Operator Projection Method Applied to the Single-Particle Green’s Function in the Hubbard Model

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A new non-perturbative framework for many-body correlated systems is formulated by extending the operator projection method (OPM). This method offers a systematic expansion which enables us to project into the low-energy structure after extracting the higher-energy hierarchy. This method also opens a way to systematically take into account the effects of collective excitations. The Mott-Hubbard metal-insulator transition in the Hubbard model is studied by means of this projection beyond the second order by taking into account magnetic and charge fluctuations in the presence of the high-energy Mott-Hubbard structure. At half filling, the Mott-Hubbard gap is correctly reproduced between the separated two bands. Near half filling, strongly renormalized low-energy single-particle excitations coexisting with the Mott-Hubbard bands are shown to appear. The significance of the momentum-dependent self-energy in the results is stressed.

KEYWORDS: metal-insulator transition, Hubbard model, projection operator

In spite of a long history, a satisfactory theoretical description of strongly correlated electrons remains open because of the difficulty in reproducing their rich hierarchy structures in energy and momentum. The properties near the metal-insulator transitions (MITs) provide a typical challenge. It is required to correctly describe both a high-energy incoherent structure of the “Hubbard bands” with the Mott gap and the low-energy coherent excitations. The low-energy part must be severely renormalized with strong momentum dependence. It is also required to treat magnetic and charge fluctuations.

The dynamical mean field theory (DMFT) reproduces both the incoherent Hubbard bands and the quasiparticle structure. On the other hand, numerical simulations have revealed an important aspect of the MIT in the two-dimensional Hubbard model, i.e., nearly dispersionless fermions around the \((\pi, 0)\) and \((0, \pi)\) momenta. This suggests that the momentum dependence of the single-particle self-energy, which is completely neglected in the DMFT, is significant in real finite-dimensional systems. The momentum dependence of the low-energy structure appears from collective modes under the influence of high-energy incoherence. Such hierarchy can not be properly treated in the perturbative or one-loop analyses of the self-energy and the dynamical susceptibilities, because the high-energy structure such as the Mott-Hubbard bands is missing.

In this letter, we propose a systematic expansion which incorporates both the coherent and incoherent structure in the energy hierarchy of single-particle excitations. By applying the operator projection method (OPM) to the single-particle Green’s function, our framework allows us to systematically project out the high-energy structure and sequentially extract the low-energy coherent excitations. The low-energy coherence appears with the strongly momentum dependent self-energy due to two-particle collective fluctuations.

The OPM first developed by Nakajima,\(^9\) Zwanzig,\(^10\) and Mori\(^11\) is based on the equation of motion\(^12\) with a moment expansion of a correlation function. The main procedure of this method is to decompose the time-derivative of an operator into the term projected onto itself and the remaining new operator. The OPM involves repeatedly applying this procedure to the newly created operators. Then, the OPM allows one to construct a continued-fraction expansion of a correlation function. The expansion is suited for systematically evaluating the energy hierarchy structure from high to low energies. Similar equation-of-motion (EQM) approaches supplemented with various decoupling schemes and/or other approximations have been intensively studied for strongly correlated models such as the Hubbard\(^2\) and the \(t-J\) models.\(^13\) For the Hubbard model, the Hubbard bands are reproduced from the first three, i.e., the zeroth-, first- and second-order moments of the Green’s function. In principle, the low-energy band appears in the fourth order, although a systematic and correct expansion has not yet been carried out. In this letter, we show that the OPM up to the second order, supplemented with the self-energy in the second-order
projection which is referred to as the second-order self-energy, makes it possible to correctly reproduce the hierarchy: the Hubbard bands as well as the renormalized low-energy bands. We note that our calculated second-order self-energy gives an evaluation of the fourth-order moment. The OPM based on the equation of motion is a non-perturbative treatment and works from the weakly correlated limit $U/n(2 - n)/t \to 0$ to the strongly correlated limit $U/n(2 - n)/t \to \infty$.

