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Boundary Energy of a Bose Gas in One Dimension*

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By the superposition of Bethe's wave functions, using the Lieb's solution for the system of identical bosons interacting in one dimension via a δ-function potential, we construct the wave function of the corresponding system enclosed in a box by imposing the boundary condition that the wave function must vanish at the two ends of an interval. Coupled equations for the energy levels are derived, and approximately solved in the thermodynamic limit in order to calculate the boundary energy of this Bose gas in its ground state. The method of superposition is also applied to the analogous problem of the Heisenberg-Ising chain (not the ring).

I. INTRODUCTION

Let us consider the system of N identical bosons in one dimension interacting via a two-body δ-function potential of strength $2c$. In the repulsive case $c>0$, the extensive properties are obtained by enclosing the system in a finite region of space. In one dimension, the simplest way of enclosing the system is to put the N particles on a circle of length L, avoiding boundary considerations, which are replaced by periodicity conditions. This problem has been solved by Lieb and Liniger[1] using Bethe's wave function.[2] A more "physical" way of enclosing the system is to enclose the particles in a box; in our case this means that the wave function must be zero at the two ends of an interval L. This problem too can be solved using Lieb and Liniger's and Bethe's method. An application is made by calculating the boundary energy of the boson gas in its ground state. Boundary energy will be defined as the energy difference between the box system and the periodic system of same length and density in the thermodynamic limit. This coincides with the usual definition of boundary energy as the coefficient of L^0 in the development of the energy as a function of the length L of the interval.

II. ELEMENTARY SOLUTION

We recall briefly the known results and introduce the notion of "elementary solution" of the Schrödinger equation:

$$-\sum_{i=1}^{N}\frac{\partial^2\psi}{\partial x_i^2}+2c\sum_{i<j}\delta(x_i-x_j)\psi=E\psi. \quad (1)$$

For the Bose system, an elementary solution is a continuous symmetric function of the coordinates $x_1, \ldots, x_N$ (or $x \in R_N$) obeying the Schrödinger equation (1) in R_N. Bethe's method gives us a continuous set of elementary solutions $\psi_{\{k\}}(x)$ parametrized by a set $\{k\}$ of N distinct numbers $k_1, k_2, \ldots, k_N$:

$$\psi_{\{k\}}(x)=\sum_P a(P)\exp\left(i\sum_{l=1}^{N}k_{Pl}x_l\right) \quad (2)$$

in the domain D, $x_1<x_2<\cdots<x_N$.

The sum is taken over all the permutations P of order N. The coefficients $a(P)$ are given here in a rational form:

$$a(P)=\prod_{i<j}\left(1+\frac{ic}{k_{Pi}-k_{Pj}}\right), \quad (3)$$

which shows clearly the continuous transformation of $\psi_{\{k\}}$ from a permanent ($c=0$) to a determinant ($c^{-1}=0$) when c increases from zero to infinity. The corresponding energy eigenvalue is

$$E_{\{k\}}=\sum_{i=1}^{N}k_i^2. \quad (4)$$

The periodicity conditions are expressed by the following relation:

$$\psi(x_1=0,\ x_2,\ldots,x_N)\equiv\psi(x_2,\ x_3,\ \ldots,x_N,x_1=L),\qquad x\in D. \quad (5)$$

It turns out that ψ can be chosen as a particular $\psi_{\{k\}}$ if the coefficients $a(P)$ satisfy

$$a(PC)e^{ik_{P1}L}=a(P)\quad\text{for all } P, \quad (6)$$

where C is the cyclic permutation $(12\cdots N)$. From Eqs. (3) and (6), we obtain Lieb and Liniger's system of coupled equations

$$k_iL=2\pi n_i+\textstyle\sum_j\psi_{ij},\quad i=[1,N] \quad (7)$$

with n_i integers and the following definition of the phases ψ_{ij}:

$$\tan\tfrac{1}{2}\psi_{ij}=c/(k_i-k_j),\qquad \psi_{ij}=-\psi_{ji}. \quad (8)$$

III. QUANTUM NUMBERS

Yang and Yang[3] have shown the uniqueness of the solution of Eq. (7) for each given permissible set of quantum numbers. We give here an intuitive argument based on the continuity in c in order to determine the integers $\{n\}$ simply. We will show that there exists a continuous sheet of the function $\psi_{ij}(c)$ which goes to zero with c. There the integers $n_i=\lim k_iL/2\pi$ as $c\to 0$ are the quantum numbers of a noninteracting Bose gas with cyclic boundary conditions and the permissible sets must be the sets of N nondecreasing integers:

$$-\infty<n_1\le n_2\le\cdots\le n_N<\infty.$$

For $n_i\neq n_j$, we choose the sheet of ψ_{ij} which in the neighborhood of $c=0$ behaves like

$$\psi_{ij}\propto[c/(n_i-n_j)]L/2\pi. \quad (9)$$

It remains to examine the case where some n are equal. Choose, for example, the ground state of total momentum zero:

$$n_i=0\quad\text{for all } i. \quad (10)$$

In the vicinity of $c=0$, we look for a solution of the type

$$k_i=(2c/L)^{1/2}q_i+O(c),\quad i=[1,N] \quad (11)$$

where all the q_i have to be distinct. Hence we find the possible sheet

$$\psi_{ij}\propto(2cL)^{1/2}(q_i-q_j)+O(c). \quad (12)$$

From Eqs. (7) and (10), the q_i must satisfy

$$q_i=+\sum_{j(\neq i)}\frac{1}{q_i-q_j}. \quad (13)$$

This gives us a precise idea of the distribution of the pseudomomenta k in the limit $c\to+0$. From Eq. (13) we recognize the q_i as the zeros of Hermite polynomials of degree N, which satisfy

$$H''(q)-2qH'(q)+2NH(q)=0. \quad (14)$$

Thus the q_i are distinct real numbers and the ψ_{ij} all have the assumed behavior $\psi_{ij}\to 0$ when $c\to 0$.

