Anomalous paramagnetic phase of the Hubbard model

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A strong-coupling regime of the Hubbard model around half filling is investigated in the Hartree-Fock random-phase approximation. At half filling, besides a normal solution that gives rise to antiferromagnetic instability at $T=T_{\mathrm{N}}^{\mathrm{RPA}}\sim U$, we find a solution representing the paramagnetic phase of the Mott insulator, for which we obtain the Néel temperature $T_{\mathrm{N}}\sim J$ in three-dimensional lattices. The solution is interpreted as the ferromagnetic band insulator depolarized by spin wave, the bound state of a particle-hole pair. Similarly, an anomalous metallic phase is derived from the Nagaoka ferromagnetic state. We evaluate T_{N} as a function of doping concentration x to find that it vanishes at $x\simeq 0.05$ for $U/6t=4$ in a simple cubic lattice. [S0163-1829(99)00604-9]

I. INTRODUCTION

Normal-state properties of the underdoped region of high-T_c cuprates have attracted a lot of current interest. It is experimentally and theoretically suggested that the metallic state adjacent to an insulating antiferromagnetic phase is so anomalous that it is better interpreted as a doped Mott insulator than as a conventional metal described by Fermi-liquid theory. In the former, an electric current is regarded to be carried by holes doped in a parent magnetic insulator, as in doped semiconductors. This feature is adequately embodied in the t-J model, but, unfortunately, it has not yet been reached a consensus whether a conventional perturbation theory starting from an uncorrelated normal metal is adequate or not as a canonical framework to attack this problem.

In this paper, we study a paramagnetic phase of the single-band Hubbard model,

$$H=-t\sum_{\langle i,j\rangle,\sigma} c_{i\sigma}^{\dagger}c_{j\sigma}+U\sum_{i}\hat{n}_{i\uparrow}\hat{n}_{i\downarrow}, \tag{1}$$

particularly in the strong-coupling regime $U\gg W$, where W is the bandwidth $W\simeq 4dt$. For one electron per site, it is well known that the model is mapped to the antiferromagnetic Heisenberg model,

$$\tilde{H}=2J\sum_{\langle i,j\rangle}\left(\hat{\mathbf{S}}_i\cdot\hat{\mathbf{S}}_j-\frac{1}{4}\right), \tag{2}$$

with the coupling constant $J\equiv 2t^2/U$. This is a model for an insulating magnet, while the model (1) generally describes itinerant electron systems.

The antiferromagnetic coupling $J\propto U^{-1}$ is usually derived by means of the second-order virtual processes, which are operative for the otherwise decoupled localized spins.[1] In short, this is perturbation theory in U^{-1} around the insulating limit $U=\infty$, in contrast to the conventional perturbation theory from a metallic side $U=0$. We note that this kind of derivation of J, though physically sound, presupposes one of the essential properties inherent in magnetic insulators, that electrons do not move around freely so that they are well described in real-space representation at the outset. For the same reason, anomalous properties of doped systems had better be justified without recourse to the t-J model, since the property of our concern, that of an anomalous metal as a doped insulator, is already incorporated in that model. As it is still controversial if the two approaches, from the strong- and weak-coupling limits, are compatible with each other, it is highly desirable to clarify how insulating and anomalous metallic properties dictated by superexchange interactions are derived in the conventional-diagram technique based on the formal perturbation theory in powers of U. This problem is addressed in this paper.

To begin with, let us note several points, which are related to the subject and results of this paper. First, the model (2) is rewritten

$$\tilde{H}=\sum_{q}\omega_q\tilde{b}_q^{\dagger}\tilde{b}_q+2J\sum_{\langle i,j\rangle}\tilde{b}_i^{\dagger}\tilde{b}_i\tilde{b}_j^{\dagger}\tilde{b}_j, \tag{3}$$

$$\omega_q=-J\sum_{\bar{\delta}}(1-e^{iq\bar{\delta}}), \tag{4}$$

in terms of the Holstein-Primakoff bosons,

$$2\hat{S}_{zi}=1-2\tilde{b}_i^{\dagger}\tilde{b}_i,\quad \hat{S}_i^{+}=\tilde{b}_i,\quad \hat{S}_i^{-}=\tilde{b}_i^{\dagger}, \tag{5}$$

