit of $p_o >> p$ and

$$I_E(p) \equiv \int_{p_0}^{p_2} j_0(q/p)\,\frac{q^2 dq}{E^0_q}$$

$$\simeq 2mp^2\left[\frac{1}{p_0}\cos(p_0/p) - \frac{1}{p_2}\cos(p_2/p)\right]$$

in the limit of $p << p_o, p_2$. The worse case is when $\cos(p_o/p) = +1$, $\cos(p_2/p) = -1$; therefore

$$I_E(p) \leq 2mp^2\left(\frac{1}{p_0} + \frac{1}{p_2}\right) < 4mp^2\frac{1}{p_0}$$

and the ratio of the two terms is

$$\frac{I_E(p)}{I_\Delta(p)} \leq 2\sqrt{\frac{2}{\pi}}\sqrt{\frac{p}{p_0}}$$

which is very small in the limit $p << p_o$.

To solve the nonlinear integral equation, (5.18)(5.22), we assume the form

$$\Delta'_p = A_0 p^{\alpha_0} \qquad (5.23)$$

Substituting (5.23) into (5.18)(5.22), we get

$$A_0^4 p^{\alpha_0} = -\frac{V_0^2}{\pi^5 \hbar^6 \beta_0^2}\, p^{6-3\alpha_0}\left[\int_0^\infty \frac{dy}{y^{7-3\alpha_0}}\left(j_0(y)-1\right)\right]\times \left[\int_0^\infty \frac{dx}{x^{\alpha_0-2}}\, j_0(x)\right]^3$$

where we have put $x = rq/\hbar$, $y = rp/\hbar$ and $\beta_0 = (k_B T_0)^{-1}$. The integrals within the braces are numbers independent of p , so the exponent α_0 is determined by the equation $\alpha_0 = 6 - 3\alpha_0$ or $\alpha_0 = 3/2$. Furthermore, A_0 is given by[98]

$$A_0^4 = \frac{2}{15\pi^3}\left(\frac{V_0}{\beta_0 \hbar^3}\right)^2 \quad . \qquad (5.24)$$

Therefore the solution for $0 \leq p \ll p_0$ is (recall $v_{T_0} = \beta_0 V_0 / \lambda^3_{T_0}$)

$$\Delta_p' = \left(\frac{2}{15\pi^3}\right)^{1/4} \sqrt{v_{T_0}}\left(\lambda_{T_0}\frac{p}{\hbar}\right)^{3/2} k_B T_0 \quad . \qquad (5.25)$$

We note that the $p^{3/2}$ — spectrum is wholly dependent upon the presence of interactions.

The relative magnitudes of p_0 and p_2 is of some interest as they give an estimate of the strength of the interaction allowable for our system. There are three distinct cases: (a) $p_0 \gg p_2$; (b) $p_0 \sim p_2$; (c) $p_0 \ll p_2$. The first case we do not know anything about since our equation is not valid for $p \sim p_2$. The next two cases are amenable to our analysis, and are considered below within an expanded context.

Note that our system is characterized by five quantities: (a) the number density, n ; (b) the integral or strength of the potential, $V_o = \int V(r) d^3 r$; (c) the range of the potential, r_f ; (d) the mass of the particle, m ; (e) the temperature of the system, T . From these five quantities, four lengths can be formed:

r_f = range of the potential
$n^{-1/3}$ = average interparticle distance
a_s = scattering length
λ_T = thermal wavelength

From the offset, we have assumed that the potential is short-ranged, i.e. $r_f n^{1/3}$, $r_f a_s^{-1}$, $r_f \lambda_T^{-1} << 1$. Note that the transition temperature for the ideal Bose gas is given by $k_B T_o^i = 3.31 \hbar^2 n^{2/3}/m$, so that $\lambda_{T_o} n^{1/3} \sim (T_o^i/T_o)^{\frac{1}{2}} \sim 1$. The only ratio that has not been estimated is $n^{1/3} a_s$, and it will be determined by the relative magnitude of p_o and p_2 .

To see this, we note that p_o may be approximated by $A_o p_o^{3/2} = \epsilon^o_{p_o}$ and p_2 by $\beta_o \epsilon^o_{p_2} = 1$. Therefore the relations $p_o \sim p_2$ and $p_o << p_2$ can be translated to $\beta_o \epsilon^o_{p_o} \sim 1$ and $\beta_o \epsilon^o_{p_o} << 1$ respectively. But

$$\beta_o \epsilon^o_{p_o} = 8 m^3 \beta_o A_o^4 = \frac{16}{15\pi^3} \frac{V_o^2 m^3}{\beta_o \hbar^6} \sim 16 (n^{1/3} a_s)^2 ,$$

where we approximated $\beta_o \sim \beta_o^i$ in the last step. Thus $p_o \sim p_2$ is equivalent to $n^{1/3} a_s \sim \frac{1}{4}$ and $p_o << p_2$ to $n^{1/3} a_s << \frac{1}{4}$. Therefore the above calculation is good for weakly-coupled or low density systems up to $n^{1/3}a_s \sim \frac{1}{4}$. For liquid helium-4, we have $n^{1/3}a_s \sim 0.7$, thus $p_0 \sim p_2 \sim \hbar\,(2\,\text{Å})^{-1}$.

It would seem that for a very weakly-coupled or low-density system, the region $p_0 \ll p \ll p_2$ would be amenable to our analysis. We show now that this thought is incorrect. Consider again the function $D(\hbar/p)$, eq. (5.21). In the region $p_0 \ll p \ll p_2$, the first integral of (5.21) is negligible, while the second integral approaches $\pi/2$. However the second integral is the contributions from $q \sim p_2$ which is unacceptable since it is in clear contradiction with our initial assumption in making the Very Dense State limit. Furthermore, if we went ahead with $D(r)$ approximated by the second integral in (5.21), then the r-integration of eq. (5.18) does not converge. Thus for only $p \ll p_0$, can we say that the main contribution to the self-energy is from intermediate states which are very dense. Otherwise contributions come from intermediate states of all occupations.

b. Above the Transition

We begin by defining some momenta. First, we define p_0 by formally the same equation as for $\eta \to 0$, i.e. $\Delta'_{p_0} = \epsilon^0_{p_0}$, where Δ'_p satisfies the integral equation (5.18,19) with $\eta > 0$. Second, we define p_η by $\Delta'_{p_\eta} = \eta$.

With these definitions, we now attempt to reduce eqs. (5.18,19) as much as possible for the various regions in momentum space. First, for $p \ll p_0$, the ϵ^0_q term in $D(r)$ can be neglected as before, so that eq. (5.19) can be written

$$D(r) = \int_0^\infty j_0\left(\frac{rq}{\hbar}\right) \frac{q^2\,dq}{\Delta'_q + \eta} \quad . \tag{5.26}$$

In the subregion $p_\eta << p << p_o$ which exists for very small η, we further reduce eq. (5.26) to

$$D(r) = \int_0^\infty dq\, j_0\left(\frac{rq}{\hbar}\right) \frac{q^2}{\Delta'_q} \quad . \tag{5.27}$$

This is justified by estimating $D(\hbar/p)$

$$D\left(\frac{\hbar}{p}\right) \simeq \int_0^{p_\eta} dq\, \frac{q^2}{\eta}\, j_0(q/p) + \int_{p_\eta}^{p_0} dq\, \frac{q^2}{\Delta'_q}\, j_0(q/p) \quad ,$$

and the first integral is very small for $p >> p_\eta$. The solution to (5.18,27) is just the $p^{3/2}$-spectrum, $\Delta'_p = A_o p^{3/2}$, where A_o is given by eq. (5.24) with $\beta_0 \rightarrow \beta$.

In the subregion $0 \leq p << p_\eta$, we must consider eq. (5.26) as it stands, for although the η term is larger than Δ'_q, but Δ'_q is needed for convergence. However, eq. (5.26) has an exponential decay in r for large values of r. To see this, we note the evenness of the integrand, so that eq. (5.26) can be written

$$D(r) = \frac{1}{2}\left(\frac{\hbar}{r}\right)^3 \mathrm{Im} \int_{-\infty}^{\infty} \frac{x e^{ix}\, dx}{\Delta'(\hbar x/r) + \eta} \quad , \tag{5.28}$$

where we wrote $x = rq/\hbar$ and Im denotes the imaginary part. In general $\Delta'(y) \sim y^n$, and a branch point appears at $x = 0$ with poles off the real axis since $\eta > 0$. Closing the contour in the upper half plane, we pick up the poles in the upper half plane satisfying $c(\hbar\varkappa/r)^n + \eta = 0$. Therefore

$$D(r) \sim e^{-\frac{r}{\hbar}\eta} \qquad r \to \infty,\ \eta > 0\ . \tag{5.29}$$

Eq. (5.29) is in mark contrast with the asymptotic behavior of D(r) for $\eta = 0$, in which we find

$$D(r) \sim \frac{1}{r^{3/2}} \qquad r \to \infty,\ \eta = 0\ . \tag{5.30}$$

Eq. (5.30) is another manifestation of the macroscopic occupation of the zero momentum state which leads to an infinite-ranged correlation in position space, while eq. (5.29) testifies towards the absence of such correlation. Because of the exponential behavior of D(r) for large r, we can obtain the solution to the integral equation (5.18,26) in the subregion $p \ll p_\eta$ by expanding in eq. (5.18)

$$j_0\left(\frac{rp}{\hbar}\right) - 1 = -\frac{1}{6}\left(\frac{rp}{\hbar}\right)^2 + \cdots$$

to obtain

$$\Delta_p' = \frac{V_0^2}{6\pi^5\hbar^9\beta^2}\left(\frac{p}{\hbar}\right)^2 \int_0^\infty dr\ r^4 D^3(r) + \cdots\ ,$$

which has the solution

$$\Delta_p' = A_1 p^2 \tag{5.31}$$

with[99]

$$A_1^3 = \frac{V_0^2}{432\pi^2\hbar^6\beta^2\eta} \quad . \tag{5.32}$$

Therefore for $\eta > 0$, the energy spectrum begins with a p^2- spectrum which goes over to a $p^{3/2}$- spectrum at p_η. The $p^{3/2}$- spectrum subsists up to p_o as in the $\eta = 0$ case. Thus as η is increased, or as we get further away from the transition, the $p^{3/2}$- spectrum is "squeezed out" from the low momenta side until there is no $p^{3/2}$ left. The vanishing of the $p^{3/2}$- spectrum occurs when $p_\eta \sim p_o$. Approximating p_η by $A_1 p_\eta^2 = \eta$, we find the $p^{3/2}$- spectrum vanishing when $\eta \sim 9\,(n^{1/3}a_s)^2 k_B T_o$.

2. Imaginary Part of Self-Energy

Although the imaginary part $\Gamma(p,\omega)$ cannot be reduced in the Very Dense State limit into a form as tractable as eqs. (5.18,19) for the real part $\Delta'(p,0)$, we nevertheless can make some interesting observations concerning $\Gamma(p,\omega)$. First of all, we show that for small ω's, $\Gamma(p,\omega) \sim \omega$ in the Very Dense State limit with $\eta > 0$. Second, we calculate $\Gamma(p,\omega)$ for small p's and small ω's with $\eta = 0$.

a. Above the Transition

We begin with eq. (5.9) for $\Gamma(p,\omega)$ which can be written as

$$\Gamma(p,\omega) = \frac{1}{V^3}\sum_{p'\bar{p}\bar{p}'}{}' \Lambda(pp'\bar{p}\bar{p}') \int\frac{d\omega'}{2\pi}\int\frac{d\bar{\omega}}{2\pi}\int\frac{d\bar{\omega}'}{2\pi}\, 2\pi\delta(\omega+\omega'-\bar{\omega}-\bar{\omega}') \times$$

$$\times\, A(p'\omega')\, A(\bar{p}\bar{\omega})\, A(\bar{p}'\bar{\omega}')\, f(\omega')\, f(\bar{\omega})\, f(\bar{\omega}')\, \times$$

$$\times \left[\frac{1}{f(\bar{\omega})} + \frac{1}{f(\bar{\omega}')} - \frac{1}{f(\omega')} \right] , \qquad (5.33)$$

where we have neglected a term linear in $f(\omega)$ in anticipation of taking the Very Dense State limit and where

$$\Lambda(pp'\bar{p}\bar{p}') = \frac{1}{2}\left[V(p-\bar{p}) + V(p-\bar{p}') \right]^2 \times$$

$$\times (2\pi\hbar)^3\, \delta(p+p'-\bar{p}-\bar{p}') . \qquad (5.34)$$

We now take the Very Dense State limit, expanding the statistical factors as in (5.12). Also we assume that for small values of ω, the spectral function has the following behavior[100]

$$A(p\omega) \sim A_p\, \omega . \qquad (5.35)$$

As (5.35) is obviously only valid for small ω's, we introduce cutoffs in the ω-integration. Then eq. (5.33) becomes

$$\Gamma(p,\omega) = \frac{1}{V^3} \sum_{p'\bar{p}\bar{p}'} \bar{\Lambda}(pp'\bar{p}\bar{p}')\, (k_B T_0)^2 \times$$

$$\times \int_{-k_B T_0}^{k_B T_0} \frac{d\omega'\, d\bar{\omega}\, d\bar{\omega}'}{(2\pi)^3}\, (\bar{\omega}+\bar{\omega}'-\omega')\, 2\pi\, \delta(\omega+\omega'-\bar{\omega}-\bar{\omega}') , \qquad (5.36)$$

where $\bar{\Lambda}(pp'\bar{p}\,\bar{p}') = A_{p'}A_{\bar{p}}A_{\bar{p}'}\,\Lambda(pp'\bar{p}\,\bar{p}')$. Eq. (5.36) is trivially integrated to give

$$\Gamma(p,\omega) = \gamma_p\,\omega \tag{5.37}$$

where γ_p is independent of ω . This linear relation (5.37) should be compared with the quadratic relation, $\Gamma(p,\omega) \sim \omega^2$, for normal fermi systems near zero temperatures, as first shown by Luttinger and Ward.[101] The above proof can be easily extended to include the renormalized vertex part $V(p,\omega)$ in place of the instantaneous potential V_p . The added assumption needed is that $V(p,\omega)$ be regular about $V(p,0)$.

From eq. (2.29), we express the spectral function in terms of the imaginary part Γ ,

$$A(p,\omega) = \frac{\Gamma(p,\omega)}{[\omega-\epsilon_p^0-\Delta_p'-\eta]^2+\frac{1}{4}[\Gamma(p,\omega)]^2} \tag{5.38}$$

From eqs. (5.37)(5.38), we see that eq. (5.35) holds for all momenta as long as $\eta > 0$. Therefore we conclude that eq. (5.37) is valid above the transition. However there is a singularity in (5.38) as $p \to 0$ and $\eta \to 0$, which is due to the macroscopic occupation of the zero momenta state. We now consider the limiting case $\eta \to 0$ in more detail.

b. On the Transition

A self-consistent calculation as $\eta \rightarrow 0$ for $\Gamma(p,\omega)$ involves a formidable integral equation (5.33), which is much too complex. Therefore we settle for a non self-consistent calculation generated by assuming a quasi-particle spectral function,

$$A(p,\omega) = \begin{cases} 2\pi\,\delta(\omega - W_p) & \omega > 0 \\ 0 & \text{otherwise} \end{cases} \tag{5.39}$$

where $W_p = \Delta'_p + \epsilon^0_p$, on the right hand side of (5.33). Taking the Very Dense State limit and doing the angular integrations in momentum space, we rewrite eq. (5.33) as

$$\begin{aligned} \Gamma(p,\omega) = {} & \frac{V_0^2}{\pi^5 \hbar^9 \beta_0^2}\,\omega \int_0^\infty dr\, r^2 j_0\!\left(\frac{rp}{\hbar}\right) \times \\ & \times \int_0^\infty \frac{p'^2 dp'}{W_{p'}} j_0\!\left(\frac{rp'}{\hbar}\right) \int_0^\infty \frac{\bar{p}^2 d\bar{p}}{W_{\bar{p}}} j_0\!\left(\frac{r\bar{p}}{\hbar}\right) \times \\ & \times \int_0^\infty \frac{\bar{p}'^2 d\bar{p}'}{W_{\bar{p}'}} j_0\!\left(\frac{r\bar{p}'}{\hbar}\right) 2\pi\,\delta(\omega + W_{p'} - W_{\bar{p}} - W_{\bar{p}'})\,. \end{aligned} \tag{5.40}$$

The r-integration in eq. (5.40) can be explicitly performed, resulting in

$$\begin{aligned} & \int_0^\infty r^2 dr\, j_0\!\left(\frac{rp}{\hbar}\right) j_0\!\left(\frac{rp'}{\hbar}\right) j_0\!\left(\frac{r\bar{p}}{\hbar}\right) j_0\!\left(\frac{r\bar{p}'}{\hbar}\right) = \\ & \qquad = \frac{\hbar^4}{p p' \bar{p} \bar{p}'}\,\frac{\pi}{4}\,\frac{p'}{\hbar} \end{aligned} \tag{5.41}$$

for $p > \bar{p} > \bar{p}' > p'$ and $p + p' < \bar{p} + \bar{p}'$. However in the integration over $\bar{p}$, $\bar{p}'$, p', there are 24 terms due to the $4!$ permutations of the inequality. Fortunately, only 6 out of the 24 terms need to be considered, the rest being negligible. The 6 terms are those with p as the largest momenta:

$$\begin{array}{ll} (1) & p > \bar{p} > p' > \bar{p}' \\ (2) & p > p' > \bar{p} > \bar{p}' \end{array} \left.\vphantom{\begin{array}{l} a \\ b \end{array}}\right\} \qquad p + \bar{p}' < p' + \bar{p}$$

$$\begin{array}{ll} (3) & p > p' > \bar{p}' > \bar{p} \\ (4) & p > \bar{p}' > p' > \bar{p} \end{array} \left.\vphantom{\begin{array}{l} a \\ b \end{array}}\right\} \qquad p + \bar{p} < p' + \bar{p}'$$

$$\begin{array}{ll} (5) & p > \bar{p}' > \bar{p} > p' \\ (6) & p > \bar{p} > \bar{p}' > p' \end{array} \left.\vphantom{\begin{array}{l} a \\ b \end{array}}\right\} \qquad p + p' < \bar{p} + \bar{p}'$$

Pictorially, these six inequalities define the six tetrahedrons which compose the solid cube of length p in the $(p', \bar{p}, \bar{p}')$ space. See Fig. 10. Hence when we integrate over these six regions, we are integrating over those values of $(p' \; \bar{p} \; \bar{p}')$ which yield the major contribution in the Very Dense State limit. Further simplification can be had if we notice the symmetry between $\bar{p}$ and $\bar{p}'$ in the integrand. Pictorially, this means that the integrand on the cube in $(p' \; \bar{p} \; \bar{p}')$ space is symmetrical about the plane defined by the main diagonal and the diagonal on the $\bar{p} \; \bar{p}'$ face. Also we neglect in W_p to obtain

$$\Gamma(p,\omega) = \frac{V_0^2}{2\pi^4 \hbar^6 \beta_0^2} \; \frac{\omega}{p} \quad \times$$

$$\times \Bigg[\int_{p/2}^{p} \frac{\bar{p}\,d\bar{p}}{\Delta'_{\bar{p}}} \int_{p-\bar{p}}^{\bar{p}} \frac{p'\,dp'}{\Delta'_{p'}} \int_{0}^{\bar{p}+p'-p} \frac{\bar{p}'^2\,d\bar{p}'}{\Delta'_{\bar{p}'}} \; 2\pi\,\delta(\omega + \Delta'_{p'} - \Delta'_{\bar{p}} - \Delta'_{\bar{p}'}) \; +$$

$$+ \int_{p/2}^{p} \frac{p'\,dp'}{\Delta'_{p'}} \int_{p-p'}^{p'} \frac{\bar{p}'\,d\bar{p}'}{\Delta'_{\bar{p}'}} \int_{0}^{\bar{p}'+p'-p} \frac{\bar{p}^2\,d\bar{p}}{\Delta'_{\bar{p}}} \; 2\pi\,\delta(\omega + \Delta'_{p'} - \Delta'_{\bar{p}} - \Delta'_{\bar{p}'}) \; +$$

$$+ \int_{p/2}^{p} \frac{\bar{p}'\,d\bar{p}'}{\Delta'_{\bar{p}'}} \int_{p-\bar{p}'}^{\bar{p}'} \frac{\bar{p}\,d\bar{p}}{\Delta'_{\bar{p}}} \int_{0}^{\bar{p}+\bar{p}'-p} \frac{p'^2\,dp'}{\Delta'_{p'}} \; 2\pi\,\delta(\omega + \Delta'_{p'} - \Delta'_{\bar{p}} - \Delta'_{\bar{p}'}) \Bigg] .$$

To do the δ-function integration, we change variables to $\Delta'_p = A_o p^{3/2}$, i.e. for an arbitrary function $f(p)$

$$\int \frac{p^2\,dp}{\Delta'_p} f(p) = \frac{2}{3A_o^2} \int d\Delta'_p \, f(p) \quad .$$

Note that the limitation to the cube in $(p' \; \bar{p} \; \bar{p}')$ is consistent with the setting of Δ'_p equal to $A_o p^{3/2}$. The δ-function is trivially integrated, and the resulting three integrals are equal. Therefore in the small ω region

$$\Gamma(p,\omega) = 15 \, \frac{\omega}{p} \times \int_{p/2}^{p} \frac{dp'}{\sqrt{p'}} \int_{p-p'}^{p'} \frac{d\bar{p}}{\sqrt{\bar{p}}}$$

which gives

$$\Gamma(p,\omega) = \frac{15}{2}(4-\pi)\,\omega \tag{5.43}$$

which is valid for $p \ll p_o$. Therefore as $\eta \to 0$, we find $\gamma_p = \frac{15}{2}\,(4 - \pi)$, independent of p for $p \ll p_o$.

3. Spectral Function and Green's Function

From eqs. (5.38)(5.37), we may explicitly write down the spectral function for $\beta\omega << 1$, i.e.

$$A(p,\omega) = \frac{\gamma_p \omega}{[\omega - W_p]^2 + \frac{1}{4}\gamma_p^2 \omega^2} \tag{5.44}$$

where

$$\gamma_p = \frac{15}{2}(4-\pi) \qquad \text{as} \quad \eta \to 0 \ .$$

First we show that the low frequencies exhaust the identity

$$\int_{-\infty}^{\infty} \frac{d\omega}{2\pi} \, \frac{A(p,\omega)}{\beta\omega} = \frac{1}{\beta W_p} \tag{5.45}$$

We have

$$\begin{aligned} \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} \, \frac{A(p,\omega)}{\beta\omega} &= \frac{\gamma_p}{2\pi\beta} \int_{-\infty}^{\infty} \frac{d\omega}{(\frac{1}{4}\gamma_p^2 + 1)\omega^2 - 2W_p\omega + W_p^2} \\ &= \frac{\gamma_p}{2\pi\beta} \, \frac{2}{\gamma_p W_p} \left[\tan^{-1} \frac{2(1+\frac{1}{4}\gamma_p^2)\omega - 2W_p}{\gamma_p W_p} \right]_{-\infty}^{\infty} \\ &= \frac{1}{\beta W_p} \ . \end{aligned} \tag{5.46}$$

Eq. (5.39) demonstrate the consistency of the Very Dense State limit. To demonstrate the validity of the Very Dense State limit, we note that for $\beta\omega << 1$, $\beta\Gamma(p,\omega) << 1$, so that the width of the spectral function is contained in the small ω interval. The condition on the peak of the spectral function is always satisfied if $p_0 \lesssim p_1$. Hence the "continuity" conditions are satisfied.

Now we show that the low frequencies do not exhaust the sum rule

$$\int_{-\infty}^{\infty} \frac{d\omega}{2\pi} A(p,\omega) = 1 \quad . \tag{5.47}$$

We write

$$\int_{-\infty}^{\infty} \frac{d\omega}{2\pi} A(p,\omega) = \int_{-\omega_c}^{\omega_c} \frac{d\omega}{2\pi} \; \frac{\gamma_p \omega}{(\frac{1}{4}\gamma_p^2+1)\omega^2 + W_p\omega + W_p^2}$$

where ω_c is introduced as a cutoff for the logarithmic singularity at infinity. As we want to include as much as possible of the peak at W_p, we set $\omega_c >> W_p$. Then

$$\int_{-\infty}^{\infty} \frac{d\omega}{2\pi} A(p,\omega) = \frac{1}{\frac{1}{4}\gamma_p^2+1} \left\{ 1 + \frac{1}{2} \ln \left[\frac{(\frac{1}{4}\gamma_p^2+1)\,\omega_c^2 - 2W_p\omega_c}{(\frac{1}{4}\gamma_p^2+1)\,\omega_c^2 + 2W_p\omega_c} \right] \right\}$$

$$\simeq \frac{1}{\frac{1}{4}\gamma_p^2+1} \qquad \text{for } \omega_c >> W_p \quad . \tag{5.48}$$

In the particular case $\eta \longrightarrow 0$, $1/(1 + \frac{1}{4}\gamma_p^2) \simeq 0.1$. Therefore the sum rule is far from being exhausted.

Eq. (5.48) can also be obtained from the analytic Green's function and Herglotz Theorem.[102] Herglotz Theorem[103] states that if, in the upper half plane ($\mathrm{Im}\, z > 0$), $G(z)$ is analytic, $\mathrm{Im}\, G(z) > 0$,

$\lim_{z\to\infty}\left[z\,G(z)\right] = c_0$ (a real constant), then

$$G(z) = \int_{-\infty}^{\infty}\frac{d\omega}{2\pi}\,\frac{A(\omega)}{z-\omega} \qquad \mathrm{Im}\, z > 0$$

and

$$\int_{-\infty}^{\infty}\frac{d\omega}{2\pi}\,A(\omega) = c_0 \;.$$

In our case, the analytic Green's function can be written, for $|\beta z| << 1$, as

$$G(p,z) = \frac{1}{z - W_p - i\frac{1}{2}\gamma_p z} \quad ; \quad z = \omega + i\delta \;. \qquad (5.49)$$

Eq. (5.48) is then obtained from (5.49) by applying Herglotz Theorem to (5.49) and noting that $c_o = 1/(1 + \frac{1}{4}\gamma_p^2)$.

