Short-Range Antiferromagnetic Correlation Effect on Conduction Electrons in Two-Dimensional Strongly Correlated Electron Systems

Takao Morinari

Graduate School of Human and Environmental Studies, Kyoto University, Kyoto 606-8501, Japan
(Dated: November 25, 2019)

We investigate magnetic polarons in two-dimensional strongly correlated electron systems, where conduction electrons interact with antiferromagnetically interacting localized spins. Starting from a basic model, we derive a simplified model with the help of spin Green’s function and a perturbation analysis. A strong coupling analysis is applied to the model, where the sum of the scattering wave vectors is approximated to be $(\pi, \pi)$ or zero, using the equation of motion for the conduction electron Green’s function, and we discuss the pseudogap-like behavior associated with the suppression of the quasiparticle weights and the crossover from the large magnetic polaron to the small magnetic polaron. In the antiferromagnetic long-range ordered state, the spectral weight of the conduction electrons has a form of broad humps due to Franck-Condon broadening associated with the multi-magnon scattering. The band folding feature due to the $(\pi, \pi)$ scattering disappears as we increase the number of the magnons involved in the multi-magnon scattering.

I. INTRODUCTION

In the hole doped cuprate high-temperature superconductors,\(^1\) one of the key correlations is the antiferromagnetic (AF) correlation, which is long-ranged in the parent compound but short-ranged in moderately doped compounds. For the purpose of understanding the physics of the cuprates, especially the enigmatic pseudogap state, we need to clarify to what extent it is understood on the basis of the AF correlation. Although this is less ambitious goal, it is not an easy task because of the strong electronic correlation which makes the parent compound a charge-transfer insulator.\(^2\)

In Ref. 3, it was pointed out that there is a close relationship between the pseudogap and the short-range AF correlation: The magnetic-torque measurement result,\(^4\) whose characteristic temperature coincides with the pseudogap temperature determined by other experiments, has a non-trivial scaling relationship with the AF spin susceptibility.\(^3\) A pseudogap behavior associated with the short-range AF correlation has been discussed in numerical simulations, such as extended versions of dynamical mean-field theory\(^5\)-\(^9\) and quantum Monte Carlo simulations.\(^7,8\)

In experiments, the Fermi surface topology changes abruptly from arcs\(^10\) to closed contours in Bi\(_2\)Sr\(_2\)CaCu\(_3\)O\(_{8+\delta}\) as observed in scanning tunneling microscopy,\(^11\) where the arcs end at the AF zone boundary. In angle-resolved photoemission spectroscopy, the AF zone boundary effect is clearly seen in the electron doped cuprate,\(^12,13\) while it just gives a terminating point of Fermi arcs in the hole doped cuprate. A possible interpretation is the difference in the range of the AF correlation length.\(^14\)

In this paper we investigate the effect of the short-range AF correlation on conduction electrons. We focus on low doping systems. The subject has been studied as a magnetic polaron formed in the $t$-$J$ model\(^15\)-\(^22\) or in the Hubbard model\(^23\)-\(^26\) with the AF correlation. Although there are powerful numerical simulations mentioned above, it is useful to study the system in a different way in order to examine limitations in the numerical simulations arising from the momentum resolution.\(^27\)

Here, we take a strong coupling approach on the basis of the equation of motion for the Green’s function. We start with a model consisting of conduction electrons and antiferromagnetically interacting localized spins with an exchange coupling between them. We introduce these degrees of freedom as separate fields to focus on the interaction effect between them. From the analysis of the second order perturbation theory, we find that the coupling between the conduction electrons and the magnons takes the largest value at the scattering wave vector $Q = (\pi, \pi)$. (Hereafter, we take the lattice constant unity.) On the basis of this observation, we propose a simplified model, which is similar to the Holstein model\(^28,29\) for the polaron problem.\(^30\) The difference is just the scattering wave vector. The advantage of our approach is that one can control the strength of the magnetic correlation effect by varying the number of magnons and there is no limitation arising from the momentum resolution.

The rest of the paper is organized as follows. In Sec. II we describe our model. In Sec. III we examine the short-range AF correlation. We propose a simplified model to describe the system. A strong coupling analysis is applied to the simplified model. We derive a general formula to investigate the electron Green’s function. And then, we introduce a dilute magnon approximation applicable for low-temperatures. In Sec. IV we present the numerical calculation results. In Sec. V we summarize the result.

II. MODEL

We consider a strongly correlated two-dimensional electron system consisting of conduction electrons and localized moments. We assume that there is a strong exchange interaction between the conduction electron spins and the localized moments. The model is taken as the low-energy effective theory for multi-orbital Hubbard models: Some of the electrons are localized due to a
strong on-site Coulomb repulsion, and form the localized moments. It is possible to derive a similar model starting from a single band model, such as the Hubbard model or the t-J model, by introducing localized moments through a Storatonovich-Hubbard transformation or applying a slave-particle formalism. In order to make the situation simple, we introduce the conduction electrons and the localized moments as separate fields.

The Hamiltonian is given by

\[
H = \sum_{k,\sigma} \xi_k c_k^{\dagger} c_k + \frac{K}{\sqrt{N}} \sum_{k,q} S_q \cdot (c_{k+q}^{\dagger} \sigma c_k) + H_{\text{spin}},
\]

where the energy dispersion of the conduction electron, \(\varepsilon_k\), minus the chemical potential, \(\mu\), is denoted by \(\xi_k = \varepsilon_k - \mu\). We consider a square lattice, and \(\varepsilon_k\) is given by

\[
\varepsilon_k = -2t (\cos k_x + \cos k_y) - 4t_1 \cos k_x \cos k_y - 2t_2 (\cos 2k_x + \cos 2k_y),
\]

with \(t\) the nearest neighbor hopping parameter, \(t_1\) the second nearest neighbor hopping parameter, and \(t_2\) the third nearest neighbor hopping parameter. The creation operator of the conduction electron with the wave vector \(k\) and spin \(\sigma\) is denoted by \(c_k^{\dagger}\). The localized spin moment at site \(j\) is denoted by \(S_j\). For the value of the spins of the localized moments, we assume one-half. The Fourier transform of \(S_j\) is denoted by \(S_q\) with \(q\) the wave vector.

