Thermodynamics of a OneDimensional System of Bosons with Repulsive DeltaFunction Interaction

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Thermodynamics of a One-Dimensional System of Bosons with Repulsive Delta-Function Interaction

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The equilibrium thermodynamics of a one-dimensional system of bosons with repulsive delta-function interaction is shown to be derivable from the solution of a simple integral equation. The excitation spectrum at any temperature T is also found.

I. INTRODUCTION

The ground-state energy of a system of N bosons with repulsive delta-function interaction in one dimension with periodic boundary condition was calculated by Lieb and Liniger.[1] The Hamiltonian for the system is

$$H = -\sum_1^N \frac{\partial^2}{\partial x_i^2} + 2c \sum_{i>j} \delta(x_i - x_j), \quad c > 0, \quad (1)$$

and the periodic box has length L. Using Bethe's hypothesis[2] they showed that the k's in the hypothesis satisfy

$$(-1)^{N-1} \exp(-ikL) = \exp\left[i \sum_{k'} \theta(k' - k)\right], \quad (2)$$

where

$$\theta(k) = -2 \tan^{-1}(k/c), \quad -\pi < \theta < \pi. \quad (3)$$

Taking the logarithm of (2) is a somewhat subtle process. In this paper we shall first discuss this point and show that *all* states of (1) are given by Bethe's hypothesis with real k's. The main purpose of the paper is to then evaluate the thermodynamical properties of the system at a finite temperature T.

While we try to maintain mathematical rigor in the rest of the paper, it is to be emphasized that Secs. III and IV are far from rigorous.

II. PROOF OF BETHE'S HYPOTHESIS FOR ALL STATES

We first take the logarithm of (2):

$$kL = 2\pi I_k + \sum_{k'} \theta(k - k'), \quad (4)$$

where

$$I_k = \text{integer}, \quad \text{if } N = \text{odd},$$
$$I_k + \tfrac{1}{2} = \text{integer}, \quad \text{if } N = \text{even}. \quad (5)$$

Now, for any set of real I's, $I_1, I_2, \cdots, I_N$, Eq. (4) has a unique real solution for the k's, $k_1, k_2, \cdots, k_N$. The proof of this statement (similar to but simpler than the proof of a corresponding statement[3] for the Heisenberg–Ising problem) follows. Let

$$\theta_1(k) = \int_0^k \theta(k) \, dk.$$

Define

$$B(k_1, \cdots, k_N) = \tfrac{1}{2} L \sum_1^N k_j^2 - 2\pi \sum_1^N I_j k_j$$
$$- \tfrac{1}{2} \sum_{j,S} \theta_1(k_j - k_S). \quad (6)$$

Equation (4) is the condition for the extrema of B. Now the second-derivative matrix B_2 of B is positive-definite. [The first sum in (6) contributes a positive-definite part to B_2. The second sum contributes nothing. Each term in the third sum is negative-semidefinite, since $\theta_1''(k) = \theta'(k) < 0$.] Furthermore for large values of $\sum k^2$, $B \to \tfrac{1}{2} L(\sum k^2)$. Thus, B has one and *only one* extremum, namely, a minimum.

It is further clear from this argument that the solution above represents a point S in k space which moves continuously as c^{-1} is changed. [In fact, $dk_j/d(c^{-1})$ can be computed.] Now when $c^{-1} = 0$, $\theta_1 = 0$ and the minimum of B occurs at

$$k_j = 2\pi I_j/L. \quad (7)$$

Now the problem with $c^{-1} = 0$ is the problem of free particles with the condition that $\psi = 0$ whenever $x_i = x_j$ (any $i \neq j$). All eigenfunctions of H for this problem are easily seen to be the same as that of free fermions in the segment $0 \leq x_1 \leq x_2 \leq x_3 \leq \cdots \leq x_N \leq L$. Thus, when $c^{-1} = 0$, all eigenfunctions are of Bethe's form, with the k's given by (7) and with all the I's different.

[1] E. Lieb and W. Liniger, Phys. Rev. **130**, 1605 (1963).
[2] H. A. Bethe, Z. Physik **71**, 205 (1931).
[3] C. N. Yang and C. P. Yang, Phys. Rev. **150**, 321 (1966).

By a continuity argument with respect to c^{-1} we obtain the following:

Theorem: For any set of I's satisfying (5), no two of which are identical, there is a unique set of real k's satisfying (4), with no two k's being identical. With this set of k's, one eigenfunction of H, of Bethe's form, can be constructed. The totality of such eigenfunctions form a complete set for the boson system.

The numbers I are quantum numbers for the problem.