The density of zeros of $H_N(q)$ is asymptotically given by the semicircle law

$$\rho(q) = (1/\pi)(2N - q^2)^{1/2}. \tag{15}$$

This gives us the density of pseudomomenta k:

$$\rho(k) = (L/2\pi c)(4c\rho - k^2)^{1/2}, \tag{16}$$

with $\rho = N/L$, in the limit c very small. This distribution is very peaked. The corresponding leading term for the ground-state energy is

$$E/N = \int k^2 \rho(k)\,dk \propto (c\rho) \tag{17}$$

The limit $c \to 0$ has to be understood for a finite system before we take the thermodynamic limit. Nevertheless, it coincides with the dominant term in the energy per particle of the corresponding infinite system.[1]

Finally we give here the correspondence between the $\{n\}$ and the $\{I\}$ introduced by Yang. Since the noncrossing of the k has been proved by this author,[3] we have

$$\psi_{ij} = -2\tan^{-1}(k_i - k_j)/c + \pi\epsilon(k_i - k_j),$$

and thus we write Eq. (7)

$$k_i L = 2\pi I_i - 2\textstyle\sum_j \tan^{-1}(k_i - k_j)/c, \tag{7$'$}$$

with

$$I_i = n_i + i - \tfrac{1}{2}(N+1), \quad i = [1, N].$$

Thus the quantum numbers I_i are integer or half-integer according to the parity of N, with the condition

$$I_1 < I_2 < \cdots < I_N.$$

IV. ELEMENTARY SOLUTION ON SEMI-INFINITE AXIS

The boundary conditions for the Boson wave function $\psi(x)$ in a box are twofold:

$$\psi(x_1 = 0, x_2, \ldots, x_N) \equiv 0, \tag{18}$$

$$\psi(x_1, x_2, \ldots, x_N = L) \equiv 0, \tag{19}$$

where the x_1 are in the region $\overline{D}$, $0 \le x_1 \le x_2 \le \cdots \le x_N \le L$.

The idea is to construct elementary solutions of the Schrödinger equation on the semi-infinite axis $x_i \ge 0$, or $x \in R_N^+$, solutions which have to verify Eq. (18) on the boundary $x_1 = 0$ of the fundamental domain D^+, $0 < x_1 < x_2 < \cdots < x_N < \infty$. Using McGuire's optical analogy[4] for the general problem of particles in δ interaction, it is natural to construct the wave function ψ by superposition of all the elementary waves $\psi_{\{k\}}$ obtained by reflection at the wall $x = 0$. Such an elementary solution is written $\psi_{\{|k|\}}(x)$ and is associated with a set of N distinct "positive" numbers $|k_i|$. "Positive" means only belonging to the same complex half-plane. If the k are real, we can choose

$$0 < |k_1| < |k_2| < \cdots < |k_N|. \tag{20}$$

Therefore we define the 2^N sets

$$\{k\} = \{k_1, k_2, \ldots, k_N\} \quad \text{with } k_i = \epsilon_i |k_i|, \ \epsilon_i = \pm 1. \tag{21}$$

All the states $\psi_{\{k\}}$ have the same energy and we look for a solution of the form

$$\psi_{\{|k|\}}(x) = \sum_{\epsilon_1\epsilon_2\cdots\epsilon_N} A(\epsilon_1\epsilon_2\cdots\epsilon_N)\psi_{\{k\}}(x). \tag{22}$$

The condition (18) gives us

$$\sum_{\{\epsilon\}} A\{\epsilon\} \sum_P \prod_{i<j}\left(1 + \frac{ic}{k_{Pi} - k_{Pj}}\right) \times e^{i(k_{P2}x_2 + \cdots + k_{PN}x_N)} \equiv 0. \tag{23}$$

Thus we are only free to sum over ϵ_{P1} when P and also the other ϵ are fixed. This gives the 2^{N-1} relations

$$A(\epsilon_1 \cdots \epsilon_{P1} \cdots \epsilon_N) \prod_{\beta(\ne P1)}\left(1 + \frac{ic}{k_{P1} - k_\beta}\right) + A(\epsilon_1 \cdots -\epsilon_{P1} \cdots \epsilon_N) \prod_{\beta(\ne P1)}\left(1 + \frac{ic}{-k_{P1} - k_\beta}\right) = 0, \tag{24}$$

which must be true for any $\{k\}$ and P. It is sufficient to choose

$$A(\epsilon_1\epsilon_2\cdots\epsilon_N) = \prod_{i<j}\left(1 - \frac{ic}{k_i + k_j}\right)\epsilon_1\epsilon_2\cdots\epsilon_N \times (k_i + k_j \equiv \epsilon_i|k_i| + \epsilon_j|k_j|). \tag{25}$$