The second term in the right-hand side of Eq. (1) describes the AF exchange coupling between the localized spins and the conduction electron spins with the coupling constant \(K\). The number of the lattice sites is denoted by \(N\). The conduction electron spin is denoted by using a two-component operator, \(c_k^{\dagger} = (c_{k^x}^{\dagger}, c_{k^y}^{\dagger})\). The components of the three dimensional vector \(\sigma = (\sigma_x, \sigma_y, \sigma_z)\) are the Pauli matrices. The last term in Eq. (1) describes the interaction between the localized spins. Here, we consider the AF Heisenberg model on the square lattice:

\[
H_{\text{spin}} = J \sum_{\langle i,j \rangle} S_i \cdot S_j,
\]

where the summation is taken over pairs of nearest neighbor sites and \(J(>0)\) is the exchange interaction.

III. EFFECT OF THE AF SHORT-RANGE CORRELATION ON CONDUCTION ELECTRONS

A. Antiferromagnetic Short-Range Order

We may expect that there are various phases, including the AF long-range ordered phase, the ferromagnetic metallic phase like manganese oxides, the Fermi liquid phase, etc., where the Hamiltonian (1) is applied with taking a suitable set of parameters. Here, we focus on a metallic phase without AF long-range order. In the presence of the conduction electrons, one may expect that the exchange interaction \(J\) is reduced from the original value. So, \(J\) must be replaced by an effective exchange interaction depending on the concentration of the conduction electrons. Hereafter, we denote this effective exchange interaction by the same symbol \(J\) to make the notation simple. In addition, the dynamics of the localized spins can be affected by the conduction electrons. To make the situation simple, we assume that the number of conduction electrons is small, and we neglect the effect of the conduction electrons on the localized spin dynamics.

We are interested in finite temperatures where a mean field approach, for example, a Schwinger boson mean field theory and a modified spin-wave theory, is not reliable. These mean field theories provide an accurate description of the ground state properties, while they fail to describe features for \(T > T_0\) with \(T_0 \sim 0.7J\) in particular, a broad peak in the temperature dependence of the spin-susceptibility. The spin-spin correlation associated with this broad peak is described by the Green’s function method. So, we use this formulation for the description of the localized spins. The formulation is briefly reviewed in Appendix A.

B. The Second Order Perturbation Theory

Now we examine the effect of AF short-range order on the conduction electrons. Theoretically challenging point is that the conduction electrons strongly coupled with the localized spins. Therefore, we need to apply a strong coupling analysis. In general, we need both higher-order terms and some kind of self-consistent calculation for any strong coupling analysis. However, this is a formidable task because rapidly increases the number of summations of the wave vectors and the Matsubara frequencies. So, we need to introduce some approximation. For the purpose of carrying out a strong coupling analysis, we take the following strategy: First, we apply the standard second order perturbation theory to the system. We examine the result and try to extract essential properties. And then, we construct a simplified model, to which one can apply a strong coupling analysis with the help of some approximation.

We consider the Matsubara Green’s function for the conduction electron with wave vector \(k\) and spin \(\sigma\), which is given by

\[
G_{k\sigma}(\tau) = -\left\langle T_\tau c_{k\sigma}(\tau) c_{k\sigma}^{\dagger}(0) \right\rangle,
\]

with \(\tau\) the imaginary time. Here, \(T_\tau\) is the imaginary time ordering operator and \(c_{k\sigma}(\tau) = \exp(\tau H) c_{k\sigma} \exp(-\tau H)\) with the Hamiltonian being given by Eq. (1).

We take the second term in Eq. (1) as the perturbation as if the coupling constant \(K\) were a small parameter. It is easy to find that the first-order electron self-energy
vanishes. The second-order electron self-energy is given by

\[ \Sigma_{\mathbf{k}\sigma}^{(2)} (i\omega_n) = \frac{3K^2}{2\beta N} \sum_{i\Omega_n} \sum_q D_q (i\Omega_n) G_{\mathbf{k}+\mathbf{q},\sigma} (i\omega_n + i\Omega_n), \]

where \( \beta = 1/T \) and the magnon propagator, which is presented in Appendix A, is given by

\[ D_q (i\Omega_n) = -\frac{4Jc_1 (1 - \gamma_q)}{(i\Omega_n)^2 - \omega_q^2}, \]

where \( \gamma_q = (\cos q_x + \cos q_y)/2 \) and \( c_1 \) is the spin-spin correlation between the nearest neighbor sites, which is defined by \( c_1 = 2\langle S_i^+ S_j^- \rangle \) with \( i \) and \( j \) being nearest neighbor sites. Here, we set the Boltzmann constant \( k_B = 1 \). Carrying out the summation over the Matsubara frequency \( \Omega_n = 2\pi n/\beta \) with \( n \) an integer, we obtain

\[ \Sigma_{\mathbf{k}\sigma}^{(2)} (i\omega_n) = \frac{K^2}{N} \sum_q g_q \left[ \frac{n_B (\omega_q) + f (\xi_{k+q})}{i\omega_n - \xi_{k+q} + \omega_q} + \frac{n_B (\omega_q) + 1 - f (\xi_{k+q})}{i\omega_n - \xi_{k+q} - \omega_q} \right], \]

with \( n_B \) the Bose-Einstein distribution function and \( f \) the Fermi-Dirac distribution function. The \( \mathbf{q} \) dependent coupling is given by

\[ g_q = \frac{3|c_1|J (1 - \gamma_q)}{\omega_q}. \]

The expression of \( \Sigma_{\mathbf{k}\sigma}^{(2)} (i\omega_n) \) is a familiar result found in an electron-boson coupled system.\(^{42}\)

### C. The Simplified Model

An important point about Eq. (7) is that the right-hand side is independent of the spin of the conduction electron. This is distinct from the case with the AF long-range ordered state where we need to study each spin state separately.\(^{15-18}\) Another important point is that there is no need to distinguish even sites and odd sites. In the presence of the AF long-range order, we need to distinguish them separately. In addition, the wave vector takes the values in the full Brillouin zone, and not restricted to the reduced magnetic Brillouin zone.

In Eq. (7), the information about the short-range AF order is included through the magnon dispersion \( \omega_q \) and the \( \mathbf{q} \)-dependent coupling \( g_q \). The self-energy (7) itself has a standard form where conduction electrons couple with bosonic excitations.\(^{42}\) In Fig. 1, we show \( \mathbf{q} \) dependence of \( g_q \) for different temperatures. The crucial point here is that \( g_q \) exhibits a sharp peak at \( \mathbf{q} = (\pi, \pi) \).