III. ENERGY AND ENTROPY FOR A SYSTEM WITH $N = \infty$

We now consider the problem for $N = \infty$ and $L = \infty$ at a fixed density $D = N/L$. For the ground state, the quantum numbers I/L form[1] a uniform lattice between $-D/2$ and $D/2$. The k's then form[1] a non-uniform distribution between a maximum k and a minimum k. For an excited state, (5) shows that the quantum numbers I/L are still on the same lattice, but not all lattice sites are taken, and the limits $-D/2$ and $D/2$ are no longer respected. We shall call the omitted lattice sites J_j/L. We would want to define corresponding "omitted k values" to be called holes. This can be easily done: Given the I's, Eq. (4) defines the set of k's as proved in the last section. Now,

$$Lh(p) \equiv pL - \sum_{k'} \theta(p - k') \qquad (8)$$

is a continuous monotonic function of p. At $p = \pm\infty$, it is equal to $\pm\infty$. Those values of p where $Lh(p) = 2\pi I$ are k's. Those values of p where $Lh(p) = 2\pi J$ will be defined as holes.

For a large system, there is thus a density distribution of holes as well as one of k's:

$$L\rho(k)\, dk = \text{No. of } k\text{'s in } dk,$$
$$L\rho_h(k)\, dk = \text{No. of holes in } dk. \qquad (9)$$

By definition, the number of k's and holes in the interval dk is the number of times $Lh(k)$ ranges over values $2\pi I$ and $2\pi J$ in this interval.

Thus,

$$\frac{dh(k)}{dk} = 2\pi(\rho + \rho_h) \equiv 2\pi f(k). \qquad (10a)$$

Equation (8) gives

$$h(k) = k - \int_{-\infty}^{\infty} \theta(k - k')\rho(k')\, dk'. \qquad (10b)$$

Differentiation with respect to k gives

$$2\pi f = 2\pi(\rho + \rho_h) = 1 + 2c \int_{-\infty}^{\infty} \frac{\rho(k')\, dk}{c^2 + (k - k')^2}. \qquad (11)$$

The energy per particle for the state is

$$E/N = D^{-1} \int_{-\infty}^{\infty} \rho(k)k^2\, dk, \qquad (12)$$

where

$$D = N/L = \int_{-\infty}^{\infty} \rho(k)\, dk. \qquad (13)$$

The entropy of the "state" is not zero since the existence of the omitted quantum numbers J_j allows many wavefunctions of approximately the same energy to be described by the same ρ and ρ_h. In fact, for given ρ and ρ_h, the total number of k's and holes in dk is $L(\rho + \rho_h)\, dk$, of which $L\rho\, dk$ are k's and $L\rho_h\, dk$ are holes. Thus the number of possible choices of states in dk consistent with given ρ and ρ_h is

$$\frac{[L(\rho + \rho_h)\, dk]!}{[L\rho\, dk]!\, [L\rho_h\, dk]!}.$$

The logarithm of this gives the contribution to the entropy from dk. Thus, the total entropy is, putting the Boltzman constant equal to 1,

$$S = \sum \{(L\rho\, dk + L\rho_h\, dk) \ln(\rho + \rho_h) - L\rho\, dk \ln \rho - L\rho_h\, dk \ln \rho_h\}$$

or

$$S/N = D^{-1} \int_{-\infty}^{\infty} [(\rho + \rho_h) \ln(\rho + \rho_h) - \rho \ln \rho - \rho_h \ln \rho_h]\, dk. \qquad (14)$$

IV. THERMAL EQUILIBRIUM

At temperature T, we should maximize the contribution to the partition function from the states described by ρ and ρ_h. In other words, given ρ, ρ_h is defined by (11). One then computes the contribution to the partition function

$$\exp(S - ET^{-1}), \qquad (14')$$

where S and E are given by (14) and (12). The equilibrium ρ is then obtained by maximizing this contribution when ρ is varied subject to the condition (13).

The above described procedure leads in a straightforward manner to the following condition on the equilibrium ρ:

$$-A + k^2 + T \ln \frac{\rho}{\rho_h}$$
$$- \frac{Tc}{\pi} \int_{-\infty}^{\infty} \frac{dq}{c^2 + (k - q)^2} \ln\left(1 + \frac{\rho}{\rho_h}\right) = 0,$$

where A is a Lagrange multiplier for the condition (13). Writing

$$\rho_h/\rho = \exp[\epsilon(k)/T], \qquad (15)$$

we have

$$\epsilon(k) = -A + k^2 - \frac{Tc}{\pi}\int_{-\infty}^{\infty}\frac{dq}{c^2 + (k-q)^2}$$
$$\times \ln\{1 + \exp[-\epsilon(q)/T]\}. \quad (16)$$

Equation (11) becomes

$$2\pi f(k) = 2\pi\rho(k)\{1 + \exp[\epsilon(k)/T]\}$$
$$= 1 + 2c\int_{-\infty}^{\infty}\frac{\rho(q)\,dq}{c^2 + (k-q)^2}. \quad (17)$$

It will be shown in Appendix A that (16) can be solved for ϵ by iteration. Equation (17) is then a Fredholm equation for ρ. It will be shown in Appendix B that ρ can be obtained by iteration of (17). The energy, density D, and entropy can then be obtained from (12)–(14).

