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Fermionic Perturbation Theory for the Statistical Mechanics of the Nonlinear Schrödinger Model

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A fermionic perturbation theory is developed for the statistical mechanics of the nonlinear Schrödinger model. The theory is based on an interacting-fermion picture of the Bethe wave function. The inner product of the Bethe wave function is explicitly evaluated, and a simple graphical representation of it is given. The basic equations obtained for the free energy agree with those of Yang and Yang. In particular, the present theory gives a clear-cut meaning to the ε function of Yang and Yang: It represents a fermion energy at finite temperatures.

KEY WORDS: Nonlinear Schrödinger model; statistical mechanics; Bethe Ansatz; virial expansion; inner product; graphical approach.

1. INTRODUCTION

The Bethe ansatz (BA) formulation of the thermodynamics of soluble models in one dimension was initiated by Yang and Yang[(1)] in the nonlinear Schrödinger (NLS) model described by the Hamiltonian,

$$H = \int dx [\partial_x \phi^* \partial_x \phi + c\phi^* \phi^* \phi\phi] \tag{1.1}$$

where $\phi(x)$ is a quantized boson field and c is a repulsive coupling constant. Since then, the BA method has been successfully generalized and applied to a variety of physical systems: the Heisenberg–Ising ring,[(2)] the

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Kondo problem,[3] the massive Thirring = sine-Gordon model,[4,5] and the Anderson model.[6] In spite of its great success, however, the BA formalism has involved certain ambiguities common to all the soluble models. These have to do with the two-body scattering phase shift and the physical meaning of the ε function introduced by Yang and Yang. These ambiguities, together with the so-called *exotic excitations* in some more intricate BA systems, have prevented people from reaching a more profound understanding of the soluble models in one dimension. As for the exotic excitations, it has been pointed out that they are mathematical artifacts rather than physical objects,[5] and a new thermodynamical formalism which does not invoke these excitations has recently been presented.[7]

In this paper I shall consider a fermionic perturbation theory for the statistical mechanics of the NLS model, thereby removing the ambiguities in the BA formalism. In particular, it is clear in the new theory that the ε function represents the fermion energy at finite temperatures.

It was Thacker[8] who first performed a perturbative calculation of the statistical mechanics of the NLS model. Thacker's argument, however, is based on a picture of interacting bosons in which the wave operator unitarity is violated, and therefore it is mathematically questionable—indeed, Thacker's formalism does not agree with the BA formalism. Nevertheless, as far as thermodynamic properties are concerned, Thacker's results agree with those of the BA theory. Although the new approach is also perturbative, it is now based on a picture of interacting fermions where the wave operator unitarity is guaranteed. As a result, this new approach does not contain any ambiguities and the resulting formalism agrees with the BA formalism.

I have organized the present paper as follows. In the next section, the BA formalism and the bosonic perturbation theory are briefly reviewed and some ambiguities in these theories are pointed out. In Section 3, the Bethe wave function is put in a form of interacting fermions. Thus we examine a fermionic perturbation theory from $c = \infty$ instead of the bosonic perturbation theory from $c = 0$. In this section, graphical rules are also given for calculating inner products of the Bethe wave function. In Section 4, inner products are explicitly evaluated. In Section 5, a simple graphical representation is first introduced for the evaluated inner products. Then, the virial expansion of the free energy is graphically manipulated to reproduce the BA formalism results. As will become clear below, although our fermionic wave function is correct as far as physical quantities are concerned, it is not the precise energy eigenstate of the Hamiltonian. Some remarks at the level of the Hamiltonian related to this latter point will be given in the last section.

2. REVIEW OF PREVIOUS THEORIES

Lieb and Liniger[9] first introduced the NLS model (1.1) as a theory of bosons interacting via a two-body δ-function potential of strength $2c$. Let us start with writing their Bethe wave function in a form suitable for the second quantized Hamiltonian (1.1):

$$|\psi(k_1 \cdots k_N)\rangle = \int dx_1 \cdots \int dx_N \exp\left(i \sum_{j=1}^{N} k_j x_j\right) \times \prod_{i<j} [\theta(x_i - x_j) + S_{ij}\theta(x_j - x_i)] \times \phi^*(x_1) \cdots \phi^*(x_N) |0\rangle \tag{2.1}$$

where θ is a step function and S_{ij} represents the two-body S matrix for bosons with momenta k_i and k_j. When we write the Bethe wave function as (2.1), we have introduced a convention that $\delta\theta = \delta/2$, or formally $\theta(0) = 1/2$. The two-body S matrix $S_{ij} = e^{i\delta(k_i - k_j)}$ with the two-body scattering phase shift

$$\delta(k) = 2 \tan^{-1}(c/k) \tag{2.2}$$

In the BA thermodynamics, the following integral equation for the quantity $\varepsilon(k)$ plays a central role[1]:

$$\varepsilon(k) = -\mu + k^2 + \beta^{-1} \int \frac{dq}{2\pi} \frac{\partial \tilde{\delta}(k-q)}{\partial k} \cdot \ln[1 + e^{-\beta\varepsilon(q)}] \tag{2.3}$$

where μ and β, respectively, represent the chemical potential and the inverse temperature (Boltzmann constant $= 1$), and

$$\tilde{\delta}(k) = -2 \tan^{-1}(k/c) \tag{2.4}$$

In terms of $\varepsilon(k)$, the free energy of the system is written as

$$F = \mu N_0 - L\beta^{-1} \int \frac{dk}{2\pi} \cdot \ln[1 + e^{-\beta\varepsilon(k)}] \tag{2.5}$$

where N_0 and L, respectively, represent the total particle number and the system size. The energy ΔE required for exciting n particles from $\{k_\alpha\}$ to $\{k'_\alpha\}$ $(\alpha = 1, 2,..., n)$ at thermal equilibrium can also be expressed in terms of $\varepsilon(k)$ as

$$\Delta E = \sum_{\alpha=1}^{n} [\varepsilon(k'_\alpha) - \varepsilon(k_\alpha)] \tag{2.6}$$

Equations (2.5) and (2.6) demonstrate a parallelism between the NLS model and free fermions having a one-particle energy $\varepsilon(k)$ measured from the chemical potential.

An ambiguity in the above BA formalism is that the quantity $\tilde{\delta}$ appearing in (2.3) is not equal to the two-body phase shift δ. In the existing BA literature, to the author's knowledge, the question of why $\tilde{\delta}$ instead of δ and what $\tilde{\delta}$ means has not been addressed even at the level of a plausibility argument. This ambiguity originates in imposing periodic boundary conditions on the Bethe wave function (2.1),

$$kL = 2\pi I_k + \sum_{k'} \delta(k - k') \tag{2.7}$$

where I_k is an integer. In the BA formalism, (2.7) is replaced by

$$kL = 2\pi \tilde{I}_k + \sum_{k'} \tilde{\delta}(k - k') \tag{2.8}$$

where now

$$\begin{aligned} \tilde{I}_k &= \text{integer}, \qquad \text{if} \quad N = \text{odd} \\ \tilde{I}_k + \tfrac{1}{2} &= \text{integer}, \qquad \text{if} \quad N = \text{even} \end{aligned} \tag{2.9}$$

The replacement of (2.7) by (2.8) is based on the identity[14]

$$\delta(k) = \pi \,\mathrm{sgn}(k) + \tilde{\delta}(k) \tag{2.10}$$

where $\mathrm{sgn}(k) = 1$ if $k > 0$, and -1 if $k < 0$. Now a subtle difference between (2.7) and (2.8) is that in differentiating these equations with respect to k, there arises a δ function term from $\delta(k)$ but not from $\tilde{\delta}(k)$. This difference is physically significant; the use of (2.7) instead of (2.8) leads to a wrong theory for the statistical mechanics.

In short, the BA formalism is not clear in two points: First, it is not clear why one should use $\tilde{\delta}$ instead of δ. Second, the physical meaning of the important quantity $\varepsilon(k)$ is not quite clear. The main purpose of the present paper is to clarify these points, and give a clear-cut physical meaning to $\varepsilon(k)$.