From the consideration above, we consider a simplified model with the characteristic features of \( g_q \) and \( \omega_q \), that is,

\[ H = \sum_k \xi_k c_k^\dagger c_k + \frac{g}{\sqrt{N}} \sum_{k,q} (b_q^\dagger + b_{-q}) c_k^\dagger c_k + q \]

\[ + \sum_q \Omega b_q^\dagger b_q. \]

Here, we omit the spin dependence of the conduction electrons because there is no need to distinguish the spin-up and spin-down states. The magnon excitation \( \omega_{Q+q} \) is created (annihilated) by \( b_q^\dagger \) (\( b_q \)). We neglect the dispersion of \( \omega_{Q+q} \), and take \( \omega_{Q+q} \approx \omega_Q = \Omega \) as an approximation because of the behavior of \( g_q \) as discussed above. The coupling constant \( g \) is chosen as the value of \( K^2 g_q \) at \( \mathbf{q} = Q \).

In the hole doped cuprate high-temperature superconductors, \( \Omega \) is associated with the resonance energy at the wave vector \( \mathbf{Q} = (\pi, \pi) \) observed in the neutron scattering,\(^{43-45}\) from which broad peaks disperse upward and incommensurate peaks disperse downward, resulting in the hourglass pattern.

### D. Strong Coupling Analysis

The model (9) is similar to the Holstein model for the polaron.\(^{28,29}\) The difference is just that the shift of the wave vector \( \mathbf{Q} \) at the scattering of the conduction electrons by the bosons.

Here, we are interested in the strong coupling regime for \( g \). So, we need to apply a strong coupling analysis. In the study of the Holstein model, various approaches have been applied in the strong coupling regime. Among others, the momentum average approximation\(^{16,17}\) is a
useful approach which reproduces the most reliable diagrammatic Monte Carlo results.\textsuperscript{48,49} Here, we apply a modified version of the momentum average approximation to the model (9).

Now we assume that the carrier density is low enough so that we may consider a single carrier system. Omitting the spin, \(\sigma\), the equation of motion of the Green's function (4) is given by

\[
\hat{c}_k \frac{d}{dt} \langle c_k \rangle \right|_{\omega_n} = +1. \tag{10}
\]

Here, the Hamiltonian is given by Eq. (9) and the notation is defined in Appendix A. The commutator in the right-hand side is

\[
\{c_k, \mathcal{H} \} = \varepsilon_k c_k + \frac{g}{\sqrt{N}} \sum_q (b_q^\dagger + b_q - i\omega_n) c_{k+q+Q}. \tag{11}
\]

After substituting this equation into Eq. (10), we need to compute, \( \langle b_{-q} c_{k+q+Q} \rangle \right|_{\omega_n} \) and \( \langle b_q^\dagger c_{k+q+Q} \rangle \right|_{i\omega_n} \). We consider the equation of motion of these quantities, and then repeat the similar procedure. In order to carry out the calculation in a systematic way, we define

\[
G_{n,m} (k, i\omega_n, q_1, q_2, \ldots, q_n, p_1, p_2, \ldots, p_m) = \langle b_{q_1}^\dagger \ldots b_{q_n}^\dagger b_{-p_1} \ldots b_{-p_m} c_{k+q_1} + p_1^m \rangle \right|_{i\omega_n} c_k^\dagger \right|_{\omega_n} \tag{12}
\]

where

\[
q_j^{(n)} = \sum_{j=1}^n q_j + nQ. \tag{14}
\]

The equation of motion is,

\[
\hat{c}_k \frac{d}{dt} \langle c_k \rangle \right|_{\omega_n} = +1. \tag{15}
\]

We compute the commutator in the right-hand side. Noting that there is only a single carrier, we obtain

\[
\left[ i\omega_n - \varepsilon_{k+q_1} + p_1^m \right] G_{n,m} (k, i\omega_n, q_1, \ldots, q_n, p_1, \ldots, p_m)
\]

\[
= \frac{g}{\sqrt{N}} \sum_{p_{m+1}} G_{n,m+1} (k, i\omega_n, q_1, \ldots, q_n, p_1, \ldots, p_{m+1})
\]

\[
+ \frac{g}{\sqrt{N}} \sum_{q_{m+1}} G_{n+1,m} (k, i\omega_n, q_1, \ldots, q_{n+1}, p_1, \ldots, p_m)
\]

\[
+ \frac{g}{\sqrt{N}} \sum_{j=1}^m G_{n+1,m-1} (k, i\omega_n, q_1, \ldots, q_{n+1}, p_1, \ldots, \hat{p}_j, \ldots, p_{m-j})
\]

\[
+ \delta_{m,n} \delta_q (n) \sum_{p_1^m \ldots p_1^m} (b_{q_1}^\dagger \ldots b_{q_n}^\dagger b_{-p_1} \ldots b_{-p_m}), \tag{17}
\]

where \( \hat{p}_j \) denotes that \( p_j \) is excluded. The full Green's function is given by

\[
G (k, i\omega_n) = G_{0,0} (k, i\omega_n) = G_{k}^{(0)} (i\omega_n) \left[ 1 + g \sqrt{N} g_{0,1} (k, i\omega_n) + g \sqrt{N} g_{1,0} (k, i\omega_n) \right], \tag{18}
\]

where

\[
G_{k}^{(0)} (i\omega_n) = \frac{1}{i\omega_n - \varepsilon_k}. \tag{19}
\]