where $\tilde{b}_i$ and $\tilde{b}_i^{\dagger}$ are the annihilation and creation operator of a hard-core boson. The operator $\tilde{b}_i^{\dagger}$ acts on the ferromagnetic vacuum,

$$|F\rangle=\prod_i|\uparrow_i\rangle, \tag{6}$$

to create the state $|\downarrow_i\rangle=\tilde{b}_i^{\dagger}|\uparrow_i\rangle$. The sum in Eq. (4) is taken over the nearest-neighbor vectors $\bar{\delta}$. For example, in a simple cubic lattice, we have

$$\omega_q=-2J(3-\cos q_x-\cos q_y-\cos q_z), \tag{7}$$

which takes the minimum $-12J$ at $\mathbf{q}=\mathbf{Q}=(\pi,\pi,\pi)$. The Bose-Einstein condensate of the boson $\tilde{b}_{\mathbf{Q}}^{\dagger}$ corresponds to the Néel ordered phase. Above the Néel temperature T_{N}, it is

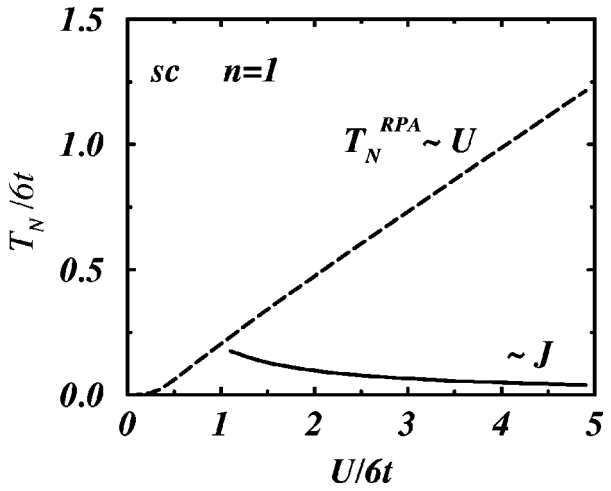

FIG. 1. The Néel temperature T_N as a function of U for the Hubbard model in a simple cubic lattice at half filling. Dashed curve, the result of the RPA. In a correct theory, T_N should decrease for $U\to\infty$, as indicated by the solid curve. See the text for the solid curve: $T_N=3.46J=6.92t^2/U$.

expected on physical grounds that the paramagnetic phase with $2\langle\hat{S}_{zi}\rangle=1-2\langle\tilde{b}_i^{\dagger}\tilde{b}_i\rangle=0$ is realized as a stable state. In this formalism, the paramagnetic state has to be maintained by means of repulsive interaction between the bosons. Thus, to prove the stability would not be a simple task theoretically, for one has to deal with the many-body problem subject to hard-core interaction. Nonetheless, it should be remarked that this formalism is formally exact, even though it is formulated on the broken symmetry state (6); in principle, the rotation symmetry of the paramagnet must be recovered in the exact result.

Second, let us review the results obtained in Ref. 2, which are used in the following discussion. We investigated the Hubbard model to show that the ferromagnetic (Nagaoka) state around half filling is destabilized by spin-wave instability. Even in the presence of a slight amount of doped holes, the spin-wave dispersion ω_q does not change so much from that of the undoped phase, for which Eq. (4) with $J\equiv 2t^2/U$ was obtained in the strong-coupling limit. Moreover, in terms of the spin wave thus obtained at half filling, we could reproduce the Heisenberg model (2).[2] In this derivation, the insulating property at half filling are evident from the outset, for all the physical states are derived from the band insulator $|F\rangle$ by exciting the ferromagnetic spin waves, which are electrically neutral. In fact, the spin wave in this context is effectively interpreted as the Holstein-Primakoff boson defined in Eq. (5). Then, as a logical consequence, we speculated that an anomalous metallic state might result from the Nagaoka state, a doped-band insulator, in the same manner as the Mott insulator at half filling is derived from a filled-band ferromagnet. The speculation can be put in other words: Is the Nagaoka state really driven to a normal metal after the spin-wave instability?