Next we briefly review the bosonic perturbation theory of Thacker. Both Thacker's and our perturbation theories are based on the virial expansion of the free energy:

$$F = \mu N_0 - \beta^{-1} \sum_{N=1}^{\infty} \lambda^N [\mathrm{Tr}_N e^{-\beta H}]_{\mathrm{conn}} \tag{2.11}$$

where $\lambda = e^{\beta\mu}$ = fugacity (or absolute activity), and $[\cdots]_{\text{conn}}$ means to take contributions from connected graphs in a graphical expansion of the trace of the Boltzmann factor $e^{-\beta H}$. The quantity $\text{Tr}_N e^{-\beta H}$ is transformed as follows[8,10,11]: First write

$$\begin{aligned}\text{Tr}_N e^{-\beta H} &= \int_C \frac{dE}{2\pi i} e^{-\beta E} \text{Tr}_N G(E) \\ &= \int_0^\infty \frac{dE}{2\pi i} e^{-\beta E} \text{Tr}_N [G^+(E+i\eta) - G(E+i\eta)] \end{aligned} \tag{2.12}$$

where $G(E) = (E-H)^{-1}$ = resolvent operator, and the contour C encloses all the poles of $G(E)$. The second expression in (2.12) is obtained by noting that the poles of $G(E)$ are only on the positive energy axis for the repulsive interaction $c>0$. Here the limit $\eta \to 0$ is understood to be taken after the thermodynamic limit. Next we expand G in terms of the free resolvent operator $G_0 = (E-H_0)^{-1}$ as

$$G = G_0 + G_0 V G_0 + \cdots \equiv \Omega G_0 \tag{2.13}$$

where V = the interaction Hamiltonian, and $\Omega = \sum_{n=0}^{\infty} (G_0 V)^n$. It is convenient to introduce an operator transition matrix T by $\Omega = 1 + G_0 T$. It is easy to show that $T = V + T G_0 V$ and the operator identity

$$T - T^\dagger = T(G_0 - G_0^\dagger)\, T^\dagger \tag{2.14}$$

With the use of $\Omega = 1 + G_0 T$ and (2.14), one can show that the following holds inside the trace operator:

$$G^\dagger - G = (G_0^\dagger - G_0)\, \Omega^\dagger \Omega = 2\pi i \delta(E - H_0)\, \Omega^\dagger \Omega \tag{2.15}$$

Substituting (2.12) and (2.15) into (2.11) gives

$$F = \mu N_0 - L\beta^{-1} \sum_{N=1}^{\infty} \lambda^N \int \frac{dk_1}{2\pi} \cdots \int \frac{dk_N}{2\pi} e^{-\beta\omega_k} \frac{\lim_{\eta\to 0} \lim_{k'\to k} W_N}{N!} \tag{2.16}$$

with

$$W_N = \frac{1}{L} \langle k' |\, \Omega^\dagger(\omega_k + i\eta)\, \Omega(\omega_k + i\eta)\, | k \rangle_{\text{conn}} \tag{2.17}$$

where $\omega_k = \sum_{j=1}^{N} k_j^2$ and $|k\rangle = |k_1 k_2 \cdots k_N\rangle$. Note that $\Omega(\omega) = U(0, -\infty)$, the Möller wave operator, and therefore the wave function $\Omega\,|k\rangle$ is obtained by an analytic continuation in the complex energy plane of the

Bethe wave function (2.1). Thus the main task is to calculate the inner product W_N in (2.17). The two limits in (2.16) have been introduced for later use.

In the bosonic perturbation theory of Thacker, the interaction Hamiltonian V is the second term on the right of (1.1) and the perturbation expansion is around $c=0$. The obtained basic equations, corresponding to (2.3) and (2.5) in the BA formalism, are[8]

$$\pi(k) = -\mu + k^2 - \beta^{-1} \int \frac{dq}{2\pi} \frac{\partial\delta(k-q)}{2k} \ln[1 - e^{-\beta\pi(q)}] \tag{2.18}$$

and

$$F = \mu N_0 + L\beta^{-1} \int \frac{dk}{2\pi} \ln[1 - e^{-\beta\pi(k)}] \tag{2.19}$$

It is easily seen that $\pi(k) \neq \varepsilon(k)$, but both the bosonic perturbation theory and the BA formalism give the same free energy. This agreement in the free energy, however, does not necessarily mean that these theories are two equivalent but different ways of approaching the NLS model. Rather, here is a fact which is unfavorable to the bosonic perturbation theory. We note a well-known property of the Bethe wave function (2.1) that the wave function identically vanishes if any two momenta coincide. In the inner product (2.17), this property appears as a violation of the wave operator unitarity. That is, for $N=2$, for example,[3]

$$0 = \langle kk|\, U^\dagger U \,|kk\rangle \neq \langle kk \mid kk\rangle \tag{2.20}$$

This means that $c=0$ is a singular point and one has no reason to expect that the perturbation calculation around this point gives a correct answer.

Our arguments in the remaining sections are also based on the virial expansion of the free energy, (2.16) and (2.17). A main difference between Thacker's approach and ours is that the latter is the perturbation calculation around $c=\infty$. Since the model at $c=\infty$, impenetrable bosons, is equivalent to free fermions,[12] our approach is in effect a fermonic per-

[3] The reader should not confuse the perturbation theory with the Bethe ansatz theory. In the latter, by imposing periodic boundary conditions, we consider an $O(L^{-1})$ shift of the momentum k. On the other hand, in the perturbation theory, we work on the unperturbed momentum space $k=(2\pi/L)x$ integer instead of imposing periodic boundary conditions. Moreover, it was shown that the unperturbed momentum labels are not changed by interactions and become momentum labels of the Bethe wave function [H. B. Thacker, *Phys. Rev. D* **11**:838 (1975); **14**:3508 (1976)]. Thus equation (2.20) precisely describes the violation of wave operator unitarity in the bosonic perturbation theory.

turbation theory. A merit of the new approach is that it guarantees the wave operator unitarity. As we will see below, this new approach removes the ambiguities in the BA formalism, and thus we can reach a more profound understanding of the statistical mechanics of the NLS model.

3. PERTURBATION THEORY FROM $c = \infty$

We start with rewriting the Bethe wave function as follows: Notice the identify (2.10), and define a new S matrix by

$$\tilde{S}_{ij} = e^{i\tilde{\delta}_{ij}} = -S_{ij} \tag{3.1}$$

The Bethe wave function (2.1) is written in terms of $\tilde{S}_{ij}$ as

$$\begin{aligned} |\psi(k_1 \cdots k_N)\rangle = \int dx_1 \cdots \int dx_N \exp\left(i \sum_{j=1}^{N} k_j x_j\right) \\ \times \prod_{i<j} [\theta(x_i - x_j) + \tilde{S}_{ij}\theta(x_j - x_i)] \\ \times \prod_{i<j} \operatorname{sgn}(x_i - x_j)\, \phi^*(x_1) \cdots \phi^*(x_N)\, |0\rangle \end{aligned} \tag{3.2}$$

Here we introduce a fermi field $\varphi(x)$ through the Jordan–Wigner transformation:

$$\varphi(x) = \exp\left(i\pi \int_x^{\infty} \phi^*\phi \, dt\right) \phi(x) \tag{3.3}$$

It is a straightforward calculation to see that the field operator $\varphi(x)$ actually obeys the fermionic anticommutation relations, and that $\phi^*(x)\,|0\rangle = \varphi^\dagger(x)\,|0\rangle$, and for $N \geqslant 2$

$$\prod_{i<j} \operatorname{sgn}(x_i - x_j)\phi^*(x_1) \cdots \phi^*(x_N)\,|0\rangle = \varphi^\dagger(x_1) \cdots \varphi^\dagger(x_N)\,|0\rangle \tag{3.4}$$

Substituting (3.4) into (3.2) gives

$$\begin{aligned} |\psi(k_1 \cdots k_N)\rangle = \int dx_1 \cdots \int dx_N \exp\left(i \sum_{j=1}^{N} k_j x_j\right) \\ \times \prod_{i<j} [1 + \tilde{\tau}_{ij}\theta(x_j - x_i)]\, \varphi^\dagger(x_1) \cdots \varphi^\dagger(x_N)\,|0\rangle \end{aligned} \tag{3.5}$$

where we have introduced a transition matrix $\tilde{\tau}_{ij}$ by $\tilde{S}_{ij} = 1 + \tilde{\tau}_{ij}$. Note that for $c = \infty$, $\tilde{\delta}_{ij} = 0$ and $\tilde{S}_{ij} = 1$ [cf. (2.4)], and hence (3.5) describes N free fermions. In general, (3.5) describes N fermions interacting via the two-body S matrix, $\tilde{S}_{ij}$. The quantity $\tilde{\delta}_{ij}$ is then regarded as the two-body phase shift. The fermionic representation of the Bethe wave function is particularly suitable for the virial expansion of the free energy, because the wave operator unitarity is clearly guaranteed in the fermionic treatment.

