PHYSICAL REVIEW B VOLUME 42, NUMBER 16 1 DECEMBER 1990

Perturbation theory of the t-J model for $t/J \ll 1$

Mamoru Uchinami*
Theoretische Physik, Eidgenössische Technische Hochschule Hönggerberg, CH-8093 Zürich, Switzerland
(Received 23 July 1990)

We apply a finite-temperature functional-integral approach by means of which Arovas and Auerbach analyzed low-dimensional Heisenberg spin models to the t-J model in the slave-fermion representation. Using a perturbation theory of the t-J model for $t \ll J$, self-consistent equations are derived for finite hole concentration that reduce to those in the case of the pure Heisenberg spin model, i.e., to those of Arovas and Auerbach, and Takahashi as a special case. Numerical solution of the corresponding self-consistent equations for the one-dimensional t-J model at sufficiently low temperature suggests that, if the transfer t is not too large, there is a phase-separation state into a hole-rich and a no-hole phase as conjectured recently by Emery *et al.*

I. INTRODUCTION

It has been clear recently that a detailed study of the motion of holes in an antiferromagnet is of fundamental importance for the understanding of the mechanism of hole-type high-T_c superconductivity.[1] The parent compounds such as La_2CuO_4 and $YBa_2Cu_3O_6$ are antiferromagnetic insulators described by the Heisenberg spin model with spin $S=\frac{1}{2}$, but when holes are introduced into the CuO_2 planes by doping, some compounds become high-T_c superconductors. It indicates that antiferromagnetic ordering probably is related to the superconductivity of holes in the metallic state. This behavior of holes in the superconducting metallic state is expected to have a strong connection with low-lying magnonlike excitation due to the creation or destruction of a spin singlet on nearest-neighbor sites in the antiferromagnetic ordering state. We are interested in investigating this connection between the holes and magnonlike excitations. As the simplest effective model for studying this problem, the t-J model was proposed.[2,3] To begin, we review briefly how the t-J model in the slave-fermion representation can be established from the one-band Hubbard model.

We focus on the one-band Hubbard model on a d-dimensional lattice. The grand canonical Hamiltonian is given by

$$H=-t\sum_{\langle i,j\rangle}\sum_{\sigma}(c_{i\sigma}^{\dagger}c_{j\sigma}+\text{H.c.})+U\sum_{i}c_{i\uparrow}^{\dagger}c_{i\uparrow}c_{i\downarrow}^{\dagger}c_{i\downarrow} -\mu\sum_{i}\sum_{\sigma}c_{i\sigma}^{\dagger}c_{i\sigma}\ . \tag{1.1}$$

Here $c_{i\sigma}(c_{i\sigma}^{\dagger})$ is the annihilation (creation) operator of an electron with spin σ ($=\uparrow$ or $\downarrow$) at lattice site i. These operators satisfy the anticommutation relation $[c_{i\sigma},c_{j\sigma'}]_{+}=\delta_{ij}\delta_{\sigma\sigma'}$. The notation $\sum_{\langle i,j\rangle}$ means summation over nearest-neighbor bonds, t denotes the transfer amplitude, and U (>0) the on-site Coulomb repulsion. The chemical potential μ is introduced to enforce the relation $\langle(1/N)\sum_i\sum_\sigma c_{i\sigma}^{\dagger}c_{i\sigma}\rangle=1-\delta$, where N is total number of lattice sites and δ is the hole concentration per site.

When we use the slave-fermion representation and neglect doubly occupied states, we can introduce two boson creation operators $a_{i\uparrow}^{\dagger}$ and $a_{i\downarrow}^{\dagger}$, and a fermion creation operator $e_i^{\dagger}$ corresponding to three basis states $c_{i\uparrow}^{\dagger}|0\rangle$, $c_{i\downarrow}^{\dagger}|0\rangle$, and $|0\rangle$ at each site i. The original electron operator $c_{i\sigma}$ is expressed by $c_{i\sigma}=e_i^{\dagger}a_{i\sigma}$, and then the completeness condition $\sum_\sigma a_{i\sigma}^{\dagger}a_{i\sigma}+e_i^{\dagger}e_i=1$ for each site i should be imposed in order to satisfy anticommutation relations of the original operators $c_{i\sigma}$ and $c_{i\sigma}^{\dagger}$. Such a formulation in a slave-fermion representation was applied to the one-band Hubbard model by Matsui[4] and to the t-J model by Yoshioka.[5] In this formulation the Hubbard model in the limit $t/U \ll 1$ is equivalent to the Heisenberg spin model in the Schwinger boson representation of spin operators. Arovas and Auerbach used such a formulation to analyze the problem of the low-dimensional quantum Heisenberg spin model.[6]

When we write the one-band Hubbard-model Hamiltonian (1.1) in the slave-fermion representation and then perform a canonical transformation which retains terms only up to the first order in t/U,[2,3] the effective Hamiltonian for $t/U \ll 1$ is given by

$$\begin{aligned}H=&-2t\sum_{\langle i,j\rangle}\sum_{\sigma}e_ie_j^{\dagger}a_{i\sigma}^{\dagger}a_{j\sigma}\\&+(J/2)\sum_{\langle i,j\rangle}\sum_{\sigma}(a_{i\sigma}^{\dagger}a_{i-\sigma}a_{j-\sigma}^{\dagger}a_{j\sigma}-a_{i\sigma}^{\dagger}a_{i\sigma}a_{j-\sigma}^{\dagger}a_{j-\sigma})\\&-\mu\left[N-\sum_i e_i^{\dagger}e_i\right],\end{aligned} \tag{1.2}$$

with $J=4t^2/U$. By defining the spin operator $\boldsymbol{\sigma}_i=(\sigma_i^x,\sigma_i^y,\sigma_i^z)$ as

$$\sigma_i^{\alpha}=(a_{i\uparrow}^{\dagger}a_{i\downarrow}^{\dagger})\sigma^{\alpha}\begin{bmatrix}a_{i\uparrow}\\a_{i\downarrow}\end{bmatrix}, \tag{1.3}$$

with Pauli spin matrices σ^{α} ($\alpha=x,y,z$) and number operator n_i as

$$n_i = \sum_\sigma a_{i\sigma}^\dagger a_{i\sigma} , \tag{1.4}$$

we can rewrite the Hamiltonian (1.2) in the following form:

$$H = -2t \sum_{\langle i,j \rangle} \sum_\sigma e_i e_j^\dagger a_{i\sigma}^\dagger a_{j\sigma} + (J/4) \sum_{\langle i,j \rangle} (\boldsymbol{\sigma}_i \cdot \boldsymbol{\sigma}_j - n_i n_j) - \mu(N - \sum_i e_i^\dagger e_i) . \tag{1.5}$$

The Hamiltonian (1.5) should, of course, be accompanied by the completeness condition $\sum_\sigma a_{i\sigma}^\dagger a_{i\sigma} + e_i^\dagger e_i = 1$ for each site i. The first term in (1.5) denotes the transfer energy characterized by the magnitude t of the transfer integral, the second one denotes the Heisenberg exchange interaction characterized by the magnitude J of exchange integral, and the last one is the chemical potential term. This effective Hamiltonian (1.5) written in slave-fermion representation is equivalent to the well-known t-J model Hamiltonian[2] written by applying the Gutzwiller projection to the original electron operators $c_{i\sigma}$ and $c_{i\sigma}^\dagger$ or to the one[3] written in the slave-boson representation. Although it is true that the t-J model describes well behaviors of the one-band Hubbard model when $t/J \gg 1$ (i.e., $t/U \ll 1$), we will see from the following discussion that it is very significant to study the t-J model Hamiltonian (1.5) for arbitrary values of t and J.

According to the Zhang-Rice mapping,[7] the t-J model Hamiltonian on a two-dimensional lattice is expected to contain sufficient physics to describe the high-T_c superconductivity of copper oxide materials. The electronic state of undoped copper oxide materials is formed from a Wannier localized orbital about each copper site which produces the copper local moment of $S=\frac{1}{2}$ because of large on-site Coulomb repulsion U. That is to say, a Mott-Hubbard-type insulator is built up. A superexchange interaction transmitted via oxygen couples nearest-neighbor copper spins. As holes are doped in the insulating copper oxide materials, oxygen holes are produced and then a spin singlet between the oxygen hole and the copper localized moment is built up because of strong antiferromagnetic exchange interaction between them due to hybridization of the copper and oxygen orbitals. The resulting singlet complex can be mapped as a hole produced in the antiferromagnetic spin system with $S=\frac{1}{2}$. The suitable model Hamiltonian describing this system of spinless holes inserted in the antiferromagnetic Heisenberg spin model is the t-J model Hamiltonian (1.5). So it is important and necessary to study the behavior of holes moving in an antiferromagnet for arbitrary values of t and J.