We take the Hubbard Hamiltonian with an electron transfer $t_{\vec{x},\vec{x}'}$ from an atomic site $\vec{x}$ to $\vec{x}'$ and the local Coulomb repulsion $U$:

$$H = -\sum_{\vec{x},\vec{x}',s} t^+_{\vec{x},\vec{x}'} c^+_{\vec{x}'} s \cdot c_{\vec{x}s} + U\sum_{\vec{x}} n_{\vec{x}\uparrow} n_{\vec{x}\downarrow} \text{ with } n_{\vec{x}s} = c^+_{\vec{x}s} c_{\vec{x}s}, \text{ or } \hat{H} = H - \mu \sum_{\vec{x}s} n_{\vec{x}s} \text{ with the chemical potential } \mu.$$

We perform the projection procedure for the electron creation and annihilation operators at an atomic site $\vec{x}$ with a spin index $s$, $c^+_{\vec{x}s}$ and $c_{\vec{x}s}$. It is useful to define the fermionic $4N$-component vector operator composed of

$$\Psi_{\vec{x}} = \left( \begin{array}{c} \sigma_0 \rho_0 + \rho_3 \frac{2}{2} - \imath \sigma_2 \rho_0 - \rho_3 \frac{2}{2} \end{array} \right) \left( \begin{array}{c} c^+_{\vec{x}\uparrow}, c_{\vec{x}\downarrow}, c^+_{\vec{x}\uparrow}, c_{\vec{x}\downarrow} \end{array} \right). \tag{1}$$

Here, $N$ is the total number of the atomic sites. $\Psi^\dagger$ is defined as the Hermitian conjugate operator of $\Psi$.

We introduce $\omega A = [A, \hat{H}]$, and $\langle A \rangle = \text{Tr}[\text{e}^{-H/T} A] / \text{Tr}[\text{e}^{-H/T}]$ at temperature $T$. We also define the response function of $\Psi$ in the $4N \times 4N$ matrix representation $K_{\Psi,\Psi^\dagger}(t)$. Its $(a,a') \otimes (\vec{x},\vec{x}')$ component is defined by

$$K^{a,a'}_{\Psi,\Psi^\dagger}(t; \vec{x}\vec{x}') = -\imath \left\{ \left[ \Psi^{a'}_{\vec{x}'}(t), \left( \Psi^\dagger_{\vec{x}} \right)^{a'} \right] \right\}_+.$$ \tag{2}

We note $K_{\Psi,\Psi^\dagger}(0) = -\imath I$ with the $4N \times 4N$ identity matrix $I$ because of the fermion anticommutation relation. The Fourier transformation of Eq. (3) gives the susceptibility $\chi_{\Psi,\Psi^\dagger}(\omega)$, which is nothing but the Green’s function $G(\omega)$. The projection procedure is defined as

$$\hat{\omega} \Psi = \varepsilon^{(1)} \Psi + \delta \hat{\omega} \Psi, \tag{3a}$$
$$\varepsilon^{(1)} = K_{\Psi,\Psi^\dagger}(0) K_{\Psi,\Psi^\dagger}^{-1}(0). \tag{3b}$$

Namely, the operator $\hat{\omega} \Psi$ is split into $\Psi$ with a component given by the equal-time correlation $K_{\Psi,\Psi^\dagger}(0)$ and the new operator $\delta \hat{\omega} \Psi$ which satisfies $K_{\Psi,\Psi^\dagger}(\omega)K_{\Psi,\Psi^\dagger}^{-1}(0) = 0$ by definition. It allows us to express the single-particle Green’s function $G(\omega) = \chi_{\Psi,\Psi^\dagger}(\omega)$ in the form of a Dyson equation as

$$G(\omega) = i \left[ G^{(0)}(\omega) - \Sigma(\omega) \right]^{-1} K_{\Psi,\Psi^\dagger}(0), \tag{4}$$
$$G^{(0)}(\omega) = \left[ \omega I - \varepsilon^{(1)} \right]^{-1}, \tag{5}$$
$$\Sigma(\omega) = -i \chi^{\text{irr}}_{\delta \omega \Psi, (\delta \omega \Psi)^\dagger}(\omega) K_{\Psi,\Psi^\dagger}^{-1}(0). \tag{6}$$