A remark which should be made before we proceed further is that (3.5) is not a precise rewriting of the Bethe wave function (2.1). The difference between (2.1) and (3.5) is in the wave amplitude when any two particles collide. This point and related questions will be discussed in the last section. Here we simply note that such a difference in the wave function does not bring about any differences in calculating physical quantities.

We now consider the inner products of the wave function (3.5). A straightforward calculation gives the following expression for W_N in (2.17):

$$W_N = \frac{1}{L} \sum_{R \in S_N} P(R) \int dx_1 \cdots \int dx_N \times \exp\left[i \sum_{j=1}^{N} (k_j - k'_{Rj})\, x_j \right] \xi(R; x_1 \cdots x_N)_{\text{conn}} \tag{3.6}$$

where S_N is the permutation group for integers 1, 2,..., N, $P(R)$ is 1 or -1 according to whether the permutation R is even or odd, and

$$\xi(R; x_1 \cdots x_N) = \prod_{(i<j) \in \varepsilon_N} [1 + \tilde{\tau}_{ij} \theta(x_j - x_i)] \times \prod_{(l<m) \in \varepsilon_N} [1 + \tilde{\tau}^*_{lm} \theta(x_{R^{-1}m} - x_{R^{-1}l})] \tag{3.7}$$

where $\varepsilon_N \equiv \{(i, j) \mid 1 \leqslant i < j \leqslant N\}$. The equation (3.7) can be simplified as follows. Look at an integer pair $i<j$. For a given permutation R, integers $l<m$ which go to integers i and j under the permutation R^{-1} are uniquely determined besides the possibilities: (i) $R^{-1}m = j$ and $R^{-1}l = i$ or (ii) $R^{-1}m = i$ and $R^{-1}l = j$. For case (i), $l = R_i$, $m = R_j$, and therefore $R_i < R_j$, and the $i<j$ pair contribution in (3.7), C^R_{ij}, is

$$\begin{aligned} C^R_{ij} &= [1 + \tilde{\tau}_{ij} \theta(x_j - x_i)][1 + \tilde{\tau}^*_{Ri,Rj} \theta(x_j - x_i)] \\ &= 1 + (\tilde{\tau}_{ij} + \tilde{\tau}^*_{Ri,Rj} + \tilde{\tau}_{ij} \tilde{\tau}^*_{Ri,Rj})\, \theta(x_j - x_i) \end{aligned} \tag{3.8a}$$

For the case (ii), on the other hand, $l = Rj$, $m = Ri$, and therefore $Rj < Ri$, and the $i<j$ pair contribution becomes

$$\begin{aligned} C^R_{ij} &= [1 + \tilde{\tau}_{ij} \theta(x_j - x_i)][1 + \tilde{\tau}^*_{Rj,Ri} \theta(x_i - x_j)] \\ &= 1 + \tilde{\tau}_{ij} \theta(x_j - x_i) + \tilde{\tau}^*_{Rj,Ri} \theta(x_i - x_j) \end{aligned} \tag{3.8b}$$

The equations (3.8a) and (3.8b) can be put together as

$$C_{ij}^R = 1 + \alpha_{ij}^R \tag{3.9}$$

with

$$\alpha_{ij}^R = \begin{cases} (\tilde{\tau}_{ij} + \tilde{\tau}^*_{Ri,Rj} + \tilde{\tau}_{ij}\tilde{\tau}^*_{Ri,Rj})\,\theta(x_j - x_i), & \text{if} \quad R_i < R_j \\ \tilde{\tau}_{ij}\theta(x_j - x_i) + \tilde{\tau}^*_{Rj,Ri}\theta(x_i - x_j), & \text{if} \quad R_j < R_i \end{cases} \tag{3.10}$$

From (3.6), (3.7), and (3.9) the inner product becomes

$$W_N = \sum_{R \in S_N} \sum_{G \subset \varepsilon_N}' D(R; G; k', k) \tag{3.11}$$

where the second sum $\sum'$ is over G such that all the N fermions are connected either statistically or dynamically, and

$$D(R; G; k', k) = \frac{1}{L} P(R) \int dx_1 \cdots \int dx_N \times \exp\left[i \sum_{j=1}^{N} (k_j - k'_{Rj})\, x_j \right] \prod_{i<j \in G} \alpha_{ij}^R \tag{3.12}$$

In light of the fact that α_{ij}^R is a step function, the following graphical representation is conjectured for the quantity $D(R; G; k', k)$:

(a) Draw N fermion lines with momenta $k_1, k_2, \ldots, k_N$ flowing in from the bottom of the graph and $k'_{R1}, k'_{R2}, \ldots, k'_{RN}$ flowing out from the top.

(b) For each pair $i < j \in G$, draw a *phonon* line connecting the fermion lines which are labeled at the bottom by k_i and k_j.

Rules for evaluating the above graph are as follows:

(i) To each phonon assign a momentum such that at each vertex, momentum conservation holds. Here it is understood that the momentum flows from bottom to top and left to right in the graph. (3.13a)

(ii) For a phonon of momentum q corresponding to the $i < j$ pair, assign a factor

$$\Gamma(R; i, j) = \begin{cases} (\tilde{\tau}_{ij} + \tilde{\tau}^*_{Ri,Rj} + \tilde{\tau}_{ij}\tilde{\tau}^*_{Ri,Rj}) \dfrac{-i}{q - i\eta}, & \text{if} \quad Ri < Rj \\ \tilde{\tau}_{ij} \dfrac{-i}{q - i\eta} + \tilde{\tau}^*_{Rj,Ri} \dfrac{i}{q + i\eta}, & \text{if} \quad Rj < Ri \end{cases} \tag{3.13b}$$

where η is an infinitesimal positive number.

(iii) The quantity $D(R; G; k', k)$ is then given by

$$D(R; G; k', k) = P(R) \left[\int \frac{dq_1}{2\pi} \int \frac{dq_2}{2\pi} \cdots \right] \prod_{i<j \in G} \Gamma(R; i, j) \quad (3.13c)$$

where the $q_1, q_2, \ldots$ integrations are over closed loops.

The core of the proof for the above statement is to show that the quantity

$$D_{\text{core}} = \frac{1}{L} \int dx_1 \cdots \int dx_N \exp \left[i \sum_{j=1}^{N} (k_j - k'_{Rj}) x_j \right] \times \prod_{i<j \in G} \theta(x_j - x_i) \prod_{l<m \in G'} \theta(x_l - x_m) \quad (3.14)$$

with the condition $Ri < Rj$ for $i < j \in G$ and $Rm < Rl$ for $l < m \in G'$, has the graphical representation (a) and (b) with a trivial change in the definition of Γ in (3.13b). This can be shown as follows. First note that the statement is trivial if there are no closed loops. Let us assume one closed loop, and look at a step function $\theta(x_s - x_t)$, $t < s$ and write it as

$$\theta(x_s - x_t) = \int \frac{dq}{2\pi} \cdot \left(\frac{-i}{q - i\eta} \right) \cdot e^{iq(x_s - x_t)} \quad (3.15)$$

The equation (3.14) with $\theta(x_s - x_t)$ in it replaced by $e^{iq(x_s - x_t)}$ has a graphical representation with k'_{Rs} replaced by $k'_{Rs} - q$ and k'_{Rt} by $k'_{Rt} + q$. Combining this graphical representation with the left-over factor in (3.15)

$$\int \frac{dq}{2\pi} \cdot \frac{-i}{q - i\eta}$$

we reach the statement for the case of one closed loop. An inductive proof for the general case of many closed loops is trivial from the above argument.