Next, we use the slave-fermion representation (i.e., the Schwinger boson one) to study the t-J model Hamiltonian (1.5) on a d-dimensional lattice system. Arovas and Auerbach[6] use this representation to describe the antiferromagnetic spin fluctuation accurately for low-dimensional Heisenberg spin models. The definition of the spin operator in terms of expression (1.3) exactly corresponds to the Schwinger boson representation of spin with $S=\frac{1}{2}$. It will be seen later that these Schwinger boson operators $a_{i\sigma}(\sigma=\uparrow,\downarrow)$ imply low-lying magnonlike excitations induced in the antiferromagnetic ordering background, as was suggested by Arovas and Auerbach[6] and Takahashi.[8] On the other hand, the spinless fermion operator e_i describes a hole whose motion is determined via the transfer term of the Hamiltonian (1.5). Recent experimental results[9] on various hole-type high-T_c superconductors by many different methods show a common feature that hole carriers in the CuO_2 planes induce superconductivity. These form a square lattice which possesses a strong antiferromagnetic spin correlation with $S=\frac{1}{2}$. It means that the antiferromagnetic spin correlation has something to do with the appearance of superconductivity on holes. In this respect we are very interested in studying the t-J model Hamiltonian (1.5), taking the strong antiferromagnetic spin correlation into consideration.

We proceed as follows. In Sec. II we will establish a finite-temperature functional-integral formalism in order to study the t-J model Hamiltonian (1.5) in the slave-fermion representation. In Sec. III we will develop the perturbation theory effective for $t \ll J$. In Sec. IV this perturbation theory will be applied to the one-dimensional t-J model. Section V will be devoted to conclusions and future problems.

II. FUNCTIONAL-INTEGRAL FORMALISM OF THE t-J MODEL

According to a study of the antiferromagnetic Heisenberg spin model by Arovas and Auerbach,[6] we introduce a bond operator S_{ij} for nearest-neighbor sites $\langle i,j \rangle$ defined by

$$S_{ij} \equiv a_{i\uparrow} a_{j\downarrow} - a_{i\downarrow} a_{j\uparrow} . \tag{2.1}$$

This bond operator describes the destruction of a spin singlet on nearest-neighbor sites. The grand canonical Hamiltonian (1.5) can be then rewritten in the following form:

$$H = 2t \sum_{\langle i,j \rangle} \sum_\sigma e_j^\dagger a_{i\sigma}^\dagger a_{j\sigma} e_i - (J/2) \sum_{\langle i,j \rangle} S_{ij}^\dagger S_{ij} - \mu(N - \sum_i e_i^\dagger e_i) , \tag{2.2}$$

where we have written it in the form of normal-ordered product. In addition to the Hamiltonian (2.2), the constraint of the completeness condition

$$\sum_\sigma a_{i\sigma}^\dagger a_{i\sigma} + e_i^\dagger e_i = 1 \tag{2.3}$$

should be imposed for each site i. Let us separate the lattice into two sublattices A and B. For the A sublattice we leave the operators $a_{i\sigma}$ $(\sigma=\uparrow,\downarrow)$ and e_i as they are, while for the B sublattice we introduce the new operators $b_{i\sigma}$ $(\sigma=\uparrow,\downarrow)$ and f_i via the following unitary transformation:

$$a_{i\uparrow} \to -b_{i\downarrow}, \quad a_{i\downarrow} \to b_{i\uparrow}, \quad e_i \to f_i . \tag{2.4}$$

For sublattice B, therefore, the following relationship holds between spin number operators in the original $a_{i\sigma}$, e_i and in the new $b_{i\sigma}, f_i$:

$$\sigma_i^x = -\sigma_i'^x, \quad \sigma_i^y = \sigma_i'^y, \quad \sigma_i^z = -\sigma_i'^z ,$$
$$n_i = n_i' ,$$

where we have defined the $\sigma_i'^\alpha$ ($\alpha = x,y,z$) and n_i' by

$$\sigma_i'^\alpha = (b_{i\uparrow}^\dagger b_{i\downarrow}^\dagger)\sigma^\alpha \begin{bmatrix} b_{i\uparrow} \\ b_{i\downarrow} \end{bmatrix} ,$$

and $n_i' = \sum_\sigma b_{i\sigma}^\dagger b_{i\sigma}$, respectively. As a result of the above unitary transformation, the bond operator S_{ij} is written as $S_{ij} = \sum_\sigma a_{i\sigma} b_{j\sigma}$ for the nearest-neighbor sites of the $i \in A$ and $j \in B$ sublattices, and so the grand canonical Hamiltonian (2.2) with the constrain (2.3) can be written as follows:

$$H = -2t \left[\sum_{\substack{\langle i,j \rangle \\ i\in A, j\in B}} f_j^\dagger (a_{i\uparrow}^\dagger b_{j\downarrow} - a_{i\downarrow}^\dagger b_{j\uparrow}) e_i - \sum_{\substack{\langle i,j \rangle \\ i\in B, j\in A}} e_j^\dagger (b_{i\uparrow}^\dagger a_{j\downarrow} - b_{i\downarrow}^\dagger a_{j\uparrow}) f_i \right] - J \sum_{\substack{\langle i,j \rangle \\ i\in A, j\in B}} S_{ij}^\dagger S_{ij} - \mu \left[N - \sum_{i\in A} e_i^\dagger e_i - \sum_{i\in B} f_i^\dagger f_i \right] , \tag{2.5}$$

accompanied by the constraint

$$\sum_\sigma a_{i\sigma}^\dagger a_{i\sigma} + e_i^\dagger e_i = 1 ,$$

for each site $i \in A$, and (2.6)

$$\sum_\sigma b_{i\sigma}^\dagger b_{i\sigma} + f_i^\dagger f_i = 1 ,$$

for each site $i \in B$.

Now we apply a finite-temperature functional-integral method[10] to this normal-ordered canonical Hamiltonian (2.5) with the constraint (2.6). As a simplification, we assume that a Lagrange multiplier $\lambda_i(\tau)$ for each site i, which multiplies the constraint (2.6), is time independent, spatially uniform, and takes a real value λ. When we note that the $a_{i\sigma}$'s and $b_{i\sigma}$'s are boson operators, while the e_i's and f_i's are fermion ones, the general partition function $Z_G = \mathrm{Tr}(e^{-\beta H})$, taking the above simplification of the Lagrange multiplier λ into consideration, can be written in the form of a functional integral with respect to imaginary time τ. With the inverse temperature $\beta = 1/T$, then Z_G is expressed as

$$Z_G = \int_{\substack{a(\beta)=a(0), b(\beta)=b(0) \\ e(\beta)=-e(0), f(\beta)=-f(0)}} d[\bar{a},a] d[\bar{b},b] d[\bar{e},e] d[\bar{f},f] d[\lambda] \exp\left[-\int_0^\beta d\tau L(\bar{a},a,\bar{b},b,\bar{e},e,\bar{f},f,\lambda) \right] , \tag{2.7}$$

where the imaginary time Lagrangian L is given by

$$\begin{aligned} L(\bar{a},a,\bar{b},b,\bar{e},e,\bar{f},f,\lambda) = & \sum_\sigma \left[\sum_{i\in A} \bar{a}_{i\sigma}(\tau) \frac{\partial}{\partial\tau} a_{i\sigma}(\tau) + \sum_{i\in B} \bar{b}_{i\sigma}(\tau) \frac{\partial}{\partial\tau} b_{i\sigma}(\tau) \right] + \sum_{i\in A} \bar{e}_i(\tau) \frac{\partial}{\partial\tau} e_i(\tau) + \sum_{i\in B} \bar{f}_i(\tau) \frac{\partial}{\partial\tau} f_i(\tau) \\ & -2t \left[\sum_{\substack{\langle i,j \rangle \\ i\in A, j\in B}} \bar{f}_j(\tau) [\bar{a}_{i\uparrow}(\tau) b_{j\downarrow}(\tau) - \bar{a}_{i\downarrow}(\tau) b_{j\uparrow}(\tau)] e_i(\tau) \right. \\ & \left. - \sum_{\substack{\langle i,j \rangle \\ i\in B, j\in A}} \bar{e}_j(\tau) [\bar{b}_{i\uparrow}(\tau) a_{j\downarrow}(\tau) - \bar{b}_{i\downarrow}(\tau) a_{j\uparrow}(\tau)] f_i(\tau) \right] - J \sum_{\substack{\langle i,j \rangle \\ i\in A, j\in B}} \bar{S}_{ij}(\tau) S_{ij}(\tau) \\ & + \lambda \left[\sum_{i\in A} \left[\sum_\sigma \bar{a}_{i\sigma}(\tau) a_{i\sigma}(\tau) + \bar{e}_i(\tau) e_i(\tau) - 1 \right] + \sum_{i\in B} \left[\sum_\sigma \bar{b}_{i\sigma}(\tau) b_{i\sigma}(\tau) + \bar{f}_i(\tau) f_i(\tau) - 1 \right] \right] \\ & - \mu \left[N - \sum_{i\in A} \bar{e}_i(\tau) e_i(\tau) - \sum_{i\in B} \bar{f}_i(\tau) f_i(\tau) \right] . \end{aligned} \tag{2.8}$$