Third, it is known that the Néel temperature T_N^{RPA} estimated in the random-phase approximation (RPA) turns out to be very large in the limit of strong correlation, i.e., one obtains $T_N^{RPA}\propto U$ instead of $T_N\propto J$ or $T_N=0$ depending on dimensionality of the model (2). (See Fig. 1.) In effect, this is not a problem peculiar to itinerant magnets. Nozières and Schmitt-Rink[3] showed that the transition temperature T_c of strong-coupling superconductors corresponds to the critical temperature of the Bose-Einstein condensation for independent bound pairs, which, therefore, becomes independent of the attractive interaction to form the bosonic pairs. On the other side, it is well known that the Hubbard model (1) is mapped to that with an attractive interaction by a suitable particle-hole transformation.[4] Then the Cooper pair in the attractive model is mapped back to a particle-hole bound state in a ferromagnetic vacuum, that is, the spin wave. In the repulsive model, the Bose-Einstein condensation brings about a magnetic long-range order, and the critical temperature will turn out to be of order of the hopping energy of the pair. Indeed, this is the way we estimate $T_N\sim J$ from a paramagnetic side of the phase diagram of the Hubbard model. To this end, in the next section, we start with the conventional theory of the Hartree-Fock (HF) RPA. In our theory, the formal techniques involved in the Holstein-Primakoff transformation and the mapping to the attractive model are utilized in physical context, in which the ferromagnetic reference frame is derived as a mean-field solution. Then we shall make use of the results of Ref. 2, which were primarily obtained to study the stability of the ferromagnetic ground state.[5–9]

II. MODEL

Now let us start on the main subject. For the total number N_σ of electrons with spin σ, the free energy $F(N,S_z)$ as a function of $N=N_\uparrow+N_\downarrow$ and $S_z=(N_\uparrow-N_\downarrow)/2$ is often introduced to discuss magnetism in itinerant electron systems.[10] To evaluate $F(N,S_z)$, we may deal with the Hamiltonian

$$H'=H-\mu\hat{N}-2h\hat{S}_z, \tag{8}$$

where

$$\hat{N}\equiv\sum_\sigma \hat{N}_\sigma\equiv\sum_{i,\sigma}\hat{n}_{i\sigma},\quad 2\hat{S}_z\equiv\hat{N}_\uparrow-\hat{N}_\downarrow, \tag{9}$$

and for H we use Eq. (1). Then the free energy is given by

$$F=\Omega+\mu N+2hS_z. \tag{10}$$

The Lagrange multipliers μ and h have to be determined by

$$N=-\frac{\partial\Omega}{\partial\mu},\quad 2S_z=-\frac{\partial\Omega}{\partial h}, \tag{11}$$

for given $N=\langle\hat{N}\rangle$ and $S_z=\langle\hat{S}_z\rangle$. The thermodynamic potential Ω in Eq. (10) is written

$$\Omega=\Omega_{\rm HF}+\Delta\Omega, \tag{12}$$

where the Hartree-Fock part is given by

$$\Omega_{\rm HF}=-T\sum_{k,\sigma}\ln(1+e^{-\varepsilon_{k\sigma}/T})-LUn_\uparrow n_\downarrow. \tag{13}$$

Here we defined $\varepsilon_{k\sigma}$ by

$$\varepsilon_{k\sigma}\equiv\varepsilon_k+Un_{-\sigma}-\mu-h\sigma, \tag{14}$$

and L is the total number of lattice sites. $\Delta\Omega$ includes all effects of electron correlation. In this paper, we take account

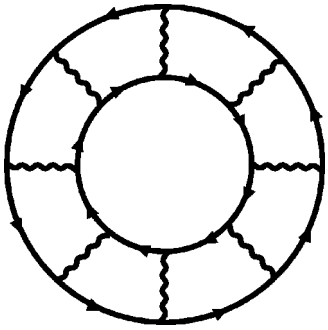

FIG. 2. An example of diagrams for the thermodynamic potential, describing particle-hole pair fluctuations.

of particle-hole pair fluctuations described by the diagrams as shown in Fig. 2, i.e., we work within the HF RPA. Then it is straightforward to derive[3]

$$\Delta\Omega = \frac{T}{2}\sum_{q,\omega_n} \ln[1 - U\chi_0^{+-}(q, i\omega_n)]. \tag{15}$$

The transverse susceptibility $\chi_0^{+-}(q,\omega)$ is given by

$$\chi_0^{+-}(q,\omega) = -\frac{1}{L}\sum_k \frac{f(\varepsilon_{k+q\downarrow}) - f(\varepsilon_{k\uparrow})}{\varepsilon_{k+q\downarrow} - \varepsilon_{k\uparrow} - \omega}, \tag{16}$$

where $f(\varepsilon)$ is the Fermi-distribution function

$$f(\varepsilon) = \frac{1}{e^{\varepsilon/T}+1}. \tag{17}$$

The longitudinal fluctuation need not be considered here, since we are not interested in the absolute value of Ω.

