The hierarchical Green function approach to the two-dimensional Hubbard model

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Abstract

By introducing multipe-site correlation functions, we propose a hierarchical Green function approach, and apply it to study the characteristic properties of a 2D square lattice Hubbard model by solving the equation of motions of a one-particle Green function and related multipe-site correlation functions. Under a cut-off approximation and taking the Fourier representation of multipe-site correlation functions, we obtain an analytical expression of one-particle Green function with static correlation functions. Then we calculate the spectral density function of electrons, and obtain that besides two main peaks corresponding to the lower and upper Hubbard bands in the spectral density function, there emerge some novel states between these two main peaks, and the total spectral weight of these emerged states is proportional to the hole doping concentration $\delta$. Meanwhile, there also emerge some collective modes related to possible charge/spin density wave and/or electronic pairing density wave ordering states. This calculation is completely consistent with the spectroscopy observations of the cuprate superconductors in normal states. On the other hand, the appearence of the static correlation functions in the one-particle Green function can be used to describe the intertwined orders observed in the normal state of the cuprate superconductors.

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I. INTRODUCTION

Since the discovery of the high $T_c$ cuprate superconducting materials\cite{1}, it is gradually realized that the strong correlation effect of electrons play a key role in understanding of the normal and superconducting states of these materials\cite{2–5}. Up to now there are a lot of experimental data and numerical simulations showing that the novel behavior of the normal states in the underdoped and optimal doped regimes of these materials\cite{6–8} originates from the strong correlation of electrons produced by the strong repulsive Coulomb interaction of electrons, and these unprecedented properties cannot be unambiguously explained by usual perturbation theory of quantum many particle systems based on the ”independent particle” (quasi-particle) assumption of the Landau Fermi liquid theory\cite{10}.

According to the present variety of experimental observations, the following aspects have been confirmed that: (1) the ”parent” of the high $T_c$ cuprate superconductors is an antiferromagnetic Mott insulator (with a 1.5eV charge-transfer energy gap) where the Cu-O plane(s) of the cuprate materials is undoped, and there is one electron on each Cu site; Hole doping rapidly suppresses the antiferromagnetic Néel order, but the optical gap does not collapse. The infrared reflectivity studies demonstrate the coexistence of the charge-transfer gap with finite optical conductivity that is transferred into the gap. Integrating the conductivity within the gap, the effective carrier density grows in proportion to the hole doping concentration\cite{11–13} $\delta$, rather than $1 - \delta$ as predicted by conventional band theory. (2) As the hole doping concentration $\delta$ reaching around $\delta_{\text{min}} \approx 5\%$, superconductivity sets in, with a transition temperature $T_c$ that grows to a maximum at about $\delta_{\text{opt}} \approx 16\%$, optimal doping, then declines for higher dopings and vanishes for $\delta_{\text{max}} \approx 27\%$. The superconducting state has a dome in the phase diagram of temperature versus hole doping level for cuprates. Materials with $\delta_{\text{min}} < \delta < \delta_{\text{opt}}$ and $\delta_{\text{opt}} < \delta < \delta_{\text{max}}$ are referred to, respectively, as ”underdoped” and ”overdoped”. For the enough large hole doping $\delta_{\text{max}} \leq \delta$, the superconductivity disappears, and the system can be represented by usual Landau Fermi liquid theory where the quasiparticle concept is established. Moreover, the superfluid density scales approximately with the hole doping concentration $\delta$ in the underdoped regime\cite{14}. Obviously, the parameter of the hole doping concentration $\delta$ play a key role in understanding of low temperature physical behavior of the cuprates, and it really sets up a bridge between an antiferromagnetic Mott insulator and the Landau Fermi liquid. (3) In the underdoped regime, at temperature just
above $T_c$, the normal state has a ”pseudogap” which is characterized by a substantial suppression of the electronic density of states at low energies that cannot be simply related to the occurrence of any form of broken symmetry, within which there are strong and ubiquitous tendencies toward several sorts of order with similar energy scales, including various forms of charge density wave (CDW), spin density wave (SDW), and possibly pairing density wave (PDW). These ”intertwined orders” make the normal state of the cuprates show ineluctable complexity [15], and remain to be understood.