We now apply a Hubbard-Stratonovich transformation to the bilinear product $\bar{S}_{ij}(\tau) S_{ij}(\tau)$ of the bond variables in (2.8). An auxiliary field $\chi_{ij}(\tau)$, which is introduced via this transformation, is also assumed to be time independent, spatially uniform, and to take a real value χ, again as a simplification. This assumption corresponds to including only an uniform mean-field state due to antiferromagnetic ordering. Consequently, we obtain the following grand partition function Z_G:

$$Z_G=\int_{\substack{a(\beta)=a(0),b(\beta)=b(0)\\ e(\beta)=-e(0),f(\beta)=-f(0)}} d[\bar{a},a]d[\bar{b},b]d[\bar{e},e]d[\bar{f},f]d[\lambda]d[\chi]\exp\left[-\beta\left[\sum_{\langle ij\rangle}(2/J)\chi^2-\mu N-\sum_i\lambda\right]\right]$$
$$\times\exp\left\{-\int_0^\beta d\tau\left[\sum_\sigma\left[\sum_{i\in A}\bar{a}_{i\sigma}(\tau)\frac{\partial}{\partial\tau}a_{i\sigma}(\tau)+\sum_{i\in B}\bar{b}_{i\sigma}(\tau)\frac{\partial}{\partial\tau}b_{i\sigma}(\tau)\right]\right.\right.$$
$$+\sum_{i\in A}\bar{e}_i(\tau)\frac{\partial}{\partial\tau}e_i(\tau)+\sum_{i\in B}\bar{f}_i(\tau)\frac{\partial}{\partial\tau}f_i(\tau)$$
$$-2t\left[\sum_{\substack{\langle i,j\rangle\\ i\in A,j\in B}}\bar{f}_j(\tau)[\bar{a}_{i\uparrow}(\tau)b_{j\downarrow}(\tau)-\bar{a}_{i\downarrow}(\tau)b_{j\uparrow}(\tau)]e_i(\tau)\right.$$
$$\left.-\sum_{\substack{\langle i,j\rangle\\ i\in B,j\in A}}\bar{e}_j(\tau)[\bar{b}_{i\uparrow}(\tau)a_{j\downarrow}(\tau)-\bar{b}_{i\downarrow}(\tau)a_{j\uparrow}(\tau)]f_i(\tau)\right]$$
$$-2\chi\sum_\sigma\left[\sum_{\substack{\langle i,j\rangle\\ i\in A,j\in B}}[a_{i\sigma}(\tau)b_{j\sigma}(\tau)+\bar{b}_{j\sigma}(\tau)\bar{a}_{i\sigma}(\tau)]\right.$$
$$\left.+\sum_{\substack{\langle i,j\rangle\\ i\in B,j\in A}}[a_{j\sigma}(\tau)b_{i\sigma}(\tau)+\bar{b}_{i\sigma}(\tau)\bar{a}_{j\sigma}(\tau)]\right]$$
$$+\lambda\sum_\sigma\left[\sum_{i\in A}\bar{a}_{i\sigma}(\tau)a_{i\sigma}(\tau)+\sum_{i\in B}\bar{b}_{i\sigma}(\tau)b_{i\sigma}(\tau)\right]$$
$$\left.\left.+(\lambda+\mu)\left[\sum_{i\in A}\bar{e}_i(\tau)e_i(\tau)+\sum_{i\in B}\bar{f}_i(\tau)f_i(\tau)\right]\right]\right\}. \tag{2.9}$$

It will be shown later that for the Heisenberg exchange interaction term in the Hamiltonian (1.5), we can describe very well low-lying antiferromagnetic magnonlike excitation even under such approximate simplifications with respect to λ and χ.

The effective grand canonical Hamiltonian which corresponds to the above grand partition function (2.9) takes the following form:

$$H_{\text{eff}}=-2t\left[\sum_{\substack{\langle i,j\rangle\\ i\in A,j\in B}}f_j^\dagger(a_{i\uparrow}^\dagger b_{j\downarrow}-a_{i\downarrow}^\dagger b_{j\uparrow})e_i-\sum_{\substack{\langle i,j\rangle\\ i\in B,j\in A}}e_j^\dagger(b_{i\uparrow}^\dagger a_{j\downarrow}-b_{i\downarrow}^\dagger a_{j\uparrow})f_i\right]$$
$$-2\chi\sum_\sigma\sum_{\substack{\langle i,j\rangle\\ i\in A,j\in B}}(a_{i\sigma}b_{j\sigma}+b_{j\sigma}^\dagger a_{i\sigma}^\dagger)+\lambda\sum_\sigma\left[\sum_{i\in A}a_{i\sigma}^\dagger a_{i\sigma}+\sum_{i\in B}b_{i\sigma}^\dagger b_{i\sigma}\right]+(\lambda+\mu)\left[\sum_{i\in A}e_i^\dagger e_i+\sum_{i\in B}f_i^\dagger f_i\right]. \tag{2.10}$$

Let us perform Fourier transformations defined by

$$a_{i\sigma}=\frac{1}{\sqrt{N/2}}\sum_{\mathbf{q}}a_{\mathbf{q}}e^{-i\mathbf{q}\cdot\mathbf{R}_i},\quad e_i=\frac{1}{\sqrt{N/2}}\sum_{\mathbf{q}}e_{\mathbf{q}}e^{-i\mathbf{q}\cdot\mathbf{R}_i},$$

for each site $i\in A$, and

$$b_{i\sigma}=\frac{1}{\sqrt{N/2}}\sum_{\mathbf{q}}b_{\mathbf{q}}e^{i\mathbf{q}\cdot\mathbf{R}_i},\quad f_i=\frac{1}{\sqrt{N/2}}\sum_{\mathbf{q}}f_{\mathbf{q}}e^{i\mathbf{q}\cdot\mathbf{R}_i},$$

for each site $i\in B$, where $\mathbf{R}_i$ denotes a lattice vector of site i and the summation $\sum_{\mathbf{q}}$ runs over half of the first Brillouin zone. The Hamiltonian (2.10) is then written as

$$H_{\text{eff}}=-t\frac{1}{N/2}\sum_{\mathbf{q}_1,\mathbf{q}_2,\mathbf{q}_3,\mathbf{q}_4}z\gamma_{\mathbf{q}_1-\mathbf{q}_3}\delta_{\mathbf{q}_1+\mathbf{q}_4-\mathbf{q}_2-\mathbf{q}_3,0}[f_{\mathbf{q}_1}^\dagger(a_{\mathbf{q}_2\uparrow}^\dagger b_{\mathbf{q}_3\downarrow}-a_{\mathbf{q}_2\downarrow}^\dagger b_{\mathbf{q}_3\uparrow})e_{\mathbf{q}_4}-e_{\mathbf{q}_1}^\dagger(b_{\mathbf{q}_2\uparrow}^\dagger a_{\mathbf{q}_3\downarrow}-b_{\mathbf{q}_2\downarrow}^\dagger a_{\mathbf{q}_3\uparrow})f_{\mathbf{q}_4}]$$
$$-\chi\sum_{\mathbf{q}}\sum_\sigma z\gamma_{\mathbf{q}}(a_{\mathbf{q}\sigma}b_{\mathbf{q}\sigma}+b_{\mathbf{q}\sigma}^\dagger a_{\mathbf{q}\sigma}^\dagger)+\lambda\sum_{\mathbf{q}}\sum_\sigma(a_{\mathbf{q}\sigma}^\dagger a_{\mathbf{q}\sigma}+b_{\mathbf{q}\sigma}^\dagger b_{\mathbf{q}\sigma})+(\lambda+\mu)\sum_{\mathbf{q}}(e_{\mathbf{q}}^\dagger e_{\mathbf{q}}+f_{\mathbf{q}}^\dagger f_{\mathbf{q}}). \tag{2.11}$$

Here z denotes number of nearest-neighbor sites, and we have defined $\gamma_{\mathbf{q}}$ by $\gamma_{\mathbf{q}}=(1/z)\sum_{\boldsymbol{\delta}}e^{-i\mathbf{q}\cdot\boldsymbol{\delta}}$, in which $\boldsymbol{\delta}$ denotes a nearest-neighbor unit vector. For the purpose of diagonalizing the corresponding Heisenberg exchange interaction term, furthermore, we introduce the following Bogoliubov transformation for $\sigma=\uparrow,\downarrow$:

$$A_{\mathbf{q}\sigma}=\cosh\theta_{\mathbf{q}}\, a_{\mathbf{q}\sigma}+\sinh\theta_{\mathbf{q}}\, b_{\mathbf{q}\sigma}^{\dagger} ,$$
$$B_{\mathbf{q}\sigma}=\cosh\theta_{\mathbf{q}}\, b_{\mathbf{q}\sigma}+\sinh\theta_{\mathbf{q}}\, a_{\mathbf{q}\sigma}^{\dagger} . \tag{2.12}$$