The obtained graphical recipe for calculating the inner product W_N is essentially the same as that in the bosonic perturbation theory.[8] By replacing the bosonic transition-matrix τ_{ij} and the bosonic exchange interaction in the latter by the fermionic $\tilde{\tau}_{ij}$ and the fermionic exchange interaction, one can get our graphical recipe. A note worth mentioning here is that our procedures in this section show how one can directly work on the Bethe wave function.

In the following section, we shall explicitly evaluate the inner product W_N. In light of the structural similarity between our graphical recipe and that in the bosonic perturbation theory, one may except to follow Thacker's procedures for evaluating W_N. However, a new reasoning shall be presented in the following section.

4. INNER PRODUCTS

Let us start with the simple cases $N=2$ and 3, which will indicate how one should work for general N. For $N=2$, we have only two graphs as shown in Fig. 1. Rules (3.13) give

$$\text{Fig. 1a} = (\tilde{\tau}_{12} + \tilde{\tau}^*_{1'2'} + \tilde{\tau}_{12}\tilde{\tau}^*_{1'2'}) \left(\frac{-i}{1-1'-i\eta}\right) \tag{4.1a}$$

$$\text{Fig. 1b} = -\left(\tilde{\tau}_{12} \frac{-i}{1-2'-i\eta} + \tilde{\tau}^*_{1'2'} \frac{i}{1-2'+i\eta}\right) \tag{4.1b}$$

where and below we abbreviate $k_i - k_j$ as either $i-j$ or k_{ij}. Noting $\tilde{\tau}_{ij} = \tilde{S}_{ij} - 1$, (2.4) and (3.1), we have

$$\lim_{\eta \to 0} \lim_{k' \to k} \text{Fig. 1a} = 0, \qquad W_{2,2} \equiv \lim_{k' \to k} \lim_{\eta \to 0} \text{Fig. 1a} = -2\Delta_{12} \tag{4.2a}$$

and

$$W_{2,1} \equiv \lim_{\eta \to 0} \lim_{k' \to k} \text{Fig. 1b} = \lim_{k' \to k} \lim_{\eta \to 0} \text{Fig. 1b} = 2\Delta_{12} \tag{4.2b}$$

where

$$\Delta_{ij} = \frac{2c}{k_{ij}^2 + c^2} \tag{4.3}$$

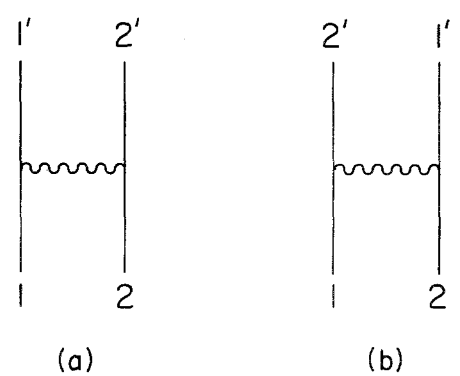

Fig. 1. Graphs for W_2.

Note the wave operator unitarity

$$W_{2,1} + W_{2,2} = 2\Delta_{12} - 2\Delta_{12} = 0 \tag{4.4}$$

which is a cancellation between the singular-type graph Fig. 1a and the nonsingular-type graph Fig. 1b. It is clear from (4.2) that in the $\lim_{\eta \to 0} \lim_{k' \to k}$, which is of thermodynamical interest [cf. (2.16)], only nonsingular-type graphs contribute. Since the two limits $\eta \to 0$ and $k' \to k$ commute for nonsingular-type graphs, one can get the quantity of thermodynamical interest,

$$W_{2,1} = \lim_{\eta \to 0} \lim_{k' \to k} W_2 = 2\Delta_{12} \tag{4.5}$$

by working either directly on the nonsingular graph or on the singular graph, thereby using the wave operator unitarity, (4.4).

The $N=2$ case examined in the above is a little bit special, and we next consider the $N=3$ case to get an insight for general N. In this case, four graphs for a given permutation R are shown in Fig. 2. We write their contribution to W_3 as $W_3(R)$. Let us first consider $R_1 =$ identify. Rules (3.13) give

$$\begin{aligned} W_3(R_1) = {} & \frac{Y_{12,12}}{2' - 2 - i\eta} \frac{Y_{13,13}}{3' - 3 - i\eta} + \frac{Y_{12,12}}{1 - 1' - i\eta} \frac{Y_{23,23}}{3' - 3 - i\eta} \\ & + \frac{Y_{13,13}}{1 - 1' - i\eta} \frac{Y_{23,23}}{2 - 2' - i\eta} \\ & + \int \frac{dq}{2\pi} \frac{Y_{12,12} Y_{13,13} Y_{23,23}}{(q - i\eta)(1 - 1' - q - i\eta)(3' - 3 - q - i\eta)} \end{aligned} \tag{4.6}$$

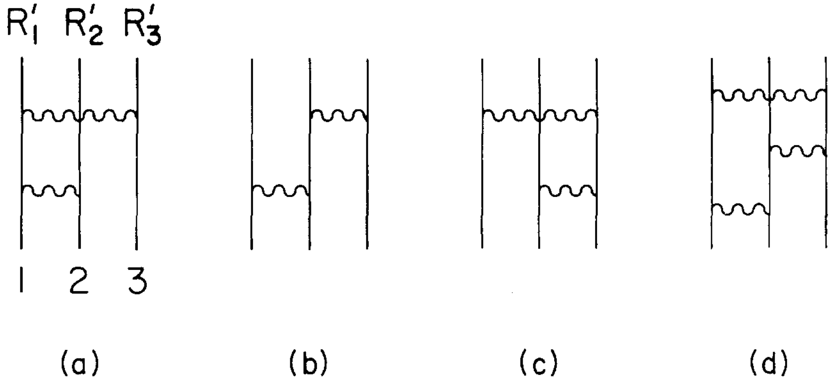

Fig. 2. Graphs for $W_3(R)$. Momentum labels in (b), (c), and (d) are the same as in (a).

where

$$Y_{ij,lm} \equiv -i(\tilde{\tau}_{ij} + \tilde{\tau}^*_{l'm'} + \tilde{\tau}_{ij}\tilde{\tau}^*_{l'm'})$$

Noting $\tilde{\tau}_{ij} = \widetilde{S}_{ij} - 1$, (2.4) and (3.1), we have

$$\begin{aligned}
W_{3,3} &\equiv \lim_{k' \to k} \lim_{\eta \to 0} W_3(R_1) \\
&= \Delta_{12}\Delta_{13} \frac{(1-2)-(1'-2')}{2'-2} \frac{(1-3)-(1'-3')}{3'-3} \\
&\quad + \Delta_{12}\Delta_{23} \frac{(1-2)-(1'-2')}{1-1'} \frac{(2-3)-(2'-3')}{3'-3} \\
&\quad + \Delta_{13}\Delta_{23} \frac{(1-3)-(1'-3')}{1-1'} \frac{(2-3)-(2'-3')}{2-2'}
\end{aligned} \tag{4.7}$$

where on the right a limit $k' \to k$ should be taken under the constraint $k_1 + k_2 + k_3 = k'_1 + k'_2 + k'_3$, i.e., momentum conservation. Similarly for R_2; $(123) \to (132)$, rules (3.13) give

$$\begin{aligned}
-W_3(R_2) &= \frac{Y_{12,13}}{3'-2-i\eta} \cdot \frac{Y_{13,12}}{2'-3-i\eta} + \frac{Y_{12,13}}{1-1'-i\eta} \\
&\quad \times \left(\frac{-i\tilde{\tau}_{23}}{2'-3-i\eta} + \frac{i\tilde{\tau}^*_{2'3'}}{2'-3+i\eta} \right) \\
&\quad + \frac{Y_{13,12}}{1-1'-i\eta} \cdot \left(\frac{-i\tilde{\tau}_{23}}{2-3'-i\eta} + \frac{i\tilde{\tau}^*_{2'3'}}{2-3'+i\eta} \right) \\
&\quad + \int \frac{dq}{2\pi} \frac{Y_{13,12}}{q-i\eta} \frac{Y_{12,13}}{1-1'-q-i\eta} \\
&\quad \times \left(\frac{-i\tilde{\tau}_{23}}{2'-3-q-i\eta} + \frac{i\tilde{\tau}^*_{2'3'}}{2'-3-q+i\eta} \right)
\end{aligned} \tag{4.8}$$