Note that in the normal fermion case where $\Gamma \sim \omega^2$ the sum rule is satisfied near zero temperature if we ignore the ω dependence of the real part. Furthermore for the fermions, the imaginary part is small with respect to the real part, i.e. for a pole at $z = \omega + i\Gamma$, the time development is

$$e^{i(\omega + i\Gamma)t} = e^{i\omega t(1 + i\Gamma/\omega)}$$

and the attenuation $(\Gamma/\omega) \sim \omega$ is small. These considerations led to the naming of the excitations in fermi systems near zero temperatures as quasi-particles. In the case of bosons, since $\Gamma \sim \omega$, no quasi-particle interpretation is warranted. Following Patashinskii and Pokrovskii,[94] we call these excitations with $\Gamma \sim \omega$ and $\Delta \sim p^{3/2}$

as low-frequency, low-momentum single-particle fluctuations. Mathematically, these excitations are represented by a pole of the single-particle analytic Green's function on the unphysical z-plane near the origin. For $p > 0$, the pole is on the unphysical sheet in the first quadrant. As $p \rightarrow 0$ the pole approaches the cut on the real axis at $z = \eta$; then as $\eta \rightarrow 0$, the pole approaches the origin and goes onto the physical sheet, which is the mathematical representation of the macroscopic occupation of the zero momentum state. Physically the excitations are fluctuations in the low-lying states as they anticipate the macroscopic occupation of the zero momentum state.

4. Macroscopic Properties

We turn from our microscopic analysis and consider its macroscopic consequences. As a beginning, we collect some thermodynamic relations for the three second-derivatives of the Gibbs potential. The isothermal compressibility κ_T is

$$\kappa_T \equiv -\frac{1}{V}\left(\frac{\partial V}{\partial P}\right)_{T,N} = -\frac{V}{N^2}\,\Omega_{\mu\mu} \tag{5.50}$$

where we wrote in shorthand $\Omega_{\mu\mu} = (\partial^2\Omega/\partial\mu^2)_{TV}$.

The isobaric coefficient of thermal expansion α_p is

$$\alpha_p \equiv \frac{1}{V}\left(\frac{\partial V}{\partial T}\right)_{PN} = -\frac{1}{N}\left[\frac{S}{N} - \frac{\Omega_{\mu T}}{\Omega_{\mu\mu}}\right]\Omega_{\mu\mu}, \tag{5.51}$$

The isobaric specific heat c_p is

$$c_p \equiv \frac{T}{\mathcal{V}}\left(\frac{\partial S}{\partial T}\right)_{pN} = c_{\mathcal{V}} - \frac{T}{\mathcal{V}}\left[\frac{S}{N} - \frac{\Omega_{\mu T}}{\Omega_{\mu\mu}}\right]^2 \Omega_{\mu\mu} \tag{5.52a}$$

where the isometric specific heat $c_{\mathcal{V}}$ is

$$c_{\mathcal{V}} \equiv \frac{T}{\mathcal{V}}\left(\frac{\partial S}{\partial T}\right)_{\mathcal{V}N} = \frac{T}{\mathcal{V}}\left[\frac{\Omega_{\mu T}^2}{\Omega_{\mu\mu}} - \Omega_{TT}\right] . \tag{5.52b}$$

Note the common occurence of the factor $\Omega_{\mu\mu}$ in eqs. (5.50,51,52).

The macroscopic properties may be obtained from the microscopic analysis by eq. (2.61) for the Massieu potential, which can be written

$$\beta\Omega = -\Phi' + \mathrm{tr}(\Sigma_1' G_1) + \mathrm{tr}\ln(-\bar{G}') \tag{5.53}$$

where Ω is the Grand potential expressed as a function of (T, $\mathcal{V}$, η), Φ' does not include the Hartree-Fock terms which have been absorbed into the free particle Green's function

$$[G_1^0(p,\zeta_\nu)]^{-1} = \zeta_\nu - \epsilon'(p) + \eta \tag{5.54}$$

$$[G_1(p,\zeta_\nu)]^{-1} = [G_1^0(p,\zeta_\nu)]^{-1} - \Sigma_1'(p,\zeta_\nu) , \tag{5.55}$$

where η and $\epsilon'(p)$ are defined by eqs. (2.110)(2.111a) respectively and

$$\Sigma_1'(p,\zeta_\nu) = \Sigma_1(p,\zeta_\nu) - \Sigma_1(0,0)$$

$$\Sigma_1'(p, \zeta_\nu) = \frac{\delta \Phi[G_1]'}{\delta G_1(p, \zeta_\nu)} \quad . \tag{5.56}$$

We first take the derivative of (5.53) with respect to η :

$$\beta \frac{\partial \Omega}{\partial \eta} = tr\left(G_1 \frac{\partial \Sigma_1'}{\partial \eta}\right) + tr\left(G_1 \frac{\partial G_1^{-1}}{\partial \eta}\right) \tag{5.57}$$

where we have used the fact that

$$\frac{\partial \Phi'}{\partial \eta} = tr\left(\Sigma_1' \frac{\partial G_1}{\partial \eta}\right) \quad .$$

From eq. (5.55), we see that

$$\frac{\partial G_1^{-1}}{\partial \eta} = -1 - \frac{\partial \Sigma_1'}{\partial \eta} \quad , \tag{5.58}$$

and eq. (5.57) becomes simply

$$\beta \frac{\partial \Omega}{\partial \eta} = -tr G_1 = \beta N . \tag{5.59}$$

Taking one more derivative with respect to η , we have from (5.58)(5.59)

$$\beta \frac{\partial^2 \Omega}{\partial \eta^2} = -tr\, G_1^2 - tr\left(G_1^2 \frac{\partial \Sigma_1'}{\partial \eta}\right) \quad . \tag{5.60}$$

The general equations are now specialized to the Very Dense State limit, which is most conveniently taken in the (p, ζ_ν) representation by setting $\zeta_\nu = 0$. We have in this manner

$$\beta\Omega = -\Phi[G(p,0)] + \sum_p \Delta'(p,0)\, G(p,0) + \qquad (5.61)$$
$$+ \sum_p \ln\left(-G^{-1}(p,0)\right)$$

$$\beta\Omega_\eta = -\sum_p G(p,0) \qquad (5.62)$$

$$\beta\Omega_{\eta\eta} = -\sum_p G^2(p,0) - \sum_p G^2(p,0)\,\frac{\partial\Delta'(p,0)}{\partial\eta} , \qquad (5.63)$$

where functionals of $G_1(p, \zeta_\nu)$ are replaced by the same functional of $G_1(p,0)$. It should be emphasized again that eqs. (5.61-63) are not the equations for a quasi-particle description of the system, although the imaginary part of the self-energy do not play an important role. The discussion of eqs. (2.115,116) applies here to eq. (5.62).

The Green's function in the Very Dense State limit can be written, from (5.49), as

$$G(p,0) = -\frac{1}{\Delta'_p + \epsilon^0_p + \eta} . \qquad (5.64)$$

We write the real part of the self-energy at $\zeta = 0$ as

$$\Delta'_p = A_1 p^2 H(p_1 - p) + A_0 p^{3/2} H(p - p_1) H(p_0 - p) + \\ + \epsilon_p^0 e^{-\lambda\beta_0 \epsilon^0 (p - p_0)} H(p - p_0) \quad , \tag{5.65a}$$

where H(p) is the Heaviside function

$$H(p) = \begin{cases} +1 & p > 0 \\ 0 & p < 0 \end{cases} \quad , \tag{5.65b}$$

λ is an arbitrary constant introduced to preserve the continuity of Δ'_p and will be taken as very large, and p_1, p_o are defined by $A_1 p_1^{\,2} = A_o p_1^{\,3/2}$ and $\epsilon^o_{p_o} = A_o p_o^{\,3/2}$ respectively. Using eqs.(5.64) (5.65), we can evaluate $\Omega_{\eta\eta}$ of (5.63). We write

$$\sum_p G^2(p) \simeq \sum_{p=0}^{p_1} G^2(p) + \sum_{p=p_1}^{p_0} G^2(p) + \sum_{p=p_0}^{p_2} G^2(p) \tag{5.66}$$

and find

$$\sum_{p=0}^{p_1} G^2(p) = \frac{v}{2\pi^2 \hbar^3 A_1^2} \Big[- \frac{p_1}{2(p_1^2 + \eta/A_1)} + \\ + \frac{1}{2} \sqrt{\frac{A_1}{\eta}} \operatorname{Arctan}\Big(p_1 \sqrt{\frac{A_1}{\eta}}\Big) \Big] \tag{5.67a}$$

$$\sum_{p=p_1}^{p_0} G^2(p) = \frac{v}{2\pi^2\hbar^3 A_0^2}\,\frac{2}{3}\left[\ln\left|\frac{p_0^{3/2}+\eta/A_0}{p_1^{3/2}+\eta/A_0}\right| + \right.$$

$$\left. + \frac{\eta}{A_0}\left(\frac{1}{p_0^{3/2}+\eta/A_0} - \frac{1}{p_1^{3/2}+\eta/A_0}\right)\right] \qquad (5.67b)$$

$$\sum_{p=p_0}^{p_2} G^2(p) = \frac{v(2m)^2}{2\pi^2\hbar^3}\left[\frac{p_0}{2(p_0^2+2m\eta)} - \right.$$

$$\left. - \frac{1}{2\sqrt{2m\eta}}\,\mathrm{Arctan}\left(\frac{p_0}{\sqrt{2m\eta}}\right)\right] - \qquad (5.67c)$$

$$-\beta_0^2 v \lambda_{T_0}^{-3} F_{1/2}(\beta\eta) .$$

In the limit $\eta \to 0$, we note that $p_1 \sim \eta^{2/3}$, $A_1 \sim \eta^{-1/3}$ so that the leading term is logarithmically divergent

$$\sum_{p} G^2(p) = \frac{v}{3\pi^2\hbar^3 A_0^2}\,\ln\left|\frac{p_0^{3/2}}{p_1^{3/2}+\eta/A_0}\right| \quad ; \quad \eta \to 0 , \qquad (5.68)$$

which comes from the integration over the $p^{3/2}$-spectrum eq. (5.67b). To complete the calculation, we note that

$$\frac{\partial \Delta'(p,0)}{\partial\eta} = \frac{\partial \Delta'_p}{\partial\eta} = \frac{\partial A_1}{\partial\eta}\, p^2 H(p_1 - p) + (\text{exponential}) \qquad ,$$

where the exponential term is negligible as $\lambda \to \infty$ and

$$\sum_{p=0}^{p_1} p^2 G^2(p) = \frac{\mathcal{V}}{2\pi^2\hbar^3 A_1^2}\left[p_1 + \frac{1}{2}\frac{\eta}{A_1}\frac{p_1}{p_1^2+\eta/A_1} - \frac{3}{4}\sqrt{\frac{\eta}{A_1}}\,\mathrm{Arctan}\left(p_1\sqrt{\frac{A_1}{\eta}}\right)\right] . \tag{5.69}$$

As $\eta \to 0$, $\sum_p G^2(p)\ (\partial \Delta'(p,0)/\partial\eta\ ) \sim 0(1)$. Therefore we have

$$\beta\Omega'_{\eta\eta} = -\frac{\mathcal{V}}{3\pi^2\hbar^3 A_0^2}\ln\left|\frac{p_0^{3/2}}{p_1^{3/2}+\eta/A_0}\right| \tag{5.70}$$

where the prime indicates just the divergent term. Using the definitions of p_0, p_1 and A_0 (5.24), we rewrite eq. (5.70) as

$$\beta\Omega'_{\eta\eta} = \sqrt{\frac{15\pi}{18}}\,\frac{\beta_0\mathcal{V}}{V_0}\ln(\beta_0\eta)\ , \quad \eta\to 0 . \tag{5.71}$$

To make contact with the macroscopic relations (5.50-52), we need to go from $(T, \mathcal{V}, \eta)$ to $(T, \mathcal{V}, \mu)$. We do this for small η only, expanding η as

$$\eta = a(\mu-\mu_0) + b(T-T_0) \tag{5.72}$$

where a and b are constants. Then

$$\Omega_{\mu\mu} = a^2\Omega_{\eta\eta}\ ;\ \Omega_{\mu T} = ab\,\Omega_{\eta\eta}\ ;\ \Omega_{TT} = b^2\Omega_{\eta\eta} . \tag{5.73}$$

Therefore eqs. (5.50-52) reduces to

$$\kappa_T = -\frac{v}{N^2}\, a^2 \Omega'_{\eta\eta} + \cdots \tag{5.74}$$

$$\alpha_p = -\frac{1}{N}\left[\frac{S}{N} - \frac{b}{a}\right] a^2 \Omega'_{\eta\eta} + \cdots \tag{5.75}$$

$$c_p = -\frac{T}{v}\left[\frac{S}{N} - \frac{b}{a}\right]^2 a^2 \Omega'_{\eta\eta} + \cdots \tag{5.76}$$

where we retained only the logarithmically divergent term. Thus we conclude that the logarithmic singularity appears in all three of the quantities κ_T, α_p, c_p, but not in c_v.

The ratio $-b/a$ can be expressed as the change in μ divided by the change in T when $\eta = 0$. In other words

$$-\frac{b}{a} = \left(\frac{\partial \mu}{\partial T}\right)_{\eta=0} = -\frac{S}{N} + \frac{v}{N}\left(\frac{\partial P}{\partial T}\right)_{\eta=0} \tag{5.77}$$

after the usual thermodynamic manipulations. Using eq. (5.77) in (5.74-76), we see that

$$\kappa_T = -\frac{v}{N^2}\, a^2 \Omega'_{\eta\eta} + \cdots \tag{5.78}$$

$$\alpha_p = -\frac{v}{N^2}\left(\frac{\partial P}{\partial T}\right)_{\eta=0} a^2 \Omega'_{\eta\eta} + \cdots \tag{5.79}$$

$$c_p = -\frac{v}{N^2}\, T\left(\frac{\partial P}{\partial T}\right)^2_{\eta=0} a^2 \Omega'_{\eta\eta} + \cdots \tag{5.80}$$

In liquid helium-4, $(\partial P/\partial T)_{\eta=0} \simeq -130$ atm/°K at $T_\lambda = 2.18$°K, which is a large number compared with $nk_B \simeq 3$ atm/°K . Therefore one would expect the logarithm singularity to be most accessible in c_p , less so in α_p , and even less so in κ_T . To make a reasonable estimate of this, one has to include the relative magnitude of the nondivergent terms.[104] We note that the ratio of the logarithm term of c_p to α_p is given by $T(\partial P/\partial T)_{\eta=0}$. Using the measured value for c_p , eq. (1.1) and α_p

$$\alpha_p = 0.0415 + 1.45\times 10^{-2} \log_{10}|T-T_\lambda| \quad \left(\frac{1}{°K}\right) ,$$

we find that $(c_p/\alpha_p)_{\log} \simeq -298$ atm. This is to be compared with the above prediction of $T_\lambda (\partial P/\partial T)_{\eta=0} \simeq -284$ atm.

A crude estimate of the width of the logarithm can be made by noting its dependence on the $p^{3/2}$-spectrum. The $p^{3/2}$-spectrum vanishes when $\eta \sim 9(n^{1/3}a_s)^2 k_B T_o$. Therefore the width of the logarithm is given by

$$\frac{T-T_0}{T_0} \sim \frac{9k_B}{b}(n^{1/3}a_s)^2 .$$

Of course the width depends on the relative magnitude of the nondivergent terms.

To determine the shift in the transition temperature, we go back to eq. (5.62)

$$N = -k_B T \sum_p G(p,0) . \tag{5.81}$$

As $\eta \longrightarrow 0$, we have

$$n = \frac{k_B T_0}{\pi^2 \hbar^3}\left[\frac{p_0^{3/2}}{3A_0} - m p_0\right] + \lambda_{T_0}^{-3}\,\zeta\left(\frac{3}{2}\right) \quad . \tag{5.82}$$

Approximating p_o by $(2mA_o)^2$ and using (5.24), we get

$$T_0 = T_0^i\left[1 - \frac{16}{3\pi^2\sqrt{15}\,\zeta(3/2)}\left(\frac{m^3 V_0^2}{\beta_0 \hbar^6}\right)^{1/2}\right]^{-2/3} \quad . \tag{5.83}$$

where T_o^i is the transition temperature for the ideal Bose gas. Treating the term involving V_o as small, we write (5.83) as

$$\frac{T_0 - T_0^i}{T_0} = 0.838\,\left(n^{1/3} a_s\right) \quad . \tag{5.84}$$

Hence the presence of the repulsive potential V_o raises the transition temperature. Recalling eq. (4.120), we see that a repulsive potential contributes both to a lowering term through the effective mass and to a raising term in the very short-ranged limit. The sign of eq. (5.84) is consistent with the hard core example, eq. (4.136).

C. Born-Collision Approximation -- (Variational Calculation)

We continue our investigation of the Born-Collision approximation above the transition by considering variational techniques. In Chapter II, we noted that in general the variation of the Massieu potential $\mathcal{W}$ with respect to the total self-energy Σ^{tot} does not have a maximal property but a stationary one. However for a special class of variations, we can show that the variation of $\mathcal{W}$ does indeed have a maximal property. We first show that the Born-Collision approximation in the Very Dense State limit is stable under arbitrary variations of a special class of self-energies. We then apply the variational techniques to the bulk limit to recover some of the results of the previous section, and finally we apply the same techniques to restricted geometry.

1. Stability in the Very Dense State Limit

We begin by recalling the general equations for first and second variations of the Massieu potential, eqs. (2.62)(2.65) respectively, and rewrite them in terms of the Grand potential Ω

$$\beta\,\delta\Omega = \sum_{p,\nu} G^2(p,\zeta_\nu)\left[\Sigma^{tot}(p\zeta_\nu) - \frac{\delta\Phi[G_1]}{\delta G(p\zeta_\nu)}\right]\delta\Sigma^{tot}(p\zeta_\nu) \tag{5.85}$$

$$\beta\,{}^2\Omega = \sum_{p,\nu} G^2(p,\zeta_\nu)\Bigg[\left(\delta\Sigma^{tot}(p\zeta_\nu)\right)^2 - \\ - \sum_{p'\zeta_{\nu'}} G^2(p'\zeta_{\nu'})\frac{\delta^2\Phi[G_1]}{\delta G(p'\zeta_{\nu'})\,\delta G(p\zeta_\nu)}\,\delta\Sigma^{tot}(p'\zeta_{\nu'})\,\delta\Sigma^{tot}(p\zeta_\nu)\Bigg] \tag{5.86}$$

where the second variation is evaluated at the point

$$\Sigma^{tot}(p\zeta_\nu) = \frac{\delta\Phi[G_1]}{\delta G(p\zeta_\nu)} \quad . \tag{5.87}$$

From eqs. (5.85-87), it can be shown that if we restrict ourselves to arbitrary variations in Σ^{tot} which are frequency independent, i.e. $\delta\Sigma^{tot}(p) = \delta\Sigma^{o}(p)$, the Ideal, Hartree, and Hartree-Fock approximations are all stable, i.e. $\delta^2\Omega > 0$. This result is to be compared with the fact that even the Ideal approximation is not stable[105] under arbitrary variations of $\Sigma^{tot}(p, \zeta_\nu)$. For the Born-Collision approximation, we find that Ω is stable in the Very Dense State limit under arbitrary variations in Δ'_p.

To demonstrate this assertion for the Born-Collision approximation, we find it convenient to absorb the Hartree-Fock terms into the free particle Green's functions, not unlike eqs. (5.53-56), viz.

$$[G_1^o(p,\zeta_\nu)]^{-1} = \zeta_\nu - \epsilon'(p) - \eta \tag{5.88}$$

$$[G_1(p,\zeta_\nu)]^{-1} = [G_1^o(p,\zeta_\nu)]^{-1} - \Sigma'(p,\zeta_\nu) \tag{5.89}$$

$$\Sigma'(p,\zeta_\nu) = \Sigma(p,\zeta_\nu) - \Sigma(0,0) \tag{5.90}$$

$$\Sigma(p,\zeta_\nu) = \frac{\delta\Phi[G_1]}{\delta G(p,\zeta_\nu)} \qquad , \tag{5.91}$$

where η and $\epsilon'(p)$ are defined by eqs. (2.110)(2.111a) respectively and Φ does not include the Hartree-Fock terms. Then eqs. (5.85) (5.86) become

$$\beta\delta\Omega = \sum_{p,\nu} G^2(p,\zeta_\nu)\left[\Sigma'(p,\zeta_\nu) - \left(\frac{\delta\Phi[G_1]}{\delta G(p\zeta_\nu)}\right)'\right]\delta\Sigma'(p\zeta_\nu) \tag{5.92}$$

$$\begin{aligned}\beta^2\delta^2\Omega = \sum_{p\nu} G^2(p\zeta_\nu)\Bigg[&\left(\delta\Sigma'(p,\zeta_\nu)\right)^2 - \\ &- \sum_{p'\zeta_{\nu'}} G^2(p'\zeta_{\nu'})\frac{\delta}{\delta G(p'\zeta_{\nu'})}\left(\frac{\delta\Phi[G_1]}{\delta G(p\zeta_\nu)}\right)'\delta\Sigma'(p'\zeta_{\nu'})\,\delta\Sigma'(p\zeta_\nu)\Bigg]\end{aligned} \tag{5.93}$$

where

$$\left(\frac{\delta\Phi[G_1]}{\delta G(p\zeta_\nu)}\right)' = \frac{\delta\Phi[G_1]}{\delta G(p,\zeta_\nu)} - \left(\frac{\delta\Phi[G_1]}{\delta G(p,\zeta_\nu)}\right)_{\substack{p=0\\ \zeta_\nu=0}} . \tag{5.94}$$

From eq. (5.5), we see that the Born-Collision part of Φ can be written in the symmetric form

$$\Phi_{BC} = -\frac{1}{4}\left(\frac{1}{-i\beta\mathcal{V}}\right)^3 \sum_{\substack{p_1p_2p_3p_4\\ \nu_1\nu_2\nu_3\nu_4}} \Lambda(\{p\}\{\nu\}) \times$$

$$\times\, G(p_1 z_{\nu_1})\, G(p_2 z_{\nu_2})\, G(p_3 z_{\nu_3})\, G(p_4 z_{\nu_4}) \;, \tag{5.95a}$$

where

$$\Lambda(\{p\},\{\nu\}) = \frac{1}{2}\left[V(p_2-p_1)+V(p_4-p_1)\right]^2 \times$$

$$\times (2\pi\hbar)^3\,\delta(p_1-p_2+p_3-p_4)\,(-i\beta)\,\delta_{\nu_1-\nu_2+\nu_3-\nu_4} \;. \tag{5.95b}$$

We now take the Very Dense State limit by setting all the $z_\nu = 0$, perform the angular integration in momentum space, and assume a very short-ranged potential to reduce (5.95) to

$$\Phi_{BC} = \frac{2V_0^2\mathcal{V}}{\beta}\;\frac{1}{4}\int_{\mathcal{V}} d^3r \left[\frac{1}{\mathcal{V}}\sum_{p'} G(p';0)\, j_0\!\left(\frac{rp'}{\hbar}\right)\right]^4 . \tag{5.96}$$

Therefore

$$\left(\frac{\delta\Phi_{Bc}[G_1]}{\delta G(p,0)}\right)' = \frac{2V_0^2}{\beta}\int_v d^3r\left[j_0\left(\frac{rp}{\hbar}\right)-1\right]\times$$

$$\times\left[\frac{1}{v}\sum_{p'}G(p'0)\,j_0\left(\frac{rp'}{\hbar}\right)\right]^3 \tag{5.97}$$

and

$$\frac{\delta}{\delta G(p'0)}\left(\frac{\delta\Phi_{Bc}}{\delta G(p0)}\right)' = \frac{6V_0^2}{\beta^2 v}\int_v d^3r\left[j_0\left(\frac{rp}{\hbar}\right)-1\right]j_0\left(\frac{rp'}{\hbar}\right)\times$$

$$\times\left[\frac{1}{v}\sum_{\bar{p}}G(\bar{p}0)\,j_0\left(\frac{r\bar{p}}{\hbar}\right)\right]^2 . \tag{5.98}$$

Hence from eqs. (5.92)(5.97), we see that the vanishing of the first variation of Ω with respect to $\delta\Sigma'(p,0) = \delta\Delta'_p$ leads directly to eq. (5.18). Substituting eq. (5.98) into (5.93), we see that the second variations can be written as

$$\beta\,\delta^2\left(\frac{\Omega}{v}\right) = \frac{1}{v}\sum_p G^2(p0)\,\delta\Delta'_p\,\delta\Delta'_p \; +$$

$$+\frac{6V_0^2}{\beta^2}\int_v d^3r\left[\frac{1}{v}\sum_{\bar{p}}G(\bar{p}0)\,j_0\left(\frac{r\bar{p}}{\hbar}\right)\right]^2\times$$

$$\times\left[\frac{1}{v}\sum_p G^2(p0)\left(1-j_0\left(\frac{rp}{\hbar}\right)\right)\delta\Delta'_p\right]\left[\frac{1}{v}\sum_{p'}G^2(p'0)\,j_0\left(\frac{rp'}{\hbar}\right)\delta\Delta'_{p'}\right] . \tag{5.99}$$

Since the p-integrations are over small p's, the integrations are all positive. Therefore $\delta^2\Omega > 0$ and Ω is minimized at the vanishing of the first variations under arbitrary variations of Δ'_p. Since the variations are arbitrary, the second functional derivative is given by

$$\beta \frac{\delta^2\Omega}{\delta \Delta_p'^2} = G^2(p0) + \frac{6V_0^2}{\beta^2 \mathcal{V}} G^4(p0) \times \\ \times \int_{\mathcal{V}} d^3r \left[1 - j_0\left(\frac{rp}{\hbar}\right)\right] j_0\left(\frac{rp}{\hbar}\right) \times \\ \times \left[\frac{1}{\mathcal{V}} \sum_{p'} G(p'0)\, j_0\left(\frac{rp'}{\hbar}\right)\right]^2 . \tag{5.100}$$

2. The Bulk Limit

In order to gain some confidence and insight into the variational technique, we now apply it to a case for which we have the solution, the bulk limit. We assume a trial self-energy of the form (5.65)

$$\Delta'_p = A_1 p^2 H(p_1 - p) + A_0 p^{3/2} H(p - p_1)\, H(p_0 - p) + \\ + \epsilon_p^0 \exp\left[-\lambda \beta_0 \epsilon^0 (p - p_0)\right] H(p - p_0) \tag{5.101}$$

where p_1 and p_0 are defined so that Δ'_p is continuous, i.e. $A_1 p_1^{\;2} = A_0 p_1^{3/2}$, $A_0 p_0^{3/2} = \epsilon^0_{p_0}$. Instead of an arbitrary variation, which as we have seen recovers the self-consistent integral equation (5.18), we assume the form (5.101) and vary A_0 and A_1 .