The boson commutation relation holds both between the $A_{\mathbf{q}\sigma}$ and $A_{\mathbf{q}\sigma}^{\dagger}$, and between $B_{\mathbf{q}\sigma}$ and $B_{\mathbf{q}\sigma}^{\dagger}$. When the coefficients $\cosh\theta_{\mathbf{q}}$ and $\sinh\theta_{\mathbf{q}}$ satisfy the relations given by

$$\cosh2\theta_{\mathbf{q}}=\frac{\lambda}{\omega_{\mathbf{q}}} , \tag{2.13a}$$

$$\sinh2\theta_{\mathbf{q}}=-\frac{\chi z\gamma_{\mathbf{q}}}{\omega_{\mathbf{q}}} , \tag{2.13b}$$

and

$$\omega_{\mathbf{q}}=[\lambda^2-(\chi z\gamma_{\mathbf{q}})^2]^{1/2} , \tag{2.13c}$$

the remaining part of the Hamiltonian (2.11) can be diagonalized except for the transfer term. The diagonalized part of the Heisenberg exchange interaction term describes a system of low-lying antiferromagnetic magnonlike excitations. After performing the Bogoliubov transformation (2.12), the effective Hamiltonian (2.11) is written as

$$H_{\text{eff}}=\sum_{\mathbf{q}}\sum_{\sigma}(\omega_{\mathbf{q}}-\lambda)+H_0(A^{\dagger},A,B^{\dagger},B,e^{\dagger}e,f^{\dagger},f)+H_1(A^{\dagger},A,B^{\dagger},B,e^{\dagger},e,f^{\dagger},f) , \tag{2.14}$$

where

$$H_0(A^{\dagger},A,B^{\dagger},B,e^{\dagger},e,f^{\dagger},f)=\sum_{\mathbf{q}}\sum_{\sigma}\omega_{\mathbf{q}}(A_{\mathbf{q}\sigma}^{\dagger}A_{\mathbf{q}\sigma}+B_{\mathbf{q}\sigma}^{\dagger}B_{\mathbf{q}\sigma})+(\lambda+\mu)\sum_{\mathbf{q}}(e_{\mathbf{q}}^{\dagger}e_{\mathbf{q}}+f_{\mathbf{q}}^{\dagger}f_{\mathbf{q}}) , \tag{2.15a}$$

and

$$\begin{aligned}
&H_1(A^{\dagger},A,B^{\dagger},B,e^{\dagger},e,f^{\dagger},f)\\
&=-t\frac{1}{N/2}\sum_{\mathbf{q}_1,\mathbf{q}_2,\mathbf{q}_3,\mathbf{q}_4} z\gamma_{\mathbf{q}_1-\mathbf{q}_3}\delta_{\mathbf{q}_1+\mathbf{q}_4-\mathbf{q}_2-\mathbf{q}_3,0}\{\cosh\theta_{\mathbf{q}_2}\cosh\theta_{\mathbf{q}_3}[f_{\mathbf{q}_1}^{\dagger}(A_{\mathbf{q}_2\uparrow}^{\dagger}B_{\mathbf{q}_3\downarrow}-A_{\mathbf{q}_2\downarrow}^{\dagger}B_{\mathbf{q}_3\uparrow})e_{\mathbf{q}_4}\\
&\qquad\qquad -e_{\mathbf{q}_4}^{\dagger}(B_{\mathbf{q}_3\uparrow}^{\dagger}A_{\mathbf{q}_2\downarrow}-B_{\mathbf{q}_3\downarrow}^{\dagger}A_{\mathbf{q}_2\uparrow})f_{\mathbf{q}_1}]\\
&+\sinh\theta_{\mathbf{q}_2}\sinh\theta_{\mathbf{q}_3}[e_{\mathbf{q}_4}^{\dagger}(B_{\mathbf{q}_2\uparrow}^{\dagger}A_{\mathbf{q}_3\downarrow}-B_{\mathbf{q}_2\downarrow}^{\dagger}A_{\mathbf{q}_3\uparrow})f_{\mathbf{q}_1}-f_{\mathbf{q}_1}^{\dagger}(A_{\mathbf{q}_3\uparrow}^{\dagger}B_{\mathbf{q}_2\downarrow}-A_{\mathbf{q}_3\downarrow}^{\dagger}B_{\mathbf{q}_2\uparrow})e_{\mathbf{q}_4}]\\
&-\cosh\theta_{\mathbf{q}_2}\sinh\theta_{\mathbf{q}_3}[f_{\mathbf{q}_1}^{\dagger}(A_{\mathbf{q}_2\uparrow}^{\dagger}A_{\mathbf{q}_3\downarrow}^{\dagger}-A_{\mathbf{q}_2\downarrow}^{\dagger}A_{\mathbf{q}_3\uparrow}^{\dagger})e_{\mathbf{q}_4}-e_{\mathbf{q}_4}^{\dagger}(A_{\mathbf{q}_3\uparrow}A_{\mathbf{q}_2\downarrow}-A_{\mathbf{q}_3\downarrow}A_{\mathbf{q}_2\uparrow})f_{\mathbf{q}_1}]\\
&-\sinh\theta_{\mathbf{q}_2}\cosh\theta_{\mathbf{q}_3}[e_{\mathbf{q}_4}^{\dagger}(B_{\mathbf{q}_2\uparrow}^{\dagger}B_{\mathbf{q}_3\downarrow}^{\dagger}-B_{\mathbf{q}_2\downarrow}^{\dagger}B_{\mathbf{q}_3\uparrow}^{\dagger})f_{\mathbf{q}_1}-f_{\mathbf{q}_1}^{\dagger}(B_{\mathbf{q}_3\uparrow}B_{\mathbf{q}_2\downarrow}-B_{\mathbf{q}_3\downarrow}B_{\mathbf{q}_2\uparrow})e_{\mathbf{q}_4}]\} .
\end{aligned} \tag{2.15b}$$

It is expected, however, that this resulting effective grand canonical Hamiltonian (2.14) describes well a system of holes interacting with antiferromagnetic magnonlike excitations. By substituting the normal-ordered form (2.14) into expression (2.9) of the grand partition function Z_G, we obtain

$$\begin{aligned}
Z_G=&\int d[\lambda]d[\chi]\exp\left\{-\beta N\left[\left[\frac{z}{J}\right]\chi^2-2\lambda-\mu+\frac{1}{2}\frac{1}{N/2}\sum_{\mathbf{q}}\sum_{\sigma}\omega_{\mathbf{q}}\right]\right\}\\
&\times\int_{\substack{a(\beta)=a(0),b(\beta)=b(0)\\ e(\beta)=-e(0),f(\beta)=-f(0)}} d[\bar{a},a]d[\bar{b},b]d[\bar{e},e]d[\bar{f},f]\\
&\times\exp\left[-\int_0^{\beta}d\tau\left\{\sum_{\sigma}\sum_{\mathbf{q}}\left[\bar{A}_{\mathbf{q}\sigma}(\tau)\left[\frac{\partial}{\partial\tau}+\omega_{\mathbf{q}}\right]A_{\mathbf{q}\sigma}(\tau)+\bar{B}_{\mathbf{q}\sigma}(\tau)\left[\frac{\partial}{\partial\tau}+\omega_{\mathbf{q}}\right]B_{\mathbf{q}\sigma}(\tau)\right]\right.\right.\\
&\qquad+\sum_{\mathbf{q}}\left[\bar{e}_{\mathbf{q}}(\tau)\left[\frac{\partial}{\partial\tau}+\lambda+\mu\right]e_{\mathbf{q}}(\tau)+\bar{f}_{\mathbf{q}}(\tau)\left[\frac{\partial}{\partial\tau}+\lambda+\mu\right]f_{\mathbf{q}}(\tau)\right]\\
&\qquad\left.\left.+H_1(\bar{A}(\tau),A(\tau),\bar{B}(\tau),B(\tau),\bar{e}(\tau),e(\tau),\bar{f}(\tau),f(\tau))\right\}\right] .
\end{aligned} \tag{2.16}$$

According to this grand partition function (2.16), we stress that holes with uniform density interact with antiferromagnetic magnonlike excitations because of the neglect of the site-i dependence of the Lagrange multiplier λ_i. This point is important later in discussing the possibility of a phase separation state into a hole-rich and a no-hole phase, which was conjectured by Emery, Kivelson, and Lin.[11]

III. PERTURBATION THEORY FOR $t/J \ll 1$

We first consider the case without the transfer term, i.e., $t=0$. In this case we can immediately calculate the functional integrals in (2.16), and then its grand partition function $Z_G|_{t=0}$ is expressed as

$$Z_G|_{t=0}=\int d[\lambda]d[\chi]\exp\left\{-\beta N\left[\left[\frac{z}{J}\right]\chi^2-2\lambda-\mu+\frac{1}{2}\frac{1}{N/2}\sum_{\mathbf{q}}\sum_{\sigma}\omega_{\mathbf{q}}\right]\right\}\left[\prod_{\mathbf{q}}\prod_{\sigma}(1-e^{-\beta\omega_{\mathbf{q}}})^{-1}\right]^2(1+e^{-\beta(\lambda+\mu)})^N . \quad (3.1)$$

