762 A. D. JANNUSSIS

The Ground-State Energy of Anisotropic Spin-Spin Interaction in One-Dimensional Chain

A. D. Jannussis *

Greek Atomic Energy Commission, Nuclear Research Center "Demokritos", Athens, Greece

(Z. Naturforsch. 24 a, 762-767 [1969]; received 25 January 1969)

In the present work the integral equation of Yang and Yang is studied by the method of moments. In general the solution of the integral equation is reducible to a linear algebraic system which can be solved only approximately. From the solution of the system the ground-state energy and the magnetization of the anisotropic spin-spin interaction in a one-dimensional chain is determined.

I. Introduction

Using a function of the type $f(\Delta, y)$, Yang and Yang ¹ recently studied the various properties of the ground-state energy of a one-dimensional chain of anisotropic spin-spin interaction. The real parameter Δ characterises the anisotropy, and for $\Delta = \pm 1$ we have the case of ferromagnetism and antiferromagnetism respectively. The magnetization per atom y is the eigenvalue of the operator

$$Y = \sigma_z/N$$
, (1)

where N in the total number of lattice sites.

In general the problems of ferromagnetism and antiferromagnetism are directly related to the eigenvalue spectrum of the operator.

$$H = -\frac{1}{2} \sum \sigma_x \, \sigma_x' + \sigma_y \, \sigma_y' + \Delta \sigma_z \, \sigma_z' \tag{2}$$

where σ are the Pauli spin matrices at a particular site $(\sigma_x{}^2 = \sigma_y{}^2 = \sigma_z{}^2 = 1)$ and σ' are the Pauli spin matrices at a neighboring site.

The problem of a quantized lattice gas is also related to the operator (2). This subject is dealt with in detail in the relevant literature 1 . The function $f(\Delta, y)$ is defined by Yang and Yang as follows:

$$f(\Delta, y) = \lim_{N \to \infty} \frac{1}{NZ}$$
 (3)

(lowest eigenvalue of H for fixed y)

which is half of the ground-state energy per bond for fixed y. Here Z is the number of nearest neighbors at each site. The existence of the limit $f(\Delta, y)$ and a number of general properties of $f(\Delta, y)$ in particular inequalities between the $f(\Delta, y)$ for one-, two- and three-dimensional lattice were proved in Ref. ². Yang and Yang confined themselves to the one-dimensional case which they examined in detail.

The one-dimensional problem was first examined by Bloch ³ and Bethe ⁴. The formation of the eigenfunctions was based on a hypothesis by Bethe which has more recently been generalized by Yang ⁵. The particular case $\Delta = -1$ (antiferromagnetic isotropic case) was considered in detailed by Hulthen ⁶, who gave an evaluation of f(-1,0) using Bethe's hypothesis.

II. Construction of the Eigenfunctions

Yang and Yang 1 consider an eigenfunction Ψ of H with m down spins and N-m up spins. Clearly

$$y = 1 - 2 m/N \tag{4}$$

and for

$$2 m \le N, \text{ is } y \ge 0. \tag{5}$$

Let x_1, x_2, \ldots, x_m (in ascending order) be the sites with down spins $(1 \le x_i \le N)$ where, according to Bethe's hypothesis, there are m unequal real numbers p_1, p_2, \ldots, p_m such that the eigenfunction Ψ is a sum of m! terms each of which is of the exponential form:

const.
$$\exp\{p P_1 x_1 + p P_2 x_2 + \ldots\}$$
 (6)

where (P_1, P_2, \ldots, P_m) is a permutation of 1, 2, $3, \ldots, m$

The eigenfunction Ψ therefore is the sum of all the possible combinations (P_1, P_2, \ldots, P_m) with

^{*} Presented address: Department of Theoretical Physics, University of Patras.

¹ C. N. Yang and C. P. Yang, Phys. Rev. **150**, 321, 327

² C. N. YANG and C. P. YANG, Phys. Rev. 147, 303 [1966].

³ F. Bloch, Z. Phys. **61**, 206 [1930]; **74**, 295 [1932].

⁴ H. A. Bethe, Z. Phys. **71**, 206 [1930]; **74**, 295 [1932].

⁵ C. N. Yang, Phys. Rev. Letters **19**, 1312 [1967].