After performing a loop integration, one can divide the right-hand side of (4.8) into two parts; one with a singular factor $(1-1'-i\eta)^{-1}$ and one without. But in doing so, note a subtlety

$$\frac{1}{(1-1'-i\eta)(2-3')} = \frac{1}{(1-1'-i\eta)(2'-3)} + \frac{1}{(2-3')(2'-3)} \tag{4.9}$$

Repeating similar calculations for R_3; $(123) \to (321)$ and R_4; $(123) \to (213)$, we find that the sum of singular-type contributions $W_{3,2}$, as (of course in the $\lim_{k'\to k}\lim_{\eta\to 0}$)

$$W_{3,2} = -2\Delta_{12}\Delta_{13}\left[\frac{(1-2)-(1'-2')}{2'-2}+\frac{(1-3)-(1'-3')}{3'-3}\right]$$
$$-2\Delta_{12}\Delta_{23}\left[\frac{(1-2)-(1'-2')}{1-1'}+\frac{(2-3)-(2'-3')}{3'-3}\right]$$
$$-2\Delta_{13}\Delta_{23}\left[\frac{(1-3)-(1'-3')}{1-1'}+\frac{(2-3)-(2'-3')}{2-2'}\right] \quad (4.10)$$

Combining (4.7) and (4.10) gives

$$W_{3,2}+W_{3,3} = -3(\Delta_{12}\Delta_{13}+\Delta_{12}\Delta_{23}+\Delta_{13}\Delta_{23}) \quad (4.11)$$

The left-over terms in the cases R_2, R_3, and R_4 and graphs from R_5; $(123)\to(231)$ and R_6; $(123)\to(312)$ are all nonsingular. For these, the two limits $k'\to k$ and $\eta\to 0$ commute. After a long but straightforward calculation, we have the contribution

$$W_{3,1} \equiv \lim_{\eta\to 0}\lim_{k'\to k} W_3 = 3(\Delta_{12}\Delta_{13}+\Delta_{12}\Delta_{23}+\Delta_{13}\Delta_{23}) \quad (4.12)$$

Let us put the above result for $N=3$ in a more appealing form. First note that, since the final result (4.11) does not depend on the way of taking limit $k'\to k$ as far as the total momentum is conserved, one can conveniently choose a special limit to get the same result. For example, taking the limit $k'=k_1+2q$, $k_2'=k_2-q$ and $k_3'=k_3-q$ with $q\to 0$ in (4.7) and (4.10) gives

$$W_{3,3} = 9\Delta_{12}\Delta_{13} \quad (4.13a)$$

and

$$W_{3,2} = -12\Delta_{12}\Delta_{13}-3\Delta_{12}\Delta_{23}-3\Delta_{13}\Delta_{23} \quad (4.13b)$$

and (4.11) follows from (4.13). Next note that, since the three terms in (4.12) are equivalent to each other in the expression (2.16) for the free energy, we can effectively write (4.12) as

$$W_{3,1} = 9\Delta^2 \quad (4.14)$$

where Δ^2 is an abbreviation of, say, $\Delta_{12}\Delta_{13}$. Similarly, (4.13) is written as

$$W_{3,2} = -18\Delta^2, \qquad W_{3,3} = 9\Delta^2 \quad (4.15)$$

With this simplified notation, the wave operator unitarity takes the form

$$W_{3,1}+W_{3,2}+W_{3,3}=(3\Delta-3\Delta)^2=0 \tag{4.16}$$

Notice a similar expression (4.4) for $N=2$.

Now we are ready to consider the case of general N. First suppose we have performed all loop integrations. Following the $N=3$ case, we then classify all terms in W_N into N groups. The first group is composed of purely nonsingular terms. Let $W_{N,1}$ denote the contribution of purely nonsingular terms in the $\lim_{k'\to k}\lim_{\eta\to 0}$. The second group is composed of those terms which have only one *infrared phonon*; hereafter a phonon is called infrared if its momentum vanishes in the limit $k'\to k$. In a similar manner as in $W_{N,1}$, we define $W_{N,2}$. And so on. In the most singular terms which belong to the last group, all $N-1$ phonons are infrared. In this way, we have N groups and their contributions,

$$\lim_{k'\to k}\lim_{\eta\to 0} W_N=W_{N,1}+W_{N,2}+\cdots+W_{N,N} \tag{4.17}$$

As a natural generalization of the above results for $N=2$ and 3, it is now conjectured that, for $i=1, 2,..., N$

$$W_{N,i}={}_{N-1}C_{i-1}(-1)^{i-1}(N\Delta)^{N-1} \tag{4.18}$$

and the wave operator unitarity takes the form

$$\sum_{i=1}^{N} W_{N,i}=(N\Delta-N\Delta)^{N-1}=0 \tag{4.19}$$

The statement (4.18) can be proved by induction. For $N=3$, (4.14) and (4.15) are nothing but (4.18). Now assume (4.18) with N replaced by $N-1$. For N, we can explicitly show below that (4.18) is true for $i=2$, 3,..., N. Then the statement (4.18) for $i=1$ follows from the wave operator unitarity. Here it is worth emphasizing that the wave operator unitarity is trivial in the present approach, because $c=\infty$ is not a singular point. Let us consider $W_{N,i}$ ($i=2, 3,..., N$). We first divide N fermions into i groups such that intergroup interactions are denoted by $i-1$ infrared phonons and intragroup interactions are nonsingular. To be specific, let X_j, $j=1$, 2,..., i denote the number of particles in the jth group. Therefore,

$$N=X_1+X_2+\cdots+X_i \tag{4.20}$$

Note that the total momentum of each group is conserved to $O(\eta)$. A convenient choice in this case for the limit $k'\to k$ is to take $k'=k-q$ for fermions which belong to the $j=2, 3,..., i$ groups. By this choice, the positions of $i-1$ infrared phonons become unique as shown by wavy lines in Fig. 3, where shaded blobs represent nonsingular interactions. For a fixed set $\{X\}$ satisfying (4.20), the contribution from graphs as shown in Fig. 3, $W_{N,i}(\{X\})$, can be evaluated as follows: First consider wavy parts $X_1 \leftrightarrow X_j$ ($j=2, 3,..., i$). The infrared phonon can connect any one of fermion lines in the first group to any one of fermion lines in the jth group. For a fixed permutation R, the total effect of such interactions, including terms originating from arbitrary number of loop integrations, can be figured out from the original expression for W_N, (3.6) and (3.7). Intergroup interactions in the present situations are described by (3.7) with i and l running over the first group and j and m the jth group. Since nonsingular interactions within the two groups are not affected by the existence of intergroup interactions of infrared type, the effect of intergroup interactions can be factorized out to be

$$\left[\prod_{i<j} (1+\tilde{\tau}_{ij})(1+\tilde{\tau}^*_{i'j'})-1\right]\frac{-i}{\sum_j (k'-k)-i\eta} \tag{4.21}$$

where i and j, respectively, runs over the first group and the jth group, and $\sum_j$ means a summation over the jth group. Since $k'=k-q$ except for the first group,

$$\sum_j (k'-k) = -qX_j \tag{4.22}$$

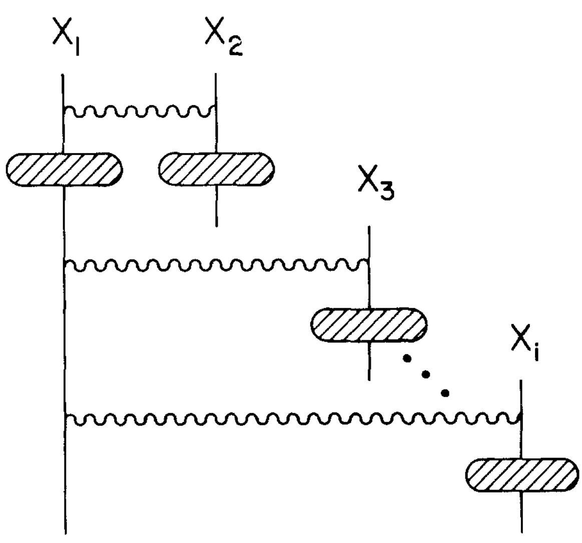

Fig. 3. Schematic representation of graphs which contribute to $W_{N,i}$.