Here, \( g_{n,m} (k, i\omega_n) \) is defined by

\[
g_{n,m} (k, i\omega_n) = \frac{1}{N^{n+m}} \sum_{q_1, \ldots, q_n, p_1, \ldots, p_m} G_{n,m} (k, i\omega_n, q_1, \ldots, q_n, p_1, \ldots, p_m). \tag{20}
\]
The recursion formula for \( g_{n,m}(\mathbf{k}, i\omega_n) \) is found from Eq. (17), and is given by

\[
g_{n,m}(\mathbf{k}, i\omega_n) = \frac{g_0}{N^{n+m+1}} \sum_{q_1, q_2, \ldots, q_{n+m+1}} G_{k+q_{n+1}+p_{m+1}}^{(0)}(i\omega_n - (m-n)\Omega) \times g_{n,m+1}(\mathbf{k}, i\omega_n, q_1, \ldots, q_n, p_1, \ldots, p_{m+1}) \\
+ \frac{g_0}{N^{n+m+1}} \sum_{q_1, q_2, \ldots, q_{n+m+1}} G_{k+q_{n+1}+p_{m+1}}^{(0)}(i\omega_n - (m-n)\Omega) \times G_{n+1,m}(\mathbf{k}, i\omega_n, q_1, \ldots, q_n, p_1, \ldots, p_{m+1}) \\
+ \frac{g_0}{N^{n+m}} \sum_{q_1, q_2, \ldots, q_{n+m}} G_{k+q_{n+1}+p_{m+1}}^{(0)}(i\omega_n - (m-n)\Omega) \times G_{n,m-1}(\mathbf{k}, i\omega_n, q_1, \ldots, q_n, p_1, \ldots, p_{m+1}) \\
+ \frac{\delta_{n,m}}{N^{n+m}} \sum_{q_1, q_2, \ldots, q_{n+m}} G_{k+q_{n+1}+p_{m+1}}^{(0)}(i\omega_n - (m-n)\Omega) \times \delta_{q_{n+1}^{(0)}+p_{m+1}^{(0)},0} \langle b_{q_1}^\dagger b_{q_2}^\dagger b_{q_n}^\dagger b_{-p_1} b_{-p_2} \ldots b_{-p_n} \rangle.
\]

(21)

Now we introduce an approximation

\[
G_{k+q_{n+1}+p_{m+1}}^{(0)}(i\omega_n - (m-n)\Omega) \simeq G_{k+Q_{n-m}}^{(0)}(i\omega_n - (m-n)\Omega).
\]

(22)

where \( Q_n = Q \) for \( n \) odd and \( Q_n = 0 \) for \( n \) even. Applying this approximation to the equation above, we find

\[
g_{n,m}(\mathbf{k}, i\omega_n) \simeq gG_{k+Q_{n-m}}^{(0)}(i\omega_n - (m-n)\Omega) \\
\times \left[ \sqrt{N} g_{n,m+1}(\mathbf{k}, i\omega_n) + \sqrt{N} g_{n+1,m}(\mathbf{k}, i\omega_n) + \frac{m}{\sqrt{N}} g_{n,m-1}(\mathbf{k}, i\omega_n) \right] \\
+ \frac{1}{N} \frac{n!}{[e^{\beta\Omega} - 1]^n} G_{k+Q_{n-m}}^{(0)}(i\omega_n) \delta_{n,m}.
\]

(23)

Here, we have used that

\[
\langle b_{q_1}^\dagger b_{q_2}^\dagger b_{q_3}^\dagger b_{q_n}^\dagger b_{-p_1} b_{-p_2} \ldots b_{-p_n} \rangle \simeq n! [n_B(\Omega)]^n
\]

(24)

where the effect of the conduction electrons is neglected in computing this quantity.

It is instructive to see the lowest order term. Within \( O(g^2) \), the Green’s function is given by

\[
G(\mathbf{k}, i\omega_n) \simeq \frac{1}{i\omega_n - \varepsilon_k - g^2 \left[ \frac{n_B(\Omega) + 1}{i\omega_n - \varepsilon_k + Q + \Omega} + \frac{n_B(\Omega)}{i\omega_n - \varepsilon_k + Q + \Omega} \right]}
\]

(25)

This is a standard result obtained for a fermion-boson coupled system.\textsuperscript{42}

### E. Dilute Magnon Approximation

Now we consider low-temperatures, where \( T \ll \Omega \), and the number of excited magnons is small. In this case, Eq. (24) with \( n > 0 \) can be neglected. For \( n > 0 \), \( g_{n,m}(\mathbf{k}, i\omega_n) \) includes the scattering process of the conduction electron absorbing \( n \) magnons. However, this kind of processes can be ignored because \( n_B(\Omega) \ll 1 \).

Under this approximation, Eq. (23) is simplified to the following form:

\[
g_m(\mathbf{k}, i\omega_n) \\
\equiv g_{0,m}(\mathbf{k}, i\omega_n) \\
\simeq gG_{k+Q_m}^{(0)}(i\omega_n - m\Omega) \\
\times \left[ \sqrt{N} g_{m+1}(\mathbf{k}, i\omega_n) + \frac{m}{\sqrt{N}} g_{m-1}(\mathbf{k}, i\omega_n) \right],
\]

(26)

and the Green’s function is given by

\[
G(\mathbf{k}, i\omega_n) = G_{\mathbf{k}}(i\omega_n) \left[ 1 + g\sqrt{N} g_1(\mathbf{k}, i\omega_n) \right].
\]

(27)

Note that \( g_0(\mathbf{k}, i\omega_n) = G(\mathbf{k}, i\omega_n) \).
From this recursion equation, we find the continued fraction form of the Green’s function:

$$G(k, i\omega_n) \simeq \frac{1}{i\omega_n - \varepsilon_k - g^2 (\varepsilon_k + Q - \Omega) - \frac{g^2}{i\omega_n - \varepsilon_k - 2\Omega} - \frac{g^2}{i\omega_n - \varepsilon_k - 2\Omega}}$$

(28)

with $\tilde{\Omega} = \Omega + i\Gamma$. The parameter $\Gamma$ is introduced to include the magnon damping effect.

This Green’s function is computed by diagonalizing the tridiagonal matrix, $H_G$, whose $i, j$ component is given by

$$(H_G)_{ij} = \varepsilon_k^{(+)\delta_{ij}} + (H_m)_{ij},$$

(29)

with

$$(H_m)_{jj} = (-1)^{j-1} \varepsilon_k^{(-)} + (j - 1) \tilde{\Omega},$$

(30)

and

$$(H_m)_{j,j+1} = (H_m)_{j+1,j} = \sqrt{fg}.$$  

(31)

Here, $\varepsilon_k^{(\pm)} = (\varepsilon_k \pm \varepsilon_{k+Q})/2$. The other components of $H_m$ are zero. The poles of the Green’s function are obtained from the eigenvalues of $H_G$ and their weights are computed from the eigenvectors of $H_G$. We compute the spectral function by analytic continuation, $i\omega_n \rightarrow \omega + i\delta$. We take $\delta$ as a parameter for the broadening of the bare conduction electron spectrum. In general, the parameters, $g$, $\Omega$, and $\delta$ are temperature dependent. Investigation of their temperature dependence requires more elaborate calculations, which is not considered in this paper.