⁶ L. Hulthen, Arkiv Mat. Astron. Fysik 26 A, No 11 [1938].

constant m, and Ψ has the following form

$$\Psi = \sum_{P} A_{p} \exp\left\{i \sum_{j} p P x_{j}\right\}. \tag{7}$$

The values of p satisfy according to 1 the following conditions

$$-\pi < p_i < \pi \quad \text{for} \quad \Delta \le -1$$
 (8)

$$-(\pi - \mu) < p_i < \pi - \mu \quad \text{for} \quad -1 \le \Delta < 1 \quad (9)$$

where
$$0 \le \mu < \pi$$
, $\cos \mu = -\Delta$. (10)

In addition they also satisfy the following non linear system:

$$p_i = 2 \pi I_i N^{-1} - N^{-1} \sum_{l=1}^{m} \Theta(p_i, p_l)$$
 (11)

where the I_i 's satisfies the relations

$$I_{1}, I_{2}, \dots, I_{m}$$

$$= \left(-\frac{m-1}{2}\right), \left(-\frac{m-1}{2} + 1\right), \dots, \left(\frac{m-1}{2} - 1\right), \left(\frac{m-1}{2}\right)$$

and the function $\Theta(p,q)$ is defined as follows

$$\Theta(p,q) = 2 \operatorname{tg}^{-1} \left(\frac{\Delta \sin \frac{1}{2} (p-q)}{\cos \frac{1}{2} (p+q) - \Delta \cos \frac{1}{2} (p-q)} \right). \tag{13}$$

The existence of a solution for (12) as well as the properties of function (13) are discussed in ¹.

Since $p_j \neq p_i$, if j > i, by continuity argument with respect to Δ , is $p_1 < p_2 \ldots < p_m$ for all Δ .

As N, $m \to \infty$ at a fixed ratio, the p's increase in number, but always lie within the interval (8), (9). In this case the number p's in an interval p to p + dp approaches according to 1.

$$N \rho(p) dp$$
, (14)

$$p = 2 \pi f - \int \Theta(p, q) \varrho(q) dq \qquad (15)$$

where f = I/N clearly

$$\mathrm{d}f/\mathrm{d}p = \varrho\left(p\right) \tag{16}$$

thus,
$$1 = 2 \pi \varrho(p) - \int \frac{\partial \Theta}{\partial p} \varrho(q) dq.$$
 (17)

The limits of integration are between -Q and Q; thus is due to the symmetric distribution of the p's about p=0, i. e.,

$$1 = 2 \pi \varrho(p) - \int_{-\rho}^{\varrho} \frac{\partial \Theta}{\partial p} \varrho(q) \, dq. \qquad (18)$$

We have obviously,

$$\frac{1}{2} (1 - y) = m/N = \int_{-0}^{Q} \varrho(p) \, dp$$
 (19)

and the function $f(\Delta, y)$ is given by

$$f(\Delta, y) = -\frac{1}{4}\Delta + \frac{1}{2}\Delta(1-y) - \int_{Q}^{Q} \rho(p) \cos p \, dp.$$
 (20)

The present problem is centered around the solution of the integral equation (20). From this equation and from relations (19) and (20) we obtain y and $f(\Delta, y)$ as functions of Q. Equations similar to (18) have been studied by a variety of methods ⁷.

The purpose of the present work is to study Eq. (18) by the method of moments ⁸ which has already been applied by the author ⁹ to solve Hulthen equations for the many-body problem in one-dimension (l. c. ¹⁰).

III. Solution of the Integral Eq. (18)

The integral kernel $\partial \Theta/\partial p$ can be expressed as a sum of three terms, namely

$$\frac{\partial \Theta}{\partial p} = -1 - \; \frac{e^{-ip}}{2\; \varDelta - e^{-ip} - e^{iq}} - \frac{e^{ip}}{2\; \varDelta - e^{ip} - e^{-iq}} \; . \eqno(21)$$

For $\Delta = 0$ it follows that $\partial \Theta/\partial p = 0$ and the solution of the Eq. (18) is known 1, namely

$$\varrho(p) = 1/2\pi, \tag{22}$$

$$Q = \frac{1}{2}\pi(1-y), \tag{23}$$

$$f(\Delta, y) = -\frac{1}{4}\Delta + \frac{1}{2}\Delta(1-y) - (1/\pi)\cos(\frac{1}{2}\pi y).$$
(24)