The thermodynamic potential per site, $\Omega_0=-(1/\beta N)\ln Z_G|_{t=0}$, in the steepest-descent approximation becomes

$$\Omega_0=\frac{z}{J}\chi^2-2\lambda-\mu+\frac{1}{2}\frac{1}{N/2}\sum_{\mathbf{q}}\sum_{\sigma}\omega_{\mathbf{q}}+\frac{1}{\beta}\frac{1}{N/2}\sum_{\mathbf{q}}\sum_{\sigma}\ln(1-e^{-\beta\omega_{\mathbf{q}}})-\frac{1}{\beta}\ln(1+e^{-\beta(\lambda+\mu)}) . \quad (3.2)$$

This expression describes a noninteracting system of antiferromagnetic magnonlike excitations and holes with uniform density. The saddle-point equations determining self-consistent values of λ_0, χ_0, and μ_0 for the case of $t=0$ are to be derived from the minimization relations $\partial\Omega_0/\partial\lambda=0$, $\partial\Omega_0/\partial\chi=0$, and the chemical potential relation $1-\delta=-\partial\Omega_0/\partial\mu$ in which δ denotes the hole concentration per site $\delta=\langle[1/(N/2)](\sum_{i\in A}e_i^\dagger e_i+\sum_{i\in B}f_i^\dagger f_i)\rangle$. Thus we have the self-consistent equations with respect to λ_0, χ_0, and μ_0:

$$1-\frac{\delta}{2}=\frac{1}{2}\sum_{\mathbf{q}}\sum_{\sigma}\cosh 2\theta_{\mathbf{q}}^0\left[\frac{1}{e^{\beta\omega_{\mathbf{q}}^0}-1}+\frac{1}{2}\right] , \quad (3.3a)$$

$$\frac{z\chi_0}{J}=-\frac{1}{2}\sum_{\mathbf{q}}\sum_{\sigma}z\gamma_{\mathbf{q}}\sinh 2\theta_{\mathbf{q}}^0\left[\frac{1}{e^{\beta\omega_{\mathbf{q}}^0}-1}+\frac{1}{2}\right] , \quad (3.3b)$$

and

$$\delta=\frac{1}{e^{\beta(\lambda_0+\mu_0)}+1} . \quad (3.3c)$$

Here $\omega_{\mathbf{q}}^0=[\lambda_0^2-(\chi_0 z\gamma_{\mathbf{q}})^2]^{1/2}$, $\cosh 2\theta_{\mathbf{q}}^0=\lambda_0/\omega_{\mathbf{q}}^0$, and $\sinh 2\theta_{\mathbf{q}}^0=-\chi_0 z\gamma_{\mathbf{q}}/\omega_{\mathbf{q}}^0$. These self-consistent equations (3.3a)–(3.3c), which have been derived by introducing the contribution of holes with uniform density, are the extension of the ones which were obtained for the antiferromagnetic Heisenberg model with spin $S=\frac{1}{2}$ by Arovas and Auerbach[6] and Takahashi.[8]

We now investigate a system of the antiferromagnetic magnonlike excitations interacting with holes with uniform density. Under the assumption of $t/J \ll 1$, now, we apply a perturbation theory to the grand partition function Z_G of (2.16). That is, let us consider the transfer term H_1 as a perturbation. As a result, we have the following perturbation formula:

$$\begin{aligned}Z_G&=\int d[\lambda]d[\chi]\exp\left\{-\beta N\left[\left[\frac{z}{J}\right]\chi^2-2\lambda-\mu+\frac{1}{2}\frac{1}{N/2}\sum_{\mathbf{q}}\sum_{\sigma}\omega_{\mathbf{q}}\right]\right\}\\&\quad\times Z_{G0}\left\langle\exp\left[-\int_0^\beta d\tau H_1(\bar{A}(\tau),A(\tau),\bar{B}(\tau),B(\tau),\bar{e}(\tau),e(\tau),\bar{f}(\tau),f(\tau))\right]\right\rangle_0\\&=\int d[\lambda]d[\chi]\exp\left\{-\beta N\left[\left[\frac{z}{J}\right]\chi^2-2\lambda-\mu+\frac{1}{2}\frac{1}{N/2}\sum_{\mathbf{q}}\sum_{\sigma}\omega_{\mathbf{q}}\right]\right\}\\&\quad\times Z_{G0}\sum_{n=0}^{\infty}\frac{(-1)^n}{n!}\int_0^\beta d\tau_1\cdots d\tau_n\langle H_1(\bar{A}(\tau_1),\ldots,f(\tau_1))\cdots H_1(\bar{A}(\tau_n),\ldots,f(\tau_n))\rangle_0 ,\end{aligned} \quad (3.4)$$

where the unperturbed grand partition function Z_{G0} is given by

$$Z_{G0}=\int_{\substack{a(\beta)=a(0),b(\beta)=b(0)\\ e(\beta)=-e(0),f(\beta)=-f(0)}} d[\bar{a},a]d[\bar{b},b]d[\bar{e},e]d[\bar{f},f]$$

$$\times\exp\left[-\int_0^\beta d\tau\left\{\sum_\sigma\sum_{\mathbf{q}}\left[\bar{A}_{\mathbf{q}\sigma}(\tau)\left[\frac{\partial}{\partial\tau}+\omega_{\mathbf{q}}\right]A_{\mathbf{q}\sigma}(\tau)+\bar{B}_{\mathbf{q}\sigma}(\tau)\left[\frac{\partial}{\partial\tau}+\omega_{\mathbf{q}}\right]B_{\mathbf{q}\sigma}(\tau)\right]\right.\right.$$

$$\left.\left.+\sum_{\mathbf{q}}\left[\bar{e}_{\mathbf{q}}(\tau)\left[\frac{\partial}{\partial\tau}+\lambda+\mu\right]e_{\mathbf{q}}(\tau)+\bar{f}_{\mathbf{q}}(\tau)\left[\frac{\partial}{\partial\tau}+\lambda+\mu\right]f_{\mathbf{q}}(\tau)\right]\right\}\right], \quad (3.5)$$

and for a certain quantity $Q(\bar{A}(\tau_1),\ldots,f(\tau_n))$ we have defined the thermal average $\langle Q\rangle_0$ in the unperturbed Hamiltonian by

$$\langle Q\rangle_0=\frac{1}{Z_{G0}}\int_{\substack{a(\beta)=a(0),b(\beta)=b(0)\\ e(\beta)=-e(0),f(\beta)=-f(0)}} d[\bar{a},a]d[\bar{b},b]d[\bar{e},e]d[\bar{f},f]$$

$$\times\exp\left[-\int_0^\beta d\tau\left\{\sum_\sigma\sum_{\mathbf{q}}\left[\bar{A}_{\mathbf{q}\sigma}(\tau)\left[\frac{\partial}{\partial\tau}+\omega_{\mathbf{q}}\right]A_{\mathbf{q}\sigma}(\tau)+\bar{B}_{\mathbf{q}\sigma}(\tau)\left[\frac{\partial}{\partial\tau}+\omega_{\mathbf{q}}\right]B_{\mathbf{q}\sigma}(\tau)\right]\right.\right.$$

$$\left.\left.+\sum_{\mathbf{q}}\left[\bar{e}_{\mathbf{q}}(\tau)\left[\frac{\partial}{\partial\tau}+\lambda+\mu\right]e_{\mathbf{q}}(\tau)+\bar{f}_{\mathbf{q}}(\tau)\left[\frac{\partial}{\partial\tau}+\lambda+\mu\right]f_{\mathbf{q}}(\tau)\right]\right\}\right]$$

$$Q(\bar{A}(\tau_1),\ldots,f(\tau_n)) . \quad (3.6)$$

At the moment it seems to be impossible to calculate systematically terms higher in order than the third order. We will take only contributions up to the second-order term of $O(t/J)^2)$ into consideration. We find immediately that the contribution of the first-order term vanishes. To calculate the second-order term, let us introduce the following single-particle thermal Green's functions:

$$\langle A_{\mathbf{q}\sigma}(\tau)\bar{A}_{\mathbf{q}'\sigma'}(\tau')\rangle_0=\langle B_{\mathbf{q}\sigma}(\tau)\bar{B}_{\mathbf{q}'\sigma'}(\tau')\rangle_0\equiv\delta_{\mathbf{q}\mathbf{q}'}\delta_{\sigma\sigma'}G_{0\mathbf{q}}(\tau-\tau') , \quad (3.7a)$$

and

$$\langle e_{\mathbf{q}}(\tau)\bar{e}_{\mathbf{q}'}(\tau')\rangle_0=\langle f_{\mathbf{q}}(\tau)\bar{f}_{\mathbf{q}'}(\tau')\rangle_0\equiv\delta_{\mathbf{q}\mathbf{q}'}g_0(\tau-\tau') . \quad (3.7b)$$

