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# Effective-potential expansion method for the many-body problem at finite temperatures. II. Application to a one-dimensional electron system with a repulsive δ-function interaction

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A one-dimensional many-electron system with a repulsive δ-function interaction is studied by the application of the variational method developed in the preceding paper [Takada and Kita, Phys. Rev. A **42**, 3242 (1990)] in order to illustrate its actual implementation. Our results on the grand potential, the entropy, and the specific heat are compared in detail with the exact ones that are calculated by the numerical solution of the coupled integral equations obtained by the Bethe ansatz.

## I. INTRODUCTION

In a previous paper[1] (hereafter referred to as I), we developed a variational scheme for calculating thermodynamic properties in an interacting many-body system. In the scheme, an effective potential $\hat{\hat{V}}$ was introduced to define a trial density matrix $\hat{\hat{\rho}}$ which was substituted to calculate the grand potential Ω in the Gibbs variational principle. In an expansion up to second order in $\hat{\hat{V}}$, we obtained an expression for Ω as

$$\begin{aligned}\Omega=\tilde{\Omega}_0+\langle\hat{H}-\hat{\hat{H}}_0\rangle_0-\int_0^{\beta}d\tau\langle\hat{\hat{V}}(\tau)(\hat{H}-\hat{\hat{H}}_0-\hat{\hat{V}})\rangle_{0C}\\+\int_0^{\beta/2}d\tau_1\int_{-\beta/2}^{0}d\tau_2\langle\hat{\hat{V}}(\tau_1)(\hat{H}-\hat{\hat{H}}_0)\hat{\hat{V}}(\tau_2)\rangle_{0C}\\-\frac{1}{2!\beta}\langle T_\tau\int_0^{\beta}d\tau_1\int_0^{\beta}d\tau_2\hat{\hat{V}}(\tau_1)\hat{\hat{V}}(\tau_2)\rangle_{0C}\,,\end{aligned}\tag{1.1}$$

where $\hat{H}$ is the Hamiltonian of the system and $\hat{\hat{H}}_0$ is a suitably chosen noninteracting Hamiltonian whose grand potential is given by $\tilde{\Omega}_0$. We refer the reader to I for the definitions of other symbols in (1.1). Basically, both $\hat{\hat{H}}_0$ and $\hat{\hat{V}}$ are determined by the Euler-Lagrange-type equations derived by the functional derivatives of (1.1).

In this paper, we apply (1.1) to a one-dimensional electron system with a repulsive δ-function interaction to illustrate how actual calculations are done in the present method. There are mainly two reasons why we are interested in the system. First, we can compare our results with the exact ones in this system. The exact solution is available in the form of the coupled equations which were derived on the basis of the Bethe ansatz.[2–5] These equations can be solved numerically to give the exact result. Second, as an extension of our work on the electron gas[6] in which the many-body effects of a long-range Coulomb repulsion are the primary concern, we make our first attempt to study those of a short-range Coulomb repulsion. In particular, we can investigate the correlation effect exclusively in the system with the δ-function interaction, because electrons with parallel spins do not interact due to the Pauli principle. Our present study may also give some light on the study of the electron correlation in the one-dimensional Hubbard model[7–10] in which the lattice structure is considered explicitly instead of the continuum nature of our system.

In Sec. II, we give the Hamiltonian of the system. In Sec. III, we make a brief review of the coupled equations for the exact result. Our numerical method to solve the equations is also explained there. We present our variational calculation in Sec. IV. For comparison, we also give the result in the second-order perturbation theory in Sec. V. The calculated results, both exact and approximate, are shown in Sec. VI. Summary and discussion are given in Sec. VII. As in I, we use units in which $\hbar=k_B=1$.

## II. HAMILTONIAN

The Hamiltonian for the system is given by

$$\hat{H}=\hat{H}_0+\hat{V}\,,\tag{2.1}$$

with

$$\hat{H}_0=\sum_{k,\sigma}\frac{k^2}{2m}\hat{c}^{\dagger}_{k\sigma}\hat{c}_{k\sigma}\,,\tag{2.2}$$

and

$$\hat{V}=V\sum_{k,k',q}\hat{c}^{\dagger}_{k+q\uparrow}\hat{c}^{\dagger}_{k'-q\downarrow}\hat{c}_{k'\downarrow}\hat{c}_{k\uparrow}\,,\tag{2.3}$$

in second quantization, where $\hat{c}_{k\sigma}$ ($\hat{c}^{\dagger}_{k\sigma}$) is the annihilation (creation) operator of an electron with momentum $k$ and spin $\sigma$ and $m$ is the mass of the electron. The total volume (or length) of the system is taken to be unity.

When we reduce units by measuring momenta and energies in terms of the Fermi momentum $k_F$ and the Fermi energy $k_F^2/2m$, respectively, we find that the system is described by only one parameter, namely, the strength of the bare interaction $V$. In our new units, the single-particle energy is represented by $k^2$ and the total number of electrons $N$ is given by $2/\pi$.

## III. EXACT SOLUTION

The exact solution for the model (2.1) at finite temperatures was obtained in the form of integral equations through the Bethe ansatz[2,11] by Takahashi[3] and Lai.[4]

The thermodynamic properties including the excitation spectrum involved in the solution were discussed in some detail by Lai.[5] Usuki *et al.*[10] reported some results on the low-temperature specific heat obtained by the numerical solution of the integral equations. However, the information of these works is limited. Here we give rather detailed numerical results of these equations for arbitrary $T$ and $V$ in the absence of the magnetic field. We present the way to obtain the numerical solution in this section.