IV. RESULT

In Fig. 2, we show the magnetic polaron energy and the quasi-particle weight as a function of $g$. Here, $(\varepsilon_k + \varepsilon_{k+Q})/2$ is taken as the origin of the energy. Then, the whole spectrum depends on $k$ through $(\varepsilon_k - \varepsilon_{k+Q})/2 \equiv \varepsilon$ with $|\varepsilon|$ being taken as the unit of energy. We clearly see a crossover from a weak coupling regime to a strong coupling regime around $g \sim 0.7$ for $\Gamma = 0$. Here, we take $M = 200$ for the maximum number of the magnons. We checked that this value is sufficiently large and the result does not change by increasing this number. The characteristic value of $g$ for the crossover decreases with increasing $\Gamma$ due to the damping of the magnons.

A similar behavior is observed when we change the value of $\Omega$. In Fig. 3, we show the magnetic polaron energy and the quasi-particle weight as a function of $g$ for different values of $\Omega$. The effect of the coupling between the conduction electron and the magnons is suppressed by increasing $\Omega$.

The small magnetic polaron behavior is clearly seen when we plot the magnetic polaron energy as a function of $\varepsilon$ as shown in Fig. 4. The band width of the original conduction electrons is reduced as we increase $g$. This behavior is associated with the crossover from a large magnetic polaron to a small magnetic polaron. We obtain almost flat dispersion for $g > 1$. We may expect that the conduction electrons localize in the presence of impurities in the small magnetic polaron regime. The situation is similar to self-trapping phenomena in the polaron physics.

The importance of including a sufficient number of magnons is clarified by investigating the spectral function. In Fig. 5 we plot the spectral function along symmetry directions. Here, the hopping parameter $t$ is taken as the unit of energy. We infer the properties of the AF long-range ordered state by taking the $\Omega \rightarrow 0$ limit. For the case of small $M$, that is, $M = 2, 4, 6$, for instance, we find a four-peak structure along the line from $(0, 0)$ to $(0, \pi)$ and near $(\pi/2, \pi/2)$ both for the AF case,
In cellular dynamical mean-field theory, two sharp bands appear inside the Mott-Hubbard bands. These two bands are absent in the single-site dynamical mean-field theory. Therefore, the appearance of these two bands is associated with the short-range spin correlations. Our Green’s function approach reproduces this feature for small $M$. But these two bands disappear for large enough $M$ as shown in Fig. 5(b) and (d). Around $(0, \pi)$ and $(\pi/2, \pi/2)$, there are no quasi-particle bands. The band energy at these wave vectors is degenerate with that with the wave vectors shifted by $(\pi, \pi)$. Therefore, many magnons are involved in the dynamics of the quasiparticles at these wave vectors. The disappearance of these two bands is due to the long-range correlation effect, which is not included either in a cellular dynamical mean-field theory or quantum Monte Carlo simulations not carried out at sufficiently lower temperatures. In the latter, the correlation length is limited to be short-ranged.

We also note that the difference between $(0, \pi)$ and $(\pi/2, \pi/2)$. As clearly seen from Fig. 5(d), the scattering effect due to magnons is much significant at $(0, \pi)$ than at $(\pi/2, \pi/2)$. The difference arises from the density of states: The density of states is large at $(0, \pi)$ compared to that at $(\pi/2, \pi/2)$. This makes the difference between the hot spot, $(0, \pi)$, and the cold spot, $(\pi/2, \pi/2)$. The lifetime of the quasiparticles is short for the former compared to the latter.

We also note that the spectra shown in Fig. 5(b) with $\Gamma = 0$ and $M = 200$ consist of a number of peaks with small separation. It was pointed out that the broad spectra observed in the ARPES measurements can be based on Franck-Condon broadening in the undoped cuprates. Similar broad spectra were obtained in a diagrammatic Monte Carlo simulation in Ref. 55 based on the $t$-$J$ model with electron-phonon coupling. Here, a similar structure is obtained from the electron-magnon coupling. For a single hole doped case, we expect that the damping effect is large in the hole dynamics. A realistic spectrum is obtained by taking a moderate value for the broadening of the bare conduction electron spectrum, $\delta_\omega$, as shown in Fig. 6. We note that the broad spectra, with the width of the order of $2J$, are associated with the electron-magnon coupling in the strong coupling regime.

The density of states is shown in Fig. 7 for different values of $g$ and in Fig. 8 for different values of $M$. The asymmetry is associated with non-zero value of $t_1$. We clearly see a pseudogap like behavior for large $g$. It should be noted that there is no Hubbard band structure because we do not include the strong correlation effect associated with the on-site Coulomb repulsion between the conduction electrons. The two-broad-peak structure for $\omega > 0$ and $\omega < 0$ is associated with the short-range AF correlation. Similar features, which are well separated from the Hubbard bands, were observed in the cellular dynamical mean-field theory. We note that there is some change in the density of states as we increase $M$. We note that in these figures the total weights decrease as we increase $g$ or $M$ because of the damping of the magnons.

V. SUMMARY

To summarize, we have proposed a simple model describing a coupling between the AF short-range correlation and the conduction electrons. The model captures the essential features of the strongly correlated electron system except for the Hubbard band. Applying a strong coupling analysis, we find a crossover from a large magnetic polaron to a small magnetic polaron. If we limit the number of magnons, $M$, small, we obtain the result similar to the cellular dynamical mean field theory. However, taking a small number for $M$ corresponds to restricting the momentum resolution. By increasing $M$, some features disappear because of the long-range AF correlation effect but a gap like feature remains. This analysis suggests that including the long-range correlation is crucial and restricting the momentum resolution can lead to incorrect results.

The strong coupling analysis given in this paper provides supplemental information for the powerful numerical techniques, like extended versions of dynamical mean-field theory and quantum Monte Carlo simulations. In those numerical calculations, the Mott-Hubbard bands are clearly obtained. However, the important feature appears in the low-energy electronic structure by including the short-range correlation effect. In general, including the short-range correlation effect is difficult in dynamical mean-field theory and quantum Monte Carlo simulations. For the former, one needs a large cluster size depending on the length of the correlation length. However, increas-
FIG. 5. (Color online) Spectral function along symmetry directions with $g = 2$ for (a) $\Omega = 0$, $\Gamma = 0$, and $M = 6$, (b) $\Omega = 0$, $\Gamma = 0$, and $M = 200$, (c) $\Omega = 0.4$, $\Gamma = 0$, and $M = 6$, (d) $\Omega = 0.4$, $\Gamma = 0.3$, and $M = 200$. The hopping parameters are $t = 1$ (unit of the energy), $t_1 = 0$, and $t_2 = 0$. The dots in (a) represent the values of $\varepsilon_k$.