Within this approximation, from Eq. (11) we get

$$N = \sum_\sigma N_\sigma = \sum_{k,\sigma} f(\varepsilon_{k\sigma}), \tag{18}$$

and

$$2S_z = -\frac{\partial\Omega}{\partial h} = N_\uparrow - N_\downarrow - \frac{\partial\Delta\Omega}{\partial h}. \tag{19}$$

The parameters μ and h are determined by these equations.

III. JUST AT HALF FILLING

In this section we discuss the case at half filling: $n = N/L = 1$.

A. Normal solution

Equations (18) and (19) with $N = L$ and $S_z = 0$ have a solution,

$$\mu = U/2, \quad h = 0, \tag{20}$$

when $n_\uparrow = n_\downarrow = 1/2$. In this case, the sum in Eq. (15) diverges at the temperature determined by

$$1 - U\chi_0^{+-}(q,0) = 1 + \frac{U}{L}\sum_k \frac{f(\varepsilon_{k+q}) - f(\varepsilon_k)}{\varepsilon_{k+q} - \varepsilon_k} = 0. \tag{21}$$

In a simple cubic lattice, the divergence first occurs at $T = T_N^{RPA}$ for $\mathbf{q} = \mathbf{Q} = (\pi,\pi,\pi)$; the dashed curve in Fig. 1 is obtained as the solution T_N^{RPA} of Eq. (21). At the low temperature $T < T_N^{RPA}$, the BCS-like mean-field solution of the antiferromagnetic phase exists.[11] In general, the mean-field theory of the magnetically ordered phase was discussed by many authors.[4,8,11–14]

B. Nontrivial solution

As is well known, the theory based on Ω_{HF} predicts ferromagnetism for $U \gtrsim W$. As a function of U, the Curie temperature T_C determined by the Stoner criterion also increases as T_N^{RPA} does; in effect, both T_C and T_N^{RPA} tend to $U/4$ for large U.[11] In particular, within the Hartree-Fock approximation, the complete ferromagnetic state, e.g., with $(n_\uparrow, n_\downarrow) = (1,0)$, is obtained as a stable phase at low temperatures $T \ll U$. This insulating state, however, is shown to bear spin waves with negative energy, so that it cannot remain stable. As we show below, the instability is readily taken into account within our approximation adopted here.

To investigate the ferromagnetic solution, we choose μ so that $\varepsilon_\uparrow < \mu < \varepsilon_\downarrow$. Then the equation $1 - U\chi_0^{+-}(q,\omega) = 0$, or

$$1 - \frac{U}{L}\sum_k \frac{1}{\varepsilon_{k+q} - \varepsilon_k + U + 2h - \omega} = 0, \tag{22}$$

has a bound-state solution, namely, the spin wave $\omega = \omega_q + 2h$ below the continuum $\eta_q(k) = \varepsilon_{k+q} - \varepsilon_k + U + 2h$. This eigenequation was discussed in Ref. 2, where it was shown that in the limit $U \to \infty$ for the tight-binding dispersion

$$\varepsilon_k = -t\sum_{\bar{\delta}} e^{ik\bar{\delta}}, \tag{23}$$

we obtain the solution (4) with $J = 2t^2/U$. In this case, we have an energy gap $\sim U$ in charge excitations. Therefore, in terms of the bound-state solution $\omega_q, \Delta\Omega$ in Eq. (15) reads

$$\Delta\Omega = T\sum_q \ln(1 - e^{-(\omega_q + 2h)/T}), \tag{24}$$

for $T \ll U$. This is the thermodynamic potential of the boson of energy ω_q and chemical potential $-2h$, the factor -2 being due to spin $S_z = -1$ of the boson. Hence, from Eq. (19) follows[3]

$$2S_z = L - \sum_q \frac{2}{e^{(\omega_q + 2h)/T} - 1}. \tag{25}$$

The parameter h should be determined by Eq. (25) for given S_z. As a result, up to an irrelevant constant, we obtain the free energy

$$F = \Delta\Omega + 2hS_z, \tag{26}$$

in which Eqs. (24) and (25) are substituted.