In Appendix C it will be shown that the maximization procedure that led to (16) can be more rigorously treated and that the conclusion of the next section can then be obtained without much algebra.

V. A = CHEMICAL POTENTIAL

We shall now show that A is the chemical potential. Multiply (16) with ρD^{-1} and integrate over k to obtain

$$A = D^{-1}\int_{-\infty}^{\infty}\rho(k^2 - \epsilon)\,dk$$
$$+ TD^{-1}\int_{-\infty}^{\infty}dq[(2\pi)^{-1} - f(q)]$$
$$\times \ln\left(1 + \exp\left\{\frac{-\epsilon(q)}{T}\right\}\right). \quad (18)$$

In this formula, the square bracket is obtained from (17). Now use (15) to rewrite (14) as

$$S/N = D^{-1}\int_{-\infty}^{\infty}(\rho + \rho_h)\ln(1 + \exp\{-\epsilon/T\})\,dk$$
$$+ (DT)^{-1}\int_{-\infty}^{\infty}\rho\epsilon\,dk. \quad (19)$$

Thus, the free energy per particle is

$$FN^{-1} = (E - TS)N^{-1} = D^{-1}\int_{-\infty}^{\infty}(k^2 - \epsilon)\rho\,dk$$
$$- TD^{-1}\int_{-\infty}^{\infty}(\rho + \rho_h)\ln[1 + \exp(-\epsilon/T)]\,dk. \quad (20)$$

Comparison of (18) and (20) gives, using $f = \rho + \rho_h$,

$$FN^{-1} = A - T(2\pi D)^{-1}\int_{-\infty}^{\infty}\ln[1 + \exp(-\epsilon/T)]\,dk. \quad (21)$$

If we now prove that the last term is $-PD^{-1}$ (where P is the pressure), then this formula demonstrates that A is the chemical potential, since by thermo-

dynamics

$$F = -PL + N \times (\text{chemical potential}).$$

Now, by (21),

$$P = -\left(\frac{\partial F}{\partial L}\right)_T$$
$$= -N\frac{\partial A}{\partial L} + \frac{TN}{2\pi D}\int_{-\infty}^{\infty}dq\,\frac{1}{1 + e^{\epsilon/T}}\left(-\frac{1}{T}\right)\frac{\partial\epsilon}{\partial A}\frac{\partial A}{\partial L}$$
$$+ \frac{T}{2\pi}\int_{-\infty}^{\infty}dk\,\ln(1 + e^{-\epsilon/T}), \quad (22)$$

where ϵ is considered a function of A defined by (16). Differentiating (16) with respect to A, we obtain

$$1 = -\left(\frac{\partial\epsilon}{\partial A}\right) + \frac{c}{\pi}\int_{-\infty}^{\infty}\frac{dq}{c^2 + (k-q)^2}\frac{(\partial\epsilon/\partial A)}{1 + e^{\epsilon(q)/T}}. \quad (23)$$

Comparing this equation with (17) we conclude, by the uniqueness of the solution of (17) (see Appendix B),

$$-\frac{\partial\epsilon}{\partial A} = 2\pi f(k) = 2\pi\rho(k)(1 + e^{\epsilon(k)/T}). \quad (24)$$

The first two terms in the expression (22) for P now cancel each other by (24) and (13). Thus,

$$P = \frac{T}{2\pi}\int_{-\infty}^{\infty}dk\,\ln(1 + e^{-\epsilon(k)/T}). \quad (25)$$

This proves the assertion that A is the chemical potential.

We shall prove in Appendix D that $P(A, T)$ is analytic in A and T. To recapitulate: ϵ is defined by (16) once A and T are given. Equation (25), then, gives P as a function of A and T. The other thermodynamic quantities are obtainable from the thermodynamic relation

$$dP = (S/L)\,dT + (N/L)\,dA. \quad (26)$$

If one wants to compute ρ, one uses either (17) or (24).