FIG. 6. (Color online) Spectral function along symmetry directions for the AF long-range ordered state ($\Omega = 0$) with the broadening $\delta = 0.3$ for the bare conduction electron spectrum. The other parameters are the same as those of Fig. 5(b).

The hopping parameters are $t = 1$ (unit of the energy), $t_1 = 0$, and $t_2 = 0$. The dots in (a) represent the values of $\varepsilon_k$.

Our analysis can be applied to understand the strong electronic correlation effect in the cuprate high-temperature superconductors. For the case of the parent compound, where a photohole is introduced in the ARPES measurements, the spectra become broad due to Franck-Condon broadening because of the strong coupling between magnons and the conduction electron. The situation is similar to the electron-phonon coupling case. Although it is natural to expect that there is contribution from the electron-phonon coupling, the major role can be played by the strong coupling between magnons and the conduction electron. As for the paramagnetic phase, a pseudogap like behavior has been obtained as shown in Fig. 5(c) and (d) and in Fig. 7.

There are several points, which are left for future re-
This suggests that a spin texture is formed around a doped hole. One possibility is a skyrmion. Including the dynamics of the spin texture can lead to a modification of the energy dispersion in the parent compound and the gap opening in the pseudogap phase. In order to study this correlation effect, we need to consider a finite number of conduction electrons.

FIG. 8. (Color online) The density of states for different values of $g$. The other parameters are $\Omega = 0.4$, $t_1 = -0.2$, $t_2 = 0$, $\Gamma = 0.3$, $M = 200$, and $\delta = 0.1$.

FIG. 7. (Color online) The density of states for different values of $M$. The other parameters are $\Omega = 0.4$, $t_1 = -0.2$, $g = 1.5$, $\Gamma = 0.3$, $\delta = 0.1$.

ACKNOWLEDGMENTS

The author thanks T. Yoshida, D. Ootsuki, and H. Yamase for helpful comments.

Appendix A: Short-Range AF Correlation

In this appendix, we review the Green’s function formalism. Suppose we consider operators $A$ and $B$ and their Matsubara Green’s function

$$G_{AB}(\tau) = -\langle T_\tau A(\tau) B(0) \rangle \equiv \langle A \mid B \rangle_\tau. \quad (A1)$$

Here, $T_\tau$ is the imaginary time ordering operator and $A(\tau) = e^{\tau H} A e^{-\tau H}$ with $H$ being the Hamiltonian and $\tau$ the imaginary time. The Fourier transform of this Green’s function is

$$G_{AB}(i\omega_n) = \int_0^\beta d\tau e^{i\omega_n \tau} \left[ -\langle T_\tau A(\tau) B(0) \rangle \right] \equiv \langle A \mid B \rangle_{i\omega_n}. \quad (A2)$$

Here, $\beta = 1/(k_B T)$ with $k_B$ the Boltzmann constant. For the case that $A$ and $B$ are bosonic operators, the Matsubara frequency is given by $\omega_n = 2\pi n/\beta$, with $n$ an integer. For the case that $A$ and $B$ are fermionic operators, the Matsubara frequency is given by $\omega_n = \pi(2n + 1)/\beta$, with $n$ an integer. Hereafter, we consider the former case. Taking the derivative of $G_{AB}(i\omega_n)$ with respect to $\tau$, and Fourier transforming, we obtain

$$i\omega_n \langle A \mid B \rangle_{i\omega_n} = \langle [A, H] \mid B \rangle_{i\omega_n} + \langle [A, B] \rangle. \quad (A3)$$

In general, we need to consider the equation of motion for the quantity $\langle [A, H] \mid B \rangle_{i\omega_n}$, which is given by

$$i\omega_n \langle [A, H] \mid B \rangle_{i\omega_n} = \langle [[A, H], H] \mid B \rangle_{i\omega_n} + \langle [A, H], B \rangle. \quad (A4)$$

Again, we need to consider the equation of motion for the first term in the right-hand side. To obtain a closed set of equations, we need to introduce a Tyablikov’s decoupling at some point.

Now we return to the spin system and apply the formalism above. We define the following Matsubara Green’s function,

$$D_{ij}(\tau) = -\langle T_\tau S_i^+ (\tau) S_j^- (0) \rangle \quad (A5)$$

with $S_j^\pm = S_j^\mp \pm i S_j^y$. Here, $S_i^\pm(\tau) = \exp (\tau H_{\text{spin}}) S_i^\pm \exp (-\tau H_{\text{spin}})$. The equation of motion is

$$i\omega_n \langle S_i^+ \mid S_j^- \rangle_{i\omega_n} = \langle [S_i^+, H_{\text{spin}}] \mid S_j^- \rangle_{i\omega_n} + \langle S_i^+, S_j^- \rangle, \quad (A6)$$

where

$$\langle S_i^+ \mid S_j^- \rangle_{i\omega_n} = \int_0^\beta d\tau D_{ij}(\tau) \exp (i\omega_n \tau). \quad (A7)$$
is the Fourier transform of \( D_{ij} (\tau) \) with \( \omega_n \) the bosonic Matsubara frequency.

The equation of motion for the first term in the right-hand side of Eq. (A6) is

\[
i\omega_n \langle [S_i^+, H_{\text{spin}}], S_j^- \rangle \rangle_{\omega_n} = \langle \langle [S_i^+, H_{\text{spin}}], S_j^- \rangle \rangle_{\omega_n} + \langle \langle [S_i^+, H_{\text{spin}}], S_j^- \rangle \rangle_{\omega_n}.
\]

(A8)

After a tedious calculation, we obtain the explicit forms for the two terms in the right-hand side of Eq. (A6) is

\[
\omega_n = \frac{\Omega}{2b} \sqrt{1 - \gamma} (1 + 2b^2 + \gamma_q)
\]

(B1)

Using \( \omega_n \), the \( q \) dependent coupling, \( g_q \), is expressed as

\[
g_q = \frac{1 - \gamma_q}{2\omega_q} \Omega g.
\]

(B2)

The parameters \( b \) and \( \Omega \) are determined from the self-consistent calculation in the AF Heisenberg model but here we take them as parameters and set \( b = 0.1 \). In this case, \( g_q^2 \) exhibits a sharp peak at \( q = (\pi, \pi) \).