The Hubbard model and the related t-J model are widely thought to capture the essential physics of a class of highly correlated systems, such as the high $T_c$ cuprate superconductors. The two-dimensional (2D) Hubbard model in a square lattice, used to describe the basic characters of high $T_c$ cuprate superconductivity [6–8, 16, 17], has been extensively studied in both analytical and numerical calculations, where there is inherent frustration between the tendency to maintain local antiferromagnetic correlations originated from the on-site strong repulsive Coulomb interaction and the doped hole itineracy.

The effective treatment of the influence of the on-site repulsive Coulomb interaction on the states of electrons is a central issue of any theoretical approach, where at the large repulsive $U$, a double occupied state on each site is strongly suppressed, and the Hilbert space of the electrons is split into two subspaces: one is composed of the unoccupied and single occupied states, and another one composed of the double occupied states that are lifted up high energy levels. In fact, there emerges a single-occupied constraint condition for electrons on each site produced by the on-site strong repulsive Coulomb interaction, which is a major difficulty faced by the present approaches. On the other hand, it is well known that in the both cases of weak $U/t_0 \ll 1$ and strong $U/t_0 \rightarrow \infty$ coupling limits, where $t_0$ is the hopping amplitude of electrons, the basic property of the ground state of the 2D square lattice Hubbard model is clear: in the former it is a Fermi liquid [18] as apart from the half filling; and in the latter it is a fully polarized ferromagnetic metallic phase [19] away from the half filling, in which there does not appear any order state.

The rich physical phenomena shown by the 2D square lattice Hubbard model really appear in the intermediate coupling, where $U$ is of order the bandwidth $W(= 8t_0)$, $U \sim W$, where there is the keen competition between the kinetic energy and the on-site repulsive Coulomb interaction of electrons. The former takes the delocalization of electrons, while the latter makes electrons localize. In this coupling range, there is still not a ubiquitous
acceptable calculations from microscopic theories. The 2D square lattice Hubbard model with intermediate coupling, likely cannot be treated using any fundamentally perturbative approach which starts with a non-interacting particle description. Beyond the present perturbation theoretical methods, the on-site Coulomb interaction of electrons had to be treated effectively before taking any approximation in analytical and numerical calculations.

In this paper, by introducing multipe-site correlation functions, we originally conceive a hierarchic Green function approach (HGFA) to study the equation of motion (EOM) of a one-particle Green function, in which the contribution of the electron correlation effect produced by the Coulomb interaction is completely represented by high order multipe-site correlation functions. In this way, by including the multipe-site correlation functions, the influence of the on-site repulsive Coulomb interaction on the states of electrons can be effectively incorporated into the one-particle Green function.

The idea of the HGFA is that, in contrast with the EOM of Green function approach that is usually written out in the phase space[20–24], we write out the EOMs of the one-particle Green function and related high order multipe-site correlation functions in the lattice space for the 2D square lattice Hubbard model, then we take the possible cut-off approximations for the highest order multipe-site correlation functions emerging in these EOMs. The two salient features of the HGFA are that: one is that the contribution coming from the on-site repulsive Coulomb interaction term can be rigorously incorporated into the EOMs, which is really represented by related hierarchical multipe-site correlation functions, and another one is that these hierarchical multipe-site correlation functions appearing in these EOMs can be classified into different levels denoted by a parameter $L$ which labels the number of electrons residing in a length (sites) scale that take part in a time evolution of an electron from initial state to final state. The multipe-site correlation functions in the same level $L$ constitute a set of linear EOMs, and in these EOMs only a few related multipe-site correlation functions belonging to the level $L + 1$ are appearing. In the lattice representation, the physical picture of a multipe-site correlation function in the level $L$ is very clear, that it represents the time evolution of an electron from the site $x_i$ at time $t_1$ to the site $x_j$ at time $t_2$ with considering the influence by the number $L$ of other electrons around this site $x_i$ at time $t_1$. It is expectant that for the higher $L$, the role of the multipe-site correlation functions in the level $L$ is weaker. This character of the multipe-site correlation functions is very helpful in taking the cut-off approximations for the highest order correlation functions appearing
in the EOMs. After the cut-off approximation, this set of EOMs of the one-particle Green function and the related multiple-site correlation functions is completely closed, and it can be solved after taking the Fourier representation of these multiple-site correlation functions.