Thus we obtain the desired elementary solution

$$\psi_{\{|k|\}} = \sum_{\{\epsilon\}}\sum_P \epsilon_1\cdots\epsilon_N \prod_{i<j}\left(1 - \frac{ic}{k_i + k_j}\right)\left(1 + \frac{ic}{k_{Pi} - k_{Pj}}\right) \times \exp[i(k_{P1}x_1 + \cdots + k_{PN}x_N)], \tag{26}$$

with $k_i = \epsilon_i |k_i|$, $k_{Pi} = \epsilon_{Pi}|k_{Pi}|$.

We notice that in expression (26), the sum is taken over the $2^N N!$ elements of the N-dimensional cube reflection group. This remark leads to the generalization developed in Sec. V, which appears as a digression.

V. BETHE'S WAVE FUNCTION ASSOCIATED WITH REFLECTION GROUP

In the two cases previously studied, the elementary symmetric solutions on the whole real axis and on half the real axis have the following common mathematical definition.

Let G be a finite reflection group acting in a Euclidean vector space R_N with scalar product (x, y). The group G is generated by a set of reflection generators g_ν ($g_\nu^2 = 1$). Let D_N be a fundamental region for G, in other words, an open domain of R_N with the properties

$$gD_N \cap D_N = 0 \quad \text{for } g\in G\ (g\neq 1), \quad \bigcup_g g\bar{D}_N = R_N\ . \tag{27}$$

Coxeter[5] has shown that D_N is a spherical simplex, bounded by a set of N planes B_ν, with normal vector n_ν, associated with the generator g_ν such that

$$g_\nu^2 = 1, \quad g_\nu B_\nu = B_\nu, \quad g_\nu n_\nu = -n_\nu\ . \tag{28}$$

D_N is defined by

$$(n_\nu, x) > 0 \quad \text{for all } \nu, \quad x\in D_N\ . \tag{29}$$

In our previous examples, the elementary wave function appears as a sum over the elements of the reflection group G:

$$\psi_{\{k\}}(x) = \sum_{g\in G} a(g)\, e^{i(gk,x)}\ , \tag{30}$$

with $k\in D_N$ and $x\in D_N$. In the "symmetric" case the solution is easily extended to the whole space R_N by the relation

$$\psi_{\{k\}}(gx) = \psi_{\{k\}}(x)\ . \tag{31}$$

The continuity of ψ at the boundary B_ν is ensured by

$$g_\nu x = x, \quad x\in B_\nu\ . \tag{32}$$

The coefficients $a(g)$ are determined by some conditions at the boundaries of D_N, which are not arbitrary and have to be consistent with the group property of G.

In the cases studied so far the conditions are of the form of a linear relation between the function ψ and its derivatives on the plane boundary B, for instance,

$$\text{(a)}\quad \text{disc}\left(\frac{d\psi(x)}{dn_\nu}\right) = 2c_\nu \psi(x)\Big|_{x\in B_\nu}\ , \quad \frac{d}{dn_\nu} = (n_\nu, \nabla) \tag{33}$$

or

$$\text{(b)}\quad \psi(x) = 0, \quad x\in \text{some } B\ . \tag{34}$$

From (30) and (33), we obtain the sufficient relations for the coefficients $a(g)$:

$$\frac{a(g_\nu g)}{a(g)} = \frac{(gk, n_\nu) + ic_\nu}{(gk, n_\nu) - ic_\nu} \tag{35}$$

for all g and generators g_ν.

We will show that these relations give $a(g)$ in terms of all the reflection operators g_α ($g_\alpha^2 = 1$) of G. (Note that the set of g_α is larger than the g_ν, which are only the generators.) This can be done by using the known properties of the finite reflection group in R_N, which are nothing else than the reflection group of the root diagram of the semisimple Lie groups.[6] Let us call α (vector in some R_N) a "positive" root in the diagram of a semisimple group Γ ["positive" is defined with respect some fixed arbitrary vector ξ in D_N such that $(\xi, \alpha) > 0$]. The root α defines a reflection g_α with respect to the hyperplane perpendicular to α at the origin:

$$g_\alpha\, \alpha = -\alpha \quad (-\alpha \text{ is a root})\ . \tag{36}$$

On the other hand, if β is a root, $g_\alpha \beta = \alpha + \beta$ is a root ($\alpha \neq \beta$). Now, if α is a positive root, $g_\nu \alpha$ is also a positive root, because from (29)

$$(\nu, \xi) > 0 \quad \text{and } (\alpha, \xi) > 0 \Rightarrow (\alpha + \nu, \xi) > 0\ .$$

Thus, if we choose

$$n_\nu = \nu/[(\nu,\nu)]^{1/2}, \quad c_\nu = c/[(\nu,\nu)]^{1/2}\ , \tag{37}$$

we can easily verify the following solution of Eq. (35) for $a(g)$:

$$a(g) = \prod_{\alpha>0}\left(1 - \frac{ic}{(gk, \alpha)}\right)\ . \tag{38}$$

From the choice of our boundary conditions (33) and (37), the function ψ is an elementary symmetric solution of the following Schrödinger equation in R_N:

$$-\Delta\psi + 2c \sum_{\alpha>0} \delta((x,\alpha))\,\psi = (k,k)\psi\ . \tag{39}$$

Thus with each semisimple Lie algebra can be associated at least one symmetric (invariant by G) Bethe wave function. It results from the invariance of the Hamiltonian (39) by G that this equation admits solutions belonging to other types of symmetry. More precisely, since the reflection group G is in some sense the commutator of Γ, the covariant solutions ψ will be representations of the corresponding semisimple Γ. But here we restrict the study to the invariant solution.