On the other hand, to $O(\eta)$, the quantity in the parenthesis in (4.21) is

$$\sum_{i<j} (\tilde{\tau}_{ij} + \tilde{\tau}^*_{i'j'} + \tilde{\tau}_{ij}\tilde{\tau}^*_{i'j'}) = \sum_{i<j} (-i\Delta)(k_i - k'_i + k'_j - k_j)$$
$$= (-i\Delta)(-qX_jN) \qquad (4.23)$$

With the use of (4.22) and (4.23), we have

$$\lim_{k' \to k} \lim_{\eta \to 0} (4.21) = -N\Delta \qquad (4.24)$$

Note that (4.24) is independent of the permutation R, and therefore we can write

$$W_{N,i}(\{X\}) = W^{\text{ns}}_{N,i}(\{X\}) \cdot W^{\text{s}}_{N,i}(\{X\}) \qquad (4.25)$$

where $W^{\text{ns}}_{N,i}(\{X\})$ represents the contribution from shaded parts (non-singular interactions), and $W^{\text{s}}_{N,i}(\{X\})$ that from singular interactions. From (4.24) we have

$$W^{\text{s}}_{N,i}(\{X\}) = (-N\Delta)^{i-1} \qquad (4.26)$$

On the other hand, since the contribution of jth shaded-blob is given by inductive assumption as $(X_j\Delta)^{X_j-1}$ [cf. (4.18)], we have

$$W^{\text{ns}}_{N,i}(\{X\}) = \prod_{j=1}^{i} (X_j\Delta)^{X_j-1} \qquad (4.27)$$

Finally some combinatories to reach the quantity $W_{N,i}$: For a given set $\{X\}$, the number of ways of choosing X_1 fermions out of N fermions is ${}_NC_{X_1}$; the number of ways of choosing X_2 fermions out of $N-X_1$ fermions is ${}_{N-X_1}C_{X_2}$, etc. Taking into account a reduction factor $(i!)^{-1}$ for over-counting, we find the number of ways of dividing N fermions into i groups as

$$C_{N,i}(\{X\}) = {}_NC_{X_1} \cdot {}_{N-X_1}C_{X_2} \cdots {}_{X_i}C_{X_i}(i!)^{-1} \qquad (4.28)$$

Multiplying (4.25) by (4.28) and summing over possible sets $\{X\}$ gives

$$W_{N,i} = (-1)^{i-1}\Delta^{N-1} \sum_{\{X\}} \frac{N!}{X_1!\,X_2!\cdots X_i!} \cdot \frac{N^{i-1}}{i!} \prod_{j=1}^{i} X_j^{X_j-1} \qquad (4.29)$$

where $\sum_{\{X\}}$ means a summation over the sets $\{X\}$ which satisfy (4.20). In the Appendix, it is proved that[4]

$$\sum_{\{X\}} \frac{N!}{X_1!\, X_2! \cdots X_i!} \frac{N^{i-1}}{i!} \prod_{j=1}^{i} X_j^{X_j - 1} = {}_{N-1}C_{i-1} N^{N-1} \tag{4.30}$$

Thus, $W_{N,i}$ is given by (4.18), completing the inductive proof of (4.18).

5. FREE ENERGY

In Section 4, we have come a rather long way to evaluate inner products. The remaining procedures to reach the free energy are, (A) to represent the quantity $\lim_{\eta \to 0} \lim_{k' \to k} W_N = W_{N,1}$ in terms of *0-phonon tree graphs*, and (B) to perform a graphical summation of (2.16). 0-phonon tree graphs were first considered by Thacker in his bosonic perturbation theory.[8] Our 0-phonon tree graph below is the same as that of Thacker except in two points. First, the 0-phonon propagator of Thacker is $\Delta_{ij} - 2\pi\delta(k_{ij})$, whereas ours is Δ_{ij} and does not contain a δ-function term. Second, the exchange interaction is bosonic in Thacker's treatment, whereas it is fermionic in this paper. In this section, we shall carry out the two steps (A) and (B) in the above. As for the step (B), we will follow Thacker's arguments.

Step (A). A constructive definition of 0-phonon tree graphs for N fermions is the following:

(i) Draw a fermion line in the left-most place of the graph.

(ii) Draw several 0-phonons (wavy lines) which come out of the first fermion line, go rightward, and reach the next fermion lines which are different from each other.

(iii) Repeat the procedure (ii) until all the N fermion lines are connected.

(iv) To N fermion lines assign N momenta $k_1, k_2, \ldots, k_N$.

It is noted that the total number of 0-phonons is $N-1$. We assign the propagator Δ to each 0-phonon, and therefore each 0-phonon tree graph has a value Δ^{N-1}. Those 0-phonon trees which can be obtained from each other by the up-and-down of 0-phonon lines are called topologically the same. For example, (a) and (b) in Fig. 4 are topologically the same.

We now claim that

$$\sum_{N} \{\text{topologically distinct 0-phonon trees}\} = W_{N,1} \tag{5.1}$$

[4] I thank Y. Oono for carrying this out.

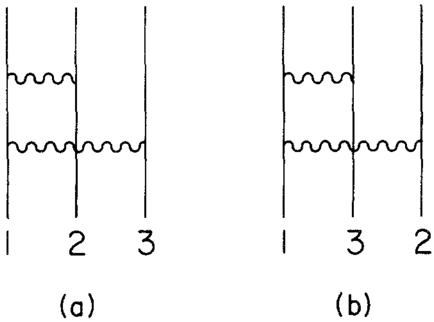

Fig. 4. Two 0-phonon trees which are topologically the same.

where $\sum_N$ means a summation for N fermions. This can be proved by induction. First it is trivially the case for $N=2$. Let us assume (5.1) for N. For $N+1$, we look at those tree graphs in which the fermion line with k_1 is in the left-most place. Let A_N denote the contribution of these graphs, then clearly

$$\sum_{N+1} \{\text{topologically distinct 0-phonon trees}\} = (N+1)\, A_N \tag{5.2}$$