The irreducible part of $\chi^{\text{irr}}_{\delta \omega \Psi, (\delta \omega \Psi)^\dagger}(\omega)$ with respect to $G^{(0)}(\omega)$ has been introduced:

$$\chi^{\text{irr}}_{\delta \omega \Psi, (\delta \omega \Psi)^\dagger}(\omega) = \left[ \chi_{\delta \omega \Psi, (\delta \omega \Psi)^\dagger}^{-1}(\omega) - i K_{\Psi,\Psi^\dagger}^{-1}(0) G^{(0)}(\omega) \right]^{-1}. \tag{7}$$

For the Hubbard model, one obtains

$$\varepsilon^{(1)}_{\vec{x},\vec{x}'} = \varepsilon^{(0)}_{\vec{x},\vec{x}'} \sigma_0 \rho_3 - U \delta_{\vec{x},\vec{x}'} \left( \left( \begin{array}{c} \delta \vec{S} \end{array} \right) \cdot \vec{\sigma} \rho_0 - \frac{\left( \Delta^s_{\vec{x}} \right)^i}{\sqrt{2}} \sigma_0 \rho_i \right), \tag{8}$$

with $\varepsilon^{(0)}_{\vec{x},\vec{x}'} = -t_{\vec{x},\vec{x}'} - (\mu - U \langle n_{\vec{x}} \rangle) \delta_{\vec{x},\vec{x}'}$, $n_{\vec{x}} = n_{\vec{x}\uparrow} + n_{\vec{x}\downarrow}$, $\delta \vec{S}^j = c^j_{\vec{x}\uparrow} \sigma_0 \rho_3 / 2$, $\Delta^s_{\vec{x}} = \frac{1}{\sqrt{2}} (c^+_{\vec{x}\uparrow} c_{\vec{x}\downarrow} + c^+_{\vec{x}\downarrow} c_{\vec{x}\uparrow})$ and $\Delta^s(\vec{x})^2 = \frac{1}{\sqrt{2}} (c^+_{\vec{x}\uparrow} c_{\vec{x}\downarrow} - c^+_{\vec{x}\downarrow} c_{\vec{x}\uparrow})$. The summation over $\vec{i} = 1$ and 2 should be taken. For the repulsively interacting model ($U > 0$), we can exclude the superconducting states with the isotropic $s$-wave pairing symmetry, $\langle \Delta^s(\vec{x})^2 \rangle = 0$. The thermal average $\langle \delta \vec{S} \rangle$, if it does not vanish, is chosen to break the symmetry in the $z$-axis, i.e., $\langle \delta \vec{S}_z \rangle = 0$. Then, Eq. (3) and $\delta \hat{\omega} \Psi$ are reduced to

$$\varepsilon^{(1)}_{\vec{x},\vec{x}'} = \varepsilon^{(0)}_{\vec{x},\vec{x}'} \sigma_0 \rho_3 - U \langle \delta \vec{S}_{\vec{x}} \rangle \delta_{\vec{x},\vec{x}'} \sigma_3 \rho_0, \tag{9a}$$
\[ \delta \omega \Psi_x = U \left( \frac{1}{2} \delta n_x \sigma_0 \rho_3 - \delta S_x^z \sigma_3 \rho_0 \right) \Psi_x, \]  
(9b)

with \( \delta n_x = n_x - \langle n_x \rangle \) and \( \delta S_x^z = S_x^z - \langle S_x^z \rangle \).

If \( \Sigma_1(\omega) \) is ignored, then the present theory is reduced to a Hartree-Fock theory. In order to calculate \( \Sigma_1(\omega) \), one can adopt perturbation expansions on a single-particle basis, one-loop approximation, long-time or short-time approximations. However, if \( \Sigma_1(\omega) \) is self-consistently determined by means of simple frameworks such as perturbation expansion or one-loop approximations, the MIT at half filling can not be reached. This is because arguments along this line always fail to give the correct high-energy behavior of the self-energy. We note that only the zeroth- and first-order moments of the Green’s function are correct in these theories. As known in the Hubbard and two-pole approximations, we need to proceed to higher-order moments, as is discussed below.