For the case $\Delta = \infty$ the solution is also known

$$\varrho(p) = (1+y)/4\pi, \tag{25}$$

$$Q = \pi (1 - y) / (1 + y), \tag{26}$$

$$f(\Delta, y) = -\frac{1}{4}\Delta + \frac{1}{2}\Delta(1-y) - \frac{1+y}{2\pi}\sin\pi \frac{1+y}{1-y}$$
(27)

In the following we will examine Eqs. (18) for all other values of the parameter Δ . Using the relations given in (21) and taking (19) into consideration,

⁷ R. Orbach, Phys. Rev. **112**, 309 [1958]. — L. R.Walker, Phys. Rev. **116**, 1089 [1959]. — R. B. Griffiths, Phys. Rev. **133**, A 768 [1964]. — J. Des Cloizeaux and J. J. Pearson, Phys. Rev. **128**, 2131 [1962]. — E. Lieb and D. Mattis, Mathematical Physics in one Dimension, Academic Press, New York—London 1966. — M. Gaudin, Phys. Letters **24** A, 55 [1967].

⁸ Chi-Yu Hu, Phys. Rev. 152, 1116 [1966]. — V. Vorobyev, Method of Moments in Applied Mathematics, Gordon and Breach Science Publ. Inc., New York 1965.

A. D. JANNUSSIS, to be published.

¹⁰ A. D. Jannussis, Phys. Rev. Letters **21**, 523 [1968].

the integral equation (18) can be written in the following form:

$$\frac{1}{2}(1+y) = 2\pi\varrho(p) + \int_{-\varrho}^{\varrho} \left\{ \frac{e^{-ip}}{2 \Delta - e^{-ip} - e^{iq}} + \frac{e^{ip}}{2 \Delta - e^{ip} - e^{-iq}} \right\} \varrho(q) dq.$$
 (28)

Expanding the integral Kernel in Fourier series with elements $e^{\pm inq}$ $(n=0,\ 1,\ 2,\ldots)$ it follows that

$$\frac{1}{2} (1+y) = 2 \pi \varrho(p) + \sum_{n=0}^{\infty} \left\{ \frac{e^{-ip}}{(2 \Delta - e^{-ip})^{n+1}} \int_{-Q}^{Q} e^{inq} \varrho(q) dq + \frac{e^{ip}}{(2 \Delta - e^{ip})^{n+1}} \right\} \int_{-Q}^{Q} e^{-inq} \varrho(q) dq$$
(29)

or

$$\frac{1}{2} (1+y) = 2 \pi \varrho(p) + \sum_{n=0}^{\infty} \left\{ \left(\frac{e^{-ip}}{(2 \Delta - e^{-ip})^{n+1}} + \frac{e^{ip}}{(2 \Delta - e^{ip})^{n+1}} \right) \int_{-Q}^{Q} \cos n \, q \, \varrho(q) \, dq + i \left(\frac{e^{-ip}}{(2 \Delta - e^{-ip})^{n+1}} - \frac{e^{ip}}{(2 \Delta - e^{ip})^{n+1}} \right) \int_{-Q}^{Q} \sin n \, q \, \varrho(q) \, dq \right\}.$$
(30)

If we define now $I_n(Q)$ and $\bar{I}_n(Q)$ the integrals

$$I_n(Q) = \int_{-Q}^{Q} \cos n \, q \, \varrho(q) \, \mathrm{d}q \,, \quad \bar{I}_m(Q) = \int \sin n \, q \, \varrho(q) \, \mathrm{d}q \tag{31}$$

then the solution of Eq. (30) has the form:

$$2 \pi \varrho(p) = \frac{1}{2} (1+y) - \sum_{n=0}^{\infty} \left\{ \left| \frac{e^{-ip}}{(2 \Delta - e^{-ip})^{n+1}} + \frac{e^{ip}}{(2 \Delta - e^{ip})^{n+1}} \right| I_n(Q) + i \left\{ \frac{e^{-ip}}{(2 \Delta - e^{-ip})^{n+1}} - \frac{e^{ip}}{(2 \Delta - e^{ip})^{n+1}} \right| \bar{I}_n(Q) \right\}.$$
(32)