According to Refs. 3 and 4, there are two sets of the coupled nonlinear integral equations. The first set for $\kappa(k)$ and $\epsilon_n(k)$ $(n=1,2,\ldots)$ is composed of

$$\kappa=k^2-\mu-\sum_{n=1}^{\infty}[n]T\ln(1+e^{-\epsilon_n/T}) , \tag{3.1}$$

$$([0]+[2])\epsilon_1=[1][-T\ln(1+e^{-\kappa/T})+T\ln(1+e^{\epsilon_2/T})] , \tag{3.2}$$

and

$$([0]+[2])\epsilon_n=[1][T\ln(1+e^{\epsilon_{n-1}/T})+T\ln(1+e^{\epsilon_{n+1}/T})] , \quad (n=2,3,\ldots) \tag{3.3}$$

with the definition of $[n]$ by

$$[n]f(k)\equiv\frac{1}{\pi}\int_{-\infty}^{\infty}\frac{nV/4}{(nV/4)^2+(k-k')^2}f(k')dk' . \tag{3.4}$$

We solve (3.1)–(3.3) iteratively. For an initial step of the iteration, we take the value of the noninteracting system for $\epsilon_n$ as

$$\epsilon_n^{(0)}(k)\equiv T\ln\left[n-\frac{1}{1+e^{(k^2-\mu)/T}}\right]\times\left[n+2-\frac{1}{1+e^{(k^2-\mu)/T}}\right] . \tag{3.5}$$

A first-iteration value $\kappa^{(1)}(k)$ for $\kappa(k)$ is obtained from (3.1) with the use of this $\epsilon_n^{(0)}(k)$. Substituting these $\kappa^{(1)}(k)$ and $\epsilon_n^{(0)}(k)$ into (3.2) and (3.3), we get a revised value $\epsilon_n^{(1)}$ for $\epsilon_n$. The integral equations (3.2) and (3.3) are solved by converting them into a set of matrix equations. We have made use of the fact that asymptotically $\epsilon_n(k)$ approaches the constant $T\ln[n(n+2)]$ as $|k|\to\infty$. The revised value $\epsilon_n^{(1)}(k)$ is employed to obtain $\kappa^{(2)}(k)$ through (3.1). This process is repeated until the difference between $\kappa^{(m)}$ and $\kappa^{(m-1)}$ becomes negligibly small. The sum over $n$ in (3.1) is truncated at some finite value $n_c$. It is checked that the obtained values for $\kappa$ and $\epsilon_n$ converge if we take $n_c\approx 10$.

With the use of $\kappa$ and $\epsilon_n$ thus obtained, the second set of the equations is given for $\rho(k)$ and $\sigma_n(k)$ as

$$(1+e^{\kappa/T})\rho=\frac{1}{2\pi}+\sum_{n=1}^{\infty}[n]\sigma_n , \tag{3.6}$$

$$([0]+[2])(1+e^{\epsilon_1/T})\sigma_1=[1](\rho+\sigma_2e^{\epsilon_2/T}) , \tag{3.7}$$

and

$$([0]+[2])(1+e^{\epsilon_n/T})\sigma_n=[1](\sigma_{n-1}e^{\epsilon_{n-1}/T}+\sigma_{n+1}e^{\epsilon_{n+1}/T}) \quad (n=2,3,\ldots) . \tag{3.8}$$

This set can also be solved iteratively. We start from the value of the noninteracting system for $\sigma_n(k)$ as

$$\sigma_n^{(0)}(k)\equiv\frac{1}{\pi}\frac{1}{1+e^{(k^2-\mu)/T}}\frac{1}{n+1+ne^{(-k^2+\mu)/T}}\times\frac{1}{n-\frac{1}{1+e^{(k^2-\mu)/T}}}\frac{1}{n+2-\frac{1}{1+e^{(k^2-\mu)/T}}} . \tag{3.9}$$

A first-iteration value for $\rho$ comes from (3.6). The subsequent procedure to obtain the convergent values for $\rho$ and $\sigma_n$ is quite similar to that mentioned for (3.1)–(3.3). Thus we will not repeat it here. The chemical potential $\mu$ is determined by the condition

$$N=\frac{2}{\pi}=\int\rho(k)dk . \tag{3.10}$$

Once the functions $\kappa$, $\rho$, $\epsilon_n$, and $\sigma_n$ are obtained, we can evaluate all the thermodynamic quantities. For example, the internal energy $E$ is calculated as

$$E=\int k^2\rho(k)dk , \tag{3.11}$$

the pressure $P=-\Omega$ is obtained by

$$P=\frac{T}{2\pi}\int\ln(1+e^{-\kappa(k)/T})dk , \tag{3.12}$$

and the entropy $S$ is given by

$$S=\frac{E-\mu N-\Omega}{T} . \tag{3.13}$$

## IV. VARIATIONAL CALCULATION

To use (1.1), let us choose $\hat{\tilde{H}}_0$ and $\hat{\tilde{V}}$ as

$$\hat{\tilde{H}}_0=\sum_{k,\sigma}\tilde{\epsilon}_k\hat{c}_{k\sigma}^{\dagger}\hat{c}_{k\sigma} , \tag{4.1}$$

and

$$\hat{\tilde{V}}=\tilde{V}\sum_q{}'\sum_{k,k'}\hat{c}_{k+q\uparrow}^{\dagger}\hat{c}_{k'-q\downarrow}^{\dagger}\hat{c}_{k'\downarrow}\hat{c}_{k\uparrow} , \tag{4.2}$$