Applying the HGFA for the 2D square lattice Hubbard model with an intermediate coupling $U$, we reveal that the one-particle Green function of electrons has the following salient characters: (1) The excitation energy spectrum of electrons is split into two subbands for a large $U$, called the lower and upper Hubbard bands, and the gap between these two bands is linear proportion to $U$; At half filling the system is a Mott insulator; As the hole doping, there emerge new states within this gap, and their total spectral weight is proportional to the hole doping concentration $\delta$; However, as taking enough large hole doping, $\delta_{\text{max}} \leq \delta$, the emerged states can fill in this gap. (2) The series of hierarchical static correlation functions are emergent in the one-particle Green function, which originate from the Coulomb interaction of electrons, and can be used to represent the contributions from possible intertwined orders appearing in the underdoped regime.

For the 2D square lattice Hubbard model, the HGFA in fact describes the intrinsic competition between the kinetic and potential energies of electrons which induces the inherent frustration between the tendency to maintain local antiferromagnetic correlations and the doped hole itineracy. As for both cases of $U = 0$ and $W = 0$, the HGFA is rigorous. In other case, the on-site Coulomb interaction can produce new multiple-site correlation functions belonging to the level $L + 1$ in the EOM of a multiple-site correlation function in the level $L$ by increasing a local factor $U \hat{n}_{\sigma}$ in a corresponding site $x_i$, where $\hat{n}_{\sigma}$ is the number operator of electrons, while the kinetic energy part of electrons is responsible to make each correlation function have a "hopping term", and to connect each EOM of a related multiple-site correlation function with others in the same level $L$ to construct a set of linear EOMs. The physics picture of the HGFA is very clear that the on-site Coulomb interaction plays the role to establish the relation between the multiple-site correlation functions in the level $L$ and those related ones belonging to the level $L + 1$, while the kinetic energy part only connects the multiple-site correlation functions in the same level $L$. Consequently there naturally appears a series of the hierarchical linear EOMs of related multiple-site correlation functions. Moreover, in this series of the hierarchical linear EOMs there emerge a series of hierarchical static correlation functions that are related to the corresponding multiple-site correlation functions. These static correlation functions can be used to describe the inho-
mogeneous states appearing in the system, and they can drastically influence the spectral density function of electrons.

The organization of the paper is as follows: we give the detail description of the HGFA in section II by using the EOM of an one-particle Green function for the Hubbard model by writing out a few EOMs of the related multipe-site correlation functions with \( L = 2 \). In section III, after taking the Fourier representation of the related multipe-site correlation functions, we solve this set of EOMs under the cutt-off approximations for the multipe-site correlation functions belonging to the level \( L = 3 \), and give an analytical expression of a one-particle Green function. In section IV, we calculate the electronic spectral density function by the one-particle Green function, and demonstrate that the total spectral weight of the emerged states within the gap between the lower and upper Hubbard bands is proportional to a hole doping concentration \( \delta \). The conclusion will be given in Section V.

II. THE EOMS OF THE ONE-PARTICLE GREEN FUNCTION AND MULTIPLE-SITE CORRELATION FUNCTIONS

The Hamiltonian of the 2D square lattice Hubbard model is that,

\[
\hat{H} = -t_0 \sum_{ij} \hat{\gamma}_{ij} \left( \hat{c}_{i\sigma}^\dagger \hat{c}_{j\sigma} + \hat{c}_{j\sigma}^\dagger \hat{c}_{i\sigma} \right) + U \sum_i \hat{n}_{i\uparrow} \hat{n}_{i\downarrow} - \mu \sum_{i\sigma} \hat{n}_{i\sigma} \tag{1}
\]

where \( \hat{c}_{i\sigma}^\dagger \) (\( \hat{c}_{i\sigma} \)) creates (annihilates) an electron with spin \( \sigma = \uparrow, \downarrow \) on site \( x_i \), \( \hat{n}_{i\sigma} = \hat{c}_{i\sigma}^\dagger \hat{c}_{i\sigma} \) is the number operator, \( \mu \) is the chemical potential, \( t_0 \) is the hopping amplitude, and \( U \) is the on-site repulsive Coulomb interaction strength. The hopping factor \( \hat{\gamma}_{ij} \) is defined as that,

\[
\hat{\gamma}_{ij} = \begin{cases} 1, & j = i + 1 \\ 0, & j \neq i + 1 \end{cases}
\]

which denotes the summation over the sites \( x_i, x_j \) only in the nearest neighbor. In order to write the EOMs of a one-particle Green function and related multipe-site correlation functions, we need the following commutation relations,