The first variation then gives us two algebraic equations for A_0 and A_1. However, because of the explicit variational form of (5.101), we run into some spurious results which we now examine in detail.

Inserting eq. (5.101) into (5.92), we obtain the first variation

$$\beta\delta\Omega = \sum_{p=0}^{P_1} G^2(p,0)\,p^2\left[A_1p^2 - \left(\frac{\delta\Phi_{BC}}{\delta G(p0)}\right)'\right]\delta A_1 + \\ + \sum_{p=P_1}^{P_0} G^2(p,0)\,p^{3/2}\left[A_0p^{3/2} - \left(\frac{\delta\Phi_{BC}}{\delta G(p0)}\right)'\right]\delta A_0 \qquad (5.102)$$

where the exponential term has been neglected. Inserting eq. (5.101) into (5.97), we find

$$\frac{\delta\Phi_{BC}'}{\delta G(p0)} = \frac{V_0^2}{\pi^5\hbar^9\beta^2}\int_0^\infty r^2dr\left[1-j_0\left(\frac{rp}{\hbar}\right)\right]D^3(r) \qquad (5.103)$$

with

$$D(r) = \int_0^{P_1}\frac{q^2dq}{A_1q^2+\eta}\,j_0\left(\frac{rq}{\hbar}\right) + \int_{P_1}^{P_0}\frac{q^2dq}{A_0q^{3/2}}\,j_0\left(\frac{rq}{\hbar}\right) + \\ + \int_{P_0}^{P_2}\frac{q^2dq}{\epsilon_q^0}\,j_0\left(\frac{rq}{\hbar}\right) , \qquad (5.104)$$

where we used the similar arguments as in the self-consistent case to reduce D(r). The second variation is obtained from (5.93)

$$\beta\delta^2\Omega = \sum_p G^2(p0)\,\delta\Delta'_p\,\delta\Delta'_p - \\ -\sum_p\sum_{p'} G^2(p0)\,G^2(p'0)\,\frac{\delta}{\delta G(p'0)}\left(\frac{\delta\Phi_{BC}}{\delta G(p0)}\right)'\delta\Delta'_{p'}\,\delta\Delta'_p \tag{5.105}$$

with

$$\delta\Delta'_{p'}\,\delta\Delta'_p = p'^2p^2\,H(p_1-p')\,H(p_1-p)\,(\delta A_1)^2 + \\ + \left[p'^{3/2}H(p'-p_1)\,H(p_0-p')\,H(p_1-p) + \right. \\ \left. + p^{3/2}H(p-p_1)\,H(p_0-p)\,H(p_1-p')\right]\delta A_0\,\delta A_1 \tag{5.106} \\ + p'^{3/2}p^{3/2}\,H(p'-p_1)\,H(p_0-p')\,H(p-p_1)\,H(p_0-p)\,(\delta A_0)^2 \;;$$

and from eq. (5.98)

$$\frac{\delta}{\delta G(p'0)}\left(\frac{\delta\Phi_{BC}}{\delta G(p0)}\right)' = -\frac{6V_0^2}{\pi^3\hbar^6\beta^2 V}\int_0^\infty r^2dr\left[1-j_0\left(\frac{rp}{\hbar}\right)\right]j_0\left(\frac{rp'}{\hbar}\right)D^2(r), \tag{5.107}$$

where D(r) is given by (5.104). The rest of this section will be spent in approximating D(r) for special cases of momentum range.

We begin by considering the limit $\eta \longrightarrow 0$, which results in $p_1 \longrightarrow 0$, $\delta A_1 \longrightarrow 0$. Therefore the vanishing of the first variation (5.102) yields

$$\beta \frac{\delta \Omega}{\delta A_0} = \sum_{p=0}^{p_0} G^2(p0)\, p^{3/2} \left[A_0 p^{3/2} - \left(\frac{\delta \Phi_{BC}}{\delta G(p0)} \right)' \right] = 0 \qquad (5.108)$$

We estimate D(r) at $r \simeq \hbar/p$:

$$D\left(\frac{\hbar}{p}\right) \simeq \frac{1}{A_0} \int_0^{p_0} q^{1/2} dq\, j_0(q/p) + 2m \int_{p_0}^{p_1} dq\, j_0(q/p)$$
$$\simeq \sqrt{\frac{\pi}{2}}\, \frac{p^{3/2}}{A_0} - \frac{p^{3/2}}{A_0} \int_{p_0/p}^{\infty} x^{1/2} j_0(x)\, dx + 2mp \int_{p_0/p}^{\infty} j_0(x)\, dx .$$

In the interval $0 < p < p_0$, we see that $D(\hbar/p)$ goes from

$$\lim_{p \to 0} D\left(\frac{\hbar}{p}\right) \simeq \sqrt{\frac{\pi}{2}}\, \frac{p^{3/2}}{A_0}$$

to

$$\lim_{p \to p_0} D\left(\frac{\hbar}{p}\right) \simeq \sqrt{\frac{\pi}{2}}\, \frac{p^{3/2}}{A_0} - \frac{p_0^{3/2}}{A_0} \left[\int_1^{\infty} x^{1/2} j_0(x)\, dx - \right.$$
$$\left. - \int_1^{\infty} j_0(x)\, dx \right] .$$

Numerical estimate of the integrals in the bracket shows their value to be $\simeq 0.008$ and therefore negligible. Hence D(r) is given by

$$D(r) \simeq \frac{1}{A_0} \left(\frac{\hbar}{r}\right)^{3/2} \int_0^{\infty} y^{1/2} dy\, j_0(y) = \frac{1}{A_0} \sqrt{\frac{\pi}{2}} \left(\frac{\hbar}{r}\right)^{3/2} \qquad (5.109)$$

Substituting (5.109) back into (5.103), we find

$$\frac{\delta \Phi'_{Bc}}{\delta G(p0)} = \frac{2}{15\pi^3}\left(\frac{V_0^2}{\beta_0^2\hbar^6}\right)\frac{p^{3/2}}{A_0^3} \quad , \tag{5.110}$$

which, when inserted into (5.108), yields eq. (5.24)

$$A_0^4 = \frac{2}{15\pi^3}\left(\frac{V_0^2}{\beta_0^2\hbar^6}\right) \quad . \tag{5.111}$$

The second variation (5.105) can be likewise calculated, and we find

$$\beta A_0^2 \, \frac{\delta^2\Omega}{\delta A_0^2} = \frac{2}{3\pi^2}\left(\frac{v p_0^3}{\hbar}\right) \geq 0 \tag{5.112}$$

which vanishes at $p_o = 0$.

We consider now the case $\eta > 0$. The vanishing of the first variation (5.102) now leads to two equations, one for A_o (5.108) and another for A_1

$$\beta \, \frac{\delta\Omega}{\delta A_1} = \sum_{p=0}^{p_1} G^2(p0)\, p^2 \left[A_1 p^2 - \left(\frac{\delta \Phi_{Bc}}{\delta G(p0)}\right)'\right] = 0 \quad . \tag{5.113}$$

We treat first the equation for A_o . In the region $p_1 < p < p_o$, we add to our previous expression for $D(r)$ in $0 < p < p_o$, eq. (5.109), corrections for the presence of $p_1 > 0$, so that

$$D(r) = \frac{1}{A_0}\sqrt{\frac{\pi}{2}}\left(\frac{\hbar}{r}\right)^{3/2} - \frac{1}{A_0}\left(\frac{\hbar}{r}\right)^{3/2}\int_0^{\frac{rp_1}{\hbar}} x^{1/2} j_0(x)\,dx \; + \\ + \frac{1}{A_1}\left(\frac{\hbar}{r}\right)\int_0^{\frac{rp_1}{\hbar}} \frac{x^2 dx\, j_0(x)}{x^2+(p_\eta r/\hbar)^2} \quad , \tag{5.114}$$

where p_η is defined by $A_1 p_\eta^2 = \eta$, which is a little smaller than p_1, and we assume $p_1 << p_0$. Numerical estimate of the two integrals in (5.114) show that the first integral dominates the second one. Therefore we approximate (5.114), just to get qualitative behavior, by

$$D(r) \simeq \frac{1}{A_0}\sqrt{\frac{\pi}{2}}\left(\frac{\hbar}{r}\right)^{3/2} - \frac{2}{3}\frac{p_1^{3/2}}{A_0}\, H\!\left(\frac{\hbar}{p_1} - r\right) \quad , \tag{5.115}$$

where the cutoff in r is introduced since the expansion of $j_0(x) \simeq 1$ is good only for $x < 1$. Treating the constant term as a perturbation, we substitute (5.115) into (5.103) to obtain

$$\left(\frac{\delta\Phi_{BC}}{\delta G(p0)}\right)' = \frac{1}{A_0^3}\,\frac{2}{15\pi^3}\left(\frac{V_0^2}{\hbar^6\beta^2}\right)\left[p^{3/2} - \frac{15}{2\pi}c_1 p_1^{3/2}\right] \quad , \tag{5.116}$$

where we have neglected a slowly varying logarithmic term in p and have defined

$$c_1 \equiv \int_0^1 \frac{dy}{y}\left(1 - j_0(y)\right) \quad . \tag{5.117}$$

Eq. (5.108) finally gives

$$A_0^4 = \frac{2}{15\pi^3}\left(\frac{V_0^2}{\hbar^6\beta^2}\right)\left[1 - \frac{15}{2\pi}\, c_1\, \frac{p_1^{3/2}}{\langle p^{3/2}\rangle_0}\right] \tag{5.118}$$

where $\langle p^{3/2}\rangle_0$ is defined by

$$\begin{aligned}\langle p^{3/2}\rangle_0 &\equiv \sum_{p=p_1}^{p_0} G^2(p0)\,p^3 \Big/ \sum_{p=p_1}^{p_0} G^2(p0)\,p^{3/2} \\ &\simeq \frac{1}{2}\left(\frac{p_0^3 - p_1^3}{p_0^{3/2} - p_1^{3/2}}\right) .\end{aligned} \tag{5.119}$$

Thus in the limit $p_1 << p_o$, we find from (5.119) that (5.118) is

$$A_0^4 = \frac{2}{15\pi^3}\left(\frac{V_0^2}{\hbar^6\beta^2}\right)\left[1 - \frac{15c_1}{\pi}\left(\frac{p_1}{p}\right)^{3/2}\right] \quad ; \tag{5.120}$$

and we see that the self-consistent solution is approached for $p_1 << p << p_o$, and the $\eta \rightarrow 0$ solution for $p_1 \longrightarrow 0$.

Now let us consider the equation for A_1 (5.113). In the region $0 < p < p_1$, we write eq. (5.114) as

$$\begin{aligned}D(r) \simeq{} & \frac{\pi}{2A_1}\,\frac{\hbar}{r}\,e^{-\frac{r}{\hbar}p_\eta} - \frac{\hbar}{A_1 r}\int_{\frac{rp_1}{\hbar}}^{\infty}\frac{x^2\,dx\,j_0(x)}{x^2+(p_\eta r/\hbar)^2} + \\ & + \frac{1}{A_0}\left(\frac{\hbar}{r}\right)^{3/2}\int_{\frac{rp_1}{\hbar}}^{\infty} x^{1/2} j_0(x)\,dx .\end{aligned} \tag{5.121}$$

Recall that we have shown that asymptotically $D(r) \sim e^{-r}$ as $r \longrightarrow \infty$. This asymptotic behavior is important in the region $0 < p < p_1$ for it is necessary for the p^2- spectrum to occur. The other two terms in eq. (5.121) do not have an exponential behavior at large r's, but a $1/r^2$ dependence. This $1/r^2$ dependence arises because of the Heaviside functions[105] in our variational form (5.101). In other words, the exact Δ'_p is smooth and yields an exponential cutoff in $D(r)$, while (5.101) is not smooth leading to $1/r^2$ asymptotic behavior of $D(r)$. Because of the importance of the exponential cutoff, we demand that the special variation satisfies it also. Therefore we neglect the two integrals in (5.121) which lead to the spurious asymptotic behavior.

From eq. (5.103), we obtain

$$\left(\frac{\delta \Phi_{BC}}{\delta G(p0)}\right)' = \frac{V_0^2}{8\pi^2\hbar^6\beta^2}\,\frac{1}{A_1^3}\;I_0(p) \qquad , \tag{5.122}$$

where

$$\begin{aligned} I_0(p) &= \int_0^\infty \frac{dy}{y}\left[1 - j_0(yp/p_\eta)\right] e^{-3y} \\ &\simeq \frac{1}{54}\left(\frac{p}{p_\eta}\right)^2\left[1 - \frac{1}{30}\left(\frac{p}{p_\eta}\right)^2 + \cdots\right] . \end{aligned} \tag{5.123}$$

Substituting eqs. (5.122)(5.123) into (5.113), we obtain to first-order

$$A_1^3 = \frac{1}{432\pi^2}\left(\frac{V_0^2}{\hbar^6\beta^2\eta}\right) . \tag{5.124}$$

The second variation may now be calculated from eqs. (5.105-107). For $0 < p , p' < p_1$, we have

$$\frac{\delta}{\delta G(p'0)}\left(\frac{\delta\Phi_{BC}}{\delta G(p0)}\right)' = -\frac{3V_0^2}{2\pi\hbar^3\beta^2\mathcal{V}A_1^2 p} \times \\ \times\int_0^\infty dx\left[1-j_0(x)\right] j_0\left(x\frac{p'}{p}\right) e^{-2xp_\eta/p} \tag{5.125}$$

which leads to

$$\frac{\delta^2\Omega}{\delta A_1^2} \geqslant 0 \tag{5.126}$$

with the equal sign when $p_1 = 0$. For $p_1 < p , p' < p_0$, we have

$$\frac{\delta}{\delta G(p'0)}\left(\frac{\delta\Phi_{BC}}{\delta G(p0)}\right)' = -\frac{3V_0^2}{\pi^2\hbar^3\beta^2A_0^3\mathcal{V}} \times \\ \times\int_0^\infty \frac{dx}{x}\left[1-j_0(x)\right] j_0\left(x\frac{p'}{p}\right) \tag{5.127}$$

which leads to elementary integrals and the explicit second variation

$$\beta A_0^2 \frac{\delta^2\Omega}{\delta A_0^2} = \frac{2}{3\pi^2}\frac{\mathcal{V}}{\hbar^3}\left(p_0^3-p_1^3\right)\left[1-\frac{15c_1}{8\pi}\left(\frac{p_1}{p_0}\right)^{3/2}\right] \geqslant 0 \tag{5.128}$$

which vanishes when $p_o \to p_1$ and reduces to (5.112) for $p_1 \to 0$. Finally we have the two mixed regions: for $0 < p < p_1 < p' < p_o$, we have (5.125); for $0 < p' < p_1 < p < p_o$, we have (5.128). Then only the range of the integration changes, and we conclude that

$$\frac{\delta^2 \Omega}{\delta A_0 \delta A_1} \geq 0 \tag{5.129}$$

with the equal sign when $p_o = p_1 = 0$.

3. The Film Geometry

With the insight gained in the bulk limit, we apply the variational techniques to the film geometry. We orient the film to be in the xy-plane, of infinite extent, with the thickness L along the z-axis. We assume the same variational form for the self-energy as in eq. (5.101) with the stipulation that the momenta are to be given by $p^2 = p_{ll}^2 + p_z^2$, with $p_{ll}^2 = p_x^2 + p_y^2$. Because of the variational form (5.101), a sum over momenta can be thought of as a total of three sums in momentum space over (1) a sphere up to p_1, (2) a spherical shell from p_1 to p_o, (3) a spherical shell from p_o to p_2. For any function f(p) where p is the magnitude of the momenta, we have the limit

$$\begin{aligned}\lim_{v\to\infty} \frac{1}{v} \sum_{p} f(p) = \frac{1}{2\pi^2\hbar^3} \Big[\int_0^{p_1} dp_z \int_{p_z}^{p_1} + p_1 \int_{p_1}^{p_o} + \\ + \int_{p_1}^{p_o} dp_z \int_{p_z}^{p_o} + p_o \int_{p_o}^{p_2} + \int_{p_o}^{p_2} dp_z \int_{p_z}^{p_2} \Big] dp\, p\, f(p) .\end{aligned} \tag{5.130}$$

As usual, we assume box quantization

$$p_z = \frac{\pi\hbar}{L} l \qquad l = 1, 2, 3, \ldots \quad . \tag{5.131}$$

Thus for finite L , eq. (5.130) becomes

$$\lim_{\substack{L_x L_y \\ \to \infty}} \frac{1}{V}\sum_{p} f(p) = \frac{1}{2\pi^2\hbar^3}\Bigg[\frac{\pi\hbar}{L}\sum_{l=1}^{l_1}\int_{\frac{\pi\hbar}{L}l}^{p_1} + \frac{\pi\hbar}{L} l_1 \int_{p_1}^{p_0} + \frac{\pi\hbar}{L}\sum_{l=l_1+1}^{l_0}\int_{\frac{\pi\hbar}{L}l}^{p_0} + \frac{\pi\hbar}{L} l_0 \int_{p_0}^{p_2} + \frac{\pi\hbar}{L}\sum_{l=l_0+1}^{l_2}\int_{\frac{\pi\hbar}{L}l}^{p_2}\Bigg] dp\, p\, f(p) \quad , \tag{5.132}$$

where l_0, l_1, l_2 are defined (in the z -direction only) by

$$p_0 = \frac{\pi\hbar}{L} l_0 \quad , \qquad p_1 = \frac{\pi\hbar}{L} l_1 \quad , \qquad p_2 = \frac{\pi\hbar}{L} l_2 \quad , \tag{5.133}$$

where the equal sign is taken to mean taking the nearest integer. Eq. (5.130) can be recovered from (5.132) by the usual limit

$$\lim_{L \to \infty} \frac{\pi\hbar}{L}\sum_{l=l_0+1}^{l_2} f(p) = \int_{p_0}^{p_2} dp_z\, f(p) \quad . \tag{5.134}$$

With these preliminaries out of the way, we consider the physical situation.

We shall consider the model in which the film is in contact (thermal and material) with the bulk system. In the bulk system, η is given by (5.17)

$$\eta_{bulk} = -\mu + \Delta_0 + 2n V_0 \quad . \tag{5.135}$$

In a film geometry, we have

$$\eta = -\mu + \Delta_0 + 2n V_0 + E_0 \tag{5.136}$$

where E_o is the additional ground state energy due to finite L . We consider the bulk system to be on the transition, i.e. $\eta_{bulk} = 0$. Therefore since the chemical potentials are equal, we have for the film geometry

$$\eta = E_0 > 0 \quad . \tag{5.137}$$

This means that at T_o , the transition temperature of the bulk system, the film has not yet reached its transition temperature because of the additional ground state energy. Hence as L decreases from its bulk value, the transition temperature decreases from T_o . For a crude estimate of this dependence, we extrapolate (5.136-137) to $\eta = 0$, which corresponds to $\eta_{bulk} = - E_o = b(T - T_o)$. Since $E_o \simeq A_1(\pi\hbar/L)^2$, we have

$$T_f - T_0 = -\frac{A_1}{b}\left(\frac{\pi\hbar}{L}\right)^2 < 0 \tag{5.138}$$

where T_f is the film transition temperature. This $1/L^2$ dependence agrees well with experimental observations (see next chapter for more discussion). However since our Born-Collision approximation has only been investigated for $\eta_{\text{bulk}} \geqslant 0$, we consider the film geometry only for $\eta \geqslant E_o$.

We now proceed with the variational calculation. As we use the same variational form (5.101) as in the bulk limit, we get the same equations as the bulk limit, eqs. (5.102-103)(5.105-107), with D(r) given by

$$D(r) = -\Big[\frac{\pi\hbar}{L} \sum_{\ell=1}^{\ell_1} \int_{\frac{\pi\hbar}{L}\ell}^{p_1} + \frac{\pi\hbar}{L}\ell_1 \int_{p_1}^{p_0} + \frac{\pi\hbar}{L} \sum_{\ell=\ell_1+1}^{\ell_0} \int_{\frac{\pi\hbar}{L}\ell}^{p_0} + \\ + \frac{\pi\hbar}{L}\ell_0 \int_{p_0}^{p_2} + \frac{\pi\hbar}{L} \sum_{\ell=\ell_0+1}^{\ell_2} \int_{\frac{\pi\hbar}{L}\ell}^{p_2} \Big] dq\, q\, j_0\left(\frac{rq}{\hbar}\right) G(q,0) . \tag{5.139}$$

As in the bulk limit, the last two terms of eq. (5.139) which integrates over the spherical shell from p_o to p_2 may be neglected. Eq. (5.139) can be further reduced to, in the region $p_1 < p < p_o$,

$$D(r) = \frac{\pi\hbar}{L} \sum_{\ell=1}^{\ell_1} \int_{\frac{\pi\hbar}{L}\ell}^{p_1} \frac{dq\, q}{A_1 q^2 + \eta} j_0\left(\frac{rq}{\hbar}\right) + \\ + \frac{\pi\hbar}{L}\ell_1 \int_{p_1}^{p_0} \frac{dq\, q}{A_0 q^{3/2}} j_0\left(\frac{rq}{\hbar}\right) + \\ + \frac{\pi\hbar}{L} \sum_{\ell=\ell_1+1}^{\ell_0} \int_{\frac{\pi\hbar}{L}\ell}^{p_0} \frac{dq\, q}{A_0 q^{3/2}} j_0\left(\frac{rq}{\hbar}\right) . \tag{5.140}$$

Note that for $\eta = E_o = A_1(\pi\hbar/L)^2$, $p_\eta = \pi\hbar/L$, and η can be neglected also from the first integral without consequences. Furthermore since $p_1 \simeq p_\eta$, we can neglect the first term and approximate the second integral by

$$D(r) = \frac{2\pi\hbar}{A_o L}\ell_1\sqrt{\frac{\hbar}{r}}\left[\sqrt{\frac{\pi}{2}} - \sqrt{\frac{rp_1}{\hbar}}\right] + \\ + \frac{\pi\hbar}{A_o L}\sqrt{\frac{\hbar}{r}}\sum_{\ell=\ell_1+1}^{\ell_0}\int_{\frac{\pi r}{L}\ell}^{\infty}\frac{dx}{x^{3/2}}\sin x \quad . \tag{5.141}$$

As L ⟶ ∞, eq. (5.141) reduces to (5.109). Note also that D(r) is independent of η; hence A_o as a result of eqs. (5.102-103) is independent of η, so that the L dependence of A_o appears only through the sum over the discrete quantum states.

We take the first-order correction to eq. (5.109) from (5.141) by letting L ⟶ ∞ but retaining the first-order term. We note that $p_1 \gtrsim p_\eta$, hence we take $p_1 = (\pi\hbar/L)\,\ell_1$ with $\ell_1 \gtrsim 1$. The sum over ℓ is approximated by the Euler-Maclaurin series to get (see Appendix E)

$$\frac{\pi\hbar}{L}\sum_{\ell=\ell_1+1}^{\infty}\int_{\left(\frac{\pi\hbar}{L}\ell\right)\frac{r}{\hbar}}^{\infty}\frac{dx}{x^{3/2}}\sin x \simeq \frac{\hbar}{r}\sqrt{\frac{\pi}{2}} - \\ - \frac{\hbar}{L}\pi\sqrt{2\pi}\left(\ell_1+\frac{1}{2}\right) + O\left(\frac{1}{L^{3/2}}\right) . \tag{5.142}$$

Therefore eq. (5.141) becomes

$$D(r) = \frac{1}{A_o}\sqrt{\frac{\pi}{2}}\left(\frac{\hbar}{r}\right)^{3/2}\left[1 - \frac{\pi r}{L}\right] + O\left(\frac{1}{L^{3/2}}\right) . \tag{5.143}$$

Treating the $1/L$ term as a perturbation, we substitute (5.143) into (5.103) to obtain

$$\left(\frac{\delta\Phi_{BC}}{\delta G(p0)}\right)' = \frac{2}{15\pi^3}\left(\frac{V_0^2}{\hbar^6\beta^2}\right)\frac{1}{A_0^3}\left[p^{3/2} - \frac{15}{2}\frac{\pi\hbar}{L}p^{1/2}\right] . \qquad (5.144)$$

The vanishing of the first variations (5.108) then leads to

$$A_0^4 = \frac{2}{15\pi^3}\left(\frac{V_0^2}{\hbar^6\beta^2}\right)\left[1 - \frac{15\pi\hbar}{2L\langle p\rangle_0}\right] \qquad (5.145)$$

where $\langle p \rangle_0$ is defined

$$\begin{aligned}\langle p\rangle_0 &\equiv \sum_{p=p_1}^{p_0} p^3 G^2(p0) \Big/ \sum_{p=p_1}^{p_0} p^2 G^2(p0)\\ &\simeq \frac{2}{3}\left(\frac{p_0^3 - p_1^3}{p_0^2 - p_1^2}\right) .\end{aligned} \qquad (5.146)$$

Thus in the $p_1 << p_0$ limit, we have from (5.146) that (5.145) is

$$A_0^4 = \frac{2}{15\pi^3}\left(\frac{V_0^2}{\hbar^6\beta^2}\right)\left[1 - \frac{45\pi}{4}\left(\frac{\hbar}{p_0 L}\right)\right] . \qquad (5.147)$$

Note that for liquid helium-4, eq. (5.147) predicts size effects to occur at $L \simeq 35\ \hbar/p_0 \simeq 70$ Å, which is of the order of magnitude of experimental observations. We note also that (5.147) predicts a narrowing of the logarithmic singularity in the specific heat. This prediction is neither proved or disproved by the experimental data as Frederikse' data[17] shows a broadening but only when the bump is almost gone.