with

$$\tilde{\epsilon}_k=k^2+\tilde{\epsilon}_0+\Delta_k . \tag{4.3}$$

Here $\tilde{V}$ is the strength of the effective potential and the prime in the sum denotes that the summation is taken under the condition of $q\neq 0$ to exclude the Hartree term. The quantity $\tilde{\epsilon}_0$ represents the chemical-potential shift due to the Hartree term. (The Fock term does not appear in the present system.) The two parameters $\tilde{\epsilon}_0$ and $\tilde{V}$ will be determined variationally. The change in the one-particle energy due to correlation is treated by $\Delta_k$. We regard $\Delta_k$ to be of order $\tilde{V}^2$ and thus we expand quantities in terms of $\Delta_k$. For example, the Fermi distribution function for $\tilde{\epsilon}_k$ is expanded as

$$\tilde{n}_k^- \equiv \langle \hat{c}_{k\sigma}^\dagger \hat{c}_{k\sigma} \rangle_0 = \frac{1}{1+e^{\beta(\tilde{\epsilon}_k-\mu)}} \approx n_k^- - \frac{\partial n_k^-}{\partial \mu}\Delta_k , \tag{4.4}$$

with

$$n_k^- = \frac{1}{1+e^{\beta(k^2-\mu_0)}} , \tag{4.5}$$

and

$$\mu_0 = \mu - \tilde{\epsilon}_0 . \tag{4.6}$$

Similarly, the grand potential for $\hat{\tilde{H}}$ is given by

$$\tilde{\Omega}_0 = \Omega_0 + 2\sum_k \Delta_k n_k^- , \tag{4.7}$$

with

$$\Omega_0 = -2T\sum_k \ln(1+e^{-\beta(k^2-\mu_0)}) . \tag{4.8}$$

From (1.1) and the above prescription, we obtain $\Omega$ to second order in $\tilde{V}^2$ as

$$\Omega = \Omega_0 - \tilde{\epsilon}_0\langle \hat{N} \rangle + V\left[\frac{\langle \hat{N} \rangle_0}{2}\right]^2 - (2V-\tilde{V})\tilde{V}W_1 + V\tilde{V}^2 W_2 + V\frac{\langle \hat{N} \rangle_0}{2}\left[\tilde{V}^2 W_{2N} - 2\sum_k \Delta_k \frac{\partial n_k^-}{\partial \mu}\right] . \tag{4.9}$$

Here $\langle \hat{N} \rangle_0$ and $\langle \hat{N} \rangle$ are, respectively, given by

$$\langle \hat{N} \rangle_0 = 2\sum_k n_k^- , \tag{4.10}$$

and

$$\langle \hat{N} \rangle = \langle \hat{N} \rangle_0 + \tilde{V}^2 W_{2N} - 2\sum_k \Delta_k \frac{\partial n_k^-}{\partial \mu} . \tag{4.11}$$

The quantities $W_1$, $W_{2N}$, and $W_2$ represent contributions from Figs. 1(a), 1(b), and 1(c), respectively. Introducing the function

$$G(\Delta;\beta) = \frac{1-e^{-(\beta/2)\Delta}}{\Delta} , \tag{4.12}$$

we can give explicit expressions for $W_1$, $W_{2N}$, and $W_2$ as

$$W_1 = \sum_q \sum_{k,k'} n_k^- n_{k+q}^+ n_{k'}^- n_{k'-q}^+ \times G(\epsilon_{k+q} - \epsilon_k + \epsilon_{k'-q} - \epsilon_{k'};\beta) , \tag{4.13}$$

$$W_{2N} = 2\sum_q \sum_{k,k'} n_k^- n_{k+q}^+ n_{k'}^- n_{k'-q}^+ (n_{k+q}^+ - n_k^-) \times G(\epsilon_{k+q} - \epsilon_k + \epsilon_{k'-q} - \epsilon_{k'};\beta)^2 , \tag{4.14}$$

and

$$W_2 = W_2^{ee} + W_2^{hh} - 2W_2^{eh} , \tag{4.15}$$

with

$$W_2^{ee} = \sum_{q,q'} \sum_{k,k'} n_k^- n_{k+q}^+ n_{k+q'}^+ n_{k'}^- n_{k'-q}^+ n_{k'-q'}^+ \times G(\epsilon_{k+q} - \epsilon_k + \epsilon_{k'-q} - \epsilon_{k'};\beta) \times G(\epsilon_{k+q'} - \epsilon_k + \epsilon_{k'-q'} - \epsilon_{k'};\beta) , \tag{4.16}$$

$$W_2^{hh} = \sum_{q,q'} \sum_{k,k'} n_k^+ n_{k+q}^- n_{k+q'}^- n_{k'}^+ n_{k'-q}^- n_{k'-q'}^- \times G(\epsilon_k - \epsilon_{k+q} + \epsilon_{k'} - \epsilon_{k'-q};\beta) \times G(\epsilon_k - \epsilon_{k+q'} + \epsilon_{k'} - \epsilon_{k'-q'};\beta) , \tag{4.17}$$

and

$$W_2^{eh} = \sum_{q,q'} \sum_{k,k'} n_k^- n_{k+q}^+ n_{k+q'}^+ n_{k'}^+ n_{k'-q}^- n_{k'-q'}^- \times G(\epsilon_{k+q} - \epsilon_k + \epsilon_{k'} - \epsilon_{k'-q};\beta) \times G(\epsilon_{k+q'} - \epsilon_k + \epsilon_{k'} - \epsilon_{k'-q'};\beta) , \tag{4.18}$$

where $\epsilon_k = k^2$ and

$$n_k^+ = 1 - n_k^- \tag{4.19}$$

At zero temperature ($\beta \rightarrow \infty$), the term $e^{-(\beta/2)\Delta}$ in (4.12) disappears and $G(\Delta;\beta)$ is nothing but $\Delta$, i.e., the energy denominator. At very high temperatures, $G(\Delta;\beta)$ approaches $1/2T$. Thus in our formalism, the crossover between the energy denominator and the temperature in the correlation effect as discussed in Sec. I of I is incorporated by the use of this function $G(\Delta;\beta)$. As a technical merit, $G(\Delta;\beta)$ is analytic at $\Delta=0$ and is favorable for numerical integrations. In fact, the term proportional to