\[
[\hat{c}_{i\sigma}, \hat{H}] = \sum_j \left( \hat{h}_{ij} - \mu \delta_{ij} \right) \hat{c}_{j\sigma} + U \hat{n}_{i\sigma} \hat{c}_{i\sigma}
\]

\[
[\hat{n}_{i\sigma}, \hat{H}] = \sum_j \hat{n}_{ij} \hat{X}_{ij\sigma}^{(-)}
\]

\[
[\hat{X}_{ij\sigma}^{(\pm)}, \hat{H}] = U \left( \hat{n}_{j\sigma} - \hat{n}_{i\sigma} \right) \hat{X}_{ij\sigma}^{(\mp)} - \sum_l \hat{h}_{il} \hat{X}_{l\sigma}^{(\mp)} + \sum_l \hat{h}_{jl} \hat{X}_{i\sigma}^{(\mp)}
\]
where \( \hat{h}_d = -t_0 (\hat{\gamma}_d + \hat{\gamma}_l) \), and the bonding operators \( \hat{X}_{ij\sigma}^{(\pm)} \) are defined as that, \( \hat{X}_{ij\sigma}^{(\pm)} = \hat{c}_{i\sigma}^{\dagger} \hat{c}_{j\sigma} \pm \hat{c}_{j\sigma}^{\dagger} \hat{c}_{i\sigma} \). These commutation relations are the basic ingredients of writing the EOMs of related multipe-site correlation functions that directly or indirectly enter the EOM of the one-particle Green function.

The one-particle Green function is defined as that,

\[
G_{ij\sigma}(t_1, t_2) = -i < T\hat{c}_{i\sigma}(t_1)\hat{c}_{j\sigma}^{\dagger}(t_2) > \\
= -i\theta(t_1 - t_2) < \hat{c}_{i\sigma}(t_1)\hat{c}_{j\sigma}^{\dagger}(t_2) > +i\theta(t_2 - t_1) < \hat{c}_{j\sigma}^{\dagger}(t_2)\hat{c}_{i\sigma}(t_1) >
\]

In the Heisenberg picture, the time dependent of the annihilation (creation) operator \( \hat{c}_{i\sigma}(t)(\hat{c}_{i\sigma}^{\dagger}(t)) \) of an electron is represented by the Hamiltonian \( \hat{H} \) of the system as that,

\[
\hat{c}_{i\sigma}(t) = e^{i\hat{H}t}\hat{c}_{i\sigma}e^{-i\hat{H}t} \\
\hat{c}_{i\sigma}(t) = e^{i\hat{H}t}\hat{c}_{i\sigma}e^{-i\hat{H}t}
\]

As applied for the Hubbard model, the EOM of the one-particle Green function reads that,

\[
\left[ (i\partial_{t_1} + \mu) \delta_{il} - \hat{h}_d \right] G_{ij\sigma}(t_1, t_2) - UF_{ij\sigma}^{(n\sigma)}(t_1, t_2) = \delta(t_1 - t_2)\delta_{ij}
\]

where, \( F_{ij\sigma}^{(n\sigma)}(t_1, t_2) = -i < T\hat{n}_{i\sigma}(t_1)\hat{c}_{i\sigma}(t_1)\hat{c}_{j\sigma}^{\dagger}(t_2) > \), is produced by the on-site Coulomb interaction, and it is a multipe-site correlation function due to the appearance of the number operator \( \hat{n}_{i\sigma}(t_1) \) in the corresponding site \( x_i \). Obviously, all correlation effects of electrons in one-particle Green function is completely coming from the contribution of the related correlation function \( F_{ij\sigma}^{(n\sigma)}(t_1, t_2) \). Physically, the correlation function \( F_{ij\sigma}^{(n\sigma)}(t_1, t_2) \) in fact describes an evolution process of an electron from a double occupied state on site \( x_i \) at time \( t_1 \) to a state on site \( x_j \) at time \( t_2 \).