The above solution is substituted into (31) whence we obtain the following linear system for determining the coefficients $I_n(Q)$ and $\bar{I}_n(Q)$:

$$\pi I_m = \frac{1}{2} (1+y) \frac{\sin m Q}{m} - \sum_{n=0}^{\infty} A_{n,m}(Q) I_n(Q),$$
 (33)

$$\pi \, \bar{I}_m \equiv \sum_{n=0}^{\infty} B_{n, m}(Q) \, \bar{I}_n(Q) \qquad \text{where}$$
 (34)

$$A_{n, m} = \frac{1}{2} \int_{-Q}^{Q} \left\{ \frac{e^{-ip}}{(2 \Delta - e^{-ip})^{n+1}} + \frac{e^{ip}}{(2 \Delta - e^{ip})^{n+1}} \right\} \cos m \, p \, \mathrm{d}p \,, \tag{35}$$

The system (34) is homogeneous and linear and the condition for the existence of a solution other than zero, is the vanishing of the determinant from which we obtain the eigenvalues of the integral kernel.

However, on account of the fact that there exists an additional condition which connects Q with y the system (34) is satisfied by a zero solution, i. e. the coefficients $\bar{I}_n(Q)$ are zero.

In other words the function $\varrho(p)$ is an even function as expected from the underlying symmetry of the problem. The integral given in (33) is calculated from the basic integral $A_{0,m}(Q)$ by differentiation with respect to 2Δ .

$$A_{n, m}(Q) = \frac{(-1)^n}{n!} \frac{\mathrm{d}^n A_{\mathbf{0}, m}(Q)}{\mathrm{d}(2 \, \Delta)^n} = \frac{(-1)^n}{2^n \cdot n!} \frac{\mathrm{d}^n A_{\mathbf{0}, m}(Q)}{\mathrm{d} \Delta^n}. \tag{37}$$

The integral $A_{0, m}(Q)$ is easily calculated and the result is written below.

$$A_{0,m}(Q) = -\frac{\sin m Q}{m} + \sum_{K=1}^{m-1} \left\{ (2 \Delta)^{K-m} - (2 \Delta)^{m-K} \right\} \frac{\sin K Q}{K} + (2 \Delta)^m \operatorname{tg}^{-1} \left(\frac{\sin Q}{2 \Delta - \cos Q} \right) - \frac{1}{(2 \Delta)^m} \operatorname{tg}^{-1} \left(\frac{2 \Delta \sin Q}{1 - 2 \Delta \cos Q} \right).$$
(38)

For $m = 0, 1, 2, \ldots$ this becomes

$$A_{0,0}(Q) = 2 \operatorname{tg}^{-1} \left(\frac{\sin Q}{2 \, \varDelta - \cos Q} \right), \qquad A_{1,0}(Q) = \frac{2 \sin Q}{4 \, \varDelta^2 - 4 \, \varDelta \cos Q + 1}, \dots$$

$$A_{0,1}(Q) = -\sin Q + 2 \, \varDelta \operatorname{tg}^{-1} \left(\frac{\sin Q}{2 \, \varDelta - \cos Q} \right) - \frac{1}{2 \, \varDelta} \operatorname{tg}^{-1} \left(\frac{2 \, \varDelta \sin Q}{1 - 2 \, \varDelta \cos Q} \right), \dots$$
(39)

The functions $A_{0,m}(Q)$ may be expanded in a power series of 2Δ or $1/2\Delta$ depending on whether 2Δ is greater or less than unity. The following series are in general valid

$$A_{0, m}(Q) = -\frac{2\sin Q}{m} - \sum_{K=1}^{m} (2\Delta)^{K} \left[\frac{\sin(m+K) Q}{m+K} + \frac{\sin(m-K) Q}{m-K} \right] - \sum_{l=1}^{\infty} (2\Delta)^{m+l} \left\{ \frac{\sin l Q}{l} + \frac{\sin(2m+l) Q}{2m+l} \right\},$$