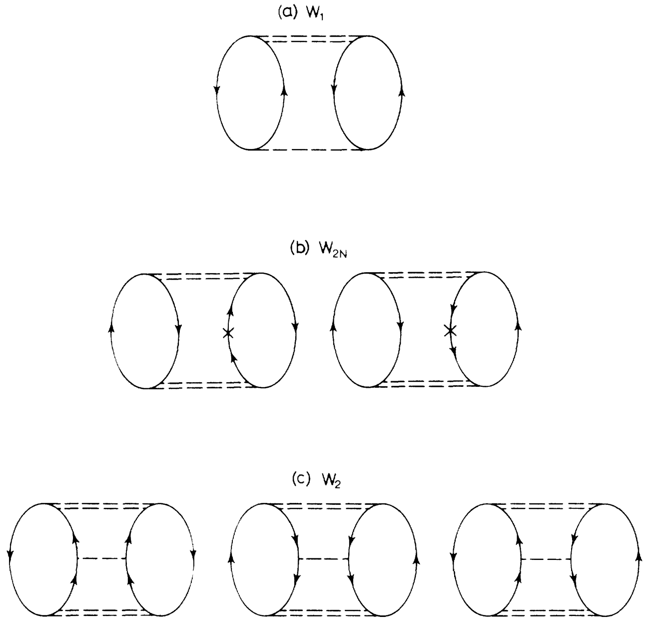

FIG. 1. Goldstone diagrams for (a) $W_1$, (b) $W_{2N}$, and (c) $W_2$.

$e^{-(\beta/2)\Delta}$ does not contribute to $W_1$ in (4.13) at any temperature, but it is included for this convenience.

There may be several ways to give $\Delta_k$, but we choose it here so as to satisfy

$$\tilde{V}^2 W_{2N} = 2\sum_k \Delta_k \frac{\partial n_k^-}{\partial \mu} \ . \tag{4.20}$$

Since it is not necessary in the following discussion, we will not give an explicit expression for $\Delta_k$ here. This choice for $\Delta_k$ is also found to be consistent with the general thermodynamic principle: If we took $\Delta_k$ to be zero, we would have got a nonzero entropy at $T=0$, because the terms in proportion to $W_{2N}$ in $\Omega$ depend on $T$ linearly at low temperatures.

From the Euler-Lagrange-type equation $\delta\Omega/\delta\tilde{V}=0$ with $\Omega$ in (4.9), we obtain an optimum value for $\tilde{V}$ as

$$\tilde{V} = \frac{1}{1+(W_2/W_1)V} V \ . \tag{4.21}$$

Note that $\tilde{V}$ is reduced from $V$ by the factor $[1+(W_2/W_1)V]^{-1}$; thus our approach from the weak-coupling limit is expected to have a wide applicable range. Similarly, noting the fact that $\tilde{\epsilon}_0$ appears in the Fermi distribution function (4.5) in the form $\mu_0=\mu-\tilde{\epsilon}_0$, we have

$$0 = \left.\frac{\delta\Omega}{\delta\tilde{\epsilon}_0}\right|_{\tilde{V}} = -\langle\hat{N}\rangle - \left.\frac{\partial\Omega}{\partial\mu}\right|_{\tilde{V}} \ . \tag{4.22}$$

This is nothing but the thermodynamic identity to relate the number of electrons to the chemical potential $\mu$. With the use of (4.11) and $\Delta_k$ in (4.20), we have an equation to determine $\mu_0$ as

$$\langle\hat{N}\rangle = \langle\hat{N}\rangle_0 = \frac{2}{\pi} \ . \tag{4.23}$$

With this $\mu_0$, $\tilde{\epsilon}_0$ is obtained from (4.22) as

$$\tilde{\epsilon}_0 = \frac{V}{2}\langle\hat{N}\rangle_0 - \frac{\tilde{V}\left[(2V-\tilde{V})\dfrac{\partial W_1}{\partial\mu} - V\tilde{V}\dfrac{\partial W_2}{\partial\mu}\right]}{\dfrac{\partial\langle\hat{N}\rangle_0}{\partial\mu}} \ . \tag{4.24}$$

Substituting these optimum values for the variational parameters, we can calculate the free energy $F$, the entropy $S$, the internal energy $E$, and the specific heat $C_V$ through the usual thermodynamic identities.

## V. SECOND-ORDER PERTURBATION THEORY

Let us present briefly the results in the perturbation theory to compare them with those in our variational method. To second order in $V$, the grand potential $\Omega(T,\mu)$ is obtained as

$$\Omega(T,\mu) = \Omega_0(T,\mu) + V\left[\frac{\langle\hat{N}\rangle_0}{2}\right]^2 - V^2\left[W_1 + \tfrac{1}{8}(\langle\hat{N}\rangle_0)^2\frac{\partial\langle\hat{N}\rangle_0}{\partial\mu}\right] , \tag{5.1}$$

where $\Omega_0(T,\mu)$ and $\langle\hat{N}\rangle_0$ are given by (4.8) and (4.10), respectively, with $\mu_0$ replaced by $\mu$. To determine the chemical potential $\mu$, let us formally expand it in $V$ as[12]

$$\mu = \mu_0 + \mu_1 + \mu_2 + \dots , \tag{5.2}$$

where the subscript denotes the corresponding order in $V$. By putting this expression into

$$N = -\left[\frac{\partial\Omega}{\partial\mu}\right]_T , \tag{5.3}$$

and expanding each term in Taylor series about the value $\mu=\mu_0$, we have

$$N = \langle\hat{N}\rangle_0(\mu_0) , \tag{5.4}$$

$$\mu_1 = VN/2 , \tag{5.5}$$

and

$$\mu_2 = -\frac{V^2\dfrac{\partial W_1}{\partial\mu_0}}{\dfrac{\partial\langle\hat{N}\rangle_0}{\partial\mu_0}} \ . \tag{5.6}$$

In the derivation of $\mu_2$, the Hartree terms should be considered carefully in the perturbation theory, because there is a strong cancellation among them. This troublesome process is avoided in our variational theory by the choice of the effective potential in (4.2).