Here $G_{0\mathbf{q}}(\tau-\tau')$ in (3.7a) and $g_0(\tau-\tau')$ in (3.7b) are given by

$$G_{0\mathbf{q}}(\tau-\tau')=e^{-\omega_{\mathbf{q}}(\tau-\tau')}[\theta(\tau-\tau'-\eta)(1+n_{\mathbf{q}})+\theta(\tau'-\tau+\eta)n_{\mathbf{q}}] ,$$

and

$$g_0(\tau-\tau')=e^{-(\lambda+\mu)(\tau-\tau')}[\theta(\tau-\tau'-\eta)(1-\tilde{n}_h)-\theta(\tau'-\tau+\eta)\tilde{n}_h] ,$$

respectively. These Green's functions have been evaluated straightforwardly by introducing the step function $\theta(\cdots)$ and the limit $\eta\rightarrow 0+$ at equal time. The expression $n_{\mathbf{q}}$ denotes the Bose distribution function $n_{\mathbf{q}}=1/(e^{\beta\omega_{\mathbf{q}}}-1)$ for an antiferromagnetic magnonlike excitation, while $\tilde{n}_h$ denotes the Fermi distribution function $\tilde{n}_h=1/(e^{\beta(\lambda+\mu)}+1)$ for a hole as a spinless fermion. By using these single-particle thermal Green's functions, we can thus write the total grand partition function Z_G up to $O((t/J)^2)$ as follows:

$$Z_G=\int d[\lambda]d[\chi]\exp\left\{-\beta N\left[\left[\frac{z}{J}\right]\chi^2-2\lambda-\mu+\frac{1}{2}\frac{1}{N/2}\sum_{\mathbf{q}}\sum_\sigma\omega_{\mathbf{q}}\right]\right\}$$

$$\times\left[\prod_{\mathbf{q}}\prod_\sigma(1-e^{-\beta\omega_{\mathbf{q}}})^{-1}\right]^2\left[1+e^{-\beta(\lambda+\mu)}\right]^N(1+Z_{G2}) , \quad (3.8)$$

where the contribution Z_{G2} of the second order in (3.8) is given as

$$Z_{G2} = -(tz)^2 \int_0^\beta d\tau_1 d\tau_2 \frac{1}{(N/2)^2} \times \sum_{\mathbf{q}_1,\mathbf{q}_2,\mathbf{q}_3,\mathbf{q}_4} \delta_{\mathbf{q}_1+\mathbf{q}_4-\mathbf{q}_2-\mathbf{q}_3,0}\, g_0(\tau_2-\tau_1) g_0(\tau_1-\tau_2) \frac{\gamma_{\mathbf{q}_1-\mathbf{q}_3}}{2}$$
$$\times \{ [\gamma_{\mathbf{q}_1-\mathbf{q}_3}(\cosh 2\theta_{\mathbf{q}_2}\cosh 2\theta_{\mathbf{q}_3}+1) - \gamma_{\mathbf{q}_1-\mathbf{q}_2}\sinh 2\theta_{\mathbf{q}_2}\sinh 2\theta_{\mathbf{q}_3}]$$
$$\times [G_{0\mathbf{q}_2}(\tau_2-\tau_1)G_{0\mathbf{q}_3}(\tau_1-\tau_2) + G_{0\mathbf{q}_2}(\tau_1-\tau_2)G_{0\mathbf{q}_3}(\tau_2-\tau_1)]$$
$$+ [\gamma_{\mathbf{q}_1-\mathbf{q}_3}(\cosh 2\theta_{\mathbf{q}_2}\cosh 2\theta_{\mathbf{q}_3}-1) - \gamma_{\mathbf{q}_1-\mathbf{q}_2}\sinh 2\theta_{\mathbf{q}_2}\sinh 2\theta_{\mathbf{q}_3}]$$
$$\times [G_{0\mathbf{q}_2}(\tau_2-\tau_1)G_{0\mathbf{q}_3}(\tau_2-\tau_1) + G_{0\mathbf{q}_2}(\tau_1-\tau_2)G_{0\mathbf{q}_3}(\tau_1-\tau_2)]\} . \tag{3.9}$$

When we introduce the following frequency representation for the bosonic Green's function $G_{0\mathbf{q}}(\tau-\tau')$ of the antiferromagnetic magnonlike excitation,

$$G_{0\mathbf{q}}(\tau-\tau') = \frac{-1}{\beta} \sum_{\omega_n} e^{-i\omega_n(\tau-\tau')} \frac{1}{i\omega_n - \omega_\mathbf{q}} ,$$

with $\omega_n = 2n\pi/\beta$, and also introduce the following one for the fermionic Green's function $g_0(\tau-\tau')$ of the hole,

$$g_0(\tau-\tau') = \frac{-1}{\beta} \sum_{\nu_n} e^{-i\nu_n(\tau-\tau')} \frac{1}{i\nu_n - (\lambda+\mu)} ,$$

with $\nu_n = (2n+1)\pi/\beta$, expression (3.9) can be written as

$$Z_{G2} = \frac{1}{2}\beta N \frac{-1}{\beta} \sum_{\nu_n} \frac{1}{i\nu_n - (\lambda+\mu)} V_{\text{eff}}^{\text{hole}}(\nu_n - \nu_n') \frac{-1}{\beta} \sum_{\nu_n} \frac{1}{i\nu_n' - (\lambda+\mu)} . \tag{3.10}$$

In (3.10) the effective potential $V_{\text{eff}}^{\text{hole}}$ that denotes interaction between holes is given by

$$V_{\text{eff}}^{\text{hole}}(\nu_n - \nu_n')$$
$$= (tz)^2 \frac{1}{(N/2)^3} \sum_{\mathbf{q}_1,\mathbf{q}_2,\mathbf{q}_3} \frac{\gamma_{\mathbf{q}_1-\mathbf{q}_3}}{2} \Bigg[[\gamma_{\mathbf{q}_1-\mathbf{q}_3}(\cosh 2\theta_{\mathbf{q}_2}\cosh 2\theta_{\mathbf{q}_3}+1) - \gamma_{\mathbf{q}_1-\mathbf{q}_2}\sinh 2\theta_{\mathbf{q}_2}\sinh 2\theta_{\mathbf{q}_3}]$$
$$\times \left[\frac{1}{e^{\beta\omega_{\mathbf{q}_2}}-1} - \frac{1}{e^{\beta\omega_{\mathbf{q}_3}}-1} \right] \left[\frac{1}{i(\nu_n-\nu_n')+\omega_{\mathbf{q}_2}-\omega_{\mathbf{q}_3}} - \frac{1}{i(\nu_n-\nu_n')-\omega_{\mathbf{q}_2}+\omega_{\mathbf{q}_3}} \right]$$
$$- [\gamma_{\mathbf{q}_1-\mathbf{q}_3}(\cosh 2\theta_{\mathbf{q}_2}\cosh 2\theta_{\mathbf{q}_3}-1) - \gamma_{\mathbf{q}_1-\mathbf{q}_2}\sinh 2\theta_{\mathbf{q}_2}\sinh 2\theta_{\mathbf{q}_3}]$$
$$\times \left[\frac{1}{e^{\beta\omega_{\mathbf{q}_2}}-1} - \frac{1}{e^{-\beta\omega_{\mathbf{q}_3}}-1} \right] \left[\frac{1}{i(\nu_n-\nu_n')+\omega_{\mathbf{q}_2}+\omega_{\mathbf{q}_3}} - \frac{1}{i(\nu_n-\nu_n')-\omega_{\mathbf{q}_2}-\omega_{\mathbf{q}_3}} \right] \Bigg] . \tag{3.11}$$

Furthermore, by summing with respect to the imaginary frequencies, calculation of (3.11) gives the following more compact form for the Z_{G2}:

$$Z_{G2} = -\beta N (tz)^2 \tilde{n}_h (1-\tilde{n}_h) \frac{1}{(N/2)^3}$$
$$\times \sum_{\mathbf{q}_1,\mathbf{q}_2,\mathbf{q}_3} \frac{\gamma_{\mathbf{q}_1-\mathbf{q}_3}}{2} \Bigg\{ [\gamma_{\mathbf{q}_1-\mathbf{q}_3}(\cosh 2\theta_{\mathbf{q}_2}\cosh 2\theta_{\mathbf{q}_3}+1) - \gamma_{\mathbf{q}_1-\mathbf{q}_2}\sinh 2\theta_{\mathbf{q}_2}\sinh 2\theta_{\mathbf{q}_3}](n_{\mathbf{q}_2} - n_{\mathbf{q}_3}) \frac{1}{\omega_{\mathbf{q}_2}-\omega_{\mathbf{q}_3}}$$
$$- [\gamma_{\mathbf{q}_1-\mathbf{q}_3}(\cosh 2\theta_{\mathbf{q}_2}\cosh 2\theta_{\mathbf{q}_3}-1) - \gamma_{\mathbf{q}_1-\mathbf{q}_2}\sinh 2\theta_{\mathbf{q}_2}\sinh 2\theta_{\mathbf{q}_3}](n_{\mathbf{q}_2} + n_{\mathbf{q}_3} + 1) \frac{1}{\omega_{\mathbf{q}_2}+\omega_{\mathbf{q}_3}} \Bigg\} . \tag{3.12}$$