We illustrate briefly these general considerations with our two examples. First consider the simplex A_{N-1} corresponding to $SU(N)$. Let e_i be an orthonormal basis in R_N; the "positive" roots of $SU(N)$ can be taken as

$$\alpha = e_i - e_j, \quad i > j, \quad i,j = [1, N]\ .$$

We have

$$(x, e_i) = x_i, \quad \delta((x,\alpha)) = \delta(x_i - x_j)\ ,$$

$$(gk, \alpha) = (gk)_i - (gk_j)\ .$$

$g_\alpha = P_{ij}$ = reflection with respect to the plane $x_i - x_j = 0$ or transposition of the permutation group $G = S_N$. The fundamental region with normal vectors

$$n_\nu = e_{i+1} - e_i, \quad i = [1, N]$$

and generators $g_\nu = P_{i,i+1}$ is determined by the inequalities

$$(n_\nu, x) > 0 \Rightarrow x_{i+1} - x_i > 0$$

$$\Rightarrow -\infty < x_1 < x_2 < \cdots < x_N < \infty .$$

We recover the familiar relations (2) and (3) of Sec. II.

The second example concerns the elementary solution on the semi-infinite real axis, constructed with the $2^N N!$ elements of the group of the hypercube or of the Cartesian frame. Two root diagrams are possible: C_N corresponding to $Sp(2N)$ and B_N corresponding to $SO(2N+1)$ with the same reflection group (Coxeter's simplex C_N). The positive roots of D_N are $e_i + e_j$ and $e_i - e_j$, $i > j$, with the supplementary roots

$$e_i \text{ for } B_N \text{ or } 2e_i \text{ for } C_N . \tag{40}$$

The generators of C_N can be taken as

$$g_{e_1}, g_{e_2 - e_1}, \ldots, g_{e_N - e_{N-1}}$$

and this gives the fundamental region $0 < x_1 < x_2 < \cdots < x_N < \infty$.

In fact, our wave function satisfying $\psi(x) = 0$ for $x_1 = 0$ is a limiting solution of the following more general Hamiltonian with potential function depending on two coupling constants b and c:

$$V(b,c) = 2b \sum_i \delta(x_i) + 2c \sum_{i<j} \delta(x_i - x_j) + \delta(x_i + x_j) . \tag{41}$$

The solution in this case is given by

$$a(g) = \prod_{i<j} \left(1 - \frac{ic}{(gk, e_i + e_j)}\right)\left(1 - \frac{ic}{(gk, e_j - e_i)}\right) \times \prod_i \left(1 - \frac{ib}{(gk, e_i)}\right) . \tag{42}$$

As in formula (38), one recognizes the product over the reflection defined by the roots (40), but with the freedom in the choice of the coefficient corresponding to the roots $+e_i$.

This corresponds to the fact that the reflection group does not completely determine the length of the roots: We can have B or C. One verifies easily that the double product $\Pi_{i<j}$ in (42) is unchanged by the transformation $g \to g_{e_1} g$. Thus

$$\frac{a(g_{e_1} g)}{a(g)} = \frac{(gk, e_1) + ib}{(gk, e_1) - ib} .$$

On the other hand, the roots $e_k \pm e_l$ and $e_{k-1} \pm e_l$ are exchanged by the generators $g_{e_k - e_{k-1}}$, unless $e_k - e_{k-1}$, which changes its sign. Finally, $g_{e_k - e_{k-1}}$ exchanges the e_k and e_{k-1} factor in the simple product Π_i in (42). Hence the conditions (35) which express boundary conditions corresponding to the Hamiltonian (41) are satisfied by the solution (42). Now our problem with the strict zero-wave-function condition at $x_1 = 0$ corresponds to the limit $b \to \infty$, and we recognize exactly the wave function (26) in the limit form of (42). The wave function restricted from the whole space to the region $x_1 > 0$ for all i does not see the part of the potential $\delta(x_i + x_j)$, and thus on the half-axis $x_i > 0$, in the limit $b \to \infty$, potential (41) is equivalent to the original one. For three values of the constant b/c, $b/c = 0, \frac{1}{2}, 1$, the solution (42) coincides with (38) corresponding to the Schrödinger equation (39), and the corresponding groups Γ are, respectively, $SO(2N)$, $Sp(2N)$, and $SO(2N+1)$.