The second-order projection gives

\[ \delta \omega \delta \omega \Psi = \varepsilon^{(21)} \Psi + \varepsilon^{(22)} \delta \omega \Psi + \delta \omega \delta \omega \Psi, \]
(10a)

\[ \varepsilon^{(21)} = K_{\delta \omega \Psi, \Psi}(0) K_{-1}^{-1}(0), \]
(10b)

\[ \varepsilon^{(22)} = K_{\delta \omega \Psi, (\delta \omega \Psi)}(0) K_{-1}^{-1}(\delta \omega \Psi, (\delta \omega \Psi))(0). \]
(10c)

From Eq. (10) one obtains the irreducible self-energy

\[ \Sigma_1(\omega) = \left[ \Sigma^{(0)}_1(\omega) - \Sigma_2(\omega) \right]^{-1} \varepsilon^{(21)}, \]
(11a)

\[ \Sigma^{(0)}_1(\omega) = \left[ \omega I - \varepsilon^{(22)} \right]^{-1}, \]
(11b)

\[ \Sigma_2(\omega) = -i \chi_{\delta \omega \Psi, (\delta \omega \Psi)}^\text{irr}(\omega) K_{-1}^{-1}(\delta \omega \Psi, (\delta \omega \Psi))(0). \]
(11c)

For the repulsive Hubbard model,

\[ \varepsilon^{(21)}_{x'x} = U^2 \delta n_{x'} \langle \delta n_x \sigma_0 \rho_3 / 2 - \delta S_x^z \sigma_3 \rho_0 \rangle^2, \]
(12a)

\[ \varepsilon^{(22)}_{x'x} = -\frac{1}{2} t'_{x'x} (\mu_2 \sigma_0 \rho_3 - \langle S_x^z \rangle \sigma_3 \rho_0) \delta n_{x'}, \]
(12b)

\[ t'_{x'x} = t_{x'x} \left( \langle \delta n_x \sigma_0 \rho_3 / 2 - \delta S_x^z \rho_3 + \Delta_{x'}^{s(s')} / \sqrt{2} \right) \]
\[ \times \left( \langle \delta n_x \sigma_0 \rho_3 / 2 - \delta S_x^z \rho_3 - \Delta_{x'}^{s(s')} \sigma_0 \rho_3 / \sqrt{2} \rangle \right) \]
\[ \times \left( \langle \delta n_x \sigma_0 \rho_3 / 2 - \delta S_x^z \sigma_3 \rho_0 \rangle^2 \right)^{-1}, \]
(12c)

\[ \mu_2 = \mu_2^{(0)} \sigma_0 + \frac{(1 - \langle n \rangle) \varepsilon_{\text{kin}} + \varepsilon_{\text{cor2}}}{\langle \delta n_x \sigma_0 \rho_3 / 2 - \delta S_x^z \sigma_3 \rho_0 \rangle^2}, \]
(12d)

\[ \varepsilon_{\text{kin}} = -\frac{1}{N} \sum_k t_{kx} \left( \langle n_{x_{kx}}(\rho_0 \rho_3 - \sigma_0 \rho_3) \right), \]
(12e)

where \( \mu_2^{(0)} = -U(1 - \frac{1}{2} \langle n \rangle) \). The kinetic energy per site summed over spins is expressed as \( E_{\text{kin}} = \frac{1}{2} \sum_{k,s} \varepsilon_{x_{kx}}(n_k \rho_3 + \rho_3) - \frac{1}{2} \sum_{k,s} t_{kx}(c_{kx}^\dagger c_{kx}^\dagger \delta n_{x_{kx}}) \). Below, a momentum independent energy shift \( \varepsilon_{\text{cor2}} \) due to two-site correlated hopping terms which take the form \( t_{x'x} c_{x_{kx}}^\dagger c_{kx}^\dagger \delta n_{x_{kx}} \) in Eq. (12b) are neglected. Then, in the case of \( \langle S_x^z \rangle = 0 \), the remaining operator becomes