Consequently, the thermodynamic potential per site, $\Omega = -(1/\beta N)\ln Z_G$, up to $O((t/J)^2)$ in the steepest-descent approximation is

$$\Omega=\left[\frac{z}{J}\right]\chi^2-2\lambda-\mu+\frac{1}{2}\frac{1}{N/2}\sum_{q}\sum_{\sigma}\omega_{q}+\frac{1}{\beta}\frac{1}{N/2}\sum_{q}\sum_{\sigma}\ln(1-e^{-\beta\omega_{q}})-\frac{1}{\beta}\ln(1+e^{-\beta(\lambda+\mu)})$$
$$+(tz)^2\bar{n}_h(1-\bar{n}_h)\frac{1}{(N/2)^3}$$
$$\times\sum_{q_1,q_2,q_3}\frac{\gamma_{q_1-q_3}}{2}\Bigg\{[\gamma_{q_1-q_3}(\cosh 2\theta_{q_2}\cosh 2\theta_{q_3}+1)-\gamma_{q_1-q_2}\sinh 2\theta_{q_2}\sinh 2\theta_{q_3}]$$
$$\times(n_{q_2}-n_{q_3})\frac{1}{\omega_{q_2}-\omega_{q_3}}-[\gamma_{q_1-q_3}(\cosh 2\theta_{q_2}\cosh 2\theta_{q_3}-1)-\gamma_{q_1-q_2}\sinh 2\theta_{q_2}\sinh 2\theta_{q_3}]$$
$$\times(n_{q_2}+n_{q_3}+1)\frac{1}{\omega_{q_2}+\omega_{q_3}}\Bigg\}. \tag{3.13}$$

The first part of the perturbation term proportional to t^2 in (3.13) gives the contribution from one magnonlike excitation, while the second part gives the contribution from two magnonlike excitations. From the thermodynamic potential Ω of (3.13) up to the second order $O(t/J)^2$), the saddle-point equations determining self-consistent values of λ, χ, and μ are to be derived by calculating the minimization relations $\partial\Omega/\partial\lambda=0$ and $\partial\Omega/\partial\chi=0$, and the chemical potential relation $1-\delta=-\partial\Omega/\partial\mu$ with hole concentration per site δ. Although we can write explicit expressions of these three self-consistent equations with respect to λ, χ, and μ, they are very complicated equations. At the moment it seems to be very difficult to treat them analytically and even numerically.

It is convenient to calculate the free energy per site F from the thermodynamic potential per site Ω by using a thermodynamic formula $F=\Omega+\mu(1-\delta)$. It enables one to compare the free energy F at sufficiently low temperature with the ground-state energy E at $T=0$.

IV. APPLICATION TO THE ONE-DIMENSIONAL CASE

We apply the formulas obtained in Sec. III to the one-dimensional t-J model. The t-J model for the case of $t=0$ (i.e., without the transfer term) describes the Heisenberg spin system together with holes with a uniform density. If the hole concentration δ is zero, it reduces to the pure Heisenberg spin model. Then the self-consistent equations (3.3a) and (3.3b) at $T=0$ can be written in a compact form by using the complete elliptic integrals $K(m)$ and $E(m)$ of the first and second kind, respectively. Taking $m=(z\chi_0/\lambda_0)^2$, we have the corresponding equations:

$$\pi=K(m)\,, \tag{4.1a}$$

$$\frac{\lambda_0}{J}=\frac{\pi-E(m)}{(\pi/2)m}\,. \tag{4.1b}$$

These equations [(4.1a) and (4.1b)] obtained for the one-dimensional antiferromagnetic Heisenberg model are equivalent to the ones which were derived by Arovas and Auerbach.[6] A solution for them is

$$\frac{\lambda_0}{J}=1.3800,\quad \frac{\chi_0}{J}=0.6793\,. \tag{4.2}$$

And then the index m which illustrates degree of gaplessness (rigorously gapless as $m=1.0$) has got $m=0.9691$. Although the excitation spectrum for the one-dimensional antiferromagnetic Heisenberg model must be rigorously gapless (i.e., des Cloizeaux-Pearson magnon spectrum) according to rigorous theory,[13] the approximation used in this paper indicates that one has obtained a very small but finite gap. We have called this excitation the antiferromagnetic magnonlike excitation because it is almost gapless. Although a rigorous value of the ground-state energy E_0 of the antiferromagnetic Heisenberg spin model is $-\ln 2$ also, the approximate value of E_0 obtained here is

$$E_0^{gs}=-0.9228 \tag{4.3}$$

which is lower than the rigorous value.

Next we examine the Heisenberg spin system in the presence of holes with a uniform density. For an arbitrary value of hole concentration δ in $0\le\delta\le 1$, we have to solve numerically the self-consistent equations (3.3a)–(3.3c) with $t=0$ at sufficiently low temperature $T/J=0.01$. The results calculated numerically for the dependence of the auxiliary field χ_0 and the Lagrange multiplier λ_0 on δ are shown in Figs. 1 and 2, respective-

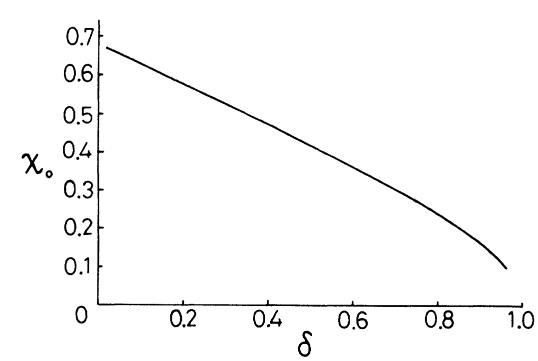

FIG. 1. Dependence of χ_0 on hole concentration δ at sufficiently low temperature $T/J=0.01$, when we consider the one-dimensional t-J model without taking the transfer part into consideration (i.e., with $t=0$).

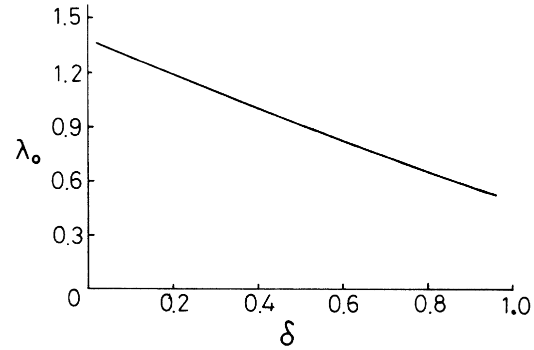

FIG. 2. Dependence of μ_0 on hole concentration δ at sufficiently low temperature $T/J = 0.01$, when we consider the one-dimensional t-J model without taking the transfer part into consideration (i.e., with $t = 0$).

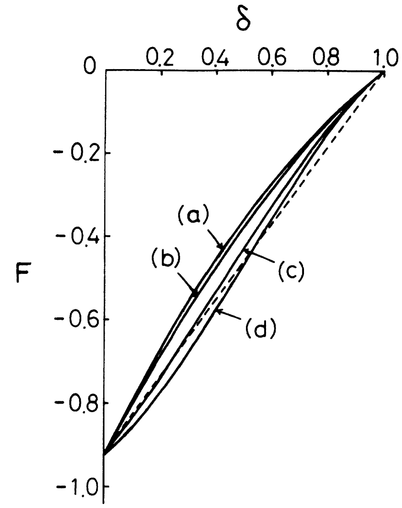

FIG. 4. Dependences of the free energy F on hole concentration δ at sufficiently low temperature $T/J = 0.01$, when we consider the one-dimensional t-J model. The curves (a), (b), (c), and (d) are the ones for the case of $t/J = 0$, 0.4, 0.8, and 1.0, respectively; the dotted straight line denotes a curve conjectured under the existence of the phase-separation state into a hole-rich and a no-hole phase.

ly. By using these numerical results of χ_0 and λ_0, the δ dependence of the index m, which represents the degree of gaplessness, is evaluated and is shown in Fig. 3. The values of χ_0 and λ_0 in the limit of $\delta = 0$ approach the corresponding values of the pure Heisenberg spin model in (4.2), respectively. Also, the value of m in the same limit approaches $m = 0.9691$. The result calculated numerically for the δ dependence of the free energy per site, $F_0 = \Omega_0 + \mu_0(1-\delta)$, at sufficiently low temperature $T/J = 0.01$, for the case of $t = 0$, is shown by (a) in Fig. 4. The limiting value of F_0 at $\delta = 0$ approaches the approximate value (4.3) of the ground-state energy of the pure Heisenberg spin model. Let us consider next the δ dependences at sufficiently low temperature $T/J = 0.01$ for the case of $t = 0$. As seen in Figs. 1 and 2, both χ_0 and λ_0 decrease almost linearly as the hole concentration δ increases from 0.02 to 0.96. The value of χ_0 is seen to rapidly approach to zero as δ becomes near one (i.e., as only holes exist), because it describes the auxiliary field for the resulting spin singlet generated with the insertion of a hole. We see from Fig. 3 that as δ increases from 0.02 to 0.96, the degree m of gaplessness deviates more and more from $m = 1$, and so the magnonlike excitation becomes more and more massive. The corresponding result on the free energy F_0 which is shown by (a) in Fig. 4 indicates an upward convex curve connected between the value $F_0 = 0$ at $\delta = 1$ and the extrapolated value of F_0 sufficiently near (4.3) at $\delta = 0$.