Unfortunately the translational invariance is lost in most of the new Hamiltonians. There is one exception corresponding to the group G_2, for which the reflection group is simply D_2^6. The corresponding potential function is

$$V = \delta(x_1 - x_2) + \delta(x_2 - x_3) + \delta(x_1 - x_3) + \delta(x_1 + x_2 - 2x_3) + \delta(x_1 + x_3 - 2x_2) + \delta(x_3 + x_2 - 2x_1),$$

where each particle interacts with the center of gravity of the other two.

We do not think that the models corresponding to the exceptional reflection groups are physically interesting. These group considerations would be fruitful, if they lead to the explicit construction of the covariant solutions $\psi_\gamma(x)$ with $\gamma x \in D_N$ belonging to a given irreducible representation of the reflection group G.

VI. COUPLED EQUATIONS FOR SPECTRUM

Now we go back to our specific problem. With the knowledge of the elementary solution $\psi_{\{|k|\}}(x)$ in the region $0 \le x_1 \le \cdots \le x_N$, we are able to impose on the wave function the second boundary condition, Eq. (19):

$$\psi(x_1, x_2, \ldots, x_N = L) \equiv 0 .$$

This gives the relation

$$\sum_{\epsilon_{PN}} \left[\prod_{i<j} \left(1 - \frac{ic}{k_{Pi} + k_{Pj}}\right)\left(1 + \frac{ic}{k_{Pi} - k_{Pj}}\right)\right] e^{ik_{PN} L} = 0 ,$$

which has to be valid for all P and $\{\epsilon\}$.

Setting $PN = \alpha$, we obtain

$$e^{2ik_\alpha L} = \prod_{\beta(\neq\alpha)} \frac{k_\beta - k_\alpha - ic}{k_\beta - k_\alpha + ic} \, \frac{k_\beta + k_\alpha + ic}{k_\beta + k_\alpha - ic} , \tag{43}$$

which must be satisfied for all α, and all possible signs of k. This last point becomes clear if we write our system in the form

$$e^{2ik_\alpha L} = \prod_{\beta(\neq\alpha)} \frac{(k_\alpha + ic)^2 - k_\beta^2}{(-k_\alpha + ic)^2 - k_\beta^2} .$$

Thus, writing k_α instead of $|k_\alpha|$, we obtain the system of coupled equations

$$k_\alpha L = \pi n_\alpha + \sum_{\beta(\neq\alpha)} \left(\tan^{-1} \frac{c}{k_\alpha - k_\beta} + \tan^{-1} \frac{c}{k_\alpha + k_\beta} \right), \tag{44}$$

with $k_\alpha > 0$, $\alpha = [1, N]$.

As in Sec. III, by applying the continuity principle in the coupling c, we deduce that the set of integers $\{n\}$ is a system of quantum numbers for free bosons in a box L:

$$1 \leq n_1 \leq n_2 \leq \cdots \leq n_N . \tag{45}$$

The system (44) is very similar to the system (7) and here we make the analogy precise. Consider (a) the N bosons system in the box $[0, L]$, and (b) the $2N$ bosons system periodic on $[0, 2L]$. Both have the same density. For the periodic system we look for a solution of the form

$$\begin{aligned} \{k\}_{2N} &\equiv \{\{-k\}_N, \{k\}_N\}, \quad k_i > 0, \ i = [1, N] \\ \{n\}_{2N} &\equiv \{\{-n\}_N, \{+n\}_N\}, \ n_i > 0, \ i = [1, N] . \end{aligned} \tag{46}$$

Thus we get exactly Eq. (44) for N bosons in the box $[0, L]$. We conclude that the energy levels of N bosons in a box L are one-half the energy of a class of levels of $2L$ - (periodic system at same density):

$$E^{\text{box } L} \{n\}_N = \tfrac{1}{2} E^{\text{cyclic } 2L} \{-n, n\}_{2N} . \tag{47}$$

The existence of real solutions for (44) is a corollary of the corresponding result[3] for Eq. (7). The ground state in the box corresponds to the excited level $\{\{-1\}_N, \{+1\}_N\}$ of the periodic gas. This allows a direct calculation of the difference

$$\Delta E = \lim (E_N^{\text{box } L} - \tfrac{1}{2} E_{2N}^{\text{cyclic } 2L}) \ \text{as } N \to \infty . \tag{48}$$

Moreover, it is shown in the Appendix that for the ground state we get

$$E_N^{\text{cyclic}} = N \text{ (energy per particle)} + O(1/N) . \tag{49}$$

Thus $\lim (\frac{1}{2} E_{2N}^{\text{cyclic}} - E_N^{\text{cyclic}}) = 0$ as $N \to \infty$ and we deduce that the quantity ΔE, to be calculated in Sec. VII, represents the boundary energy or "surface" energy of the boson gas enclosed in a box.