The second variation (5.105-107) gives

$$A_0^2\beta\,\frac{\delta^2\Omega}{\delta A_0^2} = A_0^2 \sum_{p=p_1}^{p_0} p^3 G^2(p0) \; +$$
$$+\frac{3V_0^2}{\pi^2\hbar^3\beta^2 \mathcal{V}} \sum_{p=p_1}^{p_0}\sum_{p'=p_1}^{p_0} p^{3/2} G(p0)\, p'^{3/2} G(p'0) \times \tag{5.148}$$
$$\times \int_0^\infty \frac{dx}{x}\left(1-j_0(x)\right) j_0\!\left(x\frac{p'}{p}\right)\left[1-\frac{2\pi\hbar}{pL}x\right].$$

Hence at T_0, we see that the $p^{3/2}$-spectrum can become unstable, i.e. $\delta^2\Omega/\delta A_0^2 = 0$, when L decreases to some critical L as determined by the equation (5.148). A crude estimate of this L dependence can be obtained by performing all the sums in (5.148) in the bulk limit. This procedure yields the estimate

$$\beta A_0^2\,\frac{\delta^2\Omega}{\delta A_0^2} \simeq \frac{2}{3\pi^2}\left(\frac{\mathcal{V}p_0^3}{\hbar^3}\right)\left[1-\frac{45\pi}{8}\left(\frac{\hbar}{p_0 L}\right)\right], \tag{5.149}$$

which gives the same order of magnitude for L as from (5.147). In fact, if we can extrapolate (5.149) beyond its region of validity, (5.149) predicts that the logarithmic behavior disappears at $L \simeq 35$ Å.

Now we consider the case $\eta > E_0$ or $T > T_0$. The analysis for A_0 remains essentially the same with the exception of a $p_1/p_0 << 1$ correction term as in the bulk case. We consider in detail the calculation of A_1. In the region $0 < p < p_1$, we have to remove the spurious asymptotic behavior in $D(r)$ to preserve the p^2- spectrum for $p \ll p_1$. Therefore we have

$$D(r) = \frac{\hbar\pi}{L} \sum_{\ell=1}^{\ell_1} \int_{\frac{\pi\hbar}{L}\ell}^{p_1} \frac{dq\, q}{A_1 q^2 + \eta}\, j_0\left(\frac{rq}{\hbar}\right) . \tag{5.150}$$

Application of the Euler-Maclaurin series to (5.150) leads to

$$D(r) \simeq \frac{\pi}{2A_1} \frac{\hbar}{r} e^{-p_\eta r/\hbar} \left\{ 1 + \frac{r}{L} e^{p_\eta r/\hbar} \ln \left| \frac{r}{\hbar} \sqrt{p_\eta^2 + (\pi\hbar/L)^2} \right| - \right.$$

$$\left. - \frac{\hbar}{2p_\eta L} \left[Ei\left(\frac{r p_\eta}{\hbar}\right) - e^{2p_\eta r/\hbar}\, Ei\left(-\frac{r p_\eta}{\hbar}\right) \right] \right\} , \tag{5.151}$$

where Ei(y) is the exponential integral

$$Ei(y) = \int_{-y}^{\infty} x^{-1} e^{x}\, dx .$$

Substituting (5.151) into (5.103) and expanding in terms of small p's, $p \ll p_1$, we have

$$\left(\frac{\delta \Phi_{BC}}{\delta G(p0)}\right)' = \frac{1}{432\pi^2}\left(\frac{V_0^2}{\hbar^6\beta^2\eta}\right)\frac{p^2}{A_1}\left\{1 + 27\frac{\hbar}{L}\sqrt{\frac{A_1}{\eta}}\left[I_1 + \tfrac{1}{2}I_2\right]\right\} \tag{5.152}$$

$$I_1 = \int_0^\infty dy\, y^2 e^{-2y} \ln y = 0.057 \tag{5.153a}$$

$$I_2 = \int_0^\infty dy\, y\, e^{-2y}\left[e^{y} Ei(-y) - e^{-y} Ei(y)\right] . \tag{5.153b}$$

Examination of the integrand of I_2 shows that I_2 is positive. Therefore the vanishing of the first variation (5.113) gives

$$A_1^3 = \frac{1}{432\pi^2}\left(\frac{V_0^2}{\hbar^6\beta^2\eta}\right)\left[1 + c\frac{\hbar}{L}\sqrt{\frac{A_1}{\eta}}\right] \tag{5.154}$$

where $c = 27\,(I_1 + \frac{1}{2}I_2)$ is a positive number. From eqs. (5.147) (5.154), we can draw the following conclusion about $p_0 = (2mA_0)^2$ and $p_1 = (A_0/A_1)^2$. As L decreases from its bulk value, we find that both p_0 and p_1 decrease, but whether $p_0 - p_1$ decreases or not depends on the relative magnitudes of the coefficients.

VI. MACROSCOPIC THEORIES

Thus far, we have centered our attention on microscopic theories, i.e. theories which begin with the dynamical descriptions of the elemental particles of the system. Now we turn to the complementary picture of macroscopic theories, i.e. theories which do not begin with the elemental particles of the system but with some gross, overall features of the entire system. Once again we shall use the variational approach. Instead of varying the grand potential Ω with respect to the self-energy Σ, we shall vary the Gibbs potential per volume, g, with respect to some gross order function Ψ. In order that such a variational approach be productive, we consider only the region where the order function is small so that some particular expansion of the functional $g[\Psi]$ can be made.

The general features of the theory are as follows. We first characterize the system by some order function Ψ. Next, the functional $g[\Psi]$ is constructed. Then we minimize $g[\Psi]$ with respect to Ψ, and the resulting Euler equation is used to determine the order function Ψ. The main problem of this procedure is finding suitable order function Ψ and functional form $g[\Psi]$.

Historically, Landau[107,108] was the originator of the general theory in 1937. In 1950, he and Ginzburg applied the theory to the superconductor transition[109] with great success. Eight years later, Ginzburg and Pitaevskii applied the same theory to the superfluid transition,[110] but without the magnitude of success as in the superconductor case.

We begin by reviewing the Ginzburg-Pitaevskii (GP) version of the general Landau theory and applying it to the film geometry. We show explicitly that the functional form $g[\Psi]$ assumed by GP leads to a second-order transition for the film, which is contrary to experimental observations. We next consider a modified theory which circumvents some of the difficulties of the GP theory.

A. Ginzburg-Pitaevskii Theory

The first assumption of the GP theory is that the order function $\Psi(r)$ corresponds to an "effective wave function" of the superflow component. It should be noted that this order function $\Psi(r)$ is not assumed to be the condensate wavefunction, which is quite different from that of the superflow component. Nevertheless, the order function $\Psi(r)$ is related to the condensate wavefunction in that the superfluid component exists only if there exists some long-range order which is a characteristic of the condensate. As $\Psi(r)$ is a complex wavefunction, we can write it as

$$\Psi(r) = \chi(r)\, e^{i\varphi(r)} \tag{6.1}$$

thus defining the real functions $\chi(r)$ and $\varphi(r)$ whose correspondence to the superfluid mass density $\rho_s(r)$ and the superfluid velocity $v_s(r)$ is given by

$$\rho_s(r) = m\,\chi^2(r) \tag{6.2a}$$

$$v_s(r) = \frac{\hbar}{m}\nabla\varphi(r) \quad . \tag{6.2b}$$

The second assumption involves the functional form of the Gibbs potential per volume $g[\Psi]$. We consider the system with its normal component at rest and at a temperature below but very close to the λ-transition. Then $g[\Psi]$ is assumed to be expandable in powers of Ψ, since Ψ is small. As Landau[108] has emphasized for the general theory, this analyticity assumption is the basis of the theory, and its validity is not at all obvious a priori. Keeping only the first nonvanishing terms, we have for a homogeneous system

$$g[\Psi] = g_0 - \alpha|\Psi|^2 + \frac{\beta}{2}|\Psi|^4 , \tag{6.3}$$

where α and β are expansion coefficients which are functions of pressure and temperature.[111] Any inhomogeneity can then be incorporated by retaining the first term in the expansion in terms of $\nabla\Psi$. The final GP functional form of $g[\Psi]$ is

$$g[\Psi] = g_0 - \alpha|\Psi|^2 + \frac{1}{2}\beta|\Psi|^4 - \frac{\hbar^2}{2m}|\nabla\Psi|^2 . \tag{6.4}$$

The structure of eq. (6.4) is quite evident. The first term on the right is the Gibbs potential for the normal component. The next two terms are the "potential energy" contribution from the superfluid component. The last term is the "kinetic energy" contribution from the superfluid component.

Now we vary $g[\Psi]$ with respect to Ψ in order to determine Ψ from the resulting Euler equation, which can be written

$$\left[-\frac{\hbar^2}{2m}\nabla^2-\alpha+\beta|\Psi|^2\right]\Psi(r)=0 \quad . \tag{6.5}$$

This equation, analogous to the Ginzburg-Landau equation for superconductors, is the Ginzburg-Pitaevskii (GP) equation.

The third assumption concerns the pressure and temperature dependence of the two parameters $\alpha(P,T)$ and $\beta(P,T)$. Since the transition is characterized by the solution $\Psi = 0$ above and $\Psi \neq 0$ below, $\alpha(P,T)$ must vanish on the transition. For the transition to be stable, $\beta(P,T)$ must be positive on the transition. We have then a transition line in the PT plane defined by $\alpha(P,T) = 0$. Holding pressure constant, GP assumes that $\alpha(T)$ can be expanded linearly about the transition,

$$\alpha(T)=\alpha'(T_0-T)\equiv-\alpha'\Delta T \quad . \tag{6.6}$$

There is also no a priori reason why this expansion is valid. This assumption immediately leads to the temperature dependence of ρ_s, as for a homogeneous system at equilibrium

$$|\Psi|_e^2=\frac{\alpha}{\beta}=-\frac{\alpha'}{\beta}\Delta T \; ; \qquad \Delta T\leq 0 \tag{6.7}$$

and from eq. (6.2)

$$\rho_s=-\frac{m\alpha'}{\beta}\Delta T \; ; \qquad \Delta T\leq 0 \quad . \tag{6.8}$$

Hence in the bulk limit, the Gibbs potential per volume is

$$g = g_0 - \frac{\alpha'^2}{2\beta} (\Delta T)^2 \quad ; \qquad \Delta T \leq 0 \quad . \tag{6.9}$$

From (6.9), we see that we have a second-order transition for the bulk limit.

Now we consider the film geometry and show that the GP theory yields a second-order transition as a direct consequence of the assumed functional form of $g[\Psi]$. We begin by introducing two dimensionless parameters

$$\Psi_0 \equiv \Psi / \Psi_e \qquad \Psi_e = \sqrt{\alpha/\beta} \tag{6.10a}$$

$$\xi_i \equiv x_i / \ell \qquad \ell = \hbar/(2m\alpha)^{1/2}, \quad i=1,2,3 \quad , \tag{6.10b}$$

and $(x_1\ x_2\ x_3)$ are the cartesian coordinates. Eq. (6.4) assumes the form

$$g[\Psi] = g_0 - \frac{\alpha^2}{2\beta}\left[2|\Psi_0|^2 - |\Psi_0|^4 - 2|\nabla_\xi \Psi_0|^2\right] , \tag{6.11}$$

and the resulting Euler equation is

$$\nabla_\xi \Psi_0 = \left[|\Psi_0|^2 - 1\right] \Psi_0 \quad . \tag{6.12}$$

As eq. (6.12) is a homogeneous equation, the first integral yields

$$\nabla_\xi \Psi_0 = \sqrt{\tfrac{1}{2}\Psi_0^4 - \Psi_0^2 + C} \quad , \tag{6.13}$$

where C is a constant of integration to be determined by some boundary conditions. Substituting (6.13) into (6.11), we get

$$g = g_0 - \frac{\alpha^2}{2\beta}\left[4|\Psi_0|^2 - 2|\Psi_0|^4 + C\right] . \tag{6.14}$$

We consider a film of thickness L in the z direction and infinite extent in the xy-plane. The boundary conditions are taken to be those of an impenetrable wall, viz.

$$\Psi_0(\xi) = 0 \quad \text{for} \quad \xi = 0, L/\ell \quad , \tag{6.15}$$

where $\xi = \xi_3 = z/\ell$. The formal solution of eq. (6.13) with boundary conditions (6.15) can be expressed in terms of an elliptic integral of the first kind[112]

$$\xi = \sqrt{2}\int_0^{\Psi_0} \frac{dt}{\sqrt{t^4 - 2t + 2C}} \quad , \tag{6.16}$$

which can be solved explicitly in terms of the Jacobian elliptic function of the first kind,[113] sn(u ;k)

$$\Psi_0(\xi) = \frac{\sqrt{2}\,k}{\sqrt{1+k^2}}\; sn\left(\frac{\xi}{\sqrt{1+k^2}} ; k\right) \quad , \tag{6.17}$$

where the modulus k is given by

$$\frac{L}{\ell} = 2\sqrt{1+k^2}\; K(k) \quad , \tag{6.18}$$

and K(k) is the complete elliptic function of the first kind.[112] The constant C is expressed in terms of k as

$$C = \frac{4k^2}{(1+k^2)^2} \quad . \tag{6.19}$$

The average Gibbs potential per volume for the entire film is

$$g = g_0 - \frac{\alpha^2}{2\beta}\,\frac{2}{3}\left(\frac{2\ell}{L}\right)^4 \Big[2(2+k^2)\,K^4(k) - 4(1+k^2)\,K^3(k)E(k)\Big] \quad , \tag{6.20}$$

where E(k) is the complete elliptic integral of the second kind.[112]

The transition is determined by the vanishing of the order function $\Psi(r)$, which occurs when $k = 0$. Then eq. (6.18) reads

$$L/\ell = \pi \quad , \tag{6.21}$$

which defines a film transition temperature T_f which is shifted from the bulk transition temperature T_o by the amount $\Delta T_f = T_f - T_o$ given by

$$\frac{\Delta T_f}{T_0} = -\frac{\pi^2\hbar^2}{2m\alpha' T_0}\left(\frac{1}{L^2}\right) \quad . \tag{6.22}$$

We note that eq. (6.22) has the same $1/L^2$ dependence as eq. (5.138) which was based not on the disappearance of the superfluid component but was concerned with the effect of the ground state energy.

Mathematically we expect this coincidence, as the kinetic energy term for the superfluid component in (6.4) is of the same form as the $A_1 p^2$ for small p's assumed for the ground state energy effects in (5.138).

To investigate the film transition further, we expand eqs. (6.20) (6.18) for small k's, respectively

$$g = g_0 - \frac{\alpha^2}{2\beta} \cdot \frac{3}{2}\left(\frac{\pi \ell}{L}\right)^4 k^4 + O(k^6) \tag{6.23}$$

$$\left(\frac{L}{\pi \ell}\right)^2 = 1 + \frac{3}{2} k^2 + \frac{27}{32} k^4 + O(k^6) \quad . \tag{6.24}$$

Substituting (6.24) into (6.23), we get

$$g = g_0 - \frac{\alpha^2}{2\beta} \cdot \frac{2}{3}\left(\frac{\pi \ell}{L}\right)^4 \left[\left(\frac{L}{\pi \ell}\right)^2 - 1\right]^2 \quad . \tag{6.25}$$

Since $k > 0$, we are slightly below T_f. Therefore we define $\delta T = T - T_f$, so that $\Delta T = \Delta T_f + \delta T$. Then eq. (6.25) can be rewritten as

$$g = g_0 - \left(\frac{\alpha^2}{2\beta}\right)_{T_f} \cdot \frac{2}{3}\left(\frac{\delta T}{\Delta T_f}\right)^2 \quad , \tag{6.26}$$

and we conclude that the transition at T_f is a second-order one. Actually we do not have to use the fact that $\alpha \sim \Delta T$, eq. (6.6). As long as $\alpha(T)$ is analytic about the point $\alpha(T_f)$, the order of the transition is second-order. Since $\alpha(T)$ is assumed to have a singularity only at T_o, the conclusion of a second-order transition at T_f is general, and follows solely from the functional form of $g[\Psi]$ which was assumed.

We note that very near the transition the order function $\Psi(r)$ has a spatial dependence like the ground state wavefunction for an ideal gas. To see this we need only to recall the asymptotic forms for the Jacobian elliptic function $sn(u;k)$, viz.

$$sn(u;k) = \begin{cases} \sqrt{2}\,k \sin\xi & k \to 0 \qquad (6.27a) \\ \tanh(\xi/\sqrt{2}) & k \to 1 \qquad (6.27b) \end{cases}$$

Therefore, the order function (6.17) becomes

$$\Psi_o(\xi) = \sqrt{2}\,k \sin\xi \qquad k \to 0 \tag{6.28a}$$

$$\Psi_o(\xi) = \tanh(\xi/\sqrt{2}) \qquad k \to 1 \quad . \tag{6.28b}$$

From eq. (6.28a) we see that very near the transition $\delta T \lesssim 0$, $|\delta T| \ll (\pi^2\hbar^2/2m\alpha' L^2)$, the order function behaves as a sine function with an amplitude proportional to $\sqrt{-\delta T}$. The sine behavior is a direct consequence of the kinetic energy term which always dominates very near the transition.

However in the opposite limit, not so close to the transition, $|\delta T| \gg (\pi^2\hbar^2/2m\alpha' L^2)$, eq. (6.28b) is applicable and the order function displays a "healing length" behavior as expounded by Gross[55] for the ground state wavefunction.

B. Modified Theory

There are at least three reasons why the GP version of the general Landau theory should be modified. The first is that the GP theory gives a second-order transition[114] in the bulk limit, while measurements[9] have shown a logarithmic behavior in c_p within 10^{-1}°K to 10^{-6}°K of the λ-point. The second is that the GP theory gives also a second-order transition in a film geometry, while measurements of the specific heat[17,18] has resulted in a very smooth curve at the superflow transition, indicating a high-order transition. Finally recent measurements of the superfluid component have demonstrated that ρ_s obeys the relation[11,12] $\rho_s \sim (-\Delta T)^{2/3}$ within 10^{-1}°K to 10^{-4}°K of the λ-point, while the GP version has ρ_s going as $(-\Delta T)$.

Let us first dismiss one obvious way to incorporate the logarithmic behavior of c_p near T_λ, which is to retain the same functional form for $g[\Psi]$, eq. (6.4), and change the temperature dependence of the coefficients α and β accordingly. This scheme was applied by Mattis[115] to the Ising model in two dimensions, with the following choices ($\Delta T = T - T_o$)

$$\alpha(T) = -\alpha'\Delta T\,\beta(T) \quad ; \quad \beta(T) = \beta' \ln(-\Delta T) \qquad (6.29)$$

$$|\Psi|^2 = M^8 = -\alpha'\Delta T \qquad (6.30)$$

so that

$$g = g_0 - \tfrac{1}{2}\alpha'^2\beta'(\Delta T)^2 \ln(-\Delta T)\ , \qquad (6.31)$$

where M is the magnetization. For helium, all we have to change is the identification (6.30) of the order function. But such a theory gives no shift in the transition temperature for a film, because the "kinetic energy" term is proportional to $(\Delta T)^2$ and is negligible as $\Delta T \longrightarrow 0$ compared with the "potential energy" term $\sim (\Delta T)^2 \ln(-\Delta T)$. Furthermore even if this is overlooked, the theory is unstable without the addition of a positive $|\Psi|^6$ term. Kadanoff[116] has recently written down equations similar to (6.31) for the Ising model, and the above comments are also applicable to its extension to helium.

In our microscopic calculations of the Born-Collision approximation, it was seen how the logarithmic behavior of c_p came about not because of the long-range order due to the condensate itself, but because of the anticipation by single-particle fluctuations of such an order setting in as exemplified by the applicability of the Very Dense State limit. Such observations concerning fluctuations are not new[117-119] and in fact predates any microscopic calculations. In order that such an anticipatory action be included into the macroscopic theory, a new order parameter which must be related to the number of particles in the low momenta states can be introduced. Unlike the order function $\Psi(r)$ which characterizes the long-range order of the system, this new parameter characterizes the fluctuations and must be nonzero for a neighborhood about T_λ and vanish outside. We shall not introduce such a parameter nor take into account any fluctuations[119] in any way. Hence we shall be satisfied with the attainment of a second-order transition without the logarithmic singularity from the general Landau theory.

The basis of the Landau theory is the symmetry of the system near the transition. Based on our knowledge of the symmetries of helium which we review below, we argue for a new, modified theory.

In Fig. 1, we have reproduced schematically the phases of helium. The λ-curve $[\lambda-\sigma]$ is characterized by the onset in helium II of an off-diagonal long-range order (ODLRO) of the reduced one-particle density matrix in the coordinate space representation.[52] This ODLRO is connected with a broken symmetry,[120,121] namely the phase symmetry that leads to the conservation of particle number. This symmetry is realized by the gauge group operating on the quantized field operators -- a continuous, one-parameter Abelian group. The vapor curve $[0-\lambda-K]$ is characterized by the appearance in the liquid phase of the diagonal short-range order in the reduced one-particle density matrix, as exhibited by the radial distributions from X-ray and neutron diffraction experiments. The spatial structure which gives rise to the observed diffraction patterns is quite elusive, although Keesom and Taconis[122] has suggested the space group T_d^2. Of course, liquid helium-4 does not have a crystalline structure, and the space group T_d^2 should be viewed only as a model.

The above considerations of symmetries suggest that we make the following proposal. Consider an order function Ψ (to be identified later) which characterizes the ODLRO, and construct the functional $g[\Psi]$ as

$$g[\Psi] = g_{II}[\Psi]$$
$$= g_I + A|\Psi|^2 + B|\Psi|^3 + C|\Psi|^4 + \frac{\hbar^2}{2m}|\nabla\Psi|^2 \quad . \tag{6.32}$$

We assume that the spatial structure of the liquid is such that the third-order term vanishes identically, i.e. $B = 0$. The λ -curve is then given by

$$A(P,T) = 0 \quad . \tag{6.33}$$

At the λ -point, however, the diagonal short-range order of the liquid disappears. Therefore we have the following two equations to define the λ -point.

$$\begin{cases} A(P_\lambda, T_\lambda) = 0 \\ B(P_\lambda, T_\lambda) = 0 \end{cases} \quad , \tag{6.34}$$

and the vapor curve near the λ -point is given by

$$B(P,T) = 0 \quad . \tag{6.35}$$

Therefore along the vapor curve at the λ -point, the theory has the same form as for the rest of the λ-curve. Since the vapor curve is almost at constant pressure, $c_{sat} \simeq c_p$, and c_p does not qualitatively change as one moves to higher pressure on the λ -curve.

Now we consider the identification of the order function Ψ (r). We consider the functional $g[\Psi]$ given by eq. (6.32) and vary it with respect to Ψ to yield the following Euler equation

$$-\frac{\hbar^2}{2m}\nabla^2\Psi + A\Psi + \frac{3}{2}B\Psi^2 + 2C\Psi^3 = 0 \quad , \qquad (6.36)$$

which is used to determine Ψ (r) given suitable boundary conditions. To make the identification of Ψ , we appeal to a microscopic argument. We consider the derivation of (6.36) from the equation of motion for the one-particle propagator $\tilde{G}_1$ below the transition, following the lead of Gorkov[123] who derived the Ginzburg-Landau equations. From eqs. (2.83)(2.86), we have the matrix equation of motion

$$\begin{aligned}\int_0^{-i\beta} d2\, G_0^{-1}(12)\,\tilde{G}(21') = \delta(11') + \\ + \int_0^{-i\beta} d2\, \Sigma^{tot}(12)\,\tilde{G}(21') \quad .\end{aligned} \qquad (6.37)$$

It is convenient to single out the 11 component and the 12 component respectively of eq. (6.37)

$$\begin{aligned}\int_0^{-i\beta} d2\, G_0^{-1}(12)\,\tilde{G}_{11}(21') = \delta(11') + \int_0^{-i\beta} d2\, \Sigma_{11}^{tot}(12)\,\tilde{G}_{11}(21') + \\ + \int_0^{-i\beta} d2\, \Sigma_{12}^{tot}(12)\,\tilde{G}_{12}^{+}(21')\end{aligned} \qquad (6.38a)$$

$$\int_0^{-i\beta} d2\, G_0^{-1}(12)\,\tilde{G}_{12}(21') = \int_0^{-i\beta} d2\, \Sigma_{11}^{tot}(12)\,\tilde{G}_{12}(21') + \int_0^{-i\beta} d2\, \Sigma_{12}^{tot}(12)\,\tilde{G}_{11}^{+}(21') \quad , \tag{6.38b}$$

where we have used the fact that $\tilde{G}_{21} = \tilde{G}_{12}^{+}$ and $\tilde{G}_{22} = \tilde{G}_{11}^{+}$. Now we define the "normal" one-particle Green's function[124] $G_n(12)$ which obeys the equations

$$\int_0^{-i\beta} d2\, G_0^{-1}(12)\, G_n(21') = \delta(11') + \int_0^{-i\beta} d2\, \Sigma_{11}^{tot}(12)\, G_n(21') \tag{6.39a}$$

$$\int_0^{-i\beta} d2\, G_n(12)\, G_0^{-1}(21') = \delta(11') + \int_0^{-i\beta} d2\, G_n(12)\, \Sigma_{11}^{tot}(21') \quad ; \tag{6.39b}$$

and we note that $G_n(12)$ is a propagator with no "anomalous" self-energy effects from Σ_{12}^{tot}. The operator G_o^{-1} may then be eliminated from eqs. (6.38) by folding (6.38) with $\int d3\, G_n(13)$ and using eq. (6.39b) to get the following coupled integral equations

$$\tilde{G}_{11}(11') = G_n(11') + \int_0^{-i\beta} d2\, d3\, G_n(13)\, \Sigma_{12}^{tot}(32)\, \tilde{G}_{12}^{+}(21') \tag{6.40a}$$

$$\tilde{G}_{12}(11') = \int_0^{-i\beta} d2\,d3\; G_n(13)\, \Sigma^{tot}_{12}(32)\, \tilde{G}^{+}_{11}(21') \quad . \tag{6.40b}$$

Eqs. (6.40) are precisely the integral equations from which Gorkov derived the Ginzburg-Landau equation. Gorkov inserted (6.40a) into (6.40b), expanded the resulting integral equation in powers of Σ^{tot}_{12} as the system is near the superconducting transition and Σ^{tot}_{12} is small, and obtained an equation with terms involving Σ^{tot}_{12} to the first power and a term with Σ^{tot}_{12} to the third power leading immediately to the Ginzburg-Landau equation and the identification of Ψ with Σ^{tot}_{12}. We note that it is essential in Gorkov's derivation that $G_n(12)$ be unchanged as we pass through the transition and that the only small quantity as we approach the transition from below is Σ^{tot}_{12}. Unfortunately for liquid helium-4, this is not so. In addition to the small quantity Σ^{tot}_{12}, we note that the boson system also has the condensate entering into diagrams for the self-energy Σ^{tot}_{11} whose contribution vanishes at the transition. If we write

$$\Sigma^{tot}_{11} = \tilde{\Sigma}^{tot}_{11} + \hat{\Sigma}^{tot}_{11} \tag{6.41}$$

where $\tilde{\Sigma}^{tot}_{11}$ is the total self-energy due to particles not in the condensate only and $\hat{\Sigma}^{tot}_{11}$ is the total self-energy due to the condensate, we see that in the boson system we have two small quantities near the transition: Σ_{12}^{tot} and $\hat{\Sigma}_{11}^{tot}$. We can then go back and define the normal one-particle propagator[124] $\tilde{G}_n(12)$ involving $\tilde{\Sigma}_{11}^{tot}$ instead of Σ_{11}^{tot}

$$\int_0^{-i\beta} d2\, G_0^{-1}(12)\,\tilde{G}_n(21') = \delta(11') + \int_0^{-i\beta} d2\, \tilde{\Sigma}_{11}^{tot}(12)\,\tilde{G}_n(21') \,, \tag{6.42}$$

and obtain in place of eqs. (6.40ab)

$$\tilde{G}_{11}(11') = \tilde{G}_n(11') + \int_0^{-i\beta} d2d3\, \tilde{G}_n(13)\,\hat{\Sigma}_{11}^{tot}(32)\,\tilde{G}_{11}(21') + \int_0^{-i\beta} d2d3\, \tilde{G}_n(13)\,\Sigma_{12}^{tot}(32)\,\tilde{G}_{12}^{+}(21') \tag{6.43a}$$

$$\tilde{G}_{12}(11') = \int_0^{-i\beta} d2d3\, \tilde{G}_n(13)\,\hat{\Sigma}_{11}^{tot}(32)\,\tilde{G}_{12}(21') + \int_0^{-i\beta} d2d3\, \tilde{G}_n(13)\,\Sigma_{12}^{tot}(32)\,\tilde{G}_{11}^{+}(21') \,. \tag{6.43b}$$

As there is no reason to do otherwise, we treat $\hat{\Sigma}_{11}^{tot}$ and Σ_{12}^{tot} on the same footing. Inserting eq. (6.43a) into (6.43b) and expanding in terms of $\hat{\Sigma}_{11}^{tot}$ and Σ_{12}^{tot}, we obtain

$$\tilde{G}_{12} = \tilde{G}_n \Sigma_{12} \tilde{G}_n^+ + \tilde{G}_n \Sigma_{12} \tilde{G}_n^+ \Sigma_{12}^+ \tilde{G}_n \Sigma_{12} \tilde{G}_n^+ + \\ + \tilde{G}_n \left[\hat{\Sigma}_{11} \tilde{G}_n \Sigma_{12} + \Sigma_{12} \tilde{G}_n^+ \hat{\Sigma}_{11}^+ \right] \tilde{G}_n^+ , \qquad (6.44)$$

where we have used matrix notation for the integration and suppressed the superscript tot on the total self-energies. We note that if $\hat{\Sigma}_{11}$ vanishes, then eq. (6.44) would yield Gorkov's derivation of the Ginzburg-Landau equation. For liquid helium-4, $\hat{\Sigma}_{11}$ is of the same order as Σ_{12} near the transition as was shown by Patashinskii and Pokrovskii;[94] in fact for $\eta \lesssim 0$

$$\hat{\Sigma}_{11}(p=0, z_\nu=0) = 2\Sigma_{12}(p=0; z_\nu=0) = -2\eta \ . \qquad (6.45)$$

Thus eq. (6.44) has the same dependence with Σ as eq. (6.32) has with Ψ. We conclude then that the identification of Ψ should be

$$\Psi \sim \Sigma_{12}^{tot} \sim \hat{\Sigma}_{11}^{tot} \ . \qquad (6.46)$$

To first-order in V, we find that $\Psi \sim n_o V_o$.