In order to defining multipe-site correlation functions, we introduce new composite multipe-site operators \( \hat{F}_{\{\alpha_1...\alpha_L\}}^{(A_{i_1}...A_{L})} \) that are composed of the density operators \( \hat{n}_{i\sigma} \) and the bonding operators \( \hat{X}_{il\sigma}^{(\pm)} \),

\[
\hat{F}_{\{\alpha_1...\alpha_L\}}^{(A_{i_1}...A_{L})} = \Pi_{k=1}^L \hat{A}_{\alpha_k}
\]

where \( \hat{A}_\alpha = \{ \hat{n}_{i\sigma}, \hat{n}_{i\sigma}, \hat{X}_{il\sigma}^{(-)}, \hat{X}_{il\sigma}^{(+)}, \hat{X}_{il\sigma}^{(-)}, \hat{X}_{il\sigma}^{(+)} \} \), and \( L = N_{n\sigma} + N_{n\sigma} + N_{X^+} + N_{X^+} + N_{X^+} \), where \( N_{A} \) is the number of the operator \( \hat{A}_{\alpha} \) appearing in the composite operators.
\( \widehat{F}_{\{a_1\ldots a_L\}}^{(A_1\ldots A_L)} \). With the help of these composite operators \( \widehat{F}_{\{a_1\ldots a_L\}}^{(A_1\ldots A_L)} \), we define the corresponding multi-site correlation functions \( F_{\{a_1\ldots a_L\}m\sigma}(t_1, t_2) \),

\[
F_{\{a_1\ldots a_L\}m\sigma}(t_1, t_2) = -i < T \widehat{F}_{\{a_1\ldots a_L\}}^{(A_1\ldots A_L)}(t_1) \widehat{c}_{m\sigma}(t_1) \widehat{c}_{m\sigma}^\dagger(t_2) >
\] (6)

Some of these multi-site correlation functions \( F_{\{a_1\ldots a_L\}m\sigma}(t_1, t_2) \) will enter into the series of hierarchical EOMs originated from Eq. (4), and they will construct a set of linear EOMs with the one-particle Green function \( G_{i\sigma\sigma}(t_1, t_2) \). The physics meaning of the operator \( \widehat{F}_{\{a_1\ldots a_L\}}^{(A_1\ldots A_L)} \) in the correlation function \( F_{\{a_1\ldots a_L\}m\sigma}(t_1, t_2) \) is that an electron \( \widehat{c}_{m\sigma} \) with spin \( \sigma \) at site \( x_m \) attached other electron distribution represented by the operator \( \widehat{F}_{\{a_1\ldots a_L\}} \) around the site \( x_m \), where the parameter \( L \) denotes the number of electrons residing in a length (sites) scale around this site \( x_m \) that the electrons in this scale all are involved in the time evolution process of the electron \( \widehat{c}_{m\sigma} \). Thus the correlation function \( F_{\{a_1\ldots a_L\}m\sigma}(t_1, t_2) \) in fact represents the evolution process of an electron from the initial state incorporated the influence of a definite distribution of other electrons around this electron to final state. As taking \( L = 1 \) (i.e. \( N_{e\sigma} = 1 \)), we have the correlation function \( F_{i\sigma\sigma}(t_1, t_2) = -i < T \widehat{n}_{i\sigma}(t_1) \widehat{c}_{i\sigma}(t_1) \widehat{c}_{i\sigma}^\dagger(t_2) > \), that enters into the EOM of the one-particle Green function as taking \( i = l \).

In contrast with usual correlation functions defined in the momentum space, the present multi-site correlation functions can more effectively describe the correlation effect of electrons derived from the Coulomb interaction, and the parameter \( L \) appearing in the composite operators \( \widehat{F}_{\{a_1\ldots a_L\}} \) can be used to classify the correlation functions \( F_{\{a_1\ldots a_L\}m\sigma}(t_1, t_2) \) into different levels, where the correlation functions \( F_{\{a_1\ldots a_L\}m\sigma}(t_1, t_2) \) in the same level \( L \) can constitute one or more subset of EOMs, in which only a few correlation functions belonging to the level \( L + 1 \) are emerging. For a large \( L \) (i.e. a lot of electrons in a large length scale take part in the time evolution of the electron \( \widehat{c}_{m\sigma} \)), the contribution of the correlation functions \( F_{\{a_1\ldots a_L\}m\sigma}(t_1, t_2) \) to the one-particle Green function is expectantly small, therefore we can take the cut-off approximations for those belonging to the level \( L + 1 \) that appear in the EOMs of the correlation functions in the level \( L \), and we have a closed set of the EOMs of the one-particle Green function and the related multi-site correlation functions \( F_{\{a_1\ldots a_L\}m\sigma}(t_1, t_2) \).