To evaluate A_N, we classify graphs into N groups according to the number of 0-phonons coming out of the left-most fermion line. Let P_i denote the contribution of the ith group:

$$A_N = P_1 + P_2 + \cdots + P_N \tag{5.3}$$

P_i can be evaluated as follows. First, we divide N fermions with momenta $k_2, k_3, \ldots, K_{N+1}$ into i groups, as shown schematically in Fig. 5, with X_1, $X_2, \ldots, X_i$ denoting the number of fermions in each group:

$$X_1 + X_2 + \cdots + X_i = N \tag{5.4}$$

For a fixed set $\{X\}$, there are in total

$$_N C_{X_1} \cdot {}_{N-X_1} C_{X_2} \cdot \cdots \cdot {}_{X_i} C_{X_i} \cdot (i!)^{-1} \tag{5.5}$$

ways of classifying N fermions into i groups. The reduction factor $(i!)^{-1}$ means to take only topologically distinct 0-phonon trees. Now consider the shaded parts. The jth $(j=1, 2, \ldots, i)$ shaded rectangular contributes $(X_j \Delta)^{X_j - 1}$ from the inductive assumption, and therefore in total they contribute

$$\prod_{j=1}^{i} (X_j \Delta)^{X_j - 1} \tag{5.6}$$

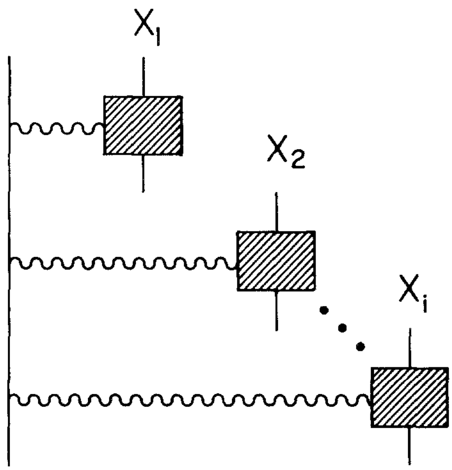

Fig. 5. Schematic representation of 0-phonon tree graphs in the ith group. Shaded rectangulars represent 0-phonon trees.

Combining (5.5) and (5.6), and taking into account Δ^i from i 0-phonons which connect the left-most fermion line to the rest of the group, we have

$$P_i = \sum_{\{X\}} \frac{N!}{X_1!\, X_2! \cdots X_i!} \frac{1}{i!} \prod_{j=1}^{i} X_j^{X_j - 1} \Delta^N \tag{5.7}$$

where $\sum_{\{X\}}$ means a summation over the sets $\{X\}$ which satisfy (5.4). With the use of (4.30), (5.7) becomes

$$P_i = {}_{N-1}C_{i-1} N^{N-i} \Delta^N \tag{5.8}$$

From (5.2), (5.3), and (5.8) we have

$$\sum_{N+1} \{\text{topologically distinct 0-phonon trees}\}$$

$$= (N+1) \sum_{i=1}^{N} {}_{N-1}C_{i-1} N^{N-i} \Delta^N = [(N+1)\Delta]^N \tag{5.9}$$

thus completing the inductive proof of (5.1).

Step (B). Substituting (5.1) into (2.16) gives

$$F = \mu N_0 - L\beta^{-1} \sum_{N=1}^{\infty} \lambda^N \int \frac{dk_1}{2\pi} \cdots \int \frac{dk_N}{2\pi} e^{-\beta\omega_k}$$

$$\times \frac{1}{N!} \sum_N \{\text{topologically distinct 0-phonon trees}\} \tag{5.10}$$

We can perform a graphical summation of (5.10) following Thacker.[8] Here it is noted that we have ignored up to now the exchange interaction between fermions, which was included in the original expression (2.17). Therefore, (5.10) should be understood to involve exchange interactions also. A tricky point, however, is that this interaction works only between fermions with the same momentum, but no two fermions in the wave vector $|k\rangle$ seem to be allowed to have the same momentum. This puzzle can be resolved by considering the free fermions. A demonstration of the virial expansion of the free energy for this simple system is found in Dashen, Ma, and Bernstein.[11] For a given N, one can easily show that the inner product due to the exchange interaction is $(-1)^{N-1}(N-1)!$, and therefore (here $\mu=0$ for simplicity),

$$\begin{aligned} F &= -L\beta^{-1} \sum_{N=1}^{\infty} \int \frac{dk}{2\pi} e^{-\beta N k^2} (-1)^{N-1} N^{-1} \\ &= -L\beta^{-1} \int \frac{dk}{2\pi} \ln(1+e^{-\beta k^2}) \end{aligned} \tag{5.11}$$

as is expected. It is now clear from (5.11) that the above puzzle is due to a series expansion of a logarithmic function in the virial expansion.

Returning to (5.10), we note that the reduction factor $(N!)^{-1}$ means to take only one of those graphs which are obtainable from each other by $N!$ permutations of momenta k. Accordingly, we have a residual reduction factor for a group of graphs which are topologically the same. In Figs. 6 and 7, graphical representation of the integrands in (5.10) are shown for $N=2$ and 3. In these graphs, trivial momentum labels are dropped and crosses represent the Boltzmann factor $e^{-\beta(k^2-\mu)}$. The dashed line in the second graph of Fig. 6 represents an exchange interaction. The factor 1/2! in the second graph of Fig. 7 is a residual reduction factor mentioned above.

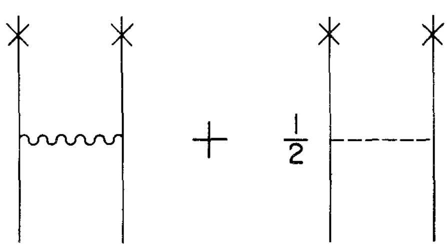

Fig. 6. Graphical representation of the integrand in (5.10) for $N=2$.

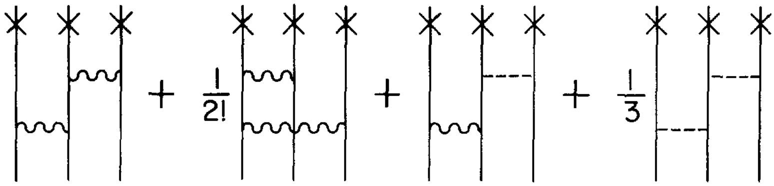

Fig. 7. Graphical representation of the integrand in (5.10) for $N=3$.

We now sum up (5.10). Performing momentum integrations except for k_1, we have

$$F=\mu N_0-L\beta^{-1}\int\frac{dk}{2\pi}\left[\zeta(k)-\frac{1}{2}\zeta(k)^2+\frac{1}{3}\zeta(k)^3-\cdots\right]$$

$$=\mu N_0-L\beta^{-1}\int\frac{dk}{2\pi}\ln[1+\zeta(k)] \qquad (5.12)$$

where a one-particle distribution function, $\zeta(k)$ is defined by Fig. 8. Defining a quantity $-\beta\tilde{\varepsilon}(k)$ by Fig. 9, we have

$$-\beta\tilde{\varepsilon}(k)=\int\frac{dq}{2\pi}\Delta(k-q)\ln[1+\zeta(q)] \qquad (5.13)$$

In terms of $-\beta\tilde{\varepsilon}(k)$,

$$\zeta(k)=e^{-\beta(k^2-\mu)}\sum_{n=0}^{\infty}\frac{1}{n!}[-\beta\tilde{\varepsilon}(k)]^n$$

$$=e^{-\beta[k^2-\mu+\tilde{\varepsilon}(k)]} \qquad (5.14)$$

It is seen from (5.12) and (5.14) that the interaction between fermions brings about only the *fermion self-energy correction* $\tilde{\varepsilon}(k)$. Substituting (5.14) into (5.12) and (5.13), and putting

$$\varepsilon(k)=k^2-\mu+\tilde{\varepsilon}(k) \qquad (5.15)$$

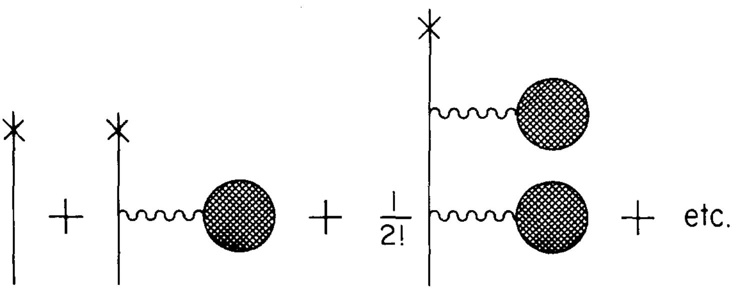

Fig. 8. Definition of $\zeta(k)$.