\[ \delta \omega \delta \omega \Psi_x \approx -U \left( \frac{1}{2} \delta n_x \sigma_0 \rho_3 - \delta S_x^z \rho_3 + \Delta_{x}^{s(s')} / \sqrt{2} \rho_3 \right), \]
\[ \delta \omega \delta \omega \Psi_x \approx -U \left( \frac{1}{2} \delta n_x \sigma_0 \rho_3 - \delta S_x^z \rho_3 + \Delta_{x}^{s(s')} / \sqrt{2} \rho_3 \right), \]
(13)

Even when \( \Sigma_2(\omega) \) is neglected, the present formalism is a generalization beyond the Hubbard I approximation because not only the Mott-Hubbard bands are reproduced but also \( \varepsilon^{(22)} \) depends on the momentum. The former fact is guaranteed, since the Pauli exclusion principle is satisfied. The latter fact modifies the single-particle dispersion in each Mott-Hubbard band. The momentum dependence of \( \varepsilon^{(22)} \)
enters the present theory through the equal-time charge, spin, isotropic s-wave pairing correlations, while these correlations are ignored in the Hubbard I approximation. In the symmetry-unbroken phase, the electron Green’s function with momentum \( \vec{k} \) and spin \( s \) reads

\[
G_{e,s}(\omega, \vec{k}) = \left[ \omega - \varepsilon_k^{(0)} - \frac{t_{\vec{k}+\vec{q}}^2 (2-\langle n \rangle)}{\omega - \varepsilon_k^{(0)}} \right]^{-1},
\]

with \( \varepsilon_k = -\tilde{t}_k - \mu_2^{(0)} - \frac{2(2-\langle n \rangle)}{\langle n \rangle + 2} \varepsilon_k^{(0)} \). Here, \( \tilde{t}_k \) is a (1,1) component of Eq. (12c). Equation (14) has a pole at \( \omega^\pm_k = (\varepsilon_k^{(0)} + \varepsilon_k^{(0)} + \Delta^{MH}_k)/2 \) in each Hubbard band with a residue \( z^\pm_k = (1 \pm (\varepsilon_k^{(0)} - \varepsilon_k^{(0)})/\Delta^{MH}_k)/2 \). Here, \( \Delta^{MH}_k = \sqrt{U^2 (2-\langle n \rangle)(2-\langle n \rangle)} + (\varepsilon_k^{(0)} - \varepsilon_k^{(0)})^2 \) is the momentum-dependent Mott-Hubbard gap. The momentum dependence diminishes as \( U/t \) diverges. It is easily found that when the collective degrees of freedom are completely frozen, i.e., \( \tilde{t}_k = 0 \), Eq. (14) recovers the Hubbard I solution at half filling. On the other hand, when equal-time two-particle correlations with the momentum \( \vec{Q} \) are significant, \( \tilde{t}_k \) behaves like \( t_{\vec{k}+\vec{Q}} \). Then, Eq. (13) smoothly connects the symmetry-broken and symmetry-unbroken phases through the growth of short-range correlations in Eq. (12c). For example, it reproduces the shadow bands in systems with well-developed short-range antiferromagnetic correlations. It can also describe other kinds of shadow bands such as nearly ferromagnetic systems. So far, few theories have reproduced such shadow-band effect even qualitatively within the one-loop approximations to \( \Sigma_1(\omega) \). Without \( \Sigma_2(\omega) \), the expectation value of the Hamiltonian as a function of \( \tilde{t}_k \) is given by

\[
\langle H \rangle = T \sum_{\omega_n, \vec{k}, s} \left[ -t_k + \frac{U \langle n \rangle}{2} + \Sigma_{1e,s}(\omega_n, \vec{k}) \right] G_{e,s}(\omega_n, \vec{k})
\]

\[
= 2 \sum_{\vec{k}, \pm} \left[ z_k^\pm \left( -t_k + \frac{U \langle n \rangle}{2} \right) + \frac{U^2 \langle n \rangle(2-\langle n \rangle)}{4 \Delta_{MH}^k} \right] f(\omega_k^\pm),
\]