On the other hand, for a system with a few electron number \( N_e \), the number of the correlation functions \( F_{\{a_1\ldots a_L\}m\sigma}(t_1, t_2) \) is finite, because the parameter \( L \) in the multipe-
site correlation functions $F_{\{\alpha_1...\alpha_L\}mp\sigma}(t_1, t_2)$ must satisfy the following condition,

$$L \leq N_e$$

(7)

Therefore, the set of EOMs of the one-particle Green function $G_{ij\sigma}(t_1, t_2)$ and the related multipe-site correlation functions $F_{\{\alpha_1...\alpha_L\}mp\sigma}(t_1, t_2)$ are automatically closed, and it can be analytically/numerically solved.

According to the above definition of the multipe-site correlation functions in Eq.(6) and with the help of Eq.(2), we can write out the EOMs of the correlation functions $F_{\{\alpha_1...\alpha_L\}mp\sigma}(t_1, t_2)$ with $L = 1$ that they enter the series of the EOM of the one-particle Green function,

$$i\partial_t F_{ij\sigma}^{(n\sigma)}(t_1, t_2) = \delta(t_1 - t_2) < \hat{n}_{i\sigma} > \delta_{jq} + UF_{ijjq\sigma}^{(n\sigma)}(t_1, t_2)$$

$$+ \sum_m \left[ h_{jm} - \mu \delta_{jm} \right] F_{im\sigma\sigma}^{(n\sigma)}(t_1, t_2) + \sum_m \hat{h}_{im} F_{imjq\sigma}^{(n\sigma)}(t_1, t_2)$$

(8)

$$i\partial_t F_{iljq\sigma}^{(X_{\pm}^\sigma)}(t_1, t_2) = \delta(t_1 - t_2) < \hat{X}_{il\sigma}^{(\pm)} > \delta_{jq} + UF_{iljq\sigma}^{(X_{\pm}^\sigma)}(t_1, t_2)$$

$$+ \sum_m \left[ h_{jm} - \mu \delta_{jm} \right] F_{imjq\sigma}^{(X_{\pm}^\sigma)}(t_1, t_2)$$

$$- \sum_m \left[ \hat{h}_{im} F_{niljq\sigma}^{(X_{\pm}^\sigma)}(t_1, t_2) - \hat{h}_{im} F_{imjq\sigma}^{(X_{\pm}^\sigma)}(t_1, t_2) \right]$$

$$+ U \left( F_{iljq\sigma}^{(n\sigma X_{\pm}^\sigma)}(t_1, t_2) - F_{iljq\sigma}^{(n\sigma X_{\pm}^\sigma)}(t_1, t_2) \right)$$

(9)

where there emerge the new multipe-site correlation functions with $L = 2$, $F_{niljq\sigma}^{(n\sigma X_{\pm}^\sigma)}(t_1, t_2)$, $F_{ijjq\sigma}^{(n\sigma X_{\pm}^\sigma)}(t_1, t_2)$ and $F_{niljq\sigma}^{(X_{\pm}^\sigma n\sigma)}(t_1, t_2)$. In the $L = 1$ level, the correlation functions $F_{ijjq\sigma}^{(n\sigma)}(t_1, t_2)$ and $F_{iljq\sigma}^{(X_{\pm}^\sigma)}(t_1, t_2)$ constitute a subset of EOMs, and they connect with the one-particle Green function $G_{ij\sigma}(t_1, t_2)$ by the correlation function $F_{ijjq\sigma}^{(n\sigma)}(t_1, t_2)$. On the other hand, other correlation functions belonging to the $L = 1$ level can be discarded because they do not enter this series of the hierarchical EOMs of the one-particle Green function and related multipe-site correlation functions.