That the order function is proportional to the "anomalous" self-energy is most interesting. First of all, Ψ vanishes for the noninteracting bose gas, even though there is ODLRO and n_o is nonzero. This fact underscores the importance of interaction on the transition; for without interaction, the transition is first-order; with interaction, the transition is second-order as we will show. Furthermore, we recall that the "anomalous" self-energy represent the interaction energy between condensate particles and the rest of the particles. We will see that it is just this interaction energy that makes the condensate energetically possible. Hence in an interacting boson system, the transition is not totally a phase-space phenomena as in the ideal gas or the first-order approximations. Finally, we note that Ψ should be interpreted neither as the wavefunction of the condensate nor of the superfluid component, but as the wavefunction of a pair of bosons (with respect to its center of mass) scattering into, out of, or by the condensate. Hence the appropriate mass is the reduced mass $\frac{1}{2}m$.

We consider the system very close to the λ-curve so that we can take $\Psi \sim n_o$. Since the condensate number density n_o has not been measured, we shall normalize Ψ in terms of the measured superfluid number density $n_s = \rho_s m^{-1}$. Let us first note that the microscopic theory[94] yields the result that near the λ-curve $n_o \sim \eta$, $\eta \lesssim 0$. This fact can be easily verified in the Born-Collision approximation applying the Very Dense State limit

$$n_o \sim \left[\sum_{p=0}^{p_\eta} \frac{1}{A_1 p^2} - \sum_{p=0}^{p_\eta} \frac{1}{A_o p^{3/2}} \right] \sim \eta \quad . \qquad (6.47)$$

Now we consider the total momentum density $\not{p}$ in the Very Dense State limit below the transition

$$p = -\frac{1}{\beta v}\sum_{p} p\,\tilde{G}_{11}(p0) \tag{6.48}$$

which clearly vanishes for a homogeneous system. We imagine that the "gas of elementary excitations" which appear once $\eta \lesssim 0$ moves relative to the liquid at an infinitesimal velocity δv. Then we can consider $\tilde{G} \simeq -W_p^{-1}$ with $W_p \longrightarrow W_p - p \cdot \delta v$. Expanding in terms of δv, taking care in subtracting out the excitations at $\eta = 0$, and setting $p = mn_s \delta v$, we find

$$n_s = \frac{1}{3m\beta}\left[\frac{1}{v}\sum_{p}\tilde{G}_{11}^{2}(p,0)\,p^2\Big|_{\eta<0} - \frac{1}{v}\sum_{p}\tilde{G}_{11}^{2}(p,0)\,p^2\Big|_{\eta=0}\right]. \tag{6.49}$$

Therefore near the transition, we can estimate (6.49) by

$$n_s \sim \left[\frac{1}{v}\sum_{p=0}^{p_\eta}\frac{p^2}{(A_1p^2)^2} - \frac{1}{v}\sum_{p=0}^{p_\eta}\frac{p^2}{(A_0p^{3/2})^2}\right] \sim \eta^{4/3}. \tag{6.50}$$

Therefore from (6.47)(6.50), we conclude that near T_λ

$$n_s^{3/2} \sim n_0^{2}. \tag{6.51}$$

With the above considerations, we normalize the order function $\Psi(r)$ as

$$|\Psi|^2 = (n_s\lambda_{T_0})^{3/2}, \tag{6.52}$$

where λ_T is the usual thermal wavelength which is introduced for dimensional reasons.

We note that eq. (6.52) is quite different from the relations between n_s and Ψ proposed recently by Josephson[125] based on the identification $\Psi \sim \langle \psi \rangle \sim \sqrt{n_0}$. Nevertheless we will show that the exponent scaling laws[126] for the critical exponents of various physical quantities as $\Delta T \rightarrow 0$ are still valid since they are independent of the identification of the order parameter.

1. The Bulk Limit

In the bulk limit, the Gibbs potential per volume is

$$g_{II}[\Psi] = g_I + A(PT)|\Psi|^2 + B|\Psi|^3 + \\ + C(PT)|\Psi|^4 \quad , \tag{6.53}$$

where for a given value of pressure P we assume the following relations, as there is no reason to do otherwise,

$$A(P,T) = A_T \Delta T \qquad A_T > 0 \tag{6.54a}$$

$$B(P,T) = B_T \Delta T \qquad B_T \gtrless 0 \tag{6.54b}$$

$$C(P,T) > 0 \tag{6.54c}$$

$$\Delta T \equiv T - T_0 < 0 \, . \tag{6.54d}$$

We center our attention on the λ-point where $g_{II}[\Psi]$ is minimized by

$$\Psi = -\frac{3}{8}\frac{B}{C} + \frac{1}{8C}\sqrt{9B^2 - 32AC} \quad . \tag{6.55}$$

Staying on the saturated vapor curve where $B = 0$, we find

$$|\Psi|^2 = -\frac{A_T}{2C}\Delta T \quad . \tag{6.56}$$

Substituting (6.56) back into (6.53), we find

$$g_{II} = g_I - \frac{A_T^2}{2C}(\Delta T)^2 , \qquad \Delta T \leq 0 \; . \tag{6.57}$$

Eqs. (6.56) and (6.52) immediately tell us that the superfluid number density is proportional to $(-\Delta T)^{2/3}$, in agreement with recent experiments.[11,12] Also eq. (6.57) tells us that the transition is second-order with a jump in the specific heat given by

$$\Delta c_p = c_{p_{II}} - c_{p_I} = T_0 \frac{A_{T_0}^2}{2C} \quad . \tag{6.58}$$

Let us determine the coefficients A_T and C numerically from comparing eqs. (6.52)(6.56)(6.58) with the experimental values[11,12] $n_s = 1.43\, n(T_o)\, (-\Delta T)^{2/3}$ and[9] $\Delta c_p = 0.759 \times 10^7$ erg/°K cm^3 . We find

$$A_{T_0} = \frac{\Delta C_p}{T_0} \frac{\Delta T}{(n_s \lambda_{T_0})^{3/2}} = 4.20 \times 10^{-17} \frac{erg}{°K} \tag{6.59a}$$

$$C = \frac{\Delta C_p}{2T_0} \frac{(\Delta T)^2}{(n_s \lambda_{T_0})^3} = 2.54 \times 10^{-40} \frac{erg}{cm^3} . \tag{6.59b}$$

In the GP theory, Ginzburg and Pitaevskii[110] found for the analogous constants $A_T = 4.5 \times 10^{-17}$ erg/°K and $C = 2 \times 10^{-40}$ erg/cm^3 . The agreement is strictly fortuitous. GP assumed the value $m\,(\partial n_s/\partial T)_{T_o} = 0.7$ gm/°K cm^3 in order to evaluate A_T and C . But from the experimental data, we see that $m(\partial n_s/\partial T)_{T_o} \sim$ $\sim (-\Delta T)^{-1/3} \longrightarrow \infty$.

Now let us consider the exponent scaling law.[126] The relation between n_s and n_o was derived using the results from the Born-Collision approximation. We shall do the same here. Consider the equal-time correlation function C(r)

$$C(r) \equiv \frac{1}{2} \langle (\psi(r)\psi^+(0) + \psi^+(0)\psi(r)) \rangle . \tag{6.60}$$

As C(r) is at equal time, it is equivalent to an instantaneous propagator. But in the Very Dense State limit we have $G(r,t=0) \sim G(r,z=0)$. Therefore in the Very Dense State limit $C(r) \sim D(r)$ where $D(r)$ is defined by eq. (5.19). The exponent scaling laws make use of the large asymptotic behavior of C(r) on the transition. From eq. (5.30), we see that on the transition

$$C(r) \sim \frac{1}{r^{3/2}} \quad ; \qquad (6.61)$$

or defining[127] η by $C(r) \sim r^{-1-\eta}$, we have $\eta = \frac{1}{2}$. If we define the critical exponents by the relations $|\Psi| \sim (-\Delta T)^{\beta}$, some coherence length $\xi \sim (-\Delta T)^{\nu'}$, $c_p \sim (-\Delta T)^{\alpha'}$, $\rho_s \sim (-\Delta T)^{\zeta}$, we can write the scaling law as $\nu' = \zeta = 2\beta - \eta\nu'$ or

$$\nu' = \zeta = \frac{2\beta}{1+\eta} \quad . \qquad (6.62)$$

We have $\eta = \beta = \frac{1}{2}$, therefore $\nu' = \zeta = 2/3$. Furthermore $\alpha' = 2 - 3\zeta$; and using $\zeta = 2/3$, we see that $\alpha' = 0$ which is the closest we will get to the logarithm. One may of course proceed backwards, beginning with the experimentally found ζ and the microscopically calculated η to deduce the value $\beta = \frac{1}{2}$ from eq. (6.62).

2. Restricted Geometries

We apply our theory now to two restricted geometries, the unsaturated films and the vycor pores.[128] In both of these cases, the Gibbs potential per volume is

$$g_{II}[\Psi] = g_I + A|\Psi|^2 + B|\Psi|^3 + C|\Psi|^4 + \frac{\hbar^2}{m}\nabla^2\Psi \quad , \qquad (6.63)$$

where the coefficients A, B, C have the properties (6.54). We note that the mass in the kinetic energy term of (6.54) is ½m by previous arguments.

We consider first the unsaturated film, oriented such that the thickness L is along the z-direction from (0, L) and the film plane is in the xy-plane. We consider the boundary conditions $\Psi(z = 0) = 0$ at the bottom of the film and $(d\Psi/dz)_{z=L} = 0$ at the free surface on the top of the film. In the GP theory, we have shown that near the transition, the order function behaves as the ideal gas wavefunction. In the interest of a simplified analysis, we assume such a form for the order function

$$\Psi(z) = \phi \sin\left(\frac{\pi z}{2L}\right) = \phi \sin \xi \quad , \tag{6.64}$$

so that the functional $g[\Psi]$ becomes a function $g(\phi)$ of the order parameter ϕ. Substituting (6.64) into (6.63), we have

$$\begin{aligned} g_{II}(\phi) = {} & g_I + A\phi^2 \sin^2\xi + B\phi^3 \sin^3\xi + \\ & + C\phi^4 \sin^4\xi + \\ & + \left(\frac{\pi}{2}\right)^2 \frac{\hbar^2}{mL^2}\phi^2 \cos^2\xi \quad , \end{aligned} \tag{6.65}$$

which when averaged across the film becomes

$$g_{II}(\phi) = g_I + \phi^2\left(\frac{A}{2} + \frac{\pi^2\hbar^2}{8mL^2}\right) + \phi^3 \frac{2}{\pi}\sqrt{\frac{2}{3}}\, B + \phi^4 \frac{C}{2} \quad . \tag{6.66}$$

Eq. (6.66) is minimized by

$$\phi = \frac{1}{4C}\left[-\frac{6}{\pi}\sqrt{\frac{2}{\pi}}\, B + \sqrt{\frac{72}{\pi^3}B^2 - 8C\left(A + \frac{\pi^2\hbar^2}{4mL^2}\right)}\ \right] . \tag{6.67}$$

The transition is characterized by ϕ vanishing, which occurs when $A + (\pi^2 \hbar^2/4mL^2)$ vanishes, for then

$$\phi = -\frac{\pi^{3/2}}{6\sqrt{2}\, B}\left(A + \frac{\pi^2\hbar^2}{4mL^2}\right) \tag{6.68}$$

yielding the transition at $T_f = T_0 + (\Delta T)_f$ with

$$(\Delta T)_f = -\frac{\pi^2\hbar^2}{4mA_T}\frac{1}{L^2} \simeq -\frac{99.6}{[L(\text{Å})]^2}\ {}^\circ K \quad , \tag{6.69}$$

which is to be compared with the corresponding equation from the GP theory

$$(\Delta T)_f \simeq -\frac{50}{[L(\text{Å})]^2}\ {}^\circ K \quad , \tag{6.70}$$

and the experimental fit[19]

$$(\Delta T)_f = -\frac{92}{[L(\text{Å})]^2}\ {}^\circ K \quad . \tag{6.71}$$

The agreement of (6.69) with the experimental (6.71) is almost too good to be true. We also note that the difference of a factor of two between the GP (6.70) and ours (6.69) is due to the identification of the order function with the "anomalous" self-energy. Finally it must be said that eqs. (6.69-71) are valid only for thick films $L \gg 3$ Å , since in the opposite region our bulk evaluations of A_T and C are dubious and the interaction of the wall which heretofore has been ignored must be included.

The order of the transition may be obtained by moving away from T_f slightly and evaluating the Gibbs potential per volume. Define δT by

$$\Delta T = T - T_0 = (\Delta T)_f + \delta T \quad .$$

Therefore eq. (6.68) becomes

$$\phi = -\frac{\pi}{6}\sqrt{\frac{3}{2}}\,\frac{A_T}{B}\,\delta T\ , \qquad \delta T \leq 0; \tag{6.72}$$

and the Gibbs potential per volume (6.66) is

$$g_{II} = g_I + \frac{\pi^2}{144}\,\frac{A_T^3}{B^2}\,(\delta T)^3\ , \qquad \delta T \leq 0\ . \tag{6.73}$$

Therefore we conclude from eq. (6.73) that we have a third-order transition in the unsaturated film at $T_f = T_o + (\Delta T)_f$. We note that the coefficient B is a constant in this case as it is evaluated at T_f. The specific heat for temperatures $\delta T << T_o$ is

$$c_{p_{II}}(L,T) = c_{p_I}(L,T) - \frac{\pi^2}{24}\frac{A_T^3}{B^2} T_f \, \delta T \,, \tag{6.74}$$

and as expected there is no jump. The theory does predict a discontinuity in the slope of $c_p(T)$, viz.

$$\left[\frac{\partial c_{p_{II}}}{\partial T} - \frac{\partial c_{p_I}}{\partial T}\right]_{T_f} = -\frac{\pi^2}{24}\frac{A_T^3}{B^2} T_f \,, \tag{6.75}$$

but its magnitude is not known as B has not been evaluated numerically.

Now we consider the second case of restricted geometry, namely that of an impenetrable pore of radius L_o and infinite in length. As the walls are impenetrable, the boundary conditions are $\Psi(r = L_o) = 0$ where we construct a cylindrical set of coordinates with z along the (infinite) length of the pore.

Again in the interest of simplicity we assume a variational form for the order parameter $\Psi(r)$, viz.

$$\Psi(r) = \phi J_0\left(a\frac{r}{L_0}\right) = \phi J_0(a\xi) \,,$$

where $J_o(\xi)$ is the zeroth-order Bessel function of the first kind with the first root at $J_o(a) = 0$ where $a = 2.405$. Going through the same procedure as for the film geometry, we find that $g(\phi)$ is minimized with respect to order parameter ϕ by

$$\phi = \frac{1}{8CK_4}\left[-3BK_3 + \sqrt{9B^2K_3^2 - 16CK_4\left(A+\frac{\hbar^2 a^2}{mL^2}\right)}\,\right], \tag{6.76}$$

where the K_n's are constants obtained from averaging over the pore

$$K_n = 2\int_0^1 \xi\, d\xi\, J_0^{\,n}(a\xi)\,. \tag{6.77}$$

The transition therefore occurs at $T_{pore} = T_0 + (\Delta T)_{pore}$ with

$$(\Delta T)_{pore} = \frac{a^2\hbar^2}{mA_T}\left(\frac{1}{L^2}\right) \simeq \frac{234}{[L(\text{Å})]^2}\,{}^\circ K\,. \tag{6.78}$$

Hence the difference between the film geometry and the pore geometry is found in the first zeros of the cosine function versus the zeroth-order Bessel function, viz. $\pi/2$ and 2.405 respectively. This result agrees well with experiments and are compared with the experimental observations in Fig. 11.

Now we consider a partially filled pore of radius L_2, filled in to radius L_1. We take as our boundary conditions

$$\Psi(r) = 0 \qquad \text{at} \quad r = L_2 \quad (\text{wall}) \tag{6.79a}$$

$$\frac{d\Psi(r)}{dr} = 0 \qquad \text{at} \quad r = L_1 \ (\text{free surface})\,. \tag{6.79b}$$

Our intuition for the form of Ψ in this case is not so good, so we derive the solution. Varying g $[\Psi]$ with respect to Ψ we get the Euler equation

$$-\frac{\hbar^2}{m}\nabla^2\Psi + A\Psi + \frac{3}{2}B\Psi^2 + 2C\Psi^3 = 0. \tag{6.80}$$

From this general equation, it can be verified that the general solution for Ψ in the film geometry is in terms of elliptic functions, which become sine functions as the transition is approached. As we have seen, for a restricted geometry the dominant role is played by the kinetic energy term, shifting the transition below that of bulk system. Hence near the transition, we work with the linearized equation

$$\left[-\frac{\hbar^2}{m}\nabla^2 + A(PT)\right]\Psi(r) = 0 \quad . \tag{6.81}$$

In the film geometry, eq. (6.81) obviously has sine function solutions. In cylindrical geometry we may write (6.81) as

$$\left[-\frac{\hbar^2}{m}\left(\frac{d^2}{dr^2} + \frac{1}{r}\frac{d}{dr}\right) + A(PT)\right]\Psi(r) = 0 \ . \tag{6.82}$$

If we introduce a new length $\ell(T)$

$$\ell(T) \equiv -\frac{\hbar^2}{mA} = -\frac{\hbar^2}{mA_T\Delta T} \tag{6.83}$$

and a dimensionless parameter $\xi = r/\ell$, we can cast (6.81) into standard form

$$\left(\frac{d^2}{d\xi^2} + \frac{1}{\xi}\frac{d}{d\xi} + 1\right)\Psi(\xi) = 0, \qquad (6.84)$$

which has general solutions of the form

$$\Psi(\xi) = C_1 J_0(\xi) + C_2 Y_0(\xi) \qquad (6.85)$$

where C_1, C_2 are constants and $Y_0(\xi)$ is the zeroth-order Weber's Bessel function of the second kind. The boundary conditions (6.79ab) become respectively

$$C_1 J_0(\xi_2) + C_2 Y_0(\xi_2) = 0 \qquad (6.86a)$$

$$C_1 J_1(\xi_1) + C_2 Y_1(\xi_1) = 0 \qquad (6.86b)$$

which result in, after eliminating one of the constants,

$$U(\xi_1, \xi_2) = J_1(\xi_1)\cdot Y_0(\xi_1) - Y_1(\xi_1)\cdot J_0(\xi_2) = 0\,. \qquad (6.87)$$

Note that if we took as our boundary conditions $\Psi(\xi_1) = \Psi(\xi_2) = 0$, we would get, instead of (6.87),

$$S(\xi_1, \xi_2) = J_0(\xi_1)Y_0(\xi_2) - Y_0(\xi_1)J_0(\xi_2) = 0\,. \qquad (6.88)$$

We define the annular radius L_0 as $L_0 = L_2 - L_1$ and $\xi_0 = L_0/\mathcal{L}$. We also define the ratio $k = L_2/L_1 > 1$ which determines the percentage of the pore filled

$$\%\ \text{filled} = 1 - 1/k^2\,. \qquad (6.89)$$

Therefore given the percentage filled, we can calculate, on the basis of (6.87) or (6.88) depending on the boundary conditions, the lowest root of ξ_0 which will then give us the shift in the transition temperature. The roots of a cross product of Bessel functions is most easily solved for by a graphical method[129,130] in which $U(\xi_1, \xi_2) = 0$ and $S(\xi_1, \xi_2) = 0$ are plotted as a function of ξ_1 and ξ_2, and the roots are given by the intersection with the $\xi_2 = k\,\xi_1$ line. Such a plot is reproduced in Fig. 12. The results thus attained for the partially-filled pore and the previous calculations for the film and pore are summarized in Table 7.

To sum up this section, we note that the new, modified theory, based on a fundamentally different identification of the order function Ψ and the assumed symmetry of the liquid phase, agrees with the experimental behavior of ρ_s and Δc_p, satisfies the exponent scaling laws, gives a second-order transition for the bulk system and a third-order one for the film, and yields shifts in the transition temperature in agreement with experimental observations.

VII. CONCLUSION

As a result of this study, we can come to the following conclusions from the microscopic viewpoint:

(a) the present state of microscopic models for liquid helium-4 is extremely primitive (Chap. III - V)

(b) the Green's function formulation is both convenient and powerful for the discussion of various approximations (Chap. II - V)

(c) no microscopic explanation for the λ-transition can be found in a simple quasi-particle picture, like the BCS model for supercorductivity (Chap. IV)

(d) no microscopic explanation for the onset of Bose-Einstein condensation is restricted geometry can be found in a zeroth or first-order theory (Chap. III, IV)

(e) the Born-Collision approximation in the Very Dense State limit offers a simple model for the λ-transition (Chap. V).

From the macroscopic viewpoint, we make these concluding remarks:

(a) the Ginzburg-Pitaevskii theory, unlike the Ginzburg-Landau theory for superconductors, has major difficulties in describing the transition in helium in particular for films (Chap VI)

(b) the new, modified theory has major qualitative and quantitative agreement with experimental observations of the transition in helium, in particular for restricted geometries (Chap. VI).

On the basis of these conclusions, we can formulate the following conjectures:

(a) the microscopic explanation of the onset of Bose-Einstein condensation in restricted geometry can be found in second-order theory, in particular the Born-Collision approximation. (A preliminary discussion of this point is contained in Appendix F)

(b) the microscopic explanation of the specific heat anomaly in helium films can be found in the Born-Collision approximation. (A preliminary indication of the "smoothing over" of the logarithm found in the bulk limit is discussed in Chap. V, section C)

(c) the microscopic explanation for the new, modified theory from the macroscopic viewpoint can be found in the Born-Collision approximation. (A partial microscopic derivation is presented in Chap. IV, section B).

Finally we have the following open questions:

(a) What would be the suitable extension below the transition of the Born-Collision approximation which does not exhibit double-valued thermodynamic functions?

(b) Is the double-value behavior connected to some general microscopic properties of the approximation?

(c) How can be logarithmic behavior be consistently incorporated into the macroscopic theory?

(d) Why is the temperature of the onset of superflow in helium films and pores lower than the temperature of the specific heat maximum?

(e) What are the effects of attractive forces on the λ-transition? It is hoped that this dissertation would be the beginning point towards the solution of these problems.

ACKNOWLEDGMENTS

It is with great pleasure that I express my gratitude to Dr. Andrew M. Sessler for suggesting the problem treated in this dissertation, for the many fruitful discussions, and for his advice and encouragement.

This work was done under the auspices of the U. S. Atomic Energy Commission.