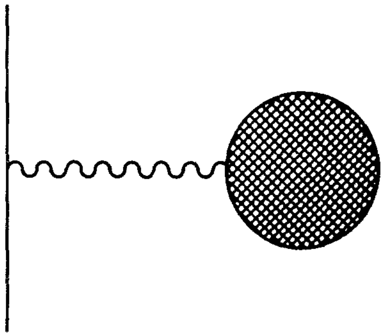

Fig. 9. Definition of $-\beta\tilde{\varepsilon}(k)$.

reproduces the basic equations (2.3) and (2.5) of the BA formalism. This shows that the ε function introduced by Yang and Yang represents the fermion energy at finite temperatures.

6. CONCLUDING REMARKS

In this paper, we have developed a fermionic perturbation theory for the statistical mechanics of the NLS model. We have understood why the two-body phase shift in the BA formalism should be $\tilde{\delta}$ instead of the bosonic phase shift δ. In particular, in the present theory, the physical meaning of the Yang and Yang ε function as the fermion energy, measured from the chemical potential, is clear.

A question which we have left untouched concerning our fermionic description is that, strictly speaking, it is incorrect at the level of the Hamiltonian and associated energy eigenstates. To look at this, let us reconsider Bethe wave function (2.1) for $N=2$. It is first noted that, owing to the singular potential, the amplitude of the Bethe wave function at $x_1 = x_2$ plays an important role in determining the two-body phase shift δ. Strictly speaking, in (3.2) for $N=2$, $\text{sgn}(0) = (1-\tilde{S}_{12})/(1+\tilde{S}_{12}) \neq 0$. Similarly, $\text{sgn}(x_1 - x_2)$ in (3.4) should be understood as $\text{sgn}(0) = -i$, and therefore $\varphi^\dagger(x)\,\varphi^\dagger(x) \neq 0$, that is, the field φ is not exactly fermionic. In this way, the description (3.5) of the Bethe wave function in terms of a *true* fermion field φ, is not exactly correct. Under the same approximation as (3.5), the boson Hamiltonian (1.1) becomes a *free* fermion Hamiltonian by the Jordan–Wigner transformation. Here it is noted that at $c=\infty$ no two bosons can come to the same place, and therefore the above description in terms of the *true* fermion field φ is correct not only for the statistical mechanics but also at the level of the Hamiltonian and associated energy eigenstates.

Now an interesting question is, if there is any soluble fermion theory which is equivalent to the NLS model at $c \neq \infty$. My answer to this question is negative owing to the following reason. If we assume the existence of such a fermion theory, it should first of all be a theory of many-components fermions. Let us consider two components for simplicity. Then, nonrelativistic, 2-components, and locally interacting theory of fermions is unique. Writing two components as φ_1 and φ_2, we have a Hamiltonian,

$$H' = \int dx[\partial_x \varphi_1^\dagger \partial_x \varphi_1 + \partial_x \varphi_2^\dagger \partial_x \varphi_2 + 2g\varphi_1^\dagger \varphi_2^\dagger \varphi_2 \varphi_1] \tag{6.1}$$

A corresponding Hamiltonian eigenstate should take a following form for two particles,

$$|\psi(k_1 k_2)\rangle' = \iint dx_1\, dx_2\, e^{i(k_1 x_1 + k_2 x_2)} \times [\theta(x_1 - x_2) + S'_{12}\theta(x_2 - x_1)]\, \varphi^\dagger(k_1, x_1)\, \varphi^\dagger(k_2, x_2)\, |0\rangle \tag{6.2}$$

where

$$\varphi^\dagger(k, x) \equiv C_k \varphi_1^\dagger(x) + S_k \varphi_2^\dagger(x) \tag{6.3}$$

A simple calculation, however, shows that the two-body S matrix S'_{12} determined so as to satisfy the Schrödinger equation,

$$H'\, |\psi(k_1 k_2)\rangle' = E\, |\psi(k_1 k_2)\rangle'$$

is different from our expectation $\tilde{S}_{12}$. Moreover, the mixing coefficients C_k and S_k can be arbitrary, indicating that (6.3) has no physical significance. In this way, it is unlikely that there is a fermion theory which is equivalent to the NLS model at $c \neq \infty$.

The above argument, however, is not necessarily unfavorable to our fermionic treatment of the NLS model, since a relativistic version of (6.1) does exist as the massive Thirring model (MTM), which is known to be soluble by Bethe ansatz.[(13)] Indeed, a system of fermions interacting via the two-body phase shift $\tilde{\delta}$ is realized as a nonrelativistic approximation of the MTM: First, as a nonrelativistic approximation, we neglect negative energy states and associated fermion–antifermion bound states. In the resulting system of interacting fermions, we next take $g = c^{-1}$ and the limit of fermion mass $\rightarrow \infty$. With this procedure, the scattering phase-shift for two fermions[(13)] becomes $\tilde{\delta}$, and we reach a system of nonrelativistic fermions interacting via the two-body phase shift $\tilde{\delta}$.

In brief, there does not seem to exist soluble fermion theory which is equivalent to the NLS model at $c \neq \infty$, but its relativistic version exists as the MTM, and a system of fermions interacting via the two-body phase shift $\tilde{\delta}$ can be deduced from the MTM under some approximations. Thus, it is tempting to say that the NLS model has a deficiency that it is nonrelativistic, and owing to this deficiency, a bosonic description is indispensable at the Hamiltonian level.

After the completion of the present paper, I have noticed a work by Creamer, Thacker, and Wilkinson,[15] in which the BA thermodynamics result was reproduced by the quantum inverse scattering technique. I still believe, however, that the fermionic character of the problem can be best understood in the present work.

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APPENDIX

Here we prove (4.30). We write (4.30) as

$$\sum_{\{X\}} \prod_{j=1}^{i} X_j^{X_j-1}/(X_1!\,X_2!\cdots X_i!) = iN^{N-i-1}/(N-i)! \tag{A1}$$

It is convenient to examine generating functions instead of (A1) itself. Multiplying (A1) by z^N and operating $\sum_{N=i}^{\infty}$ give

$$\left(\sum_{X=1}^{\infty} \frac{X^{X-1} z^X}{X!}\right)^i = \sum_{N=1}^{\infty} \frac{i(N+i-1)^{N-2}\, z^{N+i-1}}{(N-1)!} \tag{A2}$$

It is noted that since $X! \sim X^X$ for large X, the radius of convergence $\lesssim 1$ for both sides of (A2). The statement (A2) can be proved by induction with respect to i. For $i=1$, (A2) trivially holds. Assume (A2) for i. For $i+1$, we multiply the left-hand side of (A2) with $i=1$ to both sides of (A2), to obtain

$$\left(\sum_{X=1}^{\infty} \frac{X^{X-1} z^X}{X!}\right)^{i+1} = iz^i \sum_{T=1}^{\infty} z^T \sum_{X=1}^{T} \frac{(T-X+i)^{T-X-1}\, X^{X-1}}{(T-X)!\, X!} \tag{A3}$$

where we have changed variables from (N, X) to $(T=N+X, X)$. Thus, from (A2) and (A3) the statement (A2) for $i+1$ would be reached if we could show that, for arbitrary $T \geqslant 1$,

$$i \sum_{X=1}^{T} \frac{(T-X+i)^{T-X-1} X^{X-1}}{(T-X)!\, X!} = (i+1) \frac{(T+i)^{T-2}}{(T-1)!} \tag{A4}$$

as a function of i. This statement can be proved by induction with respect to T. (A4) is trivially the case for $T=1$. Now assume (A4) for T, and apply an operator $\int_1^i di$ to both sides of (A4). Under this procedure, the left-hand side of (A4) becomes

$$(i-1) \sum_{X=1}^{T+1} \frac{(T-X+i)^{T-X} X^{X-1}}{(T-X+1)!\, X!} - \frac{(T+1)^{T-1}}{T!} \tag{A5}$$

On the other hand, under the same procedure, the right of (A4) becomes

$$i \frac{(T+i)^{T-1}}{T!} - \frac{(T+1)^{T-1}}{T!} \tag{A6}$$

Equating (A5) to (A6) and replacing i by $i+1$ in the resulting equation, we arrive at (A4) with T replaced by $T+1$, thus completing the proof.

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