$$A_{0, m}(Q) = \sum_{k=1}^{m} \left(\frac{1}{2\Delta} \right)^{K} \left\{ \frac{\sin(m+K) Q}{m+K} + \frac{\sin(m-K) Q}{m-K} \right\} + \sum_{l=1}^{\infty} \left(\frac{1}{2\Delta} \right)^{m} \left\{ \frac{\sin l Q}{l} + \frac{\sin(2m+l) Q}{2m+l} \right\}.$$

$$(40)$$

From the calculated values of the coefficients $A_{n, m}(Q)$ we see that in the denominator we have the expression

$$4 \Delta^2 - 4 \Delta \cos Q + 1 \tag{41}$$

which must, in order to satisfy converge requirements, be less than unity. We assume that the series converge and proceed to a solution of the linear system (33) using the method of successive approximations.

For the zero order approximation we obtain the solution

$$\pi I_m^{(0)}(Q) = \frac{1}{2} (1+y) \frac{\sin m Q}{m}$$
 (42)

which for m = 0 gives

$$\pi I_0^{(0)}(Q) = \frac{1}{2} (1+y) \ Q = \frac{1}{2} \pi (1-y)$$

$$Q = \pi \cdot (1-y)/(1+y). \tag{43}$$

This solution is exact for $\Delta = \infty$.

As a first approximation we have the solution

$$\pi \, I_m^{(1)} \, (Q) = \tfrac{1}{2} \, (1+y) \, \left\{ \frac{\sin m \, Q}{m} - \frac{1}{\pi} \sum_{n=0}^{\infty} A_{n,\, 1}(Q) \frac{\sin n \, Q}{n} \right\} \tag{44}$$

For m = 0, 1 we obtain:

$$Q\left[1 - \frac{2}{\pi} \operatorname{tg}^{-1}\left(\frac{\sin Q}{2 \Delta - \cos Q}\right)\right]$$

$$+ \frac{i}{\pi} \sum_{n=0}^{\infty} \left\{\frac{1}{(2 \Delta - e^{-iQ})^n} - \frac{1}{(2 \Delta - e^{iQ})^n}\right\} \frac{\sin n Q}{n^2} = \pi \frac{1 - y}{1 + y}$$

$$f(\Delta, y) = -\frac{1}{4} \Delta + \frac{1}{2} \Delta (1 - y)$$

$$-\frac{1}{2 \pi} (1 + y) \left\{\sin Q - \frac{1}{\pi} \sum_{n=0}^{\infty} A_{n, 1}(Q) \frac{\sin n Q}{n}\right\}.$$
(45)

For $|2 \Delta| > 1$ we may use the following expressions

$$\frac{Q}{1 + (2/\pi) \operatorname{tg}^{-1} (\sin Q/(2\Delta - \cos Q))} = \pi \frac{1 - y}{1 + y}, \quad (47)$$

$$f(\Delta, y) = -\frac{1}{4}\Delta + \frac{1}{2}\Delta(1-y)$$

$$-\frac{1}{2\pi}\left\{ (1+y)\sin Q - (1-y)A_{0,1}(Q) \right\} \quad (48)$$

where

$$A_{0,1}(Q) = -\sin Q + 2 \, \Delta \, \text{tg}^{-1} \left(\frac{\sin Q}{2 \, \Delta - \cos Q} \right)$$

$$- \frac{1}{2 \, \Delta} \, \text{tg}^{-1} \left(\frac{\sin Q}{(1/2 \, \Delta) - \cos Q} \right).$$
(49)

Expression (47) can be written as follows:

$$y = \frac{\pi + 2 \operatorname{tg}^{-1} (\sin Q / (2 \Delta - \cos Q)) - Q}{\pi + 2 \operatorname{tg}^{-1} (\sin Q / (2 \Delta - \cos Q)) + Q}.$$
 (50)

For different values of the parameter Δ the above expression gives the exact magnetization curve. The boundary values may also be obtained from the (50), namely for y=0 gives $Q=\pi$ and for y=1 gives Q=0. Expressions for $|2\Delta|<1$ may be obtained directly by solving the integral equation (28) when the solution is expanded in powers of 2Δ or by using the first expression of relations (40).