APPENDICES

A. Asymptotic Series for an Infinite Sum of Bose-Einstein Functions

We utilize the Mellin transform technique[131] to obtain our asymptotic forms. Consider a function f(x) . Its Mellin transform is defined

$$\mathcal{F}(s) \equiv \int_0^{\infty} f(x)\, x^{s-1}\, dx, \tag{A.1a}$$

and its inverse transform is

$$f(x) = \frac{1}{2\pi i} \int_{u-i\infty}^{u+i\infty} ds\, x^{-s}\, \mathcal{F}(s) \ ; \quad u_1 < u < u_2, \tag{A.1b}$$

where s = $u + i v$ is complex with u and v real, and the limits u_1 and u_2 define a vertical strip in the complex s-plane in which the integral for $\mathcal{F}(s)$ is convergent. Now replace f(x) by f(n + a) , where n can assume integer values. We sum over n from 0 to ∞ , and interchange the order of summation and integration to get

$$\sum_{n=0}^{\infty} f(n+a) = \frac{1}{2\pi i} \int_{u-i\infty}^{u+i\infty} ds\, \zeta(s,a)\, \mathcal{F}(s) \ ; \quad u > 1, \tag{A.2}$$

where $\zeta(s,a)$ is the generalized zeta function

$$\zeta(s,a) = \sum_{n=0}^{\infty} \frac{1}{(n+a)^s} \quad .$$

The added restriction that $u > 1$ arises from the interchange of the summation and integration, which is valid only when the summation (in our case $\zeta(s,a)$) converges uniformly. Now we specialize to $a = 1$, so that $\zeta(s,a) = \zeta(s)$, the Riemann zeta function, and

$$\sum_{n=1}^{\infty} f(n) = \frac{1}{2\pi i} \int_{u-i\infty}^{u+i\infty} ds\, \zeta(s)\, \mathcal{F}(s) \, ; \qquad \begin{matrix} u_1 < u < u_2 \\ 1 < u \end{matrix} \, . \qquad \text{(A.3)}$$

The procedure is: given a summand $f(x)$, calculate its Mellin transform $\mathcal{F}(s)$, and look for poles of $\mathcal{F}(s)\,\zeta(s)$. The sum is then given by the sum of the residues of the poles plus the contribution of the arc which closes the contour.

We apply this general theory to the summand

$$f(x) = x^{2k} F_j(ax^2 + b) \qquad k = 0, 1, 2, \cdots \, ,$$

where F_j is the Bose-Einstein functions. The Mellin transform can be easily calculated to be

$$\mathcal{F}(s) = \frac{1}{2} a^{-(s/2 + k)}\, \Gamma\left(\frac{s}{2} + k\right) F_{j+k+s/2}(b) \, ; \qquad a, b, u > 0 .$$

The poles of $\mathcal{F}(s)\,\zeta(s)$ are the poles of $\Gamma(\frac{s}{2} + k)\,\zeta(s)$, since $F_{j+k+s/2}(b)$ is analytic in the entire s-plane[132] except for a singularity at $s = 2(1 - j - k)$ when $b = 0$. (This pole corresponds to the Bose-Einstein condensation). To find the poles of $\Gamma(\frac{s}{2} + k)\,\zeta(s)$, we note that[133]

$$\Gamma(\tfrac{s}{2})\cdot\zeta(s) = \frac{\pi^{s/2}}{s(s+1)} + \int_1^\infty \left(x^{\frac{1-s}{2}} + x^{s/2}\right)\frac{w(x)}{x}\,dx\ , \tag{A.4}$$

where

$$w(x) \equiv \sum_{n=1}^{\infty} e^{-\pi x n^2}\ , \tag{A.5}$$

and the integral term is analytic in the entire s-plane. From the functional equation for $\Gamma(z)$

$$z\Gamma(z) = \Gamma(z+1)\ ,$$

we can write eq. (A.4) as

$$\Gamma(\tfrac{s}{2}+k)\zeta(s) = \left[(\tfrac{s}{2}+k-1)\cdots(\tfrac{s}{2}+1)\tfrac{s}{2}\right]\times \left[\frac{\pi^{s/2}}{s(s-1)} + \int_1^\infty \left(x^{\frac{1-s}{2}} + x^{s/2}\right)\frac{w(x)}{x}\,dx\right]. \tag{A.6}$$

Therefore for $k \geq 1$, there is one pole of eq. (A.6) at s = 1 with residue

$$\frac{\sqrt{\pi}}{2}\left[(k-\tfrac{1}{2})\cdots(\tfrac{3}{2})(\tfrac{1}{2})\right] a^{-(k+1/2)} F_{j+k+1/2}(b)\ ,$$

and for $k = 0$, there is an additional pole at s = 0 with residue

$$-\tfrac{1}{2}F_j(b)\ .$$

The sum of the residue(s) at the pole(s) gives only an asymptotic series because the contribution from the contour at infinity which closes around the poles does not vanish in general, although it approaches zero as $a \longrightarrow 0+$. Hence the asymptotic series is

$$\sum_{n=1}^{\infty} n^{2k} F_j(an^2+b) \longrightarrow \frac{\sqrt{\pi}}{2}\left[(k-1/2)\cdots(3/2)(1/2)\right] a^{-(k+\frac{1}{2})} F_{j+k+1/2}(b) - \frac{1}{2} F_j(b)\, \delta_{k0} \qquad (A.7)$$

In terms of the ϕ_{jk} functions defined by

$$\phi_{jk}(\xi,\alpha) = \xi^{2k+1} \sum_{n=1}^{\infty} n^{2k} F_j\left(\frac{\pi}{4}\xi^2 n^2 + \alpha\right)$$

we rewrite eq. (A.7) as

$$\lim_{\xi\to 0} \phi_{jk}(\xi,\alpha) = \left(\frac{2}{\pi}\right)^{k} (2k-1)!!\, F_{j+k+1/2}(\alpha) - \frac{\xi}{2} F_j(\alpha)\, \delta_{k0} . \qquad (A.8)$$

We note that the above asymptotic series may also be obtained by the Fourier cosine transform technique which is embodied in the Poisson's formula. Using Poisson's formula, we find for the special case

$$\sum_{n=1}^{\infty} F_j(an^2+b) = \frac{1}{2}\sqrt{\frac{\pi}{a}}\, F_{j+1/2}(b) - \frac{1}{2} F_j(b) + + \sqrt{\frac{\pi}{a}} \sum_{m=1}^{\infty} \frac{e^{-mb}}{m^{j+1/2}}\, w\left(\frac{\pi}{ma}\right) . \qquad (A.9)$$

We can easily see from eq. (A.5) that

$$w(x) < \frac{e^{-\pi x}}{1-e^{-\pi x}} .$$

Therefore as $a \longrightarrow 0+$, the last term of eq. (A.9) is bounded by

$$\sqrt{\frac{\pi}{a}} \sum_{m=1}^{\infty} \frac{e^{-mb}}{m^{j+1/2}} e^{-\pi^2/ma} \xrightarrow[a \to 0+]{} 0 \qquad ; \; b > 0 .$$

Hence eq. (A.9) is a special case of eq. (A.7). The other cases can be likewise obtained.

B. Absence of Nontrivial Solution in Classical Limit

We verify here the assertion that there is no nontrivial solution to (3.52), i.e.

$$F_{3/2}(\alpha_b) = \bar{\xi}_b \sum_{n=1}^{\infty} F_1\left(\frac{\pi}{4}\bar{\xi}_b^2(n^2-1) + \alpha_b\right) \tag{B.1}$$

in the classical limit of large α_b where eq. (B.1) becomes

$$1 = \bar{\xi}_b \sum_{n=1}^{\infty} e^{-\frac{\pi}{4}\bar{\xi}_b^2(n^2-1)} = \bar{\xi}_b \, w\left(\tfrac{1}{4}\bar{\xi}_b^2\right) e^{-\frac{\pi}{4}\bar{\xi}_b^2} \tag{B.2}$$

where the $w(x)$ function is defined in (A.5). Recall that (x) satisfies the following equation[133]

$$1 + 2w(x) = x^{-1/2}\left[1 + w(1/x)\right] , \tag{B.3}$$

and hence has the following limit as $x \longrightarrow 0$

$$2x^{1/2} w(x) = 1 - x^{1/2} . \tag{B.4}$$

Using eq. (B.4), we verify that eq. (B.2) admits the trivial solution $\bar{\xi}_b = 0$. But we also note that $2x^{\frac{1}{2}} w(x) e^{-\pi x}$ monotonic decreases from the value 1 at $x = 0$ to zero at infinity. Hence there is no nontrivial solution to eq. (B.2) in the α_b or classical limit.

C. Integrals Involving the Bogoliubov Energy Spectrum

For ease of reference, we list here the various integrals involving the Bogoliubov energy spectrum in the $N/\mathcal{V}$ limit. We consider the following energy parameters

$$\tilde{E}(p) = \epsilon_p^0 + n_0 V_0 \tag{C.1}$$

$$F(p) = n_0 V_0 \tag{C.2}$$

$$\mathcal{E}(p) = \sqrt{\epsilon_p^0(\epsilon_p^0 + 2 n_0 V_0)} \tag{C.3}$$

and the following substitutions

$$t = \beta n_0 V_0 \tag{C.4}$$

$$x^2 = \beta \epsilon_p^0 = t\left(\sqrt{y^2+1} - 1\right) \tag{C.5}$$

$$t y = \beta \mathcal{E}(p) = x\sqrt{x^2 + 2t} \quad , \tag{C.6}$$

so that for an arbitrary function f_0 in the $N/\mathcal{V}$ limit

$$\begin{aligned} \frac{1}{\mathcal{V}} \sum_p f_0 &= \frac{1}{\lambda_T^3} \frac{4}{\sqrt{\pi}} \int_0^\infty x^2 \, dx \, f_0 \\ &= \frac{1}{\lambda_T^3} t^{3/2} \frac{2}{\sqrt{\pi}} \int_0^\infty y \, dy \left[\frac{\sqrt{y^2+1} - 1}{y^2+1}\right]^{1/2} f_0 \quad . \end{aligned} \tag{C.7}$$

We list also the asymptotic series for the integrals in the limit of small t . We have

$$\frac{1}{\beta \mathcal{V}} \sum_p \ln\left(1 + f(\mathcal{E}_p)\right) = \frac{1}{\beta \lambda_T^3} B_1(t) \tag{C.8}$$

$$\frac{1}{\mathcal{V}} \sum_p \mathcal{E}_p f(\mathcal{E}_p) = \frac{1}{\beta \lambda_T^3} B_2(t) \tag{C.9}$$

$$\frac{1}{v}\sum_{p}(u_p^2+v_p^2)f(\varepsilon_p) = \frac{1}{\lambda_T^3}\,B_3(t) \tag{C.10}$$

$$\frac{1}{2v}\sum_{p}\left[\varepsilon_p - \epsilon_p^0(u_p^2+v_p^2)\right]f(\varepsilon_p) = \frac{1}{2\beta\lambda_T^3}\,B_4(t) \tag{C.11}$$

$$\frac{1}{v}\sum_{p}f(\varepsilon_p) = \frac{1}{\lambda_T^3}\,B_5(t) \tag{C.12}$$

$$\frac{1}{v}\sum_{p}\frac{1}{\varepsilon_p}f(\varepsilon_p) = \frac{\beta}{\lambda_T^3}\,B_6(t)\quad , \tag{C.13}$$

where the functions $B_n(t)$ are defined

$$\begin{aligned} B_1(t) &= -\frac{4}{\sqrt{\pi}}\int_0^\infty x^2dx\,\ln(1-e^{-yt}) \\ &= -t^{3/2}\frac{2}{\sqrt{\pi}}\int_0^\infty dy\,y\left[\frac{\sqrt{y^2+1}-1}{y^2+1}\right]^{1/2}\ln(1-e^{-yt}) \end{aligned} \tag{C.14}$$

$$\begin{aligned} B_2(t) &= \frac{4}{\sqrt{\pi}}\int_0^\infty x^2dx\,\frac{yt}{e^{yt}-1} \\ &= t^{5/2}\frac{2}{\sqrt{\pi}}\int_0^\infty dy\,y^2\left[\frac{\sqrt{y^2+1}-1}{y^2+1}\right]^{1/2}\frac{1}{e^{yt}-1} \end{aligned} \tag{C.15}$$

$$\begin{aligned} B_3(t) &= \frac{4}{\sqrt{\pi}}\int_0^\infty x^2dx\,\frac{\sqrt{y^2+1}}{y}\,\frac{1}{e^{yt}-1} \\ &= t^{3/2}\frac{2}{\sqrt{\pi}}\int_0^\infty dy\left[\sqrt{y^2+1}-1\right]^{1/2}\frac{1}{e^{yt}-1} \end{aligned} \tag{C.16}$$

$$\begin{aligned} B_4(t) &= \frac{4}{\sqrt{\pi}}\int_0^\infty x^2dx\,\frac{x^2}{y}\,\frac{1}{e^{yt}-1} \\ &= t^{5/2}\frac{2}{\sqrt{\pi}}\int_0^\infty dy\,\frac{\left[\sqrt{y^2+1}-1\right]^{3/2}}{\sqrt{y^2+1}}\,\frac{1}{e^{yt}-1} \end{aligned} \tag{C.17}$$

$$\begin{aligned} B_5(t) &= \frac{4}{\sqrt{\pi}} \int_0^\infty x^2 dx \, \frac{1}{e^{yt}-1} \\ &= t^{3/2} \frac{2}{\sqrt{\pi}} \int_0^\infty dy \, y \left[\frac{\sqrt{y^2+1}-1}{y^2+1} \right]^{1/2} \frac{1}{e^{yt}-1} \end{aligned} \tag{C.18}$$

$$\begin{aligned} B_6(t) &= \frac{4}{\sqrt{\pi}} \int_0^\infty x^2 dx \, \frac{1}{yt} \, \frac{1}{e^{yt}-1} \\ &= t^{1/2} \frac{2}{\sqrt{\pi}} \int_0^\infty dy \left[\frac{\sqrt{y^2+1}-1}{y^2+1} \right]^{1/2} \frac{1}{e^{yt}-1} \quad . \end{aligned} \tag{C.19}$$

For small values of t , we have

$$B_1(t) = \zeta(\tfrac{5}{2}) - \zeta(\tfrac{3}{2})\, t + \tfrac{4}{3}\sqrt{2\pi}\, t^{3/2} - \tfrac{3}{2}\zeta(\tfrac{1}{2})\, t^2 + \cdots \tag{C.20}$$

$$B_2(t) = \tfrac{3}{2}\zeta(\tfrac{5}{2}) - \tfrac{1}{2}\zeta(\tfrac{3}{2})\, t + \tfrac{3}{4}\zeta(\tfrac{1}{2})\, t^2 + \cdots \tag{C.21}$$

$$B_3(t) = \zeta(\tfrac{3}{2}) - \sqrt{2\pi}\, t^{1/2} + \zeta(\tfrac{1}{2})\, t - \tfrac{4}{3}\sqrt{2\pi}\, t^{3/2} + \cdots \tag{C.22}$$

$$B_4(t) = \zeta(\tfrac{3}{2})\, t - 2\sqrt{2\pi}\, t^{3/2} + 3\zeta(\tfrac{1}{2})\, t^2 + \cdots \tag{C.23}$$

$$B_5(t) = \zeta(\tfrac{3}{2}) - 4\sqrt{\tfrac{2}{\pi}}\, t^{1/2} + \zeta(\tfrac{1}{2})\, t - \cdots \tag{C.24}$$

$$B_6(t) = t^{-1/2} - \sqrt{\tfrac{2}{\pi}}\,\zeta(\tfrac{1}{2}) + \tfrac{2}{\pi}\, t^{1/2} - (2\pi)^{-3/2}\zeta(\tfrac{3}{2})\, t + \cdots \tag{C.25}$$

D. Self-Consistent Statistical Factors and Shift in Transition Temperature

We present a very elementary example in which self-consistent statistical factors are essential to evaluating the correct shift in the transition temperature. The example is the constant energy shift model, in which the effect of the interaction is to shift all the energy levels so that the number density is given by

$$n = \frac{1}{\mathcal{V}} \sum_{p} f(\epsilon_p - \mu) \tag{D.1}$$

where

$$\epsilon_p = \epsilon_p^0 + W \tag{D.2}$$

and W is a constant. This is in fact the case in the Hartree-Fock approximation for a very short-range potential. We note that eq. (D.1) can be expressed in terms of the non-interacting statistical factor $f(\tilde{\epsilon}_p^0)$, where $\tilde{\epsilon}_p^0 = \epsilon_p^0 - \mu$, as

$$\begin{aligned} n &= \frac{1}{\mathcal{V}} \sum_{p} f(\tilde{\epsilon}_p^0) \left[1 + (1 + f(\tilde{\epsilon}_p^0)) W\beta \right]^{-1} \\ &= \frac{1}{\mathcal{V}} \sum_{p} f(\tilde{\epsilon}_p^0) \left[1 + \sum_{n=1}^{\infty} (-\beta W)^n (1 + f(\tilde{\epsilon}_p^0))^n \right] . \end{aligned} \tag{D.3}$$

Eq. (D.3) is an explicit expansion of the number density n in terms of the energy shift W. In the $N/\mathcal{V}$ limit, we can write eq. (D.3) as

$$n\lambda_T^3 = F_{3/2}(\alpha) + \beta W F'_{3/2}(\alpha) + \\ + \lambda_T^3 \frac{1}{\mathcal{V}} \sum_{n=2}^{\infty} (-\beta W)^n \sum_p f(\tilde{\epsilon}_p^o)(1+f(\tilde{\epsilon}_p^o))^n , \tag{D.4}$$

where $\alpha = -\beta\mu \geq 0$. Then for small energy shifts such that $\beta W \ll 1$, we neglect all terms with $n \geq 2$ in eq. (D.4) to get

$$n\lambda_T^3 = F_{3/2}(\alpha) + \beta W F'_{3/2}(\alpha) . \tag{D.5}$$

If we take the Hartree-Fock approximation with a very short-range potential

$$W = 2nV_0 \simeq 2\lambda_T^{-3} F_{3/2}(\alpha) V_0 \quad ; \tag{D.6}$$

and eq. (D.5) is exactly eq. (B.6) in GKW.[75] Also eq. (D.5) with W a constant or given by eq. (D.6) gives an upward shift in the transition temperature for $W > 0$, which is entirely unexpected for a constant energy shift model. The mistake lies in the truncating of the infinite series in (D.4) to get (D.5). What we have done is to expand a function into an infinite series about a singular point and to truncate the series, obliterating the original singularity in the process. The proper way to treat eq. (D.1) in the $N/\mathcal{V}$ limit is to simply write

$$n\lambda_T^3 = F_{3/2}(\alpha') \tag{D.7}$$

where $\alpha' = \beta\eta$, $\eta = -\mu + W$; and eq. (D.7) predicts no shift in the transition temperature, which is the correct result.

The above considerations may be formalized by appealing to the time-independent formulation of Balian and DeDominics,[45] in which self-consistent statistical factors are used along with unperturbed energy dinominators. Then the above example with W given by eq. (D.6) is the first-order approximation in V .

E. Application of the Euler-Maclaurin Series

The Euler-Maclaurin series for a sum can be written

$$\Delta p \sum_{\ell=n}^{m} f(p_\ell) = \int_{p_n}^{p_m} f(p)\,dp + \frac{\Delta p}{2}\left[f(p_m) - f(p_n)\right] + \sum_{\substack{i \\ \text{odd}}}^{\infty} \frac{(\Delta p)^{i+1}}{(i+1)!} B_{i+1}\left[f^{(i)}(p_m) - f^{(i)}(p_n)\right] , \tag{E.1}$$

where

$$\Delta p = p_\ell - p_{\ell-1} \; ; \quad n < \ell \leq m \tag{E.2}$$

and B_i is the i^{th} Bernoulli number. Let us apply the Euler-Maclaurin series (E.1) to the sum

$$S = \frac{\hbar\pi}{L} \sum_{\ell=1}^{\infty} f\left(\frac{\pi\hbar}{L}\ell\right) \tag{E.3}$$

where

$$f(p) = \int_{\frac{pL}{\hbar}}^{\infty} \frac{dx}{x^{3/2}} \sin x \; ; \quad p_\ell = \frac{\pi\hbar}{L}\ell \; . \tag{E.4}$$

The first two terms of eq. (E.1) leads to

$$S = \frac{\hbar}{r}\left[\int_{\frac{\pi r}{L}}^{\infty}\frac{dx}{x^{1/2}}\sin x - \frac{1}{2}\frac{\pi r}{L}\int_{\frac{\pi r}{L}}^{\infty}\frac{dx}{x^{3/2}}\sin x\right] \tag{E.5}$$

which leads to eq. (5.143) since

$$D(r) = \frac{1}{A_0}\left(\frac{\hbar}{r}\right)^{1/2} S \; . \tag{E.6}$$

The next term in the Euler-Maclaurin series (E.1) has a $1/L^{3/2}$ dependence. To see this, we note that

$$f^{(i)}(\infty) = 0 \tag{E.7}$$

$$f^{(i)}\left(\frac{\pi\hbar}{L}\right) = \left(-\frac{r}{\hbar}\right)^{i}\frac{(2i-1)!!}{2^{i}}\;\frac{\sin(\pi r/L)}{(\pi r/L)^{(2i+1)/2}}\left[1+O\left(\frac{\pi r}{L}\right)\right] \tag{E.8}$$

so that the remainder term

$$R = \sum_{\substack{i\\ \text{odd}}}^{\infty}\frac{(\Delta p)^{i+1}}{(i+1)!}B_{i+1}\left[f^{(i)}(\infty) - f^{(i)}\left(\frac{\pi\hbar}{L}\right)\right] \tag{E.9}$$

is, using eqs. (E.7,8) in (E.9)

$$R = \frac{\sin(\pi r/L)}{(\pi r/L)^{1/2}}\left(\frac{\pi\hbar}{L}\right)\sum_{\substack{i\\ \text{odd}}}^{\infty}\frac{(2i-1)!!}{(i+1)!\,2^{i}}\,B_{i+1}\left[1+O\left(\frac{\pi r}{L}\right)\right] . \tag{E.10}$$

The ratio of the remainder over the term (E.5) is $(\pi r/L)^{\frac{1}{2}}$. Since $D(r)$ is integrated over r with a peak at $r \simeq \hbar/p$, the ratio is $(\pi\hbar/pL)^{\frac{1}{2}}$. Finally the smallest momentum of interest is $\sim \hbar\,(0.1)\,\text{Å}^{-1}$; hence the expansion (E.5) is good for $L \gg 30$ Å .

F. Bose-Einstein Condensation in Restricted Geometries

In Chap. IV, sec. G, we saw how the first-order approximations were unable to change essentially the phase-space nature of the Bose-Einstein condensation as it occurs in the ideal gas. Now we consider the Born-Collision approximation as developed in Chap. V and present a tentative argument that Bose-Einstein condensation does occur in restricted geometries. We cannot demonstrate this assertion directly; therefore we proceed in a more circuitous manner. If we have a film geometry, then for low enough temperatures we are in the two-dimensional limit. If macroscopic occupation occurs in the two-dimensional limit, then we may deduce that Bose-Einstein condensation occurred at some higher temperature as there is obviously no macroscopic occupation in the high temperature or classical limit. If we have a pore geometry, then the low temperature limit is the one-dimensional limit.

We note that the structure of the self-energy for the Born-Collision approximation in the Very Dense State limit on the transition is

$$\Delta'_p \sim \sum_{p'\bar{p}\bar{p}'} \left[\delta(p+p'-\bar{p}-\bar{p}') - \delta(p'-\bar{p}-\bar{p}')\right] \frac{1}{\Delta'_{p'}\,\Delta'_{\bar{p}}\,\Delta'_{\bar{p}'}} \; . \tag{F.1}$$

If we write $\Delta'_p \sim p^{\alpha_o}$, then by counting powers we have $\alpha_o = 6-3\alpha_o$ since each summation over p brings in a p^3 factor. Thus we have the $p^{3/2}$-spectrum. Now if we were in the two-dimensional limit, then each summation over p brings in a p^2 factor, and we have $\alpha_o = 4-3\alpha_o$. Therefore in the two-dimensional limit, we have a p-spectrum. Likewise, in the one-dimensional limit, we find a $p^{\frac{1}{2}}$-spectrum.

Above the transition, we have

$$\Delta'_p \sim \sum_{p'\bar{p}\bar{p}'} \left[\delta(p+p'-\bar{p}-\bar{p}') - \delta(p'-\bar{p}-\bar{p}')\right] \times \times \left[(\Delta'_{p'}+\eta)(\Delta'_{\bar{p}}+\eta)(\Delta'_{\bar{p}'}+\eta)\right]^{-1} \quad ; \tag{F.2}$$

and for very small p's because of the convergence due to η , we can expand the δ -function

$$\delta(p+p'-\bar{p}-\bar{p}') = \delta(p'-\bar{p}-\bar{p}') + + p^2\left(\frac{\partial}{\partial p^2}\delta(p+p'-\bar{p}-\bar{p}')\right)_{p=0} + \cdots \tag{F.3}$$

to obtain a p^2-spectrum, which is independent of the dimensionality of the system.