If (5.1) is expanded about $\mu=\mu_0$, we finally obtain

$$\Omega(T,\mu) = \Omega_0(T,\mu_0) - V\left[\frac{N}{2}\right]^2 + V^2\left[-W_1 + N\frac{\dfrac{\partial W_1}{\partial\mu_0}}{\dfrac{\partial\langle\hat{N}\rangle_0}{\partial\mu_0}}\right] . \tag{5.7}$$

## VI. CALCULATED RESULTS

In Figs. 2(a) and 2(b), we have given the results for $\Omega$ divided by $N$ as a function of the bare interaction $V$ for $T=0$ and 10, respectively. (Energies are in units of the Fermi energy $k_F^2/2m$.) The curves indicated by "exact", $\tilde{V}^2$ and $V^2$ represent, respectively, the results obtained by the exact solution (3.12), our variational theory (4.9), and the second-order perturbation theory (5.7). One can see that the expansion in terms of $\tilde{V}$ is far more effective than that in $V$. The results in our approach are very close to the exact ones up to $V$ as large as 20. This wide applicability of our formula stems from the fact that the expansion parameter $\tilde{V}$ is smaller than $V$. In fact, one can see from Fig. 3 that the ratio $\tilde{V}/V$ becomes more and more reduced as $V$ is increased. The ratio increases gradually as the temperature is raised. In the high-temperature limit, $\tilde{V}$ becomes equal to $V$ and the second-order perturbation theory gives the same result as our formula. To reach that limit, however, we need a very large value of $T$ which depends, of course, on $V$.

In order to see the difference among the exact results,

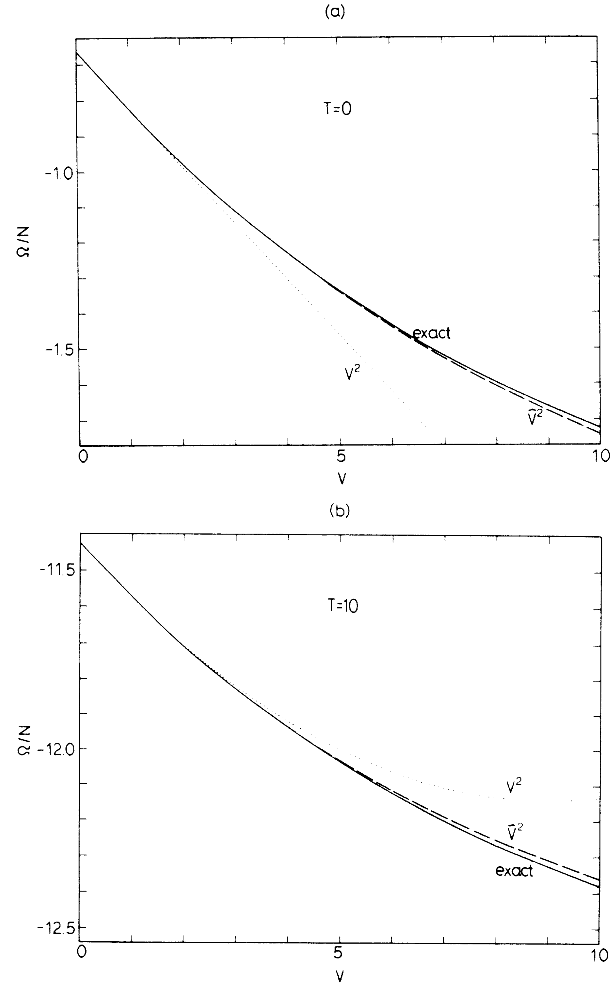

FIG. 2. The grand potential as a function of $V$ for (a) $T=0$ and (b) $T=10$. We indicate the exact results (3.12), our variational ones (4.9), and those in the usual second-order perturbation theory (5.7) by the symbols "exact", $\tilde{V}^2$, and $V^2$, respectively.

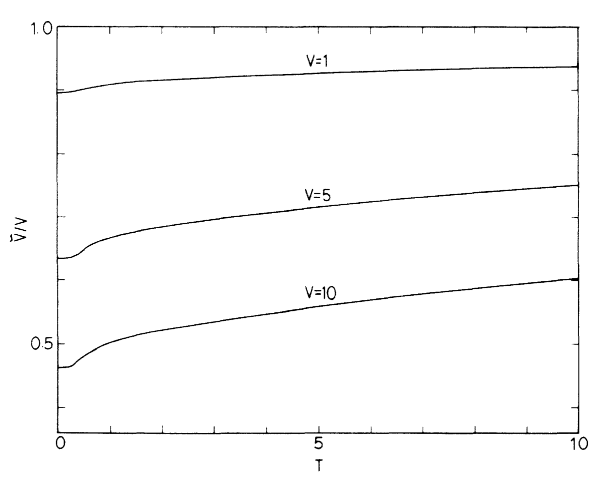

FIG. 3. Effective potential $\tilde{V}$ divided by $V$ as a function of temperature for $V=1$, 5, and 10.