The results in this case are the following:

$$Q + \frac{2 \Delta}{\pi} \{ Q \sin Q + \cos Q \ln \cos Q \} = \frac{\pi}{2} (1 - y),$$
(51)

$$f(\Delta, y) = -\frac{1}{4}\Delta + \frac{1}{2}\Delta(1-y) - \frac{\sin Q}{\pi}$$

$$-\frac{\Delta}{\pi^2} \left\{ Q^2 - \sin^2 Q + Q\sin 2 Q + 2\cos^2 Q \ln\cos Q \right\}.$$
(52)

From the results we observe that system (33) allows us to approximate the solution as close as we like and is suitable for practical calculations.

The special cases $\Delta = \pm 1$ (ferromagnetisms and antiferromagnetism) can be directly studied using (47) and (48). The case of antiferromagnetism has been recently studied by the author ⁹.

Appendix

Using the same method we will study here the system of integral equations which has been recently given by Lieb-Wu ¹¹. They are similar to the Yang and Yang ⁵ and Sutherland ¹² integral equations.

Using Lieb-Wu's symbolism the equations are as follows:

$$2 \pi \varrho(k) = 1 + \cos k \int_{-R}^{B} \frac{8 U \sigma(\Lambda) d\pi}{U^{2} + 16 (\sin k - \Lambda)^{2}}, \qquad (1)$$

$$\int_{-Q}^{Q} \frac{8 U \varrho(k) dk}{U^2 + 16 (\Lambda - \sin k)^2} = 2 \pi \sigma(\Lambda) + \int_{-B}^{B} \frac{4 U \sigma(\Lambda') d\Lambda'}{U^2 + 4 (\Lambda - \Lambda')^2}$$
(2)

where the limits are determined from the following conditions

$$\int_{-Q}^{Q} \varrho(k) \, dk = N/N_{\bar{\alpha}} \int_{-B}^{B} \sigma(\Lambda) \, d\Lambda = M/N_{\bar{\alpha}}$$
 (3, 4)

The ground-state energy of this system is given by the expression

$$E = -2 N_{\bar{\alpha}} \int_{-Q}^{Q} \varrho(k) \cos k \, dk.$$
 (5)

The case of $Q = \pi$ and $B = \infty$ has been studied by Lieb-Wu¹¹ and the solution is obtained in closed form by using Fourier transform.

Now we will confine ourselves to the case $B \leq 1$ and we will use the method of moments. From the underlying symmetry properties the functions $\varrho(k)$ and $\sigma(A)$ are even functions. Equation (1) by expanding the integral kernel in series can be written as follows:

$$2\pi \varrho(k) = 1 + i\cos k \sum_{n=0}^{\infty} \left\{ \frac{1}{(\sin k + iU/4)^{n+1}} - \frac{1}{(\sin k - iU/4)^{n+1}} \right\} \int_{-B}^{B} A^{n} \sigma(A) dA.$$
 (6)

The integral $\int_{-R}^{B} \Lambda^n \sigma(\Lambda) d\Lambda$ is non zero for even n and (6) can be written:

$$2\pi\varrho(k) = 1 + i\cos k \sum_{n=0}^{\infty} \left\{ \frac{1}{(\sin k + iU/4)^{n+1}} - \frac{1}{(\sin k - iU/4)^{n+1}} \right\} I_{2n}(B)$$
 (7)

where $I_{2n}(B)$ represents the moments:

$$I_{2n}(B) = \int_{-R}^{B} A^{2n} \, \sigma(\Lambda) \, d\Lambda \tag{8}$$

because of (7) and (8) Eq. (2) is written:

$$\frac{8 U}{2 \pi} \int_{-Q}^{Q} \frac{dk}{U^{2} + 16 (A - \sin k)^{2}} + i \frac{8 U}{2 \pi} \sum_{n=0}^{\infty} I_{2n}(B) \int_{-Q}^{Q} \frac{\cos k \, dk}{U^{2} + 16 (A - \sin k)^{2}} \left\{ \frac{1}{(\sin k + i U/4)^{2n+1}} - \frac{1}{(\sin k - i U/4)^{2n+1}} \right\}$$

$$= 2 \pi \sigma(A) + i \sum_{n=0}^{\infty} \left\{ \frac{1}{(A + i U/2)^{2n+1}} - \frac{1}{(A - i U/2)^{2n+1}} \right\} I_{2n}(B). \tag{9}$$