VII. BOUNDARY ENERGY

Let us call k_i and $\bar{k}_i$, respectively, the momenta for the $2L$-periodic and L-box system at the same density. We have the coupled equations

$$k_i L = {\sum_{j=1}^{N}}' \tan^{-1} \frac{c}{k_i - k_j} + \tan^{-1} \frac{c}{k_i + k_j}, \tag{50}$$

$$\bar{k}_i L = \pi + {\sum_{j=1}^{N}}' \tan^{-1} \frac{c}{\bar{k}_i - \bar{k}_j} + \tan^{-1} \frac{c}{\bar{k}_i + \bar{k}_j}, \quad i = [1, N] \tag{51}$$

and the surface energy

$$\Delta E = \lim \left(\sum_{i=1}^{N} (\bar{k}_i^2 - k_i^2) \right) . \tag{52}$$

We put

$$\bar{k}_i - k_i = (1/L) h(k_i) + O(1/L^2) \tag{53}$$

and we deduce from Eqs. (50) and (51) that

$$h(k_i) = \pi - \frac{c}{L} {\sum_{j=1}^{N}}' \left(\frac{h(k_i) - h(k_j)}{c^2 + (k_i - k_j)^2} + \frac{h(k_i) + h(k_j)}{c^2 + (k_i + k_j)^2} \right) \tag{54}$$

and

$$\Delta E = \lim \left(\frac{2}{L} \sum_{i=1}^{N} k_i h(k_i) \right) . \tag{55}$$

We know that in the limit $L \to \infty$, density $\rho = 2N/2L$ and the asymptotic number of k_i on the interval $[k, k+dk]$ is $2L\rho(k)dk$, where $\rho(k)$ is the solution of the Lieb integral equation

$$\rho(k) - \frac{1}{\pi} \int_{-K}^{+K} \frac{c}{(k - k')^2 + c^2} \rho(k') \, dk' = \frac{1}{2\pi} . \tag{56}$$

The parameter K is related to the density by the equation

$$\rho = \int_{-K}^{+K} \rho(k) \, dk . \tag{57}$$

The limiting form of (54) is clear. Extending for convenience the definition of $h(k)$ to negative values of the argument by

$$h(-k) = -h(k) , \tag{58}$$

we obtain

$$h(k) = \pi \epsilon(k) - 2c \int_{-K}^{+K} \frac{h(k) - h(k')}{(k - k')^2 + c^2} \rho(k') \, dk' , \tag{59}$$

with $\epsilon(k) = k/|k|$, or, by the change of function

$$g(k) = \rho(k) h(k) \ \text{(odd function)} , \tag{60}$$

we finally obtain the integral equation

$$g(k) - \frac{c}{\pi} \int_{-K}^{+K} \frac{g(k') \, dk'}{(k - k')^2 + c^2} = \tfrac{1}{2} \epsilon(k) \tag{61}$$

and the boundary energy

$$\Delta E = 2 \int_{-K}^{+K} k g(k) \, dk . \tag{62}$$

In Sec. VIII a method is described to solve approximately Eqs. (56) and (61) in the limit $c/\rho \to 0$ and thus to calculate the leading term of ΔE.

VIII. ELECTROSTATIC ANALOGY

Integral equation (56) is known in potential theory as the Love equation for the old problem of the circular disk condenser.[7] Consider two coaxial circular metallic disks of radius 1, separated by a distance a, and charged at opposite potential $\pm V_0$. In cylindric coordinates (r, z) the potential due to an axially symmetric distribution $\sigma(r)$ (on the lower plate at $z=0$, for instance) admits of the following useful representation in terms of an even real function $f(t)$:

$$V(r,z)=\int_{-1}^{+1}\frac{f(t)\,dt}{[r^2-(t+iz)^2]^{1/2}}\ . \tag{63}$$

$V(\rho, z)$ is real (f even) and harmonic outside the lower disk ($z=0$, $0\le r\le 1$). The density of charge $\sigma(r)$ is related to $f(r)$ by the Abel transform

$$\sigma(r)=-\frac{1}{\pi}\frac{d}{dr}\int_r^1\frac{f(t)t\,dt}{(t^2-r^2)^{1/2}}\ , \tag{64}$$

and the total charge on this plate is

$$Q=\int_{-1}^{+1}f(t)\,dt\ . \tag{65}$$

In the presence of the upper disk at $z=a$, density $-\sigma(r)$, the equilibrium condition on the lower disk is

$$V(\rho,0)-V(\rho,a)=V_0,\quad 0\le\rho\le 1\ . \tag{66}$$

Taking the Abel transform of Eq. (66), one obtains the Love equation for $f(t)$:

$$f(t)-\frac{a}{\pi}\int_{-1}^{+1}\frac{f(t')\,dt'}{(t-t')^2+a^2}=\frac{V_0}{\pi}\ . \tag{67}$$

This becomes Lieb and Liniger's equation after a change of scale, by choosing $V_0=\frac{1}{2}$ and $a=c/K$. The capacity of the condenser is given by Eq. (65). Between the two problems we have the correspondence

$$\rho(x)=f(x/K)\ ,$$

$$\text{density }\rho=\text{capacity}=K\int_{-1}^{+1}f(t)\,dt\ , \tag{68}$$

$$\text{energy }\epsilon=\text{second moment}$$

$$=(K^3/\rho)\int_{-1}^{+1}t^2f(t)\,dt\ . \tag{69}$$

The difficulty of the condenser problem is to find an asymptotic expansion of the capacity at small separation of the disks; by using physical arguments Kirchoff obtained

$$Q=\frac{1}{4a}+\frac{1}{4\pi}\ln\frac{16\pi}{ea}+O(1)\ , \tag{70}$$

and Hutson's method[8] gives

$$f(t)=\frac{1}{2\pi a}(1-t^2)^{1/2}+\frac{1}{4\pi^2(1-t^2)^{1/2}}\times\left(t\ln\frac{1-t}{1+t}+\ln\frac{16\pi e}{a}\right)\ . \tag{71}$$