with a fermionic Matsubara frequency \( \omega_n = (2n+1)\pi T \) and the Fermi distribution function \( f(\omega) = (e^{\omega/T} + 1)^{-1} \). The momentum-\( \vec{k} \) spin-\( s \) component of \( \Sigma_1(\omega) \) has been introduced as \( \Sigma_{1e,s}(\omega, \vec{k}) \). At \( \langle n \rangle = 1 \), we obtain \( \langle H \rangle = -\sum_{\vec{k}} t_k^2 - (t_k + \tilde{t}_k)^2/4)/U \) when \( U \gg T, t \). This includes the superexchange term through Eq. (12c).

Next, we consider the second-order self-energy \( \Sigma_2(\omega) \) by introducing decoupling approximations. Here, we can take several methods to calculate \( \Sigma_2(\omega) \): (A) the perturbation theory, (B) one-loop approximation with two-particle susceptibilities obtained by the self-consistent RPA (SCRPA), and (C) one-loop approximation with those obtained from the two-particle self-consistent (TPSC) method. In the TPSC method, irreducible vertices are determined so that the local-moment sum rule is also fulfilled for the two-particle properties, not only charge and spin correlations but also local s-wave pairing correlations. Therefore, we take the last method, (C). We note that \( \Sigma_2(\omega) \) has been evaluated within a two-site level by means of a different decoupling scheme. However, short-ranged correlations are ignored there.

Then, the second-order electronic self-energy is evaluated by means of the decoupling approximation as

\[
\Sigma_{2e}(\omega_n, \vec{k}) = \frac{2T/N}{\langle n \rangle(2-\langle n \rangle)} \sum_{m, \vec{q}} \left[ G(\omega_n - \Omega_m, \vec{k} - \vec{q}) \right]
\]

\[
\left\{ \frac{1}{2} \left[ T_{\vec{k}, \vec{q}}^2 (\chi_c(\Omega_m, \vec{q}) + \chi_s(\Omega_m, \vec{q})) + t_{\vec{k}-\vec{q}}^2 \chi_s(\Omega_m, \vec{q}) \right] \right.
\]

\[
-2t_{\vec{k}-\vec{q}} G(\Omega_m - \omega_n, \vec{q} - \vec{k}) \chi_p(\Omega_m, \vec{q}) \right\},
\]

where \( T_{\vec{k}, \vec{q}} = t_{\vec{k}-\vec{q}} - \frac{2(1-\langle n \rangle)}{\langle n \rangle(2-\langle n \rangle)} E_{\text{kin}} - t_{\vec{k}}^{(22)} \), \( \Omega_m = 2\pi m T \) is a bosonic Matsubara frequency, and \( \chi_c, \chi_s \) and \( \chi_p \) are the charge, spin, local s-wave pairing susceptibilities, respectively. The spin indices have not been included since all the variables are independent of the spin index. Within the TPSC approximation, the susceptibilities are calculated from

\[
\chi_c(\Omega_m, \vec{k}) = 2\chi_{ph}(\Omega_m, \vec{k})/[1 + \Gamma_c \chi_{ph}(\Omega_m, \vec{k})],
\]

\[
\chi_s(\Omega_m, \vec{k}) = 2\chi_{ph}(\Omega_m, \vec{k})/[1 - \Gamma_s \chi_{ph}(\Omega_m, \vec{k})],
\]

\[
\chi_{ph}(\Omega_m, \vec{k}) = \langle \hat{\rho}(\Omega_m, \vec{k}) \hat{\rho}(\Omega_m, -\vec{k}) \rangle,
\]

\[
\Gamma_c = \sum_{\vec{q}} \chi_c(\Omega_m, \vec{q}) - \sum_{\vec{q}} \chi_c(\Omega_m, -\vec{q}),
\]

\[
\Gamma_s = \sum_{\vec{q}} \chi_s(\Omega_m, \vec{q}) - \sum_{\vec{q}} \chi_s(\Omega_m, -\vec{q}).
\]
\( \chi_p(\Omega_m, \vec{k}) = \chi_{pp}(\Omega_m, \vec{k}) / [1 + \Gamma_p \chi_{pp}(\Omega_m, \vec{k})] \),