By expanding the integral kernel $1/[U^2+16(\Lambda-\sin k)^2]$ in a series of powers of $\sin k$ the above equation takes the following form:

$$\frac{i}{2\pi} \sum_{n=0}^{\infty} \left\{ \frac{1}{(A+iU/4)^{2l+1}} - \frac{1}{(A-iU/4)^{2l+1}} \right\} \int_{-Q}^{Q} \sin^{2l} k \, dk
- \frac{1}{2\pi} \sum_{l=0}^{\infty} \sum_{n=0}^{\infty} I_{2n}(B) \left\{ \frac{1}{(A+iU/4)^{2l+1}} - \frac{1}{(A-iU/4)^{2l+1}} \right\} \int_{-Q}^{Q} \sin^{2l} k \left\{ \frac{\cos k}{(\sin k+iU/4)^{2n+1}} - \frac{\cos k}{(\sin k-iU/4)^{2n+1}} \right\} dk
= 2\pi \sigma(A) + i \sum_{n=0}^{\infty} \left\{ \frac{1}{(A+iU/2)^{2n+1}} - \frac{1}{(A-iU/2)^{2n+1}} \right\} I_{2n}(B).$$
(10)

If we now multiply the above equation by A^{2m} and integrate from -B to B we obtain the equation from which the coefficients $I_{2n}(B)$ are determined.

$$\frac{1}{\pi} \sum_{l=0}^{\infty} \Gamma_{2l+1, 2m}(B, U/4) T_{2l}(Q) + \frac{1}{\pi} \sum_{l=0}^{\infty} \sum_{n=0}^{\infty} I_{2n}(B) \Gamma_{2l+1, 2m}(B, U/4) \Gamma_{2n+1, 2l}(\sin Q, U/4)
= \pi I_{2m}(B) + \sum_{n=0}^{\infty} \Gamma_{2n+1, 2m}(B, U/2) I_{2n}(B).$$
(11)

¹¹ E. Lieb and F. Wu, Phys. Rev. Letters 20, 1445 [1968].
¹² B. Sutherland, Phys. Rev. Letters 20, 98 [1968].

$$T_{2l}(Q) = \int_{0}^{Q} \sin^{2l} k \, \mathrm{d}k \tag{12}$$

and

$$\Gamma_{p,q}(B,\lambda) = \frac{i}{2} \int_{-B}^{B} x^{q} \left\{ \frac{1}{(x+i\lambda)^{p}} - \frac{1}{(x-i\lambda)^{p}} \right\} dx.$$
(13)

Various properties of the coefficient $\Gamma_{p,q}(B,\lambda)$ are cited in ¹⁰. The system of Eqs. (11) can be solved by several approximate methods. With the method of successive approximations we obtain the zero order solution

$$I_{2m}^{(0)} = \frac{1}{\pi^2} \sum_{l=0}^{\infty} \Gamma_{2l+1, 2m}(B, U/4) T_{2l}(Q).$$
 (14)

The first solution is

$$I_{2m}^{(1)}(B) = \frac{1}{\pi} \sum_{l=0}^{\infty} \Gamma_{2l+1, 2m}(B, U/4) \ T_{2l}(Q) - \frac{1}{\pi^2} \sum_{n=1}^{\infty} \sum_{q=0}^{\infty} \Gamma_{2n+1, 2m}(B, U/2) \ \Gamma_{2q+1, 2n}(B, U/4) \ T_{2q}(Q) + \frac{1}{\pi^3} \sum_{l=0}^{\infty} \sum_{n=1}^{\infty} \sum_{q=0}^{\infty} \Gamma_{2l+1, 2m}(B, U/4) \ \Gamma_{2n+1, 2l}(\sin Q, U/4) \ \Gamma_{2q+1, 2n}(B, U/4) \ T_{2q}(Q).$$

$$(15)$$

System (11) can also be solved assuming that the coefficient $I_0(B)$ is greater than all others and this for $B \leq 1$ and $U/4 \geq 1$. The coefficient $I_0(B)$ is given by the following expression

$$I_{0}(B) = \frac{1}{\pi} \cdot \frac{\sum_{l=0}^{\infty} \Gamma_{2l+1, 0}(B, U/4) \ T_{2l}(Q)}{\pi + \Gamma_{1, 0}(B, U/2) - (1/\pi) \sum_{l=0}^{\infty} \Gamma_{2l+1, 0}(B, U/4) \ \Gamma_{1, 2l}(\sin Q, U/4)}.$$
(16)