From Eqs. (68), (69), and (71) we get the density of the Bose gas as a function of K and c:

$$\rho=\frac{K^2}{4c}+\frac{K}{4\pi}\ln\left(\frac{16\pi}{e}\frac{K}{c}\right)+\cdots \tag{72}$$

and the energy particle

$$\epsilon\rho=\frac{K^4}{16c}-\frac{K^3}{6\pi}+\frac{K^3}{8\pi}\ln\left(\frac{16\pi}{e}\frac{K}{c}\right)+\cdots\ . \tag{73}$$

Eliminating K between Eqs. (72) and (73), we obtain the equation of state at zero temperature

$$\epsilon=c\rho-(4/3\pi)\rho^{1/2}c^{3/2}+\cdots\ , \tag{74}$$

which coincides with the result given by the perturbation theory of Bogoliubov previously calculated by Lieb and Liniger.[1]

Analogous methods could probably be used to transform Eq. (61) into a problem of potential theory. We only give here the dominant behavior of $g(k)$ and ΔE as c goes to zero. Following the Kac-Pollard method,[7] an approximate form of Eq. (61) (in the reduced variable $x=k/K$) is easily found:

$$\mathrm{PP}\int_{-1}^{+1}\frac{g'(y)}{y-x}\,dy=-\epsilon(x)\frac{K\pi}{2c}\ . \tag{75}$$

This can be inverted to give

$$g(y)=\frac{K}{4\pi c}\times\int_{-1}^{+1}\ln\left(\frac{1-xy-[(1-x^2)(1-y^2)]^{1/2}}{1-xy+[(1-x^2)(1-y^2)]^{1/2}}\right)\epsilon(x)\,dx\ . \tag{76}$$

Formula (62),

$$\Delta E=2K^2\int_{-1}^{+1}yg(y)\,dy\ , \tag{62'}$$

gives us the dominant term of the boundary energy

$$\Delta E\propto-\frac{K^3}{2\pi c}\frac{2\pi}{3}=-\frac{8}{3}\rho^{3/2}c^{1/2}+\cdots \tag{77}$$

in the limit $c/\rho\ll 1$.

IX. CONCLUSION

Starting from a known elementary solution of the Schrödinger equation for a boson system with a δ-function interaction, we have applied a superposition method to build up a wave function defined by $\psi=0$ boundary conditions. This constructive method led us to recognize the possibility of associating Bethe's wave function with each finite reflection group and of constructing the corresponding Hamiltonian. We do not know if the periodicity conditions are compatible with the solutions corresponding to exceptional reflection groups.

We apply this to calculate the boundary energy of the Bose gas in its ground state. The same method could be used to calculate the difference in energy between the Heisenberg-Ising chain and the ring, and possibly the boundary correction to the free energy of some two-dimensional ferroelectric system. We give here the coupled equations for the spectrum of the Hamiltonian of the anisotropic Heisenberg chain:

$$\mathcal{H}=\sum_{n=1}^{N-1} S_n^x S_{n+1}^x + S_n^y S_{n+1}^y + \rho(S_n^z S_{n+1}^z - \tfrac{1}{4}) .$$

With the notations

$$\rho=\cosh\Phi \quad \text{(in the domain } \rho>1) ,$$

$$\cot\tfrac{1}{2}k_\alpha = \coth\tfrac{1}{2}\Phi \tan\tfrac{1}{2}\xi_\alpha, \quad 0<\xi_\alpha<\pi$$

$$\cot\tfrac{1}{2}\psi(\xi) = \coth\Phi \tan\tfrac{1}{2}\xi ,$$

we have found the equation

$$k_\alpha(N+1)=\pi(\lambda_\alpha+\tfrac{1}{2})+\psi(2\xi_\alpha)$$
$$+\tfrac{1}{2}\sum_{\beta(\neq\alpha)} \psi(\xi_\alpha-\xi_\beta)+\psi(\xi_\alpha+\xi_\beta), \quad \alpha=[1,M]$$

where the quantum numbers λ_α for the ground state are probably

$$1,\ 3,\ 5,\ \ldots, N-1 \quad (N=2M) .$$

The energy is given by

$$E=\sum_{\alpha=1}^{M} (\cos k_\alpha - \cosh\Phi) .$$

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APPENDIX

We have to show that the ground-state energy of the L-periodic Bose gas behaves in the limit $N\to\infty$ like

$$E_N=\epsilon N+O(1/N) , \tag{A1}$$

where ϵ is the energy per particle given by Lieb and Liniger's equations (56) and (57) and

$$\epsilon=(1/\rho)\int_{-K}^{+K} k^2\rho(k)\,dk, \quad \rho=N/L . \tag{A2}$$

We follow exactly the proof given by Yang[9] in order to establish

$$\lim E_N/N=\epsilon \quad \text{as } N\to\infty . \tag{A3}$$

In fact, his proof gives the stronger result (A1), from which we deduce the desired formula of Sec. VI:

$$\lim[E_N(\rho)-\tfrac{1}{2}E_{2N}(\rho)]=0 \quad \text{as } N\to\infty. \tag{A4}$$