\[(16c)\]

with an approximation \( \Gamma_s = 4U \langle n_{\uparrow} n_{\downarrow} \rangle / \langle n \rangle^2 \) and the self-consistency conditions for \( \Gamma_s, \Gamma_c \) and \( \Gamma_p \) given by the local moment sum rules;

\[ T/N \sum_{m, \vec{k}} \chi_c(\Omega_m, \vec{k}) = \langle n \rangle + 2 \langle n_{\uparrow} n_{\downarrow} \rangle - \langle n \rangle^2, \]

\[ (17a) \]

\[ T/N \sum_{m, \vec{k}} \chi_s(\Omega_m, \vec{k}) = \langle n \rangle - 2 \langle n_{\uparrow} n_{\downarrow} \rangle, \]

\[ (17b) \]

\[ T/N \sum_{m, \vec{k}} \chi_p(\Omega_m, \vec{k}) = \langle n_{\uparrow} n_{\downarrow} \rangle. \]

\[ (17c) \]

\( \chi_{ph} \) and \( \chi_{pp} \) are the particle-hole and particle-particle susceptibilities calculated from the bare Green’s functions.

The calculated density of states for the Hubbard model with \( U = 4t \) and the electron transfer restricted to the nearest neighbor at the fillings \( n = 0.9 \) and \( n = 1 \) are shown in Fig. 1. The calculations have been done in the \( 32 \times 32 \) lattices with 2048 Matsubara frequencies. The metal and the Mott insulator are reproduced at \( n = 0.9 \) and \( n = 1 \), respectively, with the Hubbard bands. The emergence of a flat dispersion around \((\pi,0)\) is in agreement with the numerical results.\(^8\) It is remarkable that at \( n = 0.9 \), low-energy peaks around the magnetic Brillouin zone lie below the chemical potential and the dispersion outside the zone becomes strongly small and pinned near \( \omega = 0 \), as shown in Fig. 2, which agrees with previous results.\(^7,15\) It turns out that the growth of the equal-time antiferromagnetic (AFM) spin correlation produces such strong modification of the dispersion in the scale of \( \tilde{t} \). At \( n = 1 \), \( \tilde{t}/t \) should become \(-1\) at the zero temperature to yield the antiferromagnetism with the broken translational symmetry. In the present calculation carried out at \( T = 0.02t \), in fact, \( \tilde{t}/t = -0.84 \) for \( n = 1 \), while \( \tilde{t}/t = -0.53 \) for \( n = 0.9 \). This indicates that as
holes are doped into the Mott insulator, the shadow-band dispersion moves toward the chemical potential. However, self-consistent calculations of $\Sigma_2(\omega)$ using the TPSC method tend to weaken the SDW shadow-band structure too much and to overestimate the low-energy flat bands, as shown in Fig. 2, because the TPSC method overestimates $\Sigma_{2e}(\omega, \vec{k})$ at low frequencies. This will be improved by considering higher-order projections, as is discussed elsewhere.

We also note that in the results calculated from the (A) or (B) method, the AFM spin correlations appear to be underestimated. These give qualitatively similar results but smaller values of $|t|$. In summary, the OPM has been applied to the two-dimensional Hubbard model. Beyond the second-order projection, which correctly reproduces the first four moments and yields the two-pole approximation, the higher-order dynamics in the self-energy have been self-consistently taken into account. Then, we obtained not only the Mott insulator at half filling but also nearly dispersionless low-energy excitations pinned near the Fermi level away from half filling. This is the first analytic theory which has succeeded in describing both of the Mott-Hubbard bands and the low-energy single-particle excitations near half filling under strong short-ranged spin correlations. The OPM applied to the two-particle susceptibilities beyond the SCRPA are now under study to give more correct two-particle properties. Higher-order projections are necessary to consider the non-local pairing correlations, which are crucial in relation to the high-$T_c$ superconductivity.

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