Note that the free energy derived here is nothing but what we would obtain for the antiferromagnetic Heisenberg model (3) when boson-boson interactions are neglected. The neglect, however, brings about a problem. This is related to a difference from the case of superconductivity; in our theory S_z, unlike N, is not a given quantity but it is the quantity to

be determined so as to minimize F. For this purpose the boson-boson interaction should not be neglected, as noted in the introduction. Nonetheless, for practical purposes to discuss qualitative features of our anomalous solution, we shall assume $S_z=0$, anticipating that the state above T_N would never be ferromagnetic. Then Eq. (25) determines h as a function of T and the radius of convergence of $\Delta\Omega$ is set by the condition for the Bose-Einstein condensation,[3] or T_N is determined by $\omega_Q+2h=0$, which is tantamount to $1-U\chi_0^{+-}(Q,0)=0$. For example, in the simple-cubic lattice in the strong-coupling regime, we may use Eq. (7) to find $T_N=3.46J$; which is the solid curve in Fig. 1. This is to be compared with the result $T_N^{mf}=2zS(S+1)J/3=3J$ of the Weiss mean-field theory for the antiferromagnetic Heisenberg model (2). Moreover, it is noted that our theory correctly gives $T_N=0$ for low-dimensional systems where the Bose-Einstein condensation never occurs at finite temperature.

IV. EFFECT OF HOLE DOPING

The nontrivial solution that we saw above continues to exist even in the presence of doped holes. In this section, we consider the solution for $N<L$, or $n<1$, in the strong-coupling region $U\gg W$. Note that Eq. (19) for $N_\uparrow=N$ and $N_\downarrow=0$ does not depend on μ as $\Delta\Omega$ does not. This indicates that spin excitations are independent of the chemical potential μ. Therefore, μ is determined by Eq. (18),

$$N=N_\uparrow=\sum_k f(\varepsilon_k-\bar{\mu}), \tag{27}$$

and h is fixed by Eq. (19). In Eq. (27) we defined $\bar{\mu}\equiv\mu-h$, which may be used in place of μ to control charged excitations.

In this case, we obtain the eigenequation

$$1-\frac{U}{L}\sum_k \frac{n_k}{\varepsilon_{k+q}-\varepsilon_k+Un+2h-\omega}=0, \tag{28}$$

in which we substituted the step function n_k,

$$n_k=\begin{cases}1, & \varepsilon_k<\bar{\mu}\\ 0, & \varepsilon_k>\bar{\mu}\end{cases} \tag{29}$$

for the Fermi-distribution function $f(\varepsilon_k-\bar{\mu})$ to simplify the following calculation. Similarly, we use n_k for Eq. (27). By this replacement, we neglect the temperature dependence of the boson dispersion $\omega=\omega_q+2h$, the bound-state solution of $1-U\chi_0^{+-}(q,\omega)=0$. Equation (28) corresponds to Eq. (22) for the filled band $n=1$, and it may be regarded as the eigenequation for the spin excitation spectrum of the Nagaoka ferromagnetic state,

$$|F\rangle\equiv\prod_{\varepsilon_k<\bar{\mu}} c_{k\uparrow}^\dagger|0\rangle, \tag{30}$$

which is a doped band insulator.

As shown in the case of $n=1$, the low-energy spin-excitation properties of the system is determined by the bound-state solution ω_q. Upon hole doping, ω_q is modified

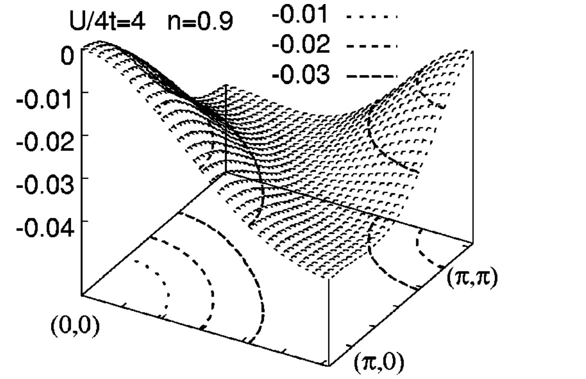

FIG. 3. The spin wave ω_q as a function of $\mathbf{q}=(q_x,q_y)$ for the Hubbard model with $U/4t=4$ and $n=0.9$ in a square lattice. The minimum lies not at $\mathbf{q}=\mathbf{Q}=(\pi,\pi)$ as for $n=1$, but at $\mathbf{q}=(\pi,0.3\pi)$. (See also Fig. 4.)