VI. SPECIAL CASES
A. $c = \infty$

The integrals in (16) and (17) do not contribute. Thus,

$$\epsilon = -A + k^2,$$
$$2\pi\rho = z\exp(-k^2/T)[1 + z\exp(-k^2/T)]^{-1},$$
$$2\pi\rho_h = [1 + z\exp(-k^2/T)]^{-1}, \quad (27)$$
$$P = T(2\pi)^{-1}\int_{-\infty}^{\infty}dk\,\ln[1 + z\exp(-k^2/T)],$$

where

$$z = \text{fugacity} = \exp(A/T).$$

These equations are those for a free Fermi gas, a result that is anticipated, as discussed in Sec. II.

B. $c = 0$

As $c \to 0$,

$$c(c^2 + x^2)^{-1} \to \pi\delta(x). \tag{28}$$

Thus, (16) gives

$$\epsilon = -A + k^2 - T \ln [1 + \exp(-\epsilon/T)]$$

or

$$\exp(-\epsilon/T) = [z^{-1} \exp(k^2/T) - 1]^{-1},$$

where we have used the fugacity defined in (27). Equation (25) now becomes

$$P = -T(2\pi)^{-1} \int_{-\infty}^{\infty} dk \ln [1 - z \exp(-k^2/T)]. \tag{29}$$

Equations (28) and (17) give

$$2\pi\rho_h = 1,$$
$$2\pi\rho = \exp(-\epsilon/T) = [z^{-1} \exp(k^2/T) - 1]^{-1}. \tag{30}$$

Equations (29) and (30) are precisely the corresponding expressions for a free Bose gas, as they should be.

C. $T = 0$

This is the case solved[1] by Lieb and Liniger.

It will be shown in Appendix A that $\epsilon(k)$ is a monotonically increasing function of k^2. At $T = 0$ assume the function to have a zero at $k^2 = q_0^2$ so that

$$\epsilon(k) < 0, \quad k^2 < q_0^2,$$
$$\epsilon(k) > 0, \quad k^2 > q_0^2, \tag{31}$$
$$\epsilon(q_0) = 0.$$

Equation (15) gives

$$\rho = 0, \quad \text{for} \quad k^2 > q_0^2,$$
$$\rho_h = 0, \quad \text{for} \quad k^2 < q_0^2. \tag{32}$$

Equations (16) and (17) become

$$\epsilon(k) = -A + k^2 + \frac{c}{\pi} \int_{-q_0}^{q_0} \frac{\epsilon(q) \, dg}{c^2 + (k - q)^2}, \tag{33}$$

$$2\pi\rho = 1 + 2c \int_{-q_0}^{q_0} \frac{\rho(q) \, dq}{c^2 + (k - q)^2}, \quad \text{for} \quad k^2 < q_0^2. \tag{34}$$

Equation (34) is the equation[1] of Lieb and Liniger. Equation (33) will be useful in the next section.

VII. EXCITATION

Consider a state S, with I's and k's satisfying

$$k_j L = 2\pi I_j + \sum_i \theta(k_j - k_i), \tag{35}$$

and a state S', with primed I's and k's satisfying

$$k_j' L = 2\pi I_j' + \sum_i \theta(k_j' - k_i'). \tag{36}$$

We consider the case where

$$I_j' = I_j, \quad \text{except when} \quad j = \alpha. \tag{37}$$

[Notice that $I_1', I_2', \cdots, I_N'$ may *not* be a monotonically increasing series, since I_α' may be any integer for $N = $ odd and any integer $+\frac{1}{2}$ for $N = $ even.]

Subtract (35) from (36) to obtain

$$(k_j' - k_j)L = \sum_i [\theta(k_j' - k_i') - \theta(k_j - k_i)]. \tag{38}$$

We now assume that, for all $j \neq \alpha$, k_j and k_j' are approximately the same. This is the same assumption as used by Lieb[4] for the excitations near the ground state (i.e., $T = 0$). We write

$$(k_j' - k_j)L = \chi(k_j), \quad j \neq \alpha.$$

Thus, we expand those terms in (38) for which $i \neq \alpha$:

$$\chi(k_j) = \sum_{i \neq \alpha} \theta'(k_j - k_i)[\chi(k_j) - \chi(k_i)]L^{-1}$$
$$+ \theta(k_j - k_\alpha') - \theta(k_j - k_\alpha) \tag{39}$$

or

$$\chi(k) = \int_{-\infty}^{\infty} \theta'(k - q)[\chi(k) - \chi(q)]\rho(q) \, dq$$
$$+ \theta(k - k_\alpha') - \theta(k - k_\alpha). \tag{40}$$