Now we calculate the number density

$$n = -k_B T \frac{1}{v} \sum_p G(p,0) \tag{F.4}$$

with G(p,0) given by

$$G(p,0) = -\frac{1}{\epsilon_p^0 + \Delta'_p + \eta} \tag{F.5}$$

and

$$\Delta'_p = A_1 p^2 H(p_1 - p) + A_0 p^{\alpha_0} H(p - p_1) H(p_0 - p) + \\ + \epsilon_p^0 \exp(-\lambda \beta_0 \epsilon^0 (p - p_0)) H(p - p_0) . \qquad (F.6)$$

To evaluate eq. (F.4), we utilize (5.132) to write, for the film geometry ($\alpha_0 = 1$) ,

$$\frac{1}{V} \sum_p G(p,0) = -\frac{1}{2\pi^2\hbar^3} \left[\frac{\pi\hbar}{L} \sum_{\ell=1}^{\ell_1} \int_{\frac{\pi\hbar}{L}\ell}^{p_1} \frac{p\,dp}{A_1 p^2 + \eta} + \right. \\ + \frac{\pi\hbar}{L} \sum_{\ell=1}^{\ell_1} \int_{p_1}^{p_0} \frac{p\,dp}{A_0 p + \eta} + \\ \left. + \frac{\pi\hbar}{L} \sum_{\ell=\ell_1+1}^{\ell_0} \int_{\frac{\pi\hbar}{L}\ell}^{p_0} \frac{p\,dp}{A_0 p + \eta} \right] , \qquad (F.7)$$

where we neglected the last two terms of (5.132) as in the bulk limit and $p_1 = A_0/A_1$, $p_0 = 2mA_0$. Now we consider the two-dimensional limit of eq. (F.7), which is to retain terms with $\ell = 1$

$$\frac{1}{V} \sum_p G(p,0) = -\frac{1}{2\pi^2\hbar^3} \frac{\pi\hbar}{L} \left[\int_{\frac{\pi\hbar}{L}}^{p_1} \frac{p\,dp}{A_1 p^2 + \eta} + \right. \\ \left. + \int_{p_1}^{p_0} \frac{p\,dp}{A_0 p + \eta} \right] , \qquad (F.8)$$

which yields, upon evaluating the integrals,

$$n = \frac{2}{\lambda_T^2 L}\left[1 - \frac{1}{2mA_1} + \frac{1}{4mA_1}\ln\left|\frac{\eta + A_0^2 A_1^{-1}}{\eta + A_1(\pi\hbar/L)^2}\right| + \right.$$

$$\left. + \frac{\eta}{2mA_0^2}\ln\left|\frac{\eta + A_0^2 A_1^{-1}}{\eta + 2mA_0^2}\right| \right] . \qquad \text{(F.9)}$$

Writing $A_1 = C\eta^{-1/3}$, $p_1 = A_0\eta^{1/3}/C$, we find the $\eta \to 0$ limit of eq. (F.9) as

$$n = \frac{2}{\lambda_T^2 L}\left[1 - \frac{\eta^{1/3}}{2mC} + \frac{2\eta^{1/3}}{4mC}\ln\left|\frac{p_1 L}{\pi\hbar}\right| + \right.$$

$$\left. + \frac{\eta}{2mA_0^2}\ln\left|\frac{\eta^{1/3}}{2mC}\right| \right] , \qquad \text{(F.10)}$$

which is finite as $\eta \to 0$. Hence Bose-Einstein condensation occurs for this film system of density n at temperatures lower than the transition temperature T_0 given by $\eta = 0$. One can likewise demonstrate that in the pore system, Bose-Einstein condensation occurs.

It should be emphasized that this calculation shows that the onset of Bose-Einstein condensation in an interacting system is not a phase-space phenomena, but is a result of the correlations at low momenta due to interactions, and hence is not determined only by the dimensionality of the system.

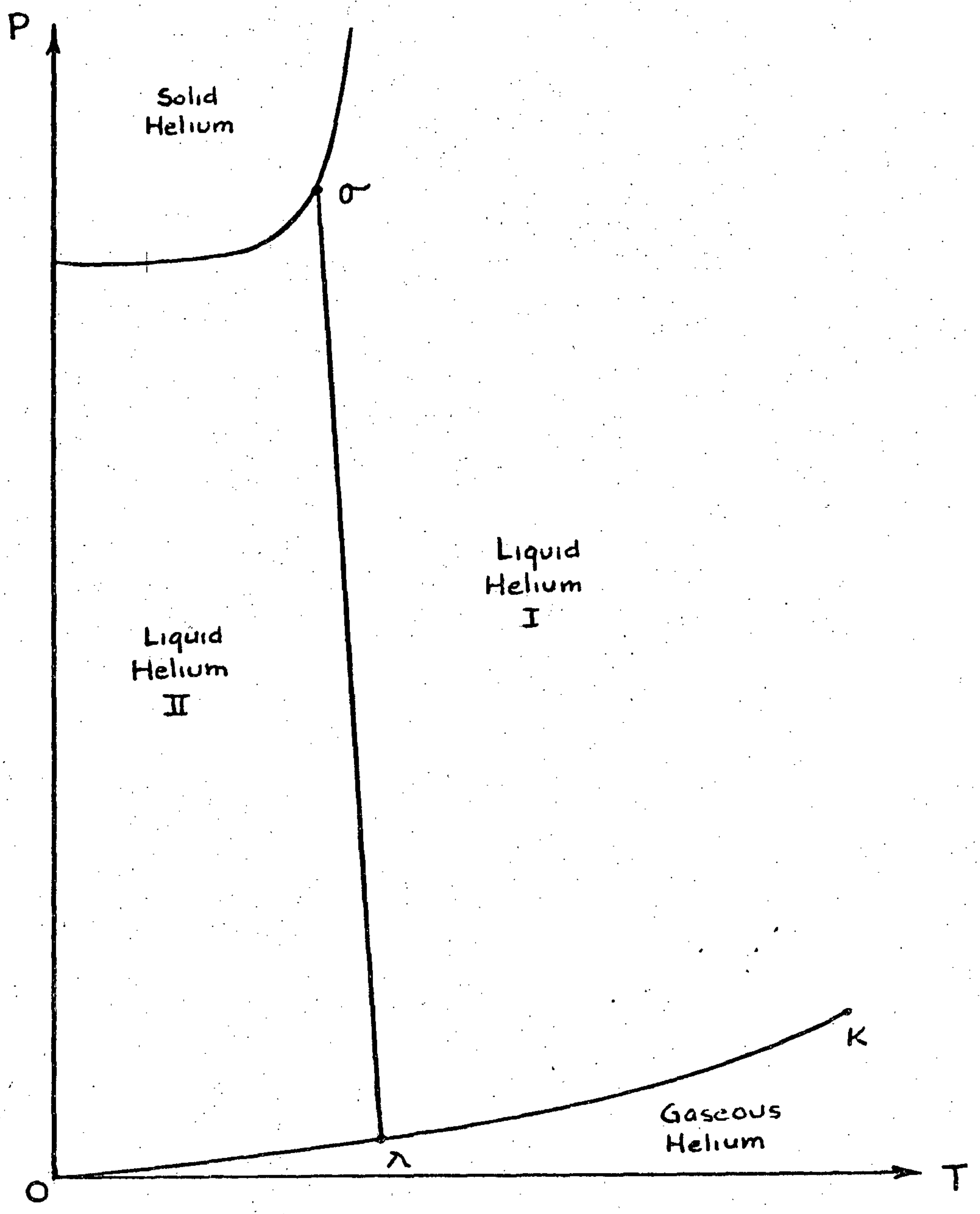

Fig. 1. Schematic Plot of the Phases of Helium-4.

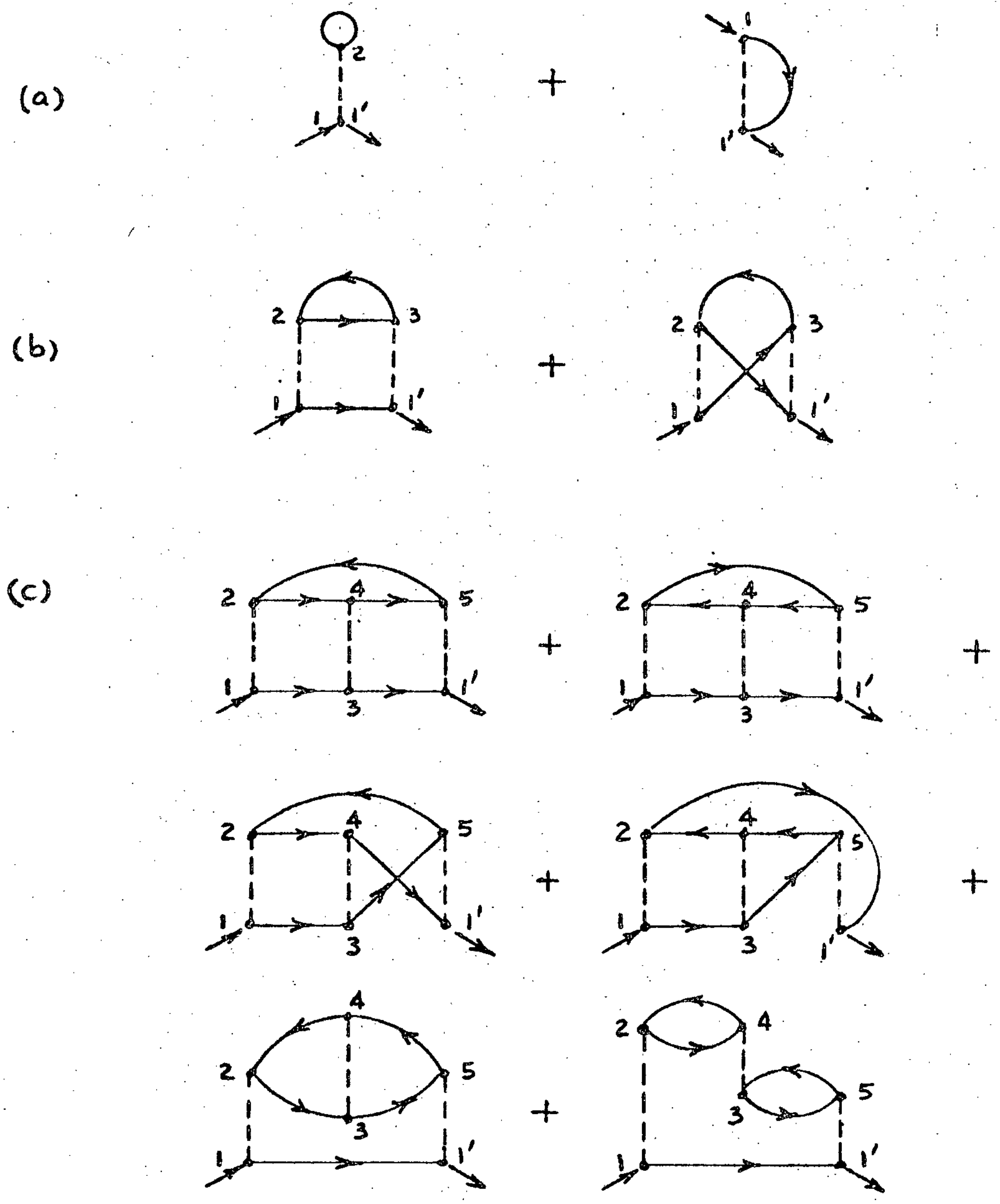

Fig. 2. Irreducible Diagrams for the Total Self-Energy

(a) first-order in V

(b) second-order in V

(c) third-order in V

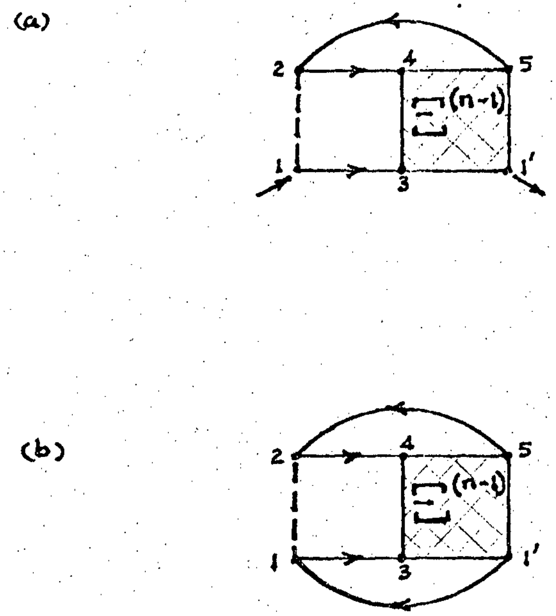

Fig. 3. nth Order Irreducible Diagrams for

(a) Total Self-Energy

(b) Functional $\Phi[G_1]$

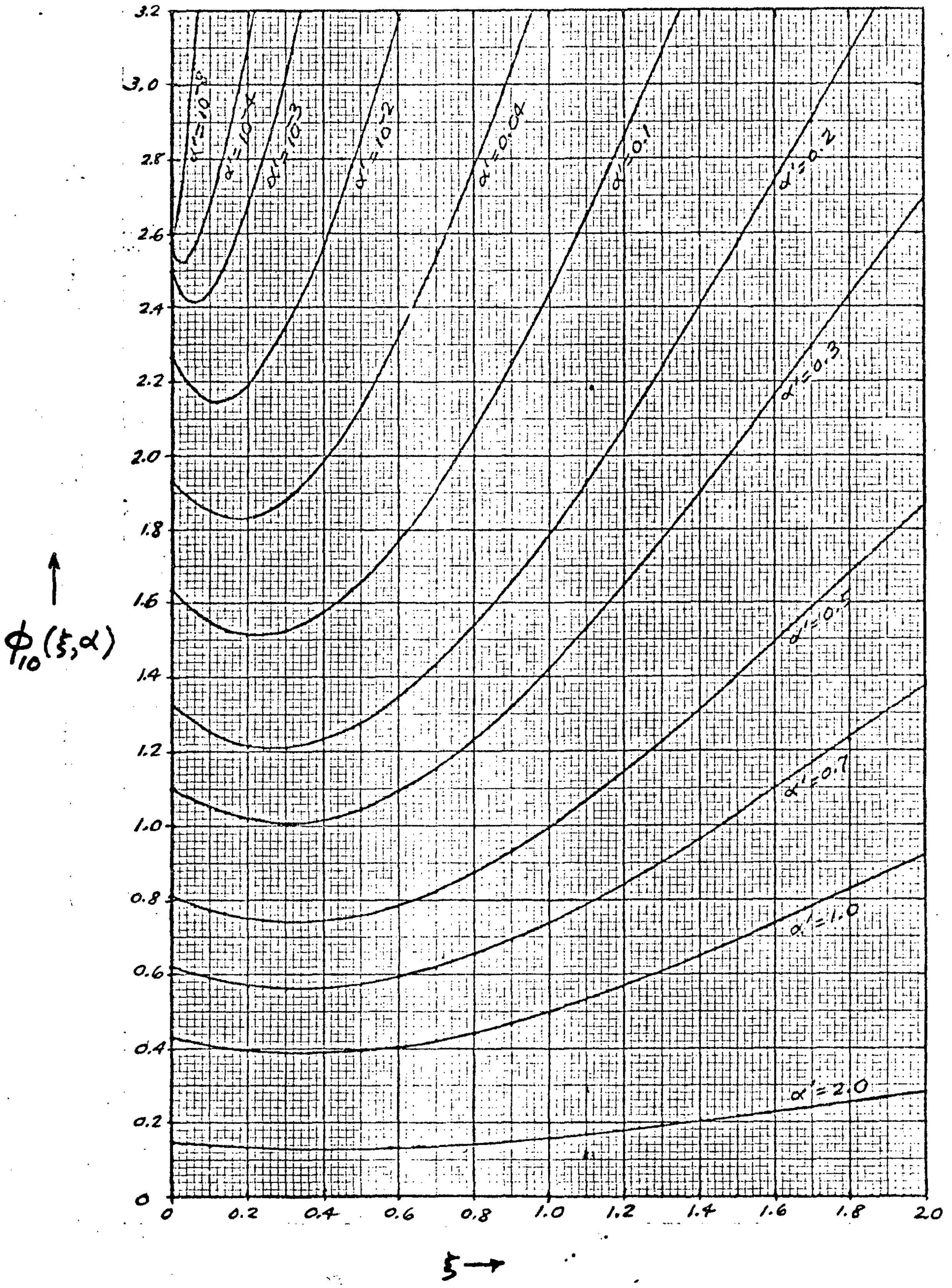

Fig. 4. The ϕ_{10} Function.

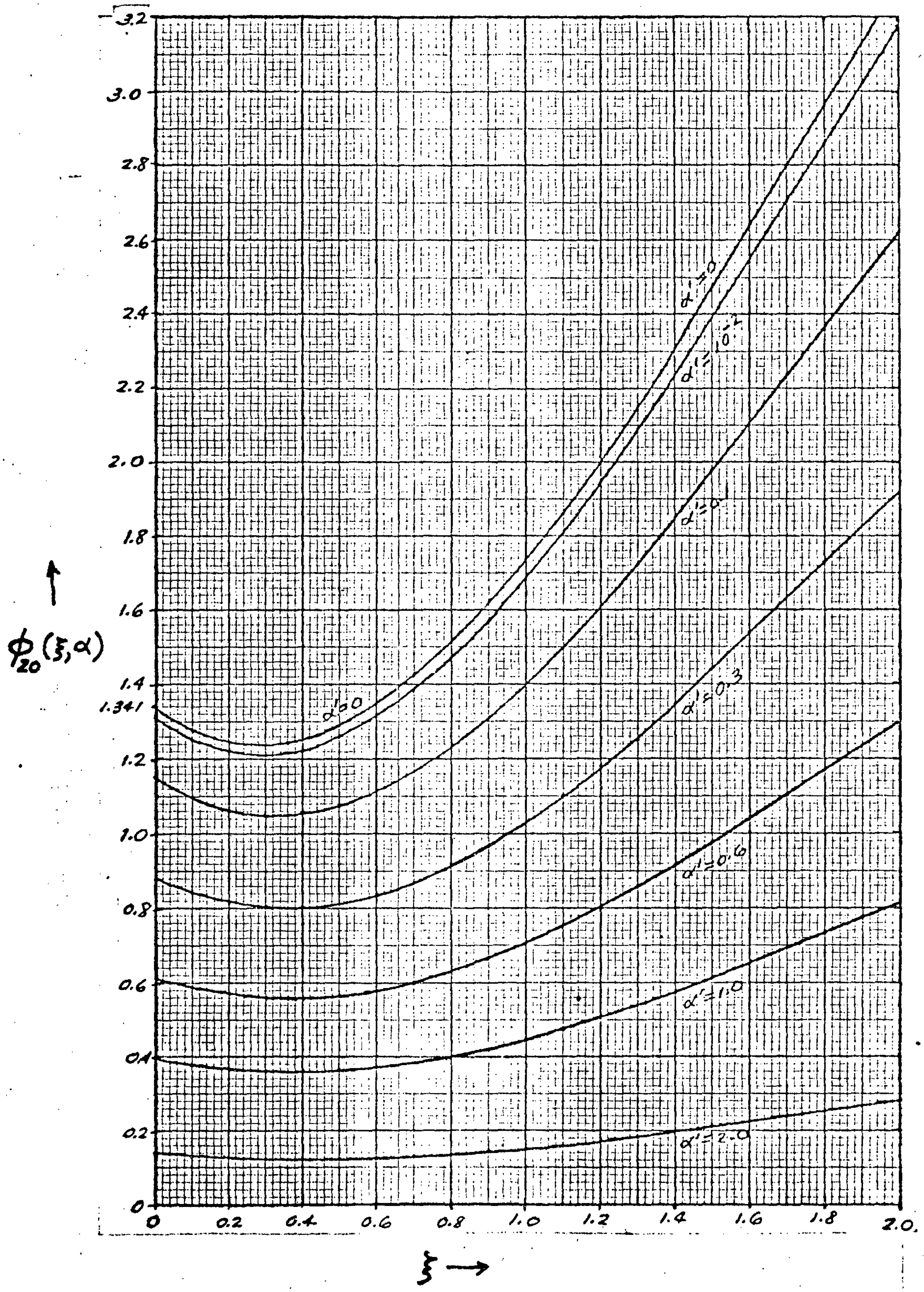

Fig. 5. The Φ_{20} Function.

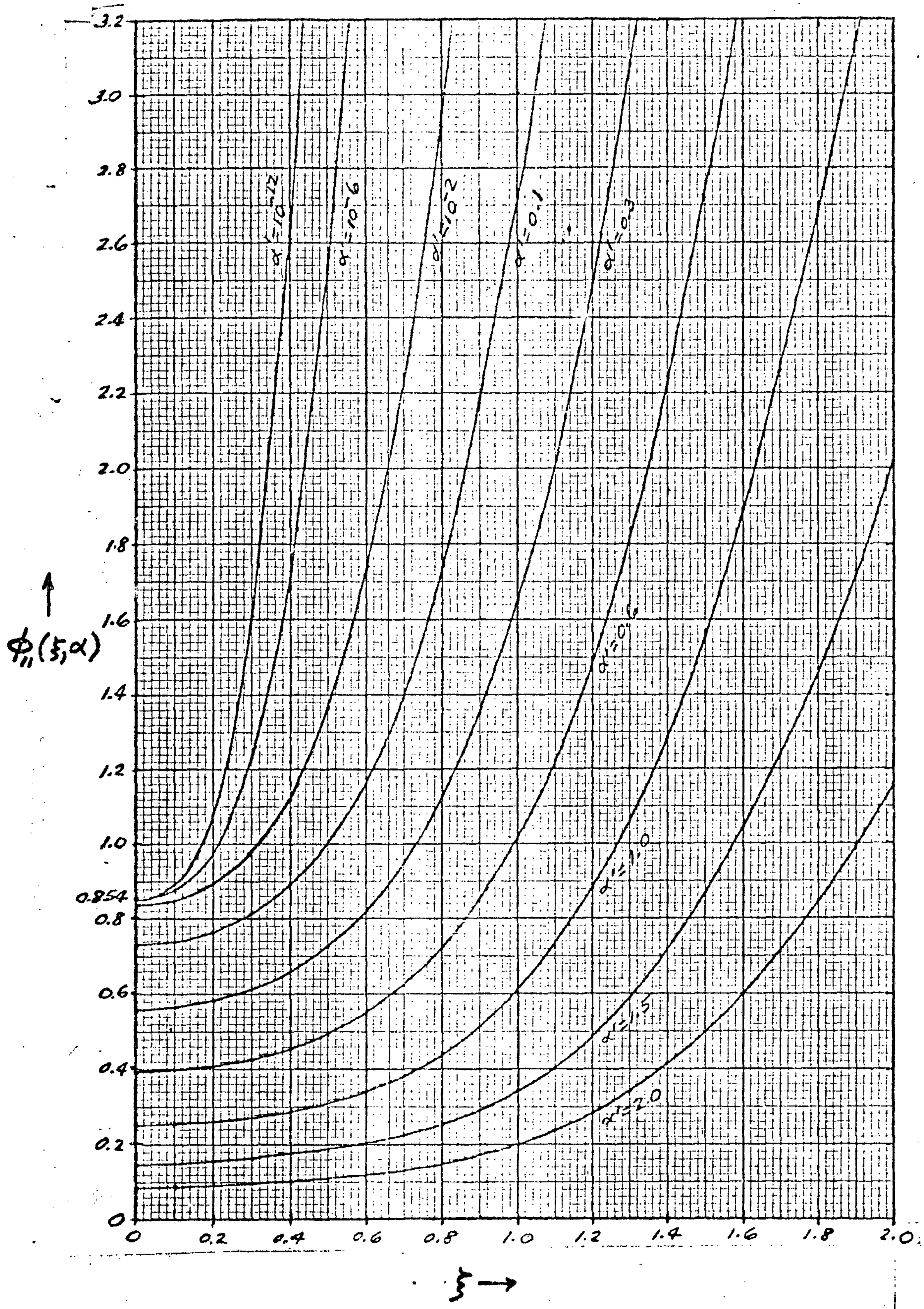

Fig. 6. The ϕ_{11} Function

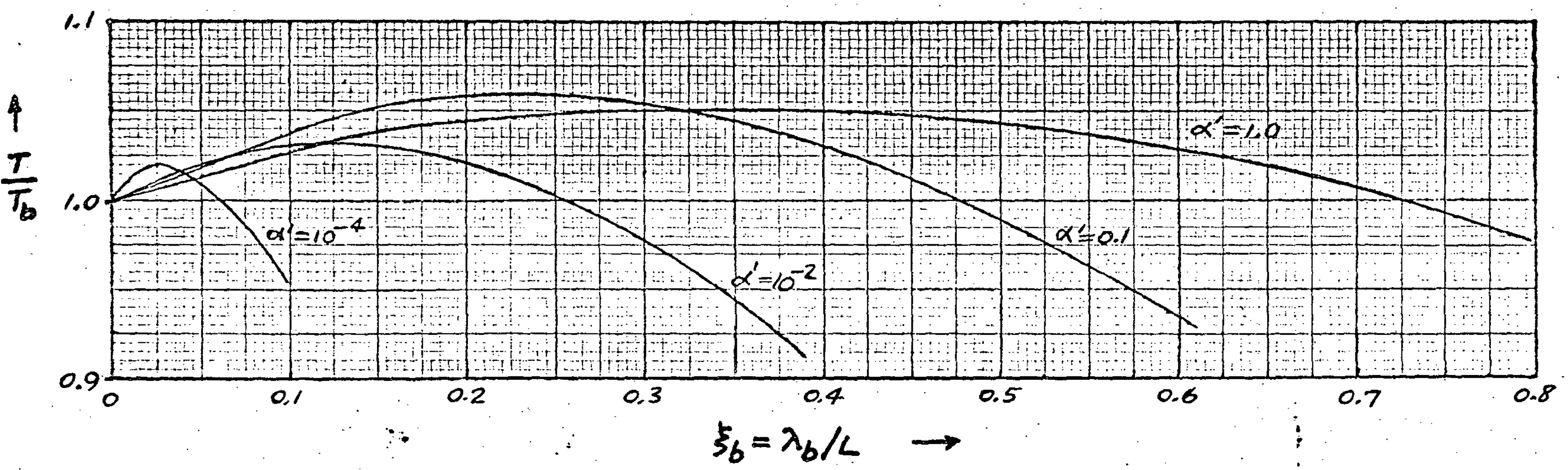

Fig. 7. Ratio of Film Temperature over Bulk Temperature at Constant Density and Ground State Occupancy

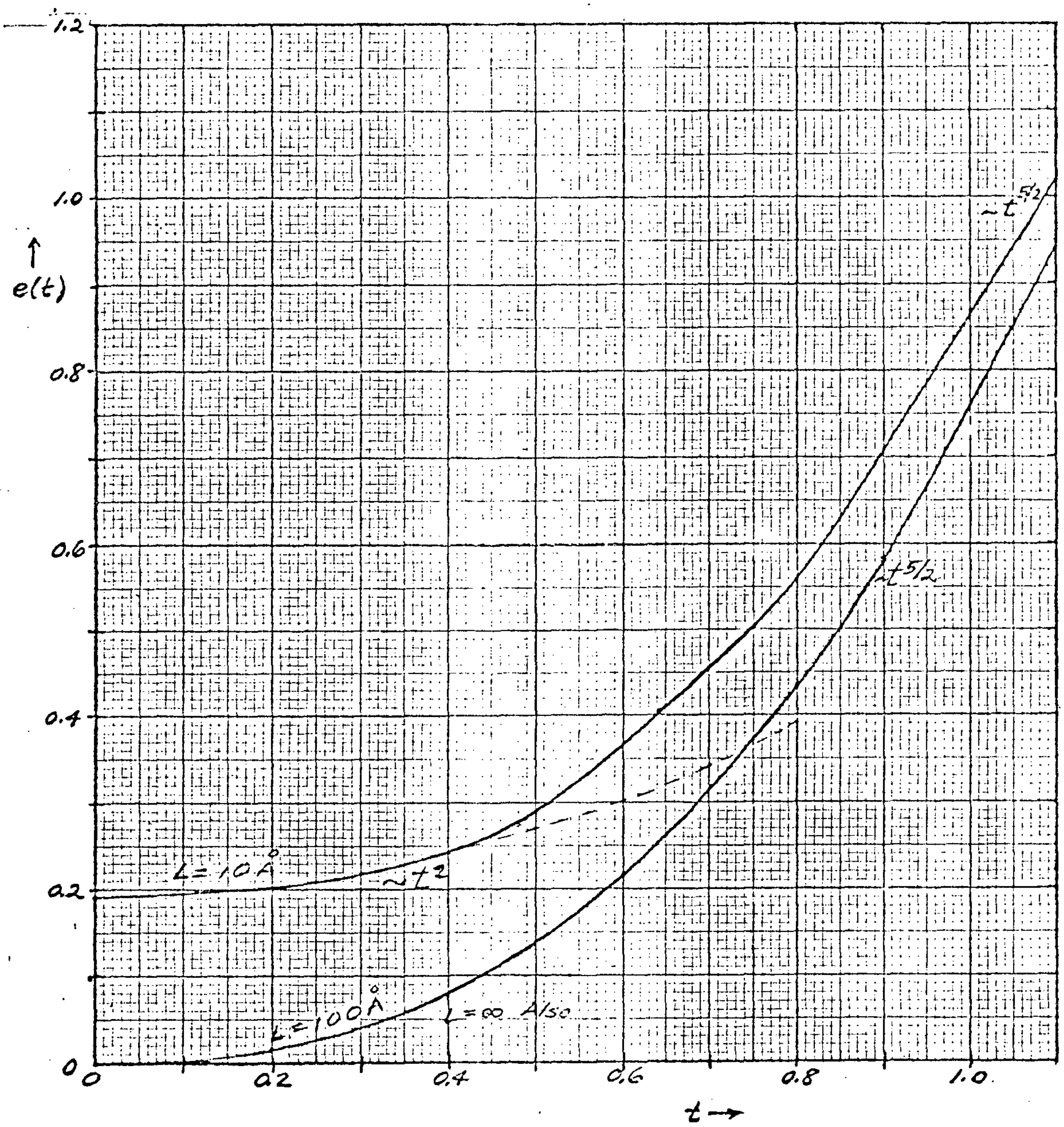

Fig. 8. Energy as a Function of Temperature for L = 10 Å and L = 100 Å .