in two ways;[2] (i) the bandwidth $\Delta\omega\equiv\max(\omega_q)-\min(\omega_q)$ is reduced and (ii) the momentum $q_{\min}$, which gives the minimum of ω_q, or $q_{\min}$ of

$$\omega_{q=q_{\min}}=\min(\omega_q),$$

shifts from $\mathbf{q}=\mathbf{Q}$ for $n=1$. It is remarked that $\Delta\omega$ is regarded as the effective superexchange coupling by $\Delta\omega=2zJ_{\rm eff}$, and $q_{\min}$ determines the spin structure, commensurate or incommensurate, of the ordered phase; see Eqs. (4) and (7) for the undoped system. To show these points explicitly, the spin-wave solution ω_q of Eq. (28) is calculated for a square lattice, with which we obtained Figs. 3 and 4.

In terms of the bound-state solution of Eq. (28), T_N is calculated as in the previous section. Assuming $S_z=0$, from Eq. (19) we obtain

$$\frac{n}{2}=\frac{1}{L}\sum_q \frac{1}{e^{(\omega_q+h)/T}-1},$$

and T_N is determined as the temperature at which the Bose-Einstein condensation occurs. In Fig. 5, the Néel temperature T_N is shown as a function of the hole density $x=1-n$. In the range of hole density shown in the figure, we found that the

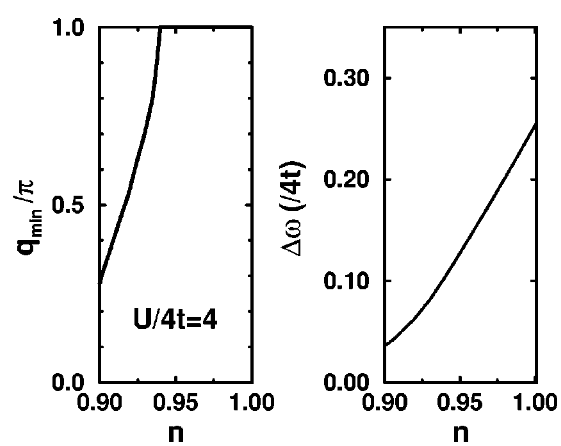

FIG. 4. The momentum $q_{\min}$ of $\mathbf{q}=(\pi,q_{\min})$, which gives the minimum of ω_q (left), and the bandwidth $\Delta\omega\equiv\max(\omega_q)-\min(\omega_q)$ (right) as a function of n in the case $U/4t=4$ of the Hubbard model in a square lattice.

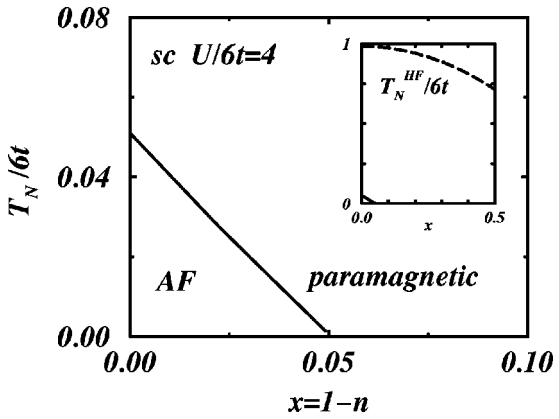

FIG. 5. The Néel temperature T_{N} of the Hubbard model $U/6t=4$ in a simple cubic lattice as a function of $x=1-n$. In the inset, the result $T_{\mathrm{N}}^{\mathrm{RPA}}$ of the Hartree-Fock approximation is displayed along with T_{N}.

minimum of ω_q remains at the zone boundary $\mathbf{q}=\mathbf{Q}$. The linear decrease of T_{N} as a function of x is due to the reduction of the bandwidth $\Delta\omega$, cf. the right of Fig. 4. In Fig. 6, we show the dispersion ω_q for a doped system in a simple cubic lattice. In this example, as in Fig. 3, the minimum is shifted from $\mathbf{q}=\mathbf{Q}$ upon hole doping, and the bottom of the band is considerably flattened. The latter is responsible for the vanishing transition temperature $T_{\mathrm{N}}\rightarrow 0$ for $x\geqslant x_{c1}\simeq 0.05$, even in three-dimensional systems.