Replacing \( \Omega \) with \( \omega_q \) and \( g \) with \( g_q \), the conduction electron Green’s function with the second order self-energy is given by

\[
G_k^{(2)} (i\omega_n) = \frac{1}{i\omega_n - \epsilon_k - \sum_q \frac{g_q^2}{\omega_n - \epsilon_{k+q} - \omega_q}}.
\]

(B3)

Figure 10 shows the spectral function along symmetry directions. Here, we set \( g = 0.5 \), which is not in the strong coupling regime, to focus on the wave vector \( q \) dependence. We see that there are no discernible changes in the spectral function except for around \((0, \pi)\). This is simply understood as the result of the average with respect to \( q \). From the behavior of \( g_q^2 \), the dominant contribution comes from \( q = (\pi, \pi) \). But in taking the average in the self-energy, this contribution is smeared out. Therefore, the spectral function with the wave vector \( q \) dependence is almost equivalent to the non-interacting case.

We note that the result shown in Fig. 10 is based on the second-order self-energy. We may expect that there are band energy changes and modification of the spectral weights at higher-order self-energies. However, there can be some cancellation at higher-order terms because of the presence of \( q \) summation in the higher-order terms. This point is left for future research.

Appendix B: The Effect of the Wave Vector \( q \) Dependence of \( g_q \) and \( \omega_q \)

In the strong coupling analysis of the self-energy, we neglected the \( q \) dependence of \( g_q \) and \( \omega_q \) in the main text. It is natural to ask how the \( q \) dependence of these parameters affects the result. Unfortunately, we are unaware of how one can examine this point: If we consider \( n \)-th order of the self-energy, we need to carry out \( q \) summation \( n \) times. Furthermore, just computing the self-energy up to a finite order is not enough to investigate the strong coupling effect. However, it is possible to examine the \( q \) dependence in the weak coupling regime. In this appendix, we consider the effect of the \( q \) dependence of \( g_q \) and \( \omega_q \) within the second-order perturbation theory.

From the Green’s function approach given in Appendix A, we find that the dispersion of the magnon excitation is given by

\[
\omega_q = \frac{\Omega}{2b} \sqrt{1 - \gamma} (1 + 2b^2 + \gamma_q)
\]

(B1)

Using \( \omega_q \), the \( q \) dependent coupling, \( g_q \), is expressed as

\[
g_q = \frac{1 - \gamma_q}{2\omega_q} \Omega g.
\]

(B2)

The parameters \( b \) and \( \Omega \) are determined from the self-consistent calculation in the AF Heisenberg model but here we take them as parameters and set \( b = 0.1 \). In this case, \( g_q^2 \) exhibits a sharp peak at \( q = (\pi, \pi) \).

Replacing \( \Omega \) with \( \omega_q \) and \( g \) with \( g_q \), the conduction electron Green’s function with the second order self-energy is given by

\[
G_k^{(2)} (i\omega_n) = \frac{1}{i\omega_n - \epsilon_k - \sum_q \frac{g_q^2}{\omega_n - \epsilon_{k+q} - \omega_q}}.
\]

(B3)

Figure 10 shows the spectral function along symmetry directions. Here, we set \( g = 0.5 \), which is not in the strong coupling regime, to focus on the wave vector \( q \) dependence. We see that there are no discernible changes in the spectral function except for around \((0, \pi)\). This is simply understood as the result of the average with respect to \( q \). From the behavior of \( g_q^2 \), the dominant contribution comes from \( q = (\pi, \pi) \). But in taking the average in the self-energy, this contribution is smeared out. Therefore, the spectral function with the wave vector \( q \) dependence is almost equivalent to the non-interacting case.

We note that the result shown in Fig. 10 is based on the second-order self-energy. We may expect that there are band energy changes and modification of the spectral weights at higher-order self-energies. However, there can be some cancellation at higher-order terms because of the presence of \( q \) summation in the higher-order terms. This point is left for future research.
FIG. 10. (Color online) The spectral function along symmetry directions computed by Eq. (B3). The values of the parameters are, \( g = 0.5 \), \( \Omega = 0.4 \), \( \tilde{b} = 0.1 \). Thick blue lines are computed by replacing \( gq \) with \( g \) and \( \omega_q \) with \( \Omega \) and not taking the \( q \) summation.