We can make the following considerations on this behavior of the free energy F_0. According to a recent study on the t-J model due to Emery, Kivelson, and Lin,[11] and Imada,[12] it is suggested that, in the region of small t/J, such a mean-field state with a uniform antiferromagnetic ordering over the whole lattice obtained above is unstable against phase separation into a hole-rich and a no-hole phase. This phase-separation state means that all of the doped holes exist in one phase, while the other phase is the undoped pure antiferromagnetic Heisenberg spin system. Under the conditions of this phase separation, we can conjecture a straight line connecting between the values at $\delta = 1$ and 0 for the δ dependence of the ground-state energy E_0. However, we find that our actual curve [Fig. 4(a)] of the case $t/J = 0$ of the free energy F_0, which is obtained at sufficiently low temperature, lies higher in energy than the expected straight line in the region of $0 < \delta < 1$. Note that the curve we have obtained is the one derived by solving numerically the self-consistent equations (3.3a)–(3.3c) under the assumption that the mean-field state is uniform over the whole lattice. We thus conclude that when we neglect the transfer term (i.e., for the case of $t = 0$), the phase-separation state conjectured by Emery, Kivelson, and Lin appears in the region of $0 < \delta < 1$.

Taking account of the transfer term, now, let us consider the case of $t \neq 0$ based on the perturbation theory developed in Sec. III. We pay attention to the expression (3.13) of the thermodynamic potential Ω up to the second order $O((t/J)^2)$ for $t/J \ll 1$. As a matter of fact, we have to solve the self-consistent equations determining

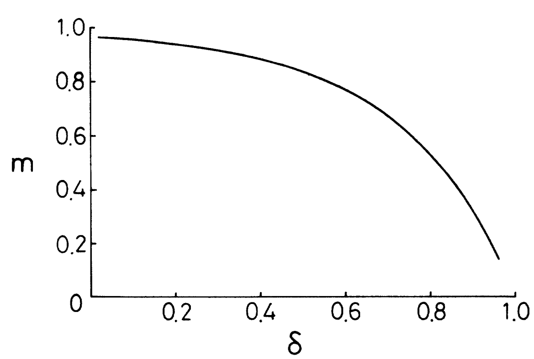

FIG. 3. Dependence of the gapless index m on hole concentration δ at sufficiently low temperature $T/J = 0.01$, when we consider the one-dimensional t-J model without taking the transfer part into consideration (i.e., with $t = 0$).

the values of λ, χ, and μ to be derived from the minimization relations $\partial\Omega/\partial\lambda=0$ and $\partial\Omega/\partial\chi=0$, and the chemical potential relation $1-\delta=-\partial\Omega/\partial\mu$ with a hole concentration δ of uniform density. But it is very difficult to solve them even numerically. By substituting the above numerical results of λ_0, χ_0, and μ_0, which we have obtained for the case of $t=0$, it is therefore possible to estimate a contribution of the second-order perturbation of t/J to the free energy $F=\Omega+\mu(1-\delta)$. Such an estimation corresponds to neglecting the renormalizations of λ, χ, and μ, which are caused by taking the transfer term into consideration. The δ dependences of the free energy F up to the second order $O((t/J)^2)$ calculated under this estimation are given in Fig. 4 for various values of $t/J=0.4$, 0,8, and 1.0 at sufficiently low temperature $T/J=0.01$. As the transfer term is introduced, we find that in the region of $0<\delta<1$ the free energy F for $t\neq 0$ becomes lower than the one F_0 at $t=0$. For comparatively large t/J there is a possibility that the free energy F becomes lower than the conjectured straight line of the phase separation state by Emery, Kivelson, and Lin[11] in the region of small δ. We then find that the contribution to lowering of the free energy is dominant at sufficiently low temperature from the term of two magnonlike excitations in (3.13). Thus for the small transfer t/J the phase-separation state is stable for arbitrary hole concentration, but we may conclude that the introduction of the large transfer t/J supports an appearance of the mean-field state, uniform over the whole lattice for small hole concentration, while the phase-separation state remains elsewhere.

V. CONCLUSIONS AND FUTURE PROBLEMS

We have extended the Arovas and Auerbach approach[6] for the Heisenberg spin model to the t-J model which has a strong possibility of describing an essential mechanism of the high-T_c superconductivity. By applying the approximation of the mean-field state with uniform antiferromagnetic ordering over the whole lattice to the J term (i.e., the Heisenberg spin part) in the t-J model, we have developed the perturbation theory with respect to the t term (i.e., the transfer one) for $t \ll J$. As a consequence we have obtained the self-consistent equations containing the hole concentration δ which are effective for $t \ll J$. Up to now, the self-consistent equations have been numerically solved only for the one-dimensional t-J model, and then the δ dependences of various physical quantities have been obtained. Specifically, the study of the contribution of the transfer part to the free energy has indicated that the two magnonlike excitations have a much more dominant contribution than the one magnonlike one at sufficiently low temperature. If the magnitude t of the transfer term is not too large, then there is not a realization of the mean-field state with uniform antiferromagnetic ordering over the whole lattice but the phase-separation state with coexisting hole-rich and no-hole phases for arbitrary hole concentration. If its magnitude t becomes large enough, we have the possibility that the uniform mean-field state appears in the region of small hole concentration, while the phase separation state remains elsewhere.

As a matter of fact, with respect to the high-T_c superconductivity, we are particularly interested in solving the corresponding self-consistent equations numerically for the two-dimensional t-J model. Although we have applied an approximation of uniform mean-field to the J term in the t-J model in the finite-temperature functional-integral formalism, it is expected that a result for the two-dimensional t-J model is a better approximation than for the one-dimensional t-J model from the point of view of mean-field theory. This is our future problem.

ACKNOWLEDGMENTS

I would like to thank the Theoretical Condensed Matter Physics Group at Eidgenössiche Technische Hochschule (ETH) for warm hospitality. I would like also to acknowledge many helpful discussions with Professor T. M. Rice and Dr. M. Ogata. I am particularly grateful to Professor T. M. Rice for many useful comments on the manuscript. The Swiss National Fond is gratefully acknowledged for financial support.

*Present address: Laboratory of Mathematics, Meiji College of Pharmacy, Nozawa, Tokyo 154, Japan.

[1]P. A. Lee, in *Mechanism of High Temperature Superconductivity*, Vol. 11 of *Springer Series in Material Science*, edited by H. Kamimura and A. Oshiyama (Springer-Verlag, Berlin, 1989), p. 383.

[2]C. Gros, R. Joynt, and T. M. Rice, Phys. Rev. B **36**, 381 (1987).

[3]Z. Zou and P. W. Anderson, Phys. Rev. B **37**, 627 (1988).

[4]T. Matsui, Int. J. Mod. Phys. B **1**, 613 (1988).

[5]D. Yoshioka, J. Phys. Soc. Jpn. **58**, 32 (1989); **58**, 1516 (1989).

[6]D. P. Arovas and A. Auerbach, Phys. Rev. B **38**, 316 (1988).

[7]F. C. Zhang and T. M. Rice, Phys. Rev. B **37**, 3759 (1988).

[8]M. Takahashi, Prog. Theor. Phys. Suppl. **87**, 233; Phys. Rev. Lett. **58**, 168 (1987); Phys. Rev. B **40**, 2494 (1989).

[9]R. Birgeneau and G. Shirane, in *Physical Properties of High Temperature Superconductors*, edited by D. M. Ginsberg (World Scientific, Singapore, 1989); H. R. Ott, in Ref. 1, p. 376.

[10]J. W. Negele and H. Orland, *Quantum Many-Particle Systems* (Addison-Wesley, Reading, MA, 1988).

[11]V. J. Emery, S. A. Kivelson, and H. Q. Lin, Phys. Rev. Lett. **64**, 475 (1990).

[12]M. Imada, *Proceedings of the International Workshop on Quantum Simulations of Condensed Matter Phenomena*, edited by J. D. Doll and J. E. Gubernatis (World Scientific, Singapore, 1990), p. 127.

[13]J. des Cloizeaux and J. J. Pearson, Phys. Rev. **128**, 2131 (1962).