V. DISCUSSION

We viewed the Mott insulator as the ferromagnetic band insulator accommodating a macroscopic number of ferromagnetic spin waves. In the same manner, the doped Mott insulator is constructed from a doped-ferromagnetic band insulator, the Nagaoka state. It was shown that the HF RPA has the solutions that substantiate this viewpoint. The condition for the Mott transition is that the system must contain as many up-spin particles as down-spin holes, i.e., $n_{\uparrow}=1-n_{\downarrow}$ or $n=n_{\uparrow}+n_{\downarrow}=1$; the insulating magnet follows when all of the particle-hole pairs are tightly bound up on the spontaneously generated ferromagnetic background. The bound states thus formed behave just as local moments. This point of view, in terms of charged-spinless fermions and neutral bosons with $S=1$ in the complete ferromagnet, embodies a kind of ''spin-charge separation.'' In the presence of the bound-state excitations, crossover from insulator to metal is caused by depolarization of the ferromagnetic vacuum, dissociation of the bound state due to the thermal effect or as a result of the vanishing-binding energy. These are realized by decreasing U, by raising temperature T, or by increasing the hole density x. Similarly, crossover from the anomalous to normal metal occurs as a result of the dissociation: The normal metal should not have the particle-hole bound-state excitation of which energy takes a minimum at finite q. The anomalous metal is anomalous because of the presence of such an excitation obeying Bose statistics. The ferromagnetic-to-paramagnetic transition of the mean-field solution, however, should not be distinctly reflected as a phase transition in physical observables, just as the results for the symmetric phases of Eq. (3) should not depend on the direction of the spin axis prescribed by $|F\rangle$ in the Holstein-Primakoff formalism. In the crossover region, we have to take account of not only the particle-hole bound states but also individual-particle spin excitations. The latter are neglected in this paper, for they have a vanishing spectral weight in the strong-coupling regime of our concern.

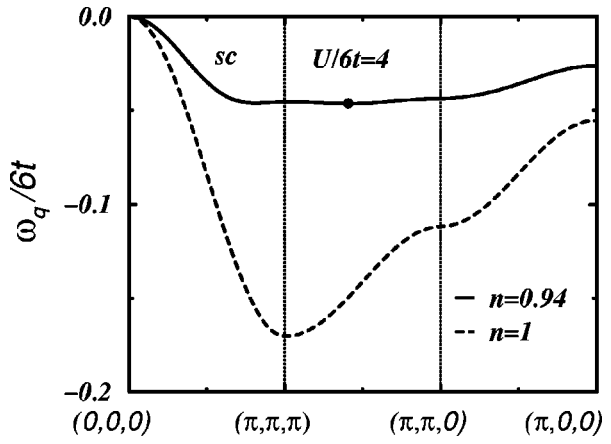

FIG. 6. For the Hubbard model with $U/6t=4$ in a simple cubic lattice, ω_q for $n=0.94$ (solid) and $n=1$ (dashed curve) are displayed as a function of $\mathbf{q}$. The dot on the solid curve indicates the minimum of ω_q.

Within the RPA, one can show that the ferromagnetic state becomes stable in an overdoped region $x\geqslant x_c^{\mathrm{RPA}}$, e.g., $x_c^{\mathrm{RPA}}\sim 0.1$ for $U/6t=4$ in a simple cubic lattice. But this is just to indicate that RPA is not a good approximation to describe that region, in which we know the bound-state solutions should disappear as a result of a sharp drop in energy of single-particle excitation spectrum;[2] the scarcity of vacant sites and a strong repulsion are responsible for the formation of the particle-hole bound pairs. In the absence of well-defined bound pairs, the ferromagnet beyond instability will be driven to a normal metal. Therefore, our theory, based on RPA, is inapplicable to the overdoped regime. We have to use a better approximation to discuss the crossover from the anomalous to normal-metal solution.