Now we differentiate (10b) and use it to evaluate the coefficient of $\chi(k)$ in (40). Writing

$$f(k)\chi(k) = g(k), \tag{41}$$

we thus obtain

$$2\pi g(k) = -\int_{-\infty}^{\infty} \theta'(k - q)g(q)$$
$$\times [1 + \exp\{+\epsilon(q)/T\}]^{-1} \, dq$$
$$+ \theta(k - k_\alpha') - \theta(k - k_\alpha) \tag{42}$$

or, explicitly,

$$g(k) = \frac{c}{\pi} \int_{-\infty}^{\infty} \frac{g(q) \, dq}{[c^2 + (k - q)^2][1 + \exp \epsilon(q)/T]}$$
$$+ \frac{1}{\pi} \tan^{-1}(k_\alpha' - k)c^{-1} - \frac{1}{\pi} \tan^{-1}(k_\alpha - k)c^{-1}. \tag{43}$$

This is a Fredholm integral equation which we shall write in operator form

$$g = Kg + G. \tag{44}$$

The momentum difference and energy difference

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[4] E. Lieb, Phys. Rev. **130**, 1616 (1963).

between the two states are

$$\Delta K = \sum_j (k'_j - k_j) = k'_\alpha - k_\alpha + \int_{-\infty}^\infty \chi(k)\rho(k)\,dk \quad (45)$$

and

$$\Delta E = \sum_j (k'^2_j - k^2_j) = k'^2_\alpha - k^2_\alpha + \int_{-\infty}^\infty \chi(k)2k\rho(k)\,dk. \quad (46)$$

We shall prove in Appendix E the following:

Theorem: The momentum difference and energy difference[5] between the two states are

$$\Delta K = h(k'_\alpha) - h(k_\alpha) \quad (47)$$

and

$$\Delta E = \epsilon_0(k'_\alpha) - \epsilon_0(k_\alpha), \quad (48)$$

where

$$\epsilon_0 = \epsilon + A \quad (49)$$

and h is an odd function of k defined by (10a). These equations are accurate to the order N^0, not just N^1. (Notice that in evaluating the thermodynamical quantities, such as the energy, we only maintain accuracy up to the order N^1.)

VIII. DISCUSSIONS

(A) It is easy to prove that, for a finite number of simultaneous excitations,

$$\Delta K = \sum_\alpha h(k'_\alpha) - \sum_\alpha h(k_\alpha), \quad (50)$$

$$\Delta E = \sum_\alpha \epsilon_0(k'_\alpha) - \sum_\alpha \epsilon_0(k_\alpha). \quad (51)$$

Thus it is tempting to regard $h(k_\alpha)$ and $\epsilon_0(k_\alpha)$ as the momentum and energy of an elementary excitation.

To be more precise, we consider a system of non-interacting fermions with its single-particle states labeled by k. The momentum and energy of a single-particle state k are taken to be $h(k)$ and $\epsilon_0(k)$, respectively. The number of single-particle states in the k interval dk is $f(k)\,dk$. Such a system of particles will be called a model system M. At a fixed fugacity z, the model system has an average number of particles in the state k given by

$$ze^{-\epsilon_0/T}[1 + ze^{-\epsilon_0/T}]^{-1}, \quad (52)$$

so that the number of particles in the interval dk is $f\,dk$ times (52), which is also the same quantity in the true system. The model system M and the true system then have the same excitation spectra at T, *provided*

only a finite number of excitations are made from thermal equilibrium. (Notice that the definition of the system M depends on h, ϵ_0, and f.)

(B) The excitation $k_\alpha \to k'_\alpha$ discussed in Sec. VII occurs with an excitation function which is proportional to a factor dependent on the method of excitation. But, in addition, it is also proportional to the number of I's in the interval dI near I_α and the number of vacancies in the interval dI' near I'_α. Thus, to excite

from $(k$ in $dk)$ to $(k'$ in $dk')$

there is an *intrinsic* excitation factor equal to

$$\rho(k)\rho_h(k')\,dk\,dk' = \rho(k)\rho(k')e^{\epsilon(k')/T}\,dk\,dk'. \quad (53)$$

APPENDIX A

We want to prove that (16) can be solved by iteration. Define the right-hand side of (16) as 0ϵ. Define further

$$\begin{aligned}
\epsilon_1 &= -A + k^2, \\
\epsilon_2 &= 0\epsilon_1, \\
\epsilon_3 &= 0\epsilon_2, \quad \text{etc.}
\end{aligned} \quad (A1)$$