If we now substitute in the above formula the sums with the corresponding integrals this becomes

$$I_0(B) = \frac{1}{\pi} \cdot \frac{\int\limits_0^Q \left\{ \operatorname{tg}^{-1} \left[\left(4/U \right) \left(B + \sin k \right) \right] + \operatorname{tg}^{-1} \left[\left(4/U \right) \left(B - \sin k \right) \right] \right\} \mathrm{d}k}{\pi + 2 \operatorname{tg}^{-1} \left(2 B/U \right) - \left(U/2 \pi \right) \int\limits_0^Q \left(\operatorname{tg}^{-1} \left[\left(4/U \right) \left(B + \sin k \right) \right] + \operatorname{tg}^{-1} \left[\left(4/U \right) \left(B - \sin k \right) \right] / \left(\sin^2 k + U^2 / 16 \right) \right) \mathrm{d}k} \ . \tag{17}$$

A convenient approximation of the integral leads to the following results:

$$I_0(B) = \frac{2\,Q}{\pi} \cdot \frac{\operatorname{tg^{-1}(4\,B/U)}}{\pi + 2\,\operatorname{tg^{-1}(2\,B/U)} - (4/\pi)\,\operatorname{tg^{-1}(4\,B/U)} \cdot \operatorname{tg^{-1}(4\,\sin\,Q/U)}} \,. \tag{18}$$

Using the known values of the coefficients $I_{2n}(B)$ in Eq. (7), integration from -Q to Q gives

$$\frac{N}{N_{\alpha}} = \frac{Q}{\pi} + \frac{2}{\pi} \cdot \frac{M}{N_{\alpha}} \operatorname{tg}^{-1} \frac{4 \sin Q}{U} - \frac{i}{2 \pi} \sum_{n=1}^{\infty} \frac{I_{2n}(B)}{n} \left\{ \frac{1}{(\sin Q + i U/4)^{2n}} - \frac{1}{(\sin Q - i U/4)^{2n}} \right\}$$
(19)

where

$$\frac{M}{N_{\alpha}} = I_0(B) = \frac{2 Q}{\pi} \frac{\text{tg}^{-1}(4 B/U)}{\pi + 2 \text{tg}^{-1}(2 B/U) - (4/\pi) \text{tg}^{-1}(4 B/U) \text{tg}^{-1}(4 \sin Q/U)}.$$
 (20)

The ground-state energy is given by

$$\pi \frac{E}{N_a} = -2\sin Q + \frac{M}{N_a} U Q - 4\frac{M}{N_a} \left(\frac{4}{U} + \frac{U}{4}\right)_0^Q \frac{\mathrm{d}k}{1 + 165 \, m^2 \, k/U^2}$$

$$-i \sum_{n=1}^{\infty} I_{2n}(B) \int_0^Q \cos^2 k \, \left\{ \frac{1}{(\sin k + i \, U/4)^{2n+1}} - \frac{1}{(\sin k - i \, U/4)^{2n+1}} \right\} \, \mathrm{d}k$$
(21)

or

$$\frac{E}{N_{\sigma}} = -\frac{2}{\pi} \sin Q + \frac{M}{N_{\sigma}} \cdot \frac{U}{\pi} \left\{ Q - \sqrt{1 + 16/U^2} \cdot \lg^{-1} \left(\sqrt{1 + 16/U^2} \cdot \lg Q \right) \right\} + \dots$$
 (22)

The formulae (19) and (20), obtained by assuming $B \le 1$, which were also given for $Q \le \pi$ and $B = \infty$, yield exactly the maximum values of $M/N_{\alpha} = 1/2$ and $N/N_{\alpha} = 1$. The energy formula (22) for $Q = \pi$ becomes $E = M U + \dots$ (23)

Knowing the energy E from (22) we can calculate the chemical potentials 11 .