In the previous section, we saw that T_{N} vanishes at the hole density $x=x_{c1}\sim 0.05$ for $U/6t=4$ in a simple cubic lattice. On the other side, as noted above, the spin waves cease to remain well defined when further holes are doped,[2] i.e., they will disappear for $x\geqslant x_{c2}(>x_{c1})$. To see this point definitely, in Fig. 7 the energy gap in the spin-excitation spectrum $\Delta\equiv\min\eta_q(k)-\min\omega_q$ obtained using the improved theory of Ref. 2 is displayed as a function of x, where $\eta_q(k)$ and ω_q represent the bottom energy of the Stoner continuum and the energy of the spin wave, respectively. As discussed above, below the dissociation temperature, i.e., for $T\lesssim\Delta/2$, we will be in the anomalous metallic phase where particle-hole pair correlations become conspicuous. Thus, the gap may be tentatively identified with the ''high-energy pseudogap'' recently observed by photoemission spectroscopy.[15] In any case, from the figure we observe $x_{c2}\sim 0.2$. Then there arises a question concerning the ground state in the range $x_{c1}\lesssim x\lesssim x_{c2}$. To settle this problem, we must solve a complicated problem of the system of interacting bosons with highly overlapping internal structures that depend on the electronic state of doped holes as well as the

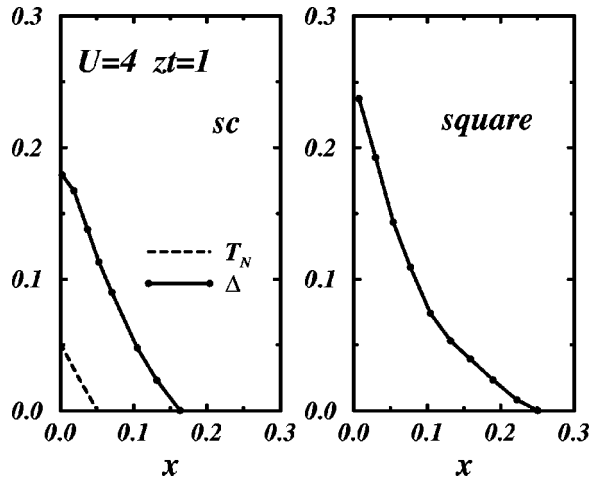

FIG. 7. The excitation gap $\Delta \equiv \min \eta_q(k) - \min \omega_q$ estimated by the improved theory of Ref. 2 is displayed as a function of $x = 1 - n$ for the Hubbard model with $U = 4$ and $zt = 1$ in a simple cubic lattice $z = 6$ and a square lattice $z = 4$. For the former T_N is drawn also with the dashed line.

configuration of the bosons themselves. Theoretically, to construct a symmetric state from a broken-symmetry phase, as proposed in this paper, is not a familiar procedure. However, we believe that such a formal device will help us to understand how things are going in the Mott insulator and the anomalous metal, even though it may not be well suited for practical purposes of calculation. Needless to say, a real matter of fact is not so simple and clear-cut as we saw above in the simple approximation. Indeed this is just an attempt to facilitate understanding of the subject of current controversy, the metallic state adjacent to the magnetic insulator, which, in fact, appears to have little resemblance to a canonical normal metal. To explain the anomalous features, we have recourse to just the two elementary notions, that a completely filled band is insulating, and that spin wave does not carry an electric current.

In summary, our approach made use of a ''defect'' of the mean-field approximation, that it predicts ferromagnetism when the on-site repulsion dominates the hopping energy. The ferromagnetic state must be made unstable either by collective or single-particle excitations. The former is relevant around half filling, while the latter is for large doping concentration. In contrast to the latter case where one will end up with a normal metal, we argue that the former case can lead to an anomalous metallic state, which may be ultimately led to antiferromagnetism, or some other unusual ground states. This argument is motivated by the fact that one can properly construct the antiferromagnetic Heisenberg model in terms of spin waves of a ferromagnetic band insulator.[2] From this point of view, we estimated the Néel temperature T_N as a function of the hole concentration x from a paramagnetic side of the phase diagram on the basis of the Hartree-Fock random-phase approximation.

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[5] With regard to the historical background of the present paper, we must mention, among others, Anderson (Ref. 6) and Kohn (Ref. 7) who speculated the metal-insulator transition at half filling in terms of spin waves of a ferromagnetic-band insulator. In the mean-field theory of Krishnamurthy *et al.* (Ref. 8), a similar view as ours was presented in different terms. In Ref. 9, the array of localized spins in the ferromagnetic Kondo lattice model, viz., the Mott insulator, was described as a filled band of a general model comprising degenerate orbitals.
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