It is easily seen that

$$\epsilon_1(k) > \epsilon_2(k) > \epsilon_3(k), \quad \text{etc.}$$

Next one can show that $\epsilon_n(k)$ is bounded from below. To do this, one proves first by induction that $\epsilon_n - k^2$ is a nondecreasing function of k^2. One then has

$$\epsilon_{n+1}(0) \geq -A - \frac{Tc}{\pi}\int_{-\infty}^\infty \frac{dq}{c^2 + q^2} \times \ln[1 + \exp\{-\epsilon_n(0)T^{-1} - q^2 T^{-1}\}]. \quad (A2)$$

Now define the right-hand side of (A2) as $f[\epsilon_n(0)]$. That is,

$$f(x) = -A + x - \frac{Tc}{\pi}\int_{-\infty}^\infty \frac{dq}{c^2 + q^2} \ln(e^{x/T} + e^{-q^2/T}). \quad (A3)$$

It is clear from (A3) that $f(x) - x$ is monotonically decreasing. It has one and only one zero. Call the zero x_0 so that

$$f(x_0) = x_0. \quad (A4)$$

The right-hand side of (A2) shows that

$$f(x) \text{ is monotonically increasing} \quad (A5)$$

and that $f(x) < -A$. Thus (A4) gives

$$-A > f(x_0) = x_0. \quad (A6)$$

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[5] In the limit $T \to 0$, the energy and momentum spectra are reducible to very simple expressions, using (31)–(34). These spectra have been obtained by Lieb in Ref. 4. Reduction to such simple equations as (33) is new.

Equations (A4), (A5), and (A6) show that

$$\epsilon_1(0) = -A > x_0,$$
$$\epsilon_2(0) \geq f[\epsilon_1(0)] > f(x_0) = x_0,$$
$$\epsilon_3(0) \geq f[\epsilon_2(0)] > f(x_0) = x_0, \quad \text{etc.}$$

Thus,

$$\epsilon_n(k) \geq \epsilon_n(0) > x_0. \tag{A7}$$

Having shown that

$$\lim_{n \to \infty} \epsilon_n(k) = \epsilon_L(k)$$

exists, one can next prove that the limit $\epsilon_L(k)$ does indeed satisfy (16). The main point is to show successively that (i), for $\epsilon > x_0$,

$$\frac{d}{d\epsilon} \ln (1 + e^{-\epsilon/T}) > -\frac{C}{T}, \quad \text{where} \quad 0 < C < 1,$$

and (ii) $\epsilon_n \to \epsilon_L$ uniformly in k.

APPENDIX B

To show that (17) can be solved by iteration we construct the symmetrized kernel

$$\mathbf{K}' = \frac{\pi^{-1}c}{c^2 + (k - q)^2} (1 + e^{\epsilon(q)/T})^{-\frac{1}{2}}(1 + e^{\epsilon(k)/T})^{-\frac{1}{2}}. \tag{B1}$$

If ψ is any normalized function and

$$\Phi = [1 + e^{\epsilon/T}]^{-\frac{1}{2}}\psi,$$

then

$$\psi^+\mathbf{K}'\psi = \Phi^+ \frac{\pi^{-1}c}{e^2 + (k - q)^2} \Phi$$
$$\leq \Phi^+\Phi \leq [1 + e^{x_0/T}]^{-1}\psi^+\psi,$$

where x_0 was defined in Appendix A. Thus, the eigenvalues of $\mathbf{K}'$ are less than unity and iteration of (17) converges.

The solution of (17) so obtained evidently satisfies

$$\rho > 0, \quad \rho_h = \rho \exp [\epsilon/T] > 0. \tag{B2}$$

APPENDIX C

(A) We treat the maximization procedure leading to (16) and (17) more rigorously here, showing that the solution of (16) and (17) indeed leads to a minimum of the free energy, i.e., a maximum of the partition function (14′).

Consider any $\rho(k)$. If $\rho(k) \geq 0$ and the $\rho_h(k)$ defined by (11) is everywhere ≥ 0, we say that ρ is in R_0. It is clear that if ρ_1 and ρ_2 are both in R_0, then $x\rho_1 + (1 - x)\rho_2$ for $0 \leq x \leq 1$ is also in R_0. Thus R_0 is convex.