our variational ones, and those in the second-order perturbation theory in more detail, we have plotted the values for the correlation part of the grand potential $\Delta\Omega/N \equiv [\Omega(T,\mu)-\Omega_0(T,\mu_0)]/N$ as a function of $T$ at $V=5$ and 10 in Fig 4. When $V$ is smaller than about 2, our variational method gives virtually the exact values for $\Omega$ in the whole temperature region. Even when $V$ is much larger than that, we have found that our method still provides the values for $\Omega$ very close to the exact ones if $T$ is larger than about $2V$. For $T$ larger than about 1, our results always satisfy the variational upper-bound property which is stated that a value for $\Omega$ estimated by a variational method should be higher than the exact value. For $V$ larger than about 2 and $T$ smaller than about 1, however, the upper-bound property is violated. This indicates that the series for $\Omega$ in $\tilde{V}$ derived in Secs. III and IV in I should not be cut off at second order in this temperature region for $V$ as strong as 2 or larger in the present system. The deviation of our value for $\Delta\Omega$ from the exact one becomes most serious at $T\approx 0.4$, though the deviation itself is at most 11% even for $V=10$. This error is much smaller than that of 55% in the second-order perturbation theory. Nevertheless, our present method as well as the second-order perturbation theory is seen to reproduce the correct qualitative behavior of $\Omega$ as a function of $T$ in the whole temperature region.

We have calculated the exact values for the entropy $S$ in detail as a function of $T$ for several values of $V$. The results for $S/N$ are given in Fig. 5. In the low-temperature region, i.e., $T$ less than about 0.2, $S$ increases in proportion to $T$. This behavior is consistent with the Landau's Fermi-liquid theory. The $T$-linear coefficient increases monotonically and approaches infinity as $V$ is increased. In the limit of $V=\infty$, it is finite, but $S/N$ it-

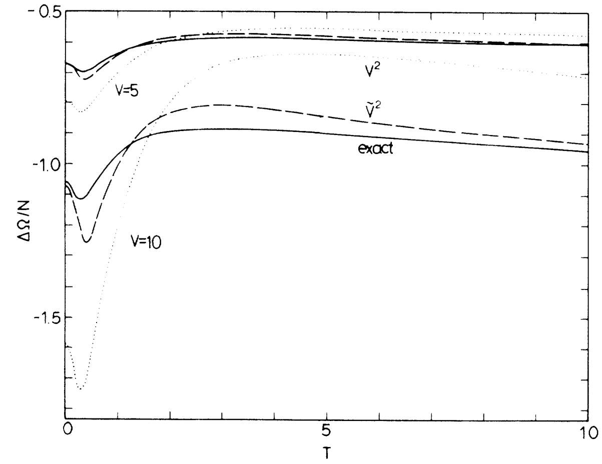

FIG. 4. Temperature dependence of the correlation part of the grand potential $\Delta\Omega/N \equiv (\Omega-\Omega_0)/N$ for $V=5$ and 10, where $\Omega_0$ is the grand potential of the noninteracting system. The results in the exact, our variational, and the second-order perturbation theories are, respectively, plotted by the solid, the dashed, and the dotted curves.

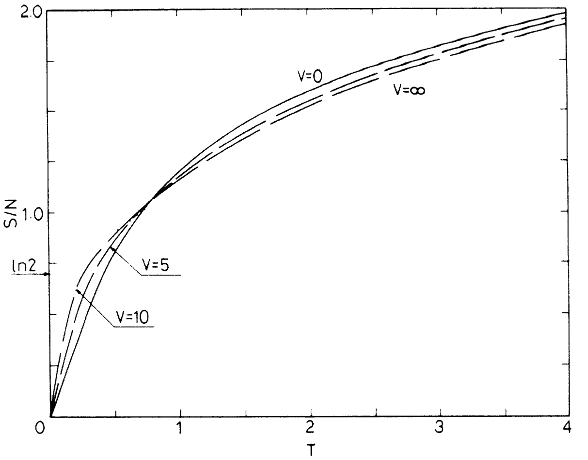

FIG. 5. The exact values for the entropy $S/N$ as a function of $T$ for $V=0$, 5, 10, and $\infty$.

self starts from ln2 which reflects the double degeneracy of the spin degrees of freedom. Contrary to the low-temperature behavior with the increase of $V$, $S$ becomes smaller than the corresponding one in the noninteracting system for $T$ larger than about 0.8. The overall feature of $S$ for $T$ less than about 1 is very similar to that in the Hubbard model.[8-10] Since the first increase of $S$ with $V$ is attributed to the spin-wave excitations in the Hubbard model, we can also explain the low-temperature behavior of $S$ in this system in terms of the same origin. This explanation is also consistent with the analysis of Lai.[5] We have plotted the results for $\Delta S/N \equiv (S-S_0)/N$ as a function of $T$ in Fig. 6 for the cases of $V=5$ and 10, where $S_0$ is the entropy of the noninteracting system. The solid and the dashed curves represent the exact and

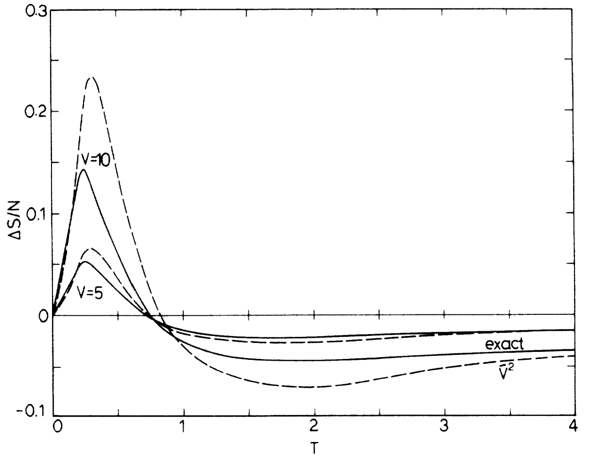

FIG. 6. The entropy $\Delta S/N \equiv (S-S_0)/N$ as a function of $T$ for $V=5$ and 10, where $S_0$ is the entropy of the noninteracting system. The solid curves represent the exact results, while the dashed ones show our variational values.