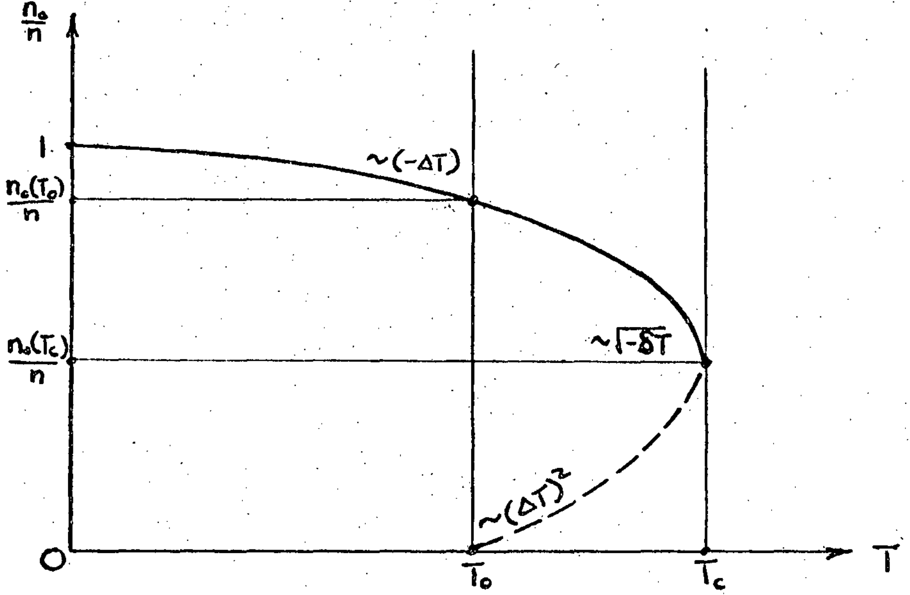

Fig. 9. Condensate Number Density as a Function of Temperature for Bogoliubov Energy Spectrum (not to scale).

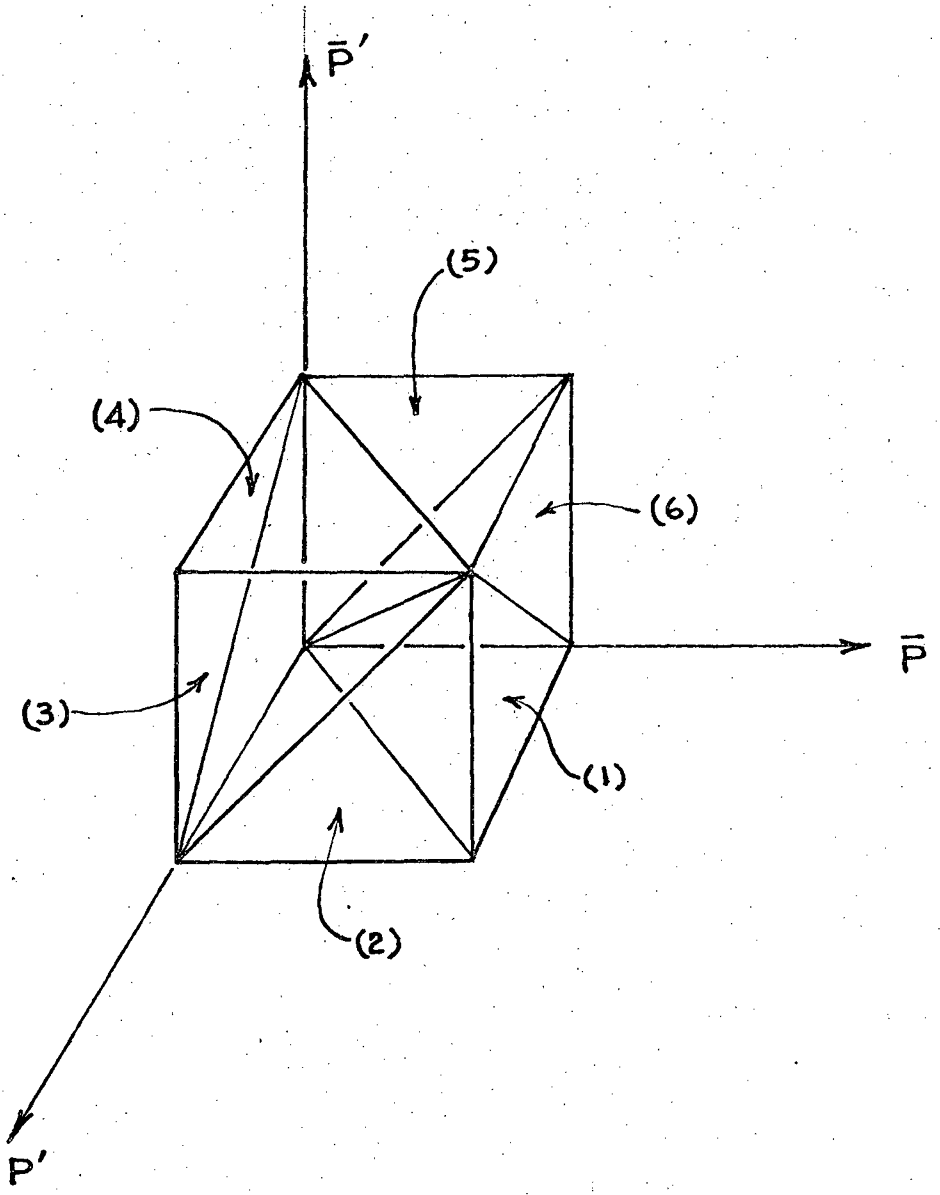

Fig. 10. Regions of Integration for Imaginary Part of Self-Energy.

Fig. 11. Comparison of Experimental Data and Theoretical Calculations.

✕ Specific Heat Maximum in Vycor Pores[19]

△ Specific Heat Maximum of Film[17,19]

○ Superflow Transition of Film[19-22]

□ Superflow Transition and Specific Heat Maximum of Vycor Pores[23]

◇ Superflow Transition in Vycor Pores[24]

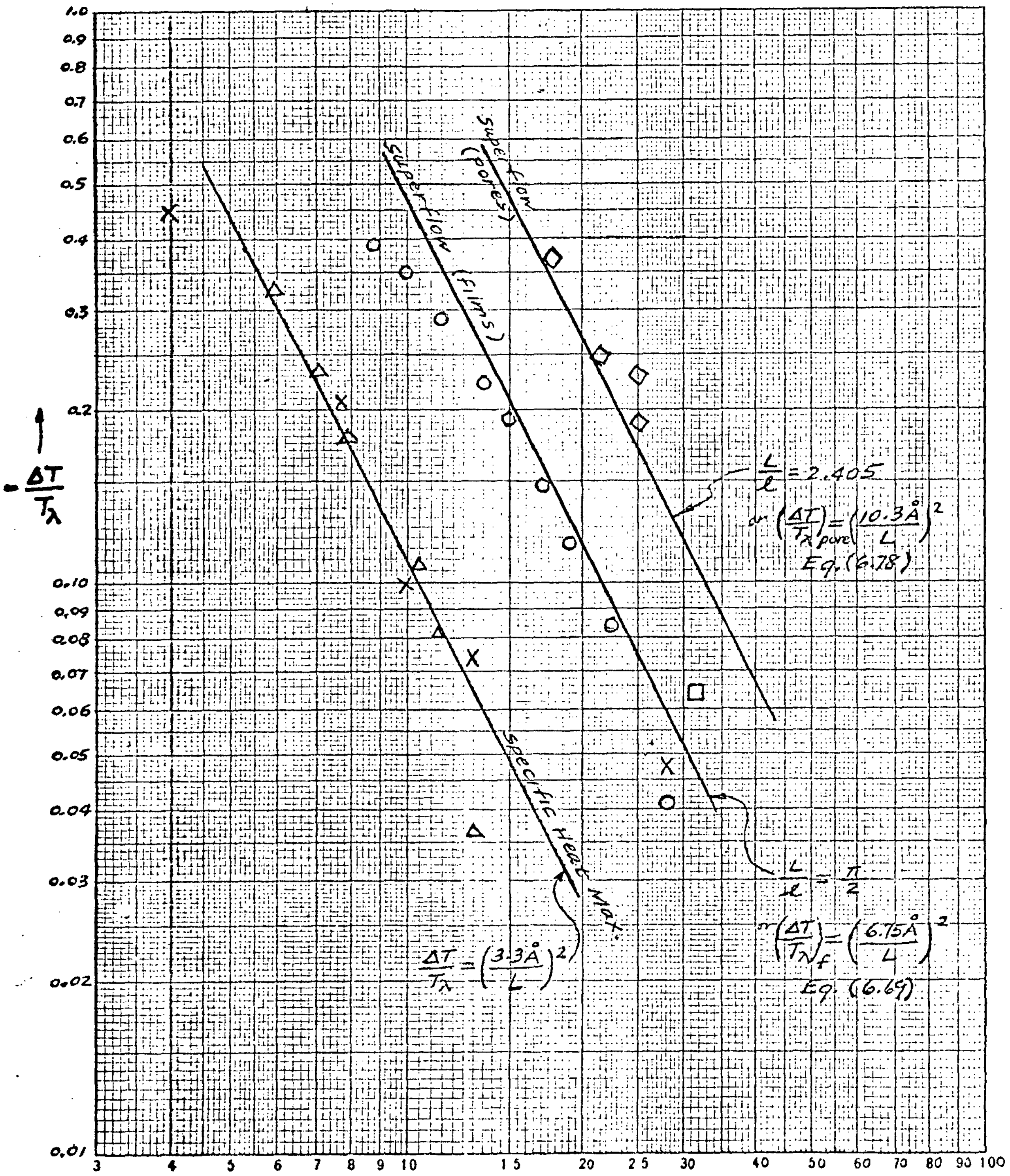

Fig. 11. Comparison of Experimental Data and Theoretical Calculations.

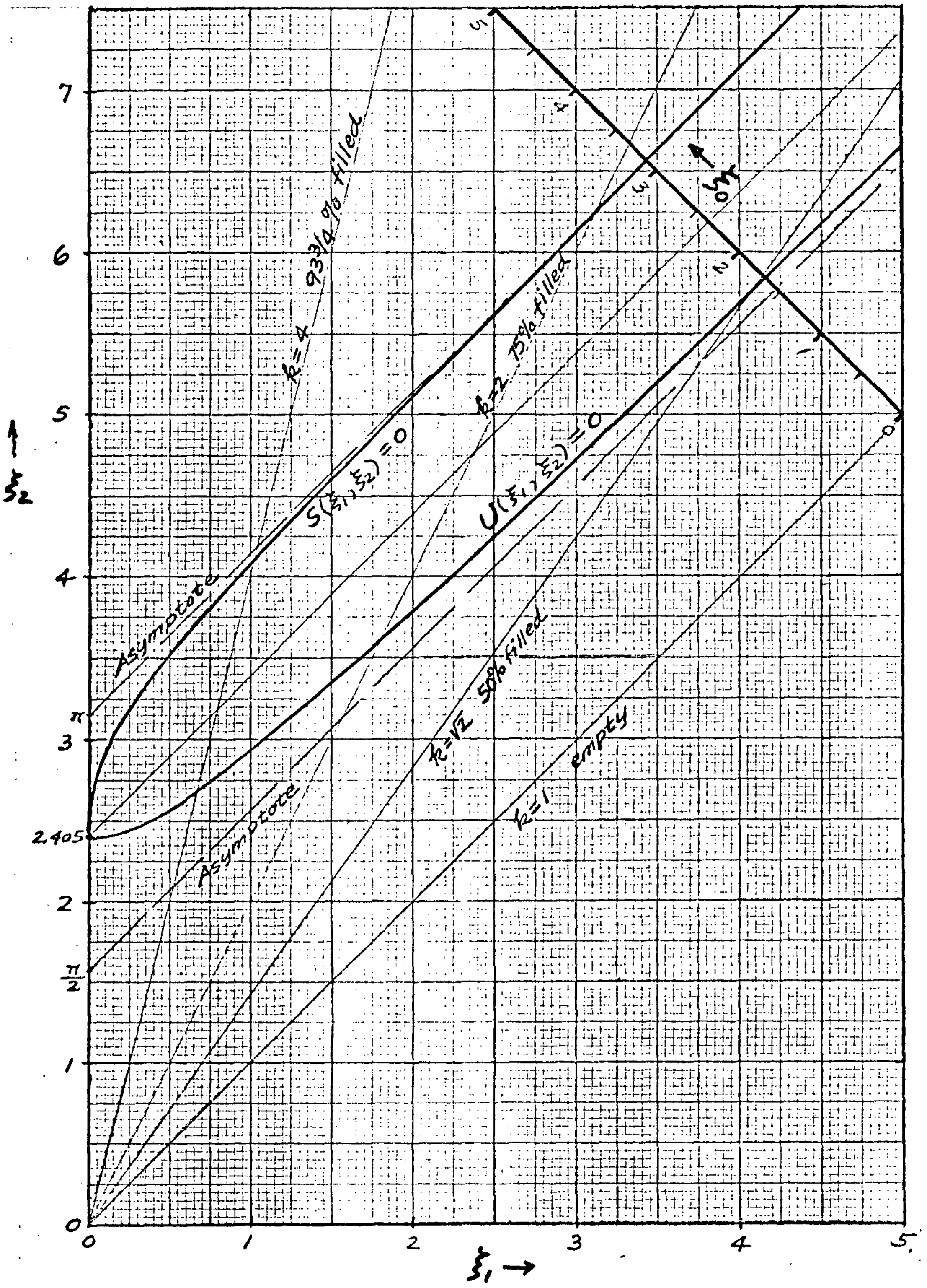

Fig. 12. Graphical Determination of the Smallest Root for a Cross-Product of Bessel Functions

TABLE 1. The ϕ_{00} Function

ξ \ α'	10^{-8}	10^{-4}	10^{-2}	0.1	1.0	10.0
0.1	0.100	0.101	0.165	0.388	0.482	0.435
0.2	0.200	0.200	0.231	0.391	0.468	0.422
0.4	0.400	0.400	0.410	0.474	0.463	0.412
0.6	0.600	0.600	0.602	0.616	0.489	0.422
0.8	0.800	0.800	0.798	0.782	0.542	0.450
1.0	1.000	1.000	0.996	0.960	0.619	0.498
1.2	1.200	1.200	1.194	1.145	0.713	0.563
1.4	1.400	1.400	1.393	1.332	0.820	0.642
1.6	1.600	1.600	1.592	1.522	0.933	0.728
1.8	1.800	1.800	1.791	1.712	1.048	0.818
2.0	2.000	2.000	1.990	1.902	1.164	0.908
2.2	2.200	2.200	2.189	2.092	1.280	0.999
2.4	2.400	2.400	2.388	2.282	1.397	1.090
2.6	2.600	2.600	2.587	2.472	1.513	1.180
2.8	2.800	2.800	2.786	2.662	1.630	1.271
3.0	3.000	3.000	2.985	2.852	1.746	1.362
	$\times 10^{8}$	$\times 10^{4}$	$\times 10^{2}$	$\times 10^{1}$	$\times 1$	$\times 10^{-4}$

TABLE 2. The ϕ_{10} Function

ξ \ α'	10^{-8}	10^{-4}	10^{-2}	0.1	1.0	10.0
0.1	0.360	0.268	2.148	1.548	4.093	4.347
0.2	0.499	0.314	2.190	1.512	3.970	4.216
0.4	0.811	0.442	2.570	1.572	3.901	4.118
0.6	1.146	0.594	3.172	1.773	4.049	4.217
0.8	1.495	0.758	3.901	2.074	4.403	4.503
1.0	1.852	0.931	4.711	2.444	4.949	4.979
1.2	2.215	1.109	5.573	2.860	5.654	5.632
1.4	2.580	1.291	6.468	3.306	6.472	6.419
1.6	2.948	1.474	7.380	3.767	7.353	7.282
1.8	3.316	1.658	8.300	4.235	8.259	8.176
2.0	3.684	1.842	9.220	4.704	9.174	9.081
2.2	4.053	2.026	10.14	5.175	10.09	9.988
2.4	4.421	2.210	11.07	5.645	11.01	10.90
2.6	4.790	2.395	11.99	6.116	11.93	11.80
2.8	5.158	2.579	12.91	6.586	12.84	12.71
3.0	5.526	2.763	13.83	7.057	13.76	13.62
	x 10^1	x 10^1	x 1	x 1	x 10^{-1}	x 10^{-5}

TABLE 3. The ϕ_{20} Function

ξ \ α'	10^{-8}	10^{-4}	10^{-2}	0.1	1.0	10.0
0.1	1.277	1.277	1.255	1.094	0.378	4.347
0.2	1.245	1.244	1.221	1.062	0.367	4.216
0.4	1.256	1.255	1.226	1.054	0.360	4.118
0.6	1.352	1.351	1.314	1.114	0.370	4.216
0.8	1.519	1.518	1.472	1.232	0.399	4.503
1.0	1.744	1.743	1.687	1.401	0.445	4.979
1.2	2.015	2.014	1.947	1.611	0.505	5.632
1.4	2.317	2.315	2.238	1.850	0.577	6.419
1.6	2.636	2.634	2.546	2.103	0.655	7.282
1.8	2.962	2.960	2.861	2.363	0.736	8.176
2.0	3.290	3.288	3.178	2.624	0.818	9.081
2.2	3.619	3.617	3.496	2.887	0.900	9.988
2.4	3.948	3.945	3.813	3.149	0.981	10.90
2.6	4.277	4.274	4.131	3.412	1.063	11.80
2.8	4.606	4.603	4.449	3.674	1.144	12.71
3.0	4.935	4.932	4.767	3.936	1.226	13.62
	x 1	x 1	x 1	x 1	x 1	x 10^{-5}

TABLE 4. The ϕ_{01} Function

α' ξ	10^{-8}	10^{-4}	10^{-2}	0.1	1.0	10.0
0.1	0.0010	0.0012	0.016	0.106	0.275	0.291
0.2	0.0080	0.0081	0.022	0.114	0.283	0.298
0.4	0.064	0.064	0.075	0.158	0.317	0.328
0.6	0.216	0.216	0.224	0.285	0.385	0.383
0.8	0.512	0.512	0.516	0.546	0.512	0.478
1.0	1.000	1.000	0.999	0.990	0.733	0.634
1.2	1.728	1.728	1.722	1.665	1.093	0.891
1.4	2.744	2.744	2.731	2.619	1.607	1.295
1.6	4.096	4.096	4.076	3.898	2.398	1.878
1.8	5.832	5.832	5.803	5.546	3.398	2.653
2.0	8.000	8.000	7.960	7.607	4.657	3.633
2.2	10.65	10.65	10.59	10.12	6.197	4.835
2.4	13.82	13.82	13.76	13.14	8.045	6.276
2.6	17.58	17.58	17.49	16.71	10.23	7.980
2.8	21.95	21.95	21.84	20.87	12.78	9.967
3.0	27.00	27.00	26.87	25.67	15.72	12.26
	$\times 10^{8}$	$\times 10^{4}$	$\times 10^{2}$	$\times 10^{1}$	$\times 1$	$\times 10^{-4}$

TABLE 5. The ϕ_{11} Function

α' ξ	10^{-8}	10^{-4}	10^{-2}	0.1	1.0	10.0
0.1	0.088	0.087	0.085	0.739	0.254	0.291
0.2	0.102	0.094	0.089	0.765	0.261	0.298
0.4	0.202	0.144	0.113	0.888	0.289	0.328
0.6	0.473	0.274	0.174	1.175	0.344	0.383
0.8	1.003	0.532	0.295	1.741	0.441	0.478
1.0	1.884	0.963	0.502	2.726	0.607	0.634
1.2	3.207	1.615	0.820	4.280	0.879	0.891
1.4	5.066	2.538	1.276	6.553	1.299	1.295
1.6	7.549	3.777	1.892	9.670	1.893	1.877
1.8	10.74	5.373	2.690	13.73	2.679	2.653
2.0	14.74	7.369	3.688	18.82	3.670	3.633
2.2	19.61	9.807	4.909	25.05	4.884	4.835
2.4	25.46	12.73	6.373	32.52	6.341	6.276
2.6	32.38	16.19	8.103	41.34	8.062	7.980
2.8	40.44	20.22	10.12	51.63	10.07	9.966
3.0	49.74	24.87	12.45	63.51	12.38	12.26
	$\times 10^{1}$	$\times 10^{1}$	$\times 10^{1}$	$\times 1$	$\times 1$	$\times 10^{-4}$

TABLE 6. The ϕ_{02} Function

α' ξ	10^{-8}	10^{-4}	10^{-2}	0.1	1.0	10.0
0.1	$1x10^{-6}$	$2x10^{-5}$	0.0016	0.014	0.049	0.056
0.2	$3x10^{-5}$	5.10^{-5}	0.0017	0.015	0.050	0.057
0.4	0.0010	0.0010	0.0029	0.017	0.055	0.063
0.6	0.0078	0.0078	0.0097	0.025	0.066	0.073
0.8	0.033	0.033	0.035	0.049	0.085	0.091
1.0	0.100	0.100	0.101	0.111	0.122	0.121
1.2	0.249	0.249	0.249	0.249	0.196	0.175
1.4	0.538	0.538	0.536	0.519	0.344	0.283
1.6	1.049	1.049	1.044	1.001	0.625	0.494
1.8	1.890	1.889	1.880	1.798	1.105	0.865
2.0	3.200	3.200	3.184	3.043	1.864	1.455
2.2	5.154	5.153	5.128	4.900	3.000	2.340
2.4	7.963	7.962	7.923	7.571	4.634	3.615
2.6	11.88	11.88	11.82	11.30	6.915	5.394
2.8	17.21	17.21	17.12	16.36	10.02	7.814
3.0	24.30	24.30	24.18	23.11	14.14	10.03
	x 10^{9}	x 10^{5}	x 10^{3}	x 10^{2}	x 10^{1}	x 10^{-3}

TABLE 7. Superflow Transition for Various Geometries and Boundary Conditions

$(\mathcal{L}^2 = -\hbar^2/mA_T\Delta T)$

Geometry	% filled	Wall Boundaries $\Psi = 0$	One Free Surface Boundary $\nabla_n \Psi = 0$
film (L = thickness)	--	$\frac{L}{\mathcal{L}} = \pi = 3.14$	$\frac{L}{\mathcal{L}} = \frac{\pi}{2} = 1.571$
pore (L = radius)	full	$\frac{L}{\mathcal{L}} = 2.405$	No free surface
pore (L_o = annular radius)	99 %	$\frac{L_o}{\mathcal{L}} = 2.98$	$\frac{L_o}{\mathcal{L}} = 2.20$
"	96 %	$\frac{L_o}{\mathcal{L}} = 3.05$	$\frac{L_o}{\mathcal{L}} = 2.08$
"	89 %	$\frac{L_o}{\mathcal{L}} = 3.09$	$\frac{L_o}{\mathcal{L}} = 1.94$
"	75 %	$\frac{L_o}{\mathcal{L}} = 3.12$	$\frac{L_o}{\mathcal{L}} = 1.80$
"	60 %	$\frac{L_o}{\mathcal{L}} = 3.13$	$\frac{L_o}{\mathcal{L}} = 1.75$
"	50 %	$\frac{L_o}{\mathcal{L}} = 3.14$	$\frac{L_o}{\mathcal{L}} = 1.7$
"	30 %	$\frac{L_o}{\mathcal{L}} = 3.14$	$\frac{L_o}{\mathcal{L}} = 1.6$
		$\rightarrow \pi$	$\rightarrow \pi/2$

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97. Note that if $\Delta'_p \sim p$, then $I_\Delta(p) \sim p^2$; and $I_\Delta(p) \sim I_\epsilon(p)$. Hence the neglect of ϵ^0_q in D(r) hinges on $\alpha_0 > 1$.

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