We define $X(L, T, A, \rho)$ by

$$X = L \int_{-\infty}^{\infty} k^2\rho \, dk + LT \int_{-\infty}^{\infty} [\rho \ln \rho + \rho_h \ln \rho_h$$
$$- (\rho + \rho_h) \ln (\rho + \rho_h)] \, dk - LA \int_{-\infty}^{\infty} \rho \, dk. \tag{C1}$$

Consider $\rho = \rho_0 + x\rho_1$ where ρ_0 and ρ_1 are independent of x. Assume ρ to be in R_0 for a real segment of x. We can take the derivatives of X with respect to x in this segment. A straightforward calculation yields

$$\frac{dX}{dx} = L \int \rho_1 \, dk \left[k^2 - A - \epsilon(k) - T \right.$$
$$\left. \times \int B(k, q) \ln (1 + e^{-\epsilon(q)/T}) \, dq \right], \tag{C2}$$

where ϵ is defined by

$$\exp (\epsilon/T) = \rho_h/\rho \tag{C3}$$

and

$$B(k, q) = \frac{\pi^{-1}c}{c^2 + (k - q)^2} = B(q, k). \tag{C4}$$

It is easy to show that

$$-T^{-1}\frac{\partial\epsilon(k)}{\partial x} = \rho^{-1}[1 + e^{-\epsilon/T}]$$
$$\times \left\{ \rho_1 - [1 + e^{\epsilon(k)/T}]^{-1} \int B(k, q)\rho_1(q) \, dq \right\}. \tag{C5}$$

Now,

$$\frac{d^2X}{dx^2} = L \int \rho_1 \, dk$$
$$\times \left\{ -\frac{\partial\epsilon(k)}{\partial x} + \int B(k, q)(1 + e^{\epsilon(q)/T})^{-1}\frac{\partial\epsilon(q)}{\partial x} \, dq \right\}. \tag{C6}$$

The double integral in (C6), after the switch $k \leftrightarrow q$, can be reduced through the use of (C5), giving

$$\frac{d^2X}{dx^2} = T^{-1}L \int \left[\frac{\partial\epsilon(k)}{\partial x} \right]^2 \rho(k)[1 + e^{-\epsilon(k)/T}]^{-1} \, dk > 0. \tag{C7}$$

By (B2), the solution of (16) and (17) gives a ρ in R_0. By (C2), at that ρ, $dX/dx = 0$.

We conclude further, from (C7), that X has a unique minimum in R_0 at the ρ given by (16) and (17).

(B) For given L, T, and A, we denote the minimum of X discussed above by $Y = Y(L, T, A)$. Clearly,

$$\frac{\partial Y}{\partial A} = -L \int \rho \, dk = -N,$$

$$\frac{\partial Y}{\partial T} = -S,$$

by (13) and (14). Further, since Y is proportional to L,

$$dY = -N\,dA - S\,dT + (Y/L)\,dL.$$

Thus,

$$d(Y + NA) = -S\,dT + (Y/L)\,dL + A\,dN.$$

But $Y + NA$ is the free energy. Thus,

$$A = \text{chemical potential}$$

and

$$Y/L = -\text{pressure}.$$

APPENDIX D

Write (16) symbolically in the form

$$\epsilon = W[A, T, \epsilon]. \tag{D1}$$

Consider two real numbers A_0, $T_0 > 0$ and let ϵ_1 be the solution of

$$\epsilon_1 = W[A_0, T_0, \epsilon_1]. \tag{D2}$$

The existence of ϵ_1 was proved in Appendix A. Now for complex values of A and T in the neighborhood of A_0, and T_0, we shall solve (D1) by iteration:

$$\epsilon_2 = W[A, T, \epsilon_1],$$
$$\epsilon_3 = W[A, T, \epsilon_2], \quad \text{etc.}$$

It can be shown that in a sufficiently small complex neighborhood R_1 of (A_0, T_0), $\epsilon_n \to \epsilon_\infty$ as $n \to \infty$, *uniformly* in k, T, and A. Since ϵ_n is analytic in A and T within R_1, so is ϵ_∞. It then easily follows that P as computed from (25) is analytic in A and T within R_1.

APPENDIX E

To prove (47) and (48) we define the kernel of (43):

$$K(k, q) = \frac{\pi^{-1}c}{[c^2 + (k - q)^2][1 + \exp \epsilon(q)/T]}. \tag{E1}$$

Equation (43) is then equivalent to

$$(1 - \mathbf{K})g = \int_{k_\alpha}^{k_\alpha'} K(k, q)[1 + \exp \epsilon(q)/T]\,dq. \tag{E2}$$

Let

$$(1 + \mathbf{L})(1 - \mathbf{K}) = 1 \tag{E3}$$

or

$$\mathbf{L} - \mathbf{K} = \mathbf{L}\mathbf{K}. \tag{E4}$$

Equation (E2) gives

$$g(k) = \int_{k_\alpha}^{k_\alpha'} L(k, q)[1 + \exp \epsilon(q)/T]\,dq. \tag{E5}$$