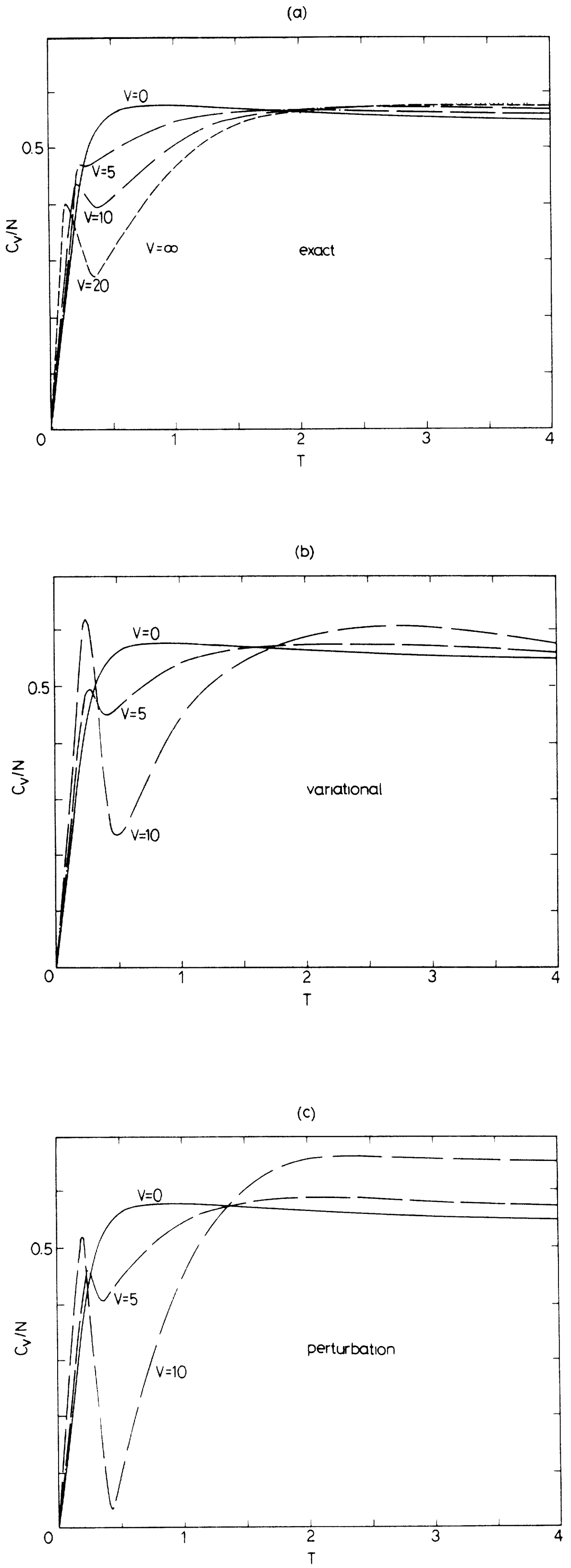

FIG. 7. Specific heat $C_V/N$ as a function of $T$. (a) Exact results for $V=0$, 5, 10, 20, and $\infty$. (b) Our variational results for $V=0$, 5, and 10. (c) Results in the second-order perturbation theory for $V=0$, 5, and 10.

our variational results, respectively. As in the case of $\Omega$, our variational method gives a qualitatively correct behavior. Quantitatively, we have obtained a large enhancement due to the spin-wave excitations in $S$ except for $T$ very close to zero. If we could have obtained a little smaller value for $\tilde{V}$, we had an even better result.

The contribution of the spin-wave excitations can be seen more easily in the curve of the specific heat as a function of $T$. The calculated results are shown for several values of $V$ in Figs. 7(a), 7(b), and 7(c) which are given, respectively, in the exact, our variational, and the second-order perturbation theories. As the exact calculation shows, the peak structure in the specific heat appears at low temperatures for $V$ larger than about 5. Such a structure is absent in both the weakly interacting ($V \approx 0$) and the "spinless" ($V = \infty$) systems in which the spin degrees of freedom do not play a role. In fact, the curve for $V = \infty$ is just the same as that for $V = 0$ if we do not plot it in $T$ but in $4T$. The peak structure in $C_V$ obtained here is very similar to that of the one-dimensional Hubbard model which has been found in both half-filled[8] and non-half-filled[9,10] cases. The broad peak in the specific heat at high temperatures ($T > 0.6$) reflects the divergence in the density of states at the band edge. This structure will disappear in higher dimensions. Note also that we need a very large $T$ in one-dimensional systems to reach the classical limit ($C_V = N/2$). Our variational method as well as the second-order perturbation theory gives a qualitatively correct behavior of the specific heat in the whole temperature region. Quantitatively, however, our results are not good for large $V$, though they are much improved over those in the perturbation theory. Here again, use of a little smaller $\tilde{V}$ would have given much better values for the specific heat.