We start with the following formula (Whittaker and Watson[10]), which is valid for an analytic function on a segment line including the points a and b $(b-a=rw)$:

$$\sum_{N=1}^{r} f(a+wn)=\frac{1}{w}\int_a^b f(x)\,dx+\tfrac{1}{2}[f(b)-f(a)] + \tfrac{1}{2}w[f'(b)-f'(a)]+O(w^2) . \tag{A5}$$

Specializing to an even function, and using the analyticity at the ends of the interval in order to shift the limits of the integral from $\tfrac{1}{2}w$, we obtain the modified formula

$$\sum_{I=-\frac{1}{2}(N-1)}^{\frac{1}{2}N-1} f\left(\frac{2\pi I}{N}\right) = \frac{L}{2\pi}\int_{-\pi N/L}^{+\pi N/L} f(x)\,dx+\frac{1}{L}R_N , \tag{A6}$$

with $|R_N|<\tfrac{1}{2}\pi|f'(\pi N/L)|+\text{const}$

For a set $\{k\}_N$ solution of the coupled equation, the function $h(p)$,

$$h(p)=p-\frac{2}{L}\sum_I \tan^{-1}\frac{p-k_I}{c} , \tag{A7}$$

is analytic on the real axis, as is the inverse function $p(h)$ with $|dp/dh|<1$. For any value of p we have

$$\frac{dh}{dp}=1+\frac{1}{L}\sum_{h=-(N-1)\pi/L}^{(N-1)\pi/L} \frac{2c}{c^2+[p-p(h)]^2} . \tag{A8}$$

Thus, using (A6), we get

$$\frac{dh}{dp}=1+\frac{c}{\pi}\int_{-\eta}^{+\eta} \frac{dp'}{(p-p')^2+c^2}\frac{dh}{dp'}+\frac{1}{L^2}R_1(p) , \tag{A9}$$

with

$$\eta=p(\pi N/L) \tag{A10}$$

and

$$|R_1(p)|<\frac{2\pi}{3c^3}\left|\frac{dp}{dh}\right|+\text{const}<\frac{2\pi}{3c^3}+\text{const} \tag{A11}$$

We obtain also the density of particles

$$\frac{2\pi N}{L}=\int_{-\eta}^{+\eta} \frac{dh(p')}{dp'}\,dp' \tag{A12}$$

and the total energy

$$E_N=L\int_{-\eta}^{+\eta} p^2\frac{dh(p)}{dp}\,dp+\frac{R_2}{L} , \tag{A13}$$

with

$$|R_2| < \tfrac{1}{12}\pi\, 2\eta\, (dp/dh)\,(\eta) + \text{const} < \tfrac{1}{6}\pi\eta + \text{const.} \quad (A14)$$

Using the existence of a bounded inverse operator of the integral operator in (A9) and the fact that η is bounded, we deduce that

$$\frac{dh}{dp} = 2\pi\rho_1(p) + O\,(1/L^2) \quad (A15)$$

and

$$E_N = L\epsilon_1\rho_1 + O(1/L)\ , \quad (A16)$$

where ρ_1 and $\rho_1(p)$ are, respectively, the density and the solution of Lieb and Liniger's equation for the value of the parameter $K_1 = \eta$; from Eqs. (A12) and (A15) we have

$$\rho_1 = \rho + O(1/L^2), \quad \rho = N/L\ . \quad (A17)$$

Since all the quantities ρ and ϵ are derivable in the parameter K, we have also

$$\epsilon_1 = \epsilon + O(1/L^2) \quad (A18)$$

and this gives, with (A16) and (A17), Eq. (A1) and the corollary (A4).

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Quantum Field Theory for Bosons with Condensed Phase at a Finite Temperature*†

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A detailed proof is given for the validity of substituting a *c* number for the zero-momentum-state operators in the quantum-field-theory approach to the many-boson problem at a finite temperature. We use a modification of the method of Kromminga and Bolsterli, and add slightly to their work for the ground-state case. The case in which the bosons which condense are themselves composite particles, as in superconductivity, is treated in this method by the artifice of coupling to a fictitious elementary boson and then letting the coupling become infinitely weak; the self-consistent formulation of Schrieffer for superconductivity can be obtained in this way.

I. INTRODUCTION

The application of quantum-field-theory methods[1] to the problems of statistical mechanics can normally be made only when the grand canonical ensemble can be used to describe the system being studied. This is because only in the grand canonical average over states for the unperturbed system can the occupation numbers of the separate single-particle states be summed over independently and the thermodynamic Wick's theorem[2] applied, whereas with the canonical average the restriction on the total particle number prevents these different occupation numbers from being independent of each other. For a system without particle number conservation, this restriction is absent, however, and the canonical ensemble average is just like the grand canonical average with the chemical potential μ set equal to zero; in this case, therefore, the quantum-field-theory methods are directly applicable in the canonical ensemble.

For the many-boson system at a temperature for which there is no condensed phase, it is quite proper to use the grand ensemble, but difficulties arise when there is a condensed phase, that is, when one single-particle state (typically the zero-momentum state) is macroscopically occupied. In this case, if the grand ensemble is used, the chemical potential for the unperturbed system, which is the reference system for this approach, has an anomalous