Now, the $\mathbf{K}'$ of (B1) is a symmetrical kernel with a symmetrical inverse kernel. From that fact we easily obtain

$$L(k, q)[1 + \exp \epsilon(q)/T] = L(q, k)[1 + \exp \epsilon(k)/T]. \tag{E6}$$

Two other useful formulas can be obtained as follows. Equation (17) can be rewritten as

$$(1 - \mathbf{K})f = (2\pi)^{-1}.$$

Operating with $1 + \mathbf{L}$ on both sides we obtain

$$f = (2\pi)^{-1} + (2\pi)^{-1}\int_{-\infty}^{\infty} L(k, q)\,dq. \tag{E7}$$

Similarly, differentiation of (16) with respect to k yields

$$\frac{d\epsilon}{dk} = 2k + \mathbf{K}\frac{d\epsilon}{dk}.$$

Thus,

$$\frac{d\epsilon}{dk} = 2k + \int_{-\infty}^{\infty} L(k, q)2q\,dq. \tag{E8}$$

Now, by (41),

$$\chi\rho = g/[1 + \exp (\epsilon/T)].$$

Thus, (45) becomes

$$\begin{aligned}
\Delta K &= k_\alpha' - k_\alpha + \int_{-\infty}^{\infty} \frac{g(k)\,dk}{1 + \exp \epsilon(k)/T} \\
&= k_\alpha' - k_\alpha + \int_{-\infty}^{\infty} dk \int_{k_\alpha}^{k_\alpha'} dq L(k, q) \\
&\quad \times [1 + \exp \epsilon(q)/T][1 + \exp \epsilon(k)/T]^{-1} \\
&= k_\alpha' - k_\alpha + \int_{-\infty}^{\infty} dk \int_{k_\alpha}^{k_\alpha'} dq L(q, k) \\
&= k_\alpha' - k_\alpha + \int_{k_\alpha}^{k_\alpha'} dq[2\pi f(q) - 1],
\end{aligned}$$

yielding (47). Similarly we derive (48).

APPENDIX F

We shall prove here rigorously that, for the ground state, the k's of Sec. II approach a distribution $L\rho(k)\,dk$ as $L \to \infty$, $N \to \infty$ proportionally. By continuing with respect to c^{-1} and the theorem of Sec. II, we know that for the ground state the I's form a close-packed set of integers or half-odd integers. We now define, as in (8),

$$h(k) = k - L^{-1}\sum_{k'} \theta(k - k'). \tag{F1}$$

Clearly,

$$\frac{dh}{dk} = 1 + \frac{2c}{L}\sum_{k'} \frac{1}{c^2 + (k - k')^2} > 1. \tag{F2}$$

Equation (F1) defines $h(k)$ for *all* real values of k. At the successive values of k_j, the successive values of $h(k_j)$ are $2\pi I_j/L$, by (4). Thus, the successive values of h form a lattice, with a lattice constant of $2\pi/L$, extending between $\pm(N - 1)\pi L^{-1}$. It is sometimes convenient to use h as the variable rather than k.

$k(h)$ is then a monotonically increasing odd function, defined for all real h, and approaches ∞ as $h \to \infty$.

Differentiation of (F1) gives, writing $dh/dk = h_1$,

$$
h_1(k) = 1 + \frac{2c}{L} \sum_{k'} \frac{1}{c^2 + (k - k')^2}
$$

$$
= 1 + \frac{c}{\pi} \int_{-N\pi/L}^{N\pi/L} \frac{1}{c^2 + (k - k')^2} \, dh' + \text{residue.}
$$

$$(F3)$$

The residue is in absolute value less than $A_1 L^{-1}$, since the integrand has a bounded derivative. Thus,

$$
h_1(k) = 1 + \frac{c}{\pi}
$$

$$
\times \int_{-Q}^{Q} \frac{1}{c^2 + (k - k')^2} h_1(k') \, dk' + O(L^{-1}),
$$

$$(F4)$$

$$
2N\pi/L = \int_{-Q}^{Q} h_1(k') \, dk'. \tag{F5}
$$

It is now possible to complete the proof. We first use $h_1 > 1$ to obtain, from (F5),

$$
Q < N\pi/L. \tag{F6}
$$

With this fixed bound for Q, the inverse kernel for the integral equation (F4) is also absolutely bounded and we obtain

$$
h_1(k) = 1(k, Q) + O(L^{-1}), \tag{F7}
$$

where $1(k, Q)$ is the solution of (F4) when $O(L^{-1})$ is deleted. Integration of (F7) gives

$$
2N\pi/L = \int_{-Q}^{Q} 1(k, Q) \, dk + O(L^{-1}). \tag{F8}
$$

Thus, for fixed N/L, as $L \to \infty$, Q approaches a limit Q_0 given by

$$
2\pi N/L = \int_{-Q_0}^{Q} 1(k, Q_0) \, dk. \tag{F9}
$$

The rest is easy.