The gradient in the curve of $S(T)$ or $C_V(T)$ at very low temperatures determines the effective mass $m^*$ for the electrons at the Fermi surface. The calculated results for $m^*$ in the exact, our variational, and the second-order perturbation theories are given as a function of $V$ in Fig. 8. The value for $m^*$ in the perturbation theory increases in proportion to $V^2$, whereas the behavior of $m^*$ in our variational calculation is different: It increases in proportion to $V^2$ for $V$ smaller than about 3 but to $V$ for $V$ larger than about 7. The exact theory gives a value between these two results. Of course, our variational result is much closer to the exact value than that in the second-order perturbation theory, but a much more sophisticated improvement seems to be necessary to obtain a correct behavior of $m^*$ as a function of $V$.

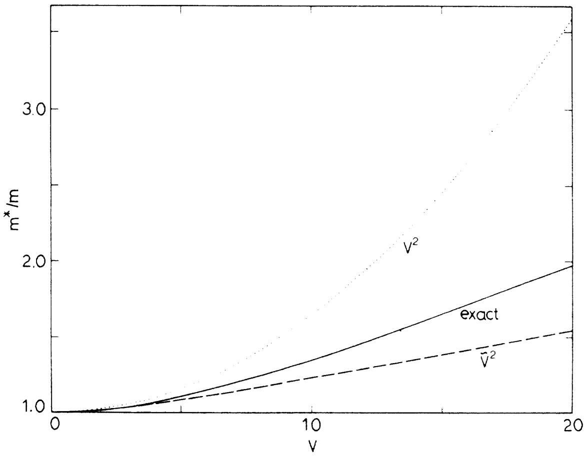

FIG. 8. The effective mass $m^*$ for the electrons near the Fermi surface at low temperatures divided by the bare mass $m$ as a function of $V$. The solid, the dashed, and the dotted curves correspond, respectively, to the results in the exact, our variational, and the second-order perturbation theories.

## VII. SUMMARY AND DISCUSSION

We have shown an example of the actual implementation of the effective-potential expansion (EPX) method at finite temperatures by applying it to the one-dimensional many-electron system with the repulsive δ-function interaction. It is demonstrated that, in spite of the calculation only up to second order in the effective potential, the EPX method is effective in very wide ranges of both $T$ and the strength of the bare potential $V$. Even in the case in which the result is not so good quantitatively, we can always obtain a qualitatively correct result. This is very important when we investigate the many-body effects in an analytic approach as in the EPX method. In order to build a new concept on the many-body effects, we do not always need a very sophisticated method to give a quantitatively very accurate result but rather a much simpler and transparent one to give at least a qualitatively correct behavior.

Since a general discussion on the problems related to the finite-temperature EPX method was given in I, we restrict ourselves to the discussion on the improvement of our method for the present system. Because the deviation of our values for $\Omega$ from the exact ones becomes largest at $T$ around 0.4 in which the contribution of the spin-wave excitations dominates, we need a better treatment for the spin fluctuations in the choice of the effective potential. For this purpose, we may give $\hat{\tilde{V}}$ as

$$\hat{\tilde{V}} = \frac{1}{8} \sum_{q,k,k'}{}' \sum_{\alpha,\beta,\gamma,\delta} [\tilde{V}_c(q)\delta_{\alpha\delta}\delta_{\beta\gamma} - \tilde{V}_s(q)\boldsymbol{\sigma}_{\alpha\delta}\cdot\boldsymbol{\sigma}_{\beta\gamma}] \times \hat{c}^\dagger_{k+q\alpha}\hat{c}^\dagger_{k'-q\beta}\hat{c}_{k'\gamma}\hat{c}_{k\delta} , \tag{7.1}$$

where $\sigma_x$, $\sigma_y$, and $\sigma_z$ are the Pauli spin matrices and the prime in the sum over $q$, $k$, and $k'$ denotes to exclude the Hartree and the Fock terms. The potentials $\tilde{V}_c(q)$ and $\tilde{V}_s(q)$ represent, respectively, the contributions from the exchange of the charge and the spin fluctuations. We can rewrite (7.1) as

$$\hat{\tilde{V}}=\frac{1}{2}\sum_{q,k,k'}{}' \frac{\tilde{V}_c(q)-\tilde{V}_s(q)}{4}(\hat{c}^{\dagger}_{k+q\uparrow}\hat{c}^{\dagger}_{k'-q\uparrow}\hat{c}_{k'\uparrow}\hat{c}_{k\uparrow}+\hat{c}^{\dagger}_{k+q\downarrow}\hat{c}^{\dagger}_{k'-q\downarrow}\hat{c}_{k'\downarrow}\hat{c}_{k\downarrow})$$
$$+\sum_{q,k,k'}{}' \frac{\tilde{V}_c(q)+\tilde{V}_s(q)+2\tilde{V}_s(k-k'+q)}{4}\hat{c}^{\dagger}_{k+q\uparrow}\hat{c}^{\dagger}_{k'-q\downarrow}\hat{c}_{k'\downarrow}\hat{c}_{k\uparrow}\ . \tag{7.2}$$

If we neglect the $q$ dependence in both $\tilde{V}_c$ and $\tilde{V}_s$, the first term in (7.2) is irrelevant and we can see that (7.2) is equivalent to (4.2) with $\tilde{V}=(\tilde{V}_c+3\tilde{V}_s)/4$. Thus the $q$ dependence is important for the improvement. However, a preliminary calculation up to second order in $\tilde{V}_s$ shows that we can obtain only a very modest improvement even with the $q$-dependent $\tilde{V}_s$. We do not think that a substantial improvement can be achieved by the fourth-order calculation either, because the spin wave is a kind of collective excitations and some kind of an infinite sum, or a calculation up to an infinite order in $\tilde{V}_s(q)$ is necessary to obtain a nearly exact result. We are planning to make an improvement by taking some partial infinite sum. However, that is beyond the scope of this paper.

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