6. M. Ferrero, P. S. Cornaglia, L. D. Leo, O. Parcollet, G. Kotliar, and A. Georges, Phys. Rev. B 80, 10.1103/physrevb.80.064501 (2009).
7. A. Macridin, M. Jarrell, T. Maier, P. R. C. Kent, and T. Uefuji, Phys. Rev. B 82, 134504 (2010).
8. G. Martinez and P. Horsch, Phys. Rev. B 46, 6435 (1992).
9. E. Manousakis, Phys. Rev. B 75, 10.1103/physrevb.75.035106 (2007).
10. M. Fujita, H. Hiraka, M. Matsuda, M. Matsuura, J. M. Tranquada, S. Wakimoto, G. Xu, and K. Yamada, J. Phys. Soc. Jpn. 81, 011007 (2012).
11. H. Matsui, T. Takahashi, T. Sato, K. Terashima, H. Ding, T. Uefuji, and K. Yamada, Phys. Rev. B 75, 10.1103/physrevb.75.224514 (2007).
12. N. P. Armitage, P. Fourrier, and R. L. Greene, Rev. Mod. Phys. 82, 2421 (2010).
13. C. Proust and L. Taillefer, Annual Review of Condensed Matter Physics 10, 409 (2019).
14. G. Martinez and P. Horsch, Phys. Rev. Lett. 63, 1318 (1989).
15. Z. B. Su, Y. M. Li, W. Y. Lai, and L. Yu, Phys. Rev. Lett. 63, 1318 (1989).
16. D. Poilblanc, H. J. Schulz, and T. Ziman, Phys. Rev. B 46, 6435 (1992).
17. E. Manousakis, Phys. Rev. B 75, 10.1103/physrevb.75.035106 (2007).
18. G. Sangiovanni, G. Rohringer, and A. Toschi, Phys. Rev. B 75, 035105 (2007).
19. G. Martinez and P. Horsch, Phys. Rev. B 44, 317 (1991).
20. M. Greiner, D. Greif, and E. Demler, Rev. Mod. Phys. 82, 10.1103/physrevb.82.155101 (2010).
21. F. Grusdt, M. Kánasz-Nagy, A. Bohrdt, C. Chiu, G. Ji, M. Greiner, D. Greif, and E. Demler, Phys. Rev. X 8, 10.1103/physrevx.8.011046 (2018).
22. F. Grusdt, A. Bohrdt, and E. Demler, arXiv preprint arXiv:1901.01113 (2019).
23. W. F. Brinkman and T. M. Rice, Phys. Rev. B 2, 1324 (1970).
24. L. Bulaevski, E. Nagaev, and D. Khomskii, Soviet Journal of Experimental and Theoretical Physics 27, 836 (1968).
25. S. A. Trugman, Phys. Rev. B 37, 1597 (1988).
26. V. V. Val’kov, D. M. Dzebisashvili, and A. F. Barabanov, JETP Letters 104, 730 (2016).
27. E. Gull, M. Ferrero, O. Parcollet, A. Georges, and A. J. Millis, Phys. Rev. B 82, 10.1103/physrevb.82.155101 (2010).
28. T. Holstein, Ann. Phys. 8, 325 (1959).
29. T. Holstein, Ann. Phys. 8, 343 (1959).
30. J. T. Devreese and A. S. Alexandrov, Rep. Prog. Phys. 72, 066501 (2009).
31. P. A. Lee, N. Nagaosa, and X.-G. Wen, Rev. Mod. Phys. 78, 17 (2006).
32. E. Dagotto, T. Hotta, and A. Moreo, Phys. Rep. 344, 1 (2001).
33. D. P. Arovas and A. Auerbach, Phys. Rev. B 38, 316 (1988).
34. M. Takahashi, Phys. Rev. B 40, 2494 (1989).
35. D. Yoshioka, J. Phys. Soc. Jpn. 58, 3733 (1989).
36. E. Manousakis, Rev. Mod. Phys. 63, 1 (1991).
37. J. Kondo and K. Yamaji, Progr. Theoret. Phys. 47, 807 (1972).
38. H. Shimahara and S. Takada, J. Phys. Soc. Jpn. 60, 2394 (1991).
39. S. Winterfeldt and D. Ihle, Phys. Rev. B 56, 5535 (1997).
40. A. Y. Zavidonov and D. Brinkmann, Phys. Rev. B 58, 12486 (1998).
41. M. V. Sadovskii, Phys. Usp. 44, 515 (2001).
42. G. D. Mahan, Many-particle physics (Springer Science & Business Media, 2013).
43. S. Hayden, H. Mook, P. Dai, T. Perring, and F. Doğan, Nature 429, 531 (2004).
44. J. Tranquada, H. Woo, T. Perring, H. Goka, G. Gu, G. Xu, M. Fujita, and K. Yamada, Nature 429, 534 (2004).
45. M. Fujita, H. Hiraka, M. Matsuda, M. Matsuura, J. M. Tranquada, S. Wakimoto, G. Xu, and K. Yamada, J. Phys. Soc. Jpn. 81, 011007 (2012).
46. M. Berciu, Phys. Rev. Lett. 97, 10.1103/physrevlett.97.036402 (2006).
47. G. L. Goodvin, M. Berciu, and G. A. Sawatzky, Phys. Rev. B 74, 10.1103/physrevb.74.245104 (2006).
48. N. V. Proko’ev and B. V. Svistunov, Phys. Rev. Lett. 81, 2514 (1998).
49. A. Mishchenko, N. Proko’ev, A. Sakamoto, and B. Svistunov, Phys. Rev. B 62, 6317 (2000).
50. A. Barabanov and L. Maksimov, Phys. Lett. A 207, 390 (1995).
51. S. Winterfeldt and D. Ihle, Phys. Rev. B 59, 6010 (1999).
52. A. M. Stoneham, J. Gavartin, A. L. Shulger, A. V. Kimmel, D. M. Ramo, H. M. Ronnow, G. Aeppli, and C. Renner, J. Phys.: Condens. Matter 19, 255208 (2007).
53. A.-M. S. Tremblay, B. Kyung, and D. Sénéchal, Low Temp. Phys. 32, 424 (2006).
54. K. M. Shen, F. Ronning, D. H. Lu, W. S. Lee, N. J. C. Ingle, W. Meevasana, F. Baumberger, A. Damascelli, N. P. Armitage, L. L. Miller, Y. Kohsaka, M. Azuma,
M. Takano, H. Takagi, and Z. X. Shen, Phys. Rev. Lett. 93, 267002 (2004).

55 A. S. Mishchenko and N. Nagaosa, Phys. Rev. Lett. 93, 036402 (2004).

56 T. Morinari, Half-skrymion theory for high-temperature superconductivity (World Scientific, 2010) Chap. 13, pp. 311–332.

57 M. Hashimoto, I. M. Vishik, R.-H. He, T. P. Devereaux, and Z.-X. Shen, Nat. Phys. 10, 483 (2014).

58 I. M. Vishik, Rep. Prog. Phys. 81, 062501 (2018).

59 T. Wu, H. Mayaffre, S. Krmer, M. Horvatić, C. Berthier, W. N. Hardy, R. Liang, D. A. Bonn, and M.-H. Julien, Nature 477, 191 (2011).

60 G. Ghiringhelli, M. L. Tacon, M. Minola, S. Blanco-Canosa, C. Mazzoli, N. B. Brookes, G. M. D. Luca, A. Frano, D. G. Hawthorn, F. He, T. Loew, M. M. Sala, D. C. Peets, M. Salluzzo, E. Schierle, R. Sutarto, G. A. Sawatzky, E. Weschke, B. Keimer, and L. Braicovich, Science 337, 821 (2012).

61 J. Chang, E. Blackburn, A. T. Holmes, N. B. Christensen, J. Larsen, J. Mesot, R. Liang, D. A. Bonn, W. N. Hardy, A. Watenphul, M. v. Zimmermann, E. M. Forgan, and S. M. Hayden, Nat. Phys. 8, 871 (2012).