To the next level $L = 2$, we need to include all correlation functions that enter this series of the hierarchical EOMs, such as, $F_{niljq\sigma}^{(n\sigma X_{\pm}^\sigma)}(t_1, t_2)$, $F_{ijjq\sigma}^{(n\sigma X_{\pm}^\sigma)}(t_1, t_2)$ and $F_{niljq\sigma}^{(X_{\pm}^\sigma n\sigma)}(t_1, t_2)$, as well as that ones emerging in their EOMs. For example, the EOM of the multipe-site correlation
functions $F_{n\sigma}^{(n_\sigma \mp \mp \mp)}(t_1, t_2)$ can be written as that,

$$i\partial_{t_1} F_{n\sigma}^{(n_\sigma \mp \mp \mp)}(t_1, t_2) = \delta(t_1 - t_2) < \{ \hat{n}_{n\sigma} \hat{c}^{\dagger}_{j\sigma}, \hat{c}^{\dagger}_{q\sigma} \} \hat{X}_{i\sigma}^{\mp} > + U F_{n\sigma}^{(n_\sigma \mp \mp \mp)(t_1, t_2)}$$

$$+ \sum_m \left( \tilde{h}_{jm} - \mu \delta_{jm} \right) F_{m\sigma}^{(n_\sigma \mp \mp \mp)}(t_1, t_2)$$

$$- \sum_m \left[ \tilde{h}_{im} F_{nm\sigma}^{(n_\sigma \mp \mp \mp)}(t_1, t_2) - \tilde{h}_{im} F_{nmj\sigma}^{(n_\sigma \mp \mp \mp)}(t_1, t_2) \right]$$

$$+ \sum_m \tilde{h}_{nm} F_{n\sigma}^{(X^\mp_X \mp \mp \mp)}(t_1, t_2)$$

$$+ U \left[ F_{n\sigma}^{(n_\sigma \mp \mp \mp)}(t_1, t_2) - F_{n\sigma}^{(n_\sigma \mp \mp \mp)}(t_1, t_2) \right]$$

(10)

where, the indexes $n, j$ of the correlation functions $F_{n\sigma}^{(n_\sigma \mp \mp \mp)}(t_1, t_2)$ are not equal to each other, $n \neq j$. In the above EOM there also emerge new correlation functions with $L = 2$, $F_{nm\sigma j\sigma}^{(X^\mp_X \mp \mp \mp)}(t_1, t_2)$, as well as some ones with $L = 3$, $F_{n\sigma}^{(n_\sigma \mp \mp \mp)}(t_1, t_2)$. Of course, following this same routine, we can write out the EOMs of correlation functions with $L = 3$ that appear in the above equations, and so on. Meanwhile, there emerge a series of static correlation functions in these hierarchical EOMs, that are corresponding to the equal time parts of these EOMs, respectively, such as, $< \hat{n}_{i\sigma} >$, $< \hat{X}_{i\sigma}^{(\pm)} >$, $< \{ \hat{n}_{n\sigma} \hat{c}_{j\sigma}, \hat{c}_{q\sigma}^{\dagger} \} \hat{X}_{i\sigma}^{\mp} >$, etc.. These static correlation functions can be used to describe a variety of possible inhomogeneous states of the system in low temperature regime, and they will strongly influence the spectral density function of electrons.

More importantly, in the above calculations, it is clearly shown that in the EOM of a multipe-site correlation function with $L$ there never emerges any multipe-site correlation function belonging to the level $L - 1$. It is an important guideline as taking any cut-off approximation for a multipe-site correlation function belonging to the high level $L + 1$.

This set of the EOMs has an obvious hierarchical structure denoted by the parameter $L$. In the EOM of the one-particle Green function $G_{lj\sigma}(\omega)$, there only emerges the correlation function $F_{i\sigma}^{(\sigma)(\omega)}$ which is produced by the on-site Coulomb interaction. In the EOM of the correlation function $F_{i\sigma}^{(\sigma)(\omega)}$, there appear the correlation functions $F_{i\sigma}^{(\sigma)(\omega)}$ and $F_{ij\sigma}^{(\sigma)(\omega)}$. The correlation function $F_{i\sigma}^{(\sigma)(\omega)}$ originates from the on-site Coulomb interaction, which can be written as, $F_{i\sigma}^{(\sigma)(\omega)} = \delta_{i\sigma} F_{i\sigma}^{(\sigma)(\omega)} + (1 - \delta_{i\sigma}) F_{i\sigma}^{(\sigma)(\omega)}$, and the correlation function $(1 - \delta_{i\sigma}) F_{i\sigma}^{(\sigma)(\omega)}$ is expectantly small as assuming the function $F_{i\sigma}^{(\sigma)(\omega)}$ varying smoothly in the lattice space; Thus in this way, the on-site Coulomb interaction of electrons is rigorously treated. While the correlation function $F_{ijkl\sigma}^{(\sigma)(\omega)}$ comes
from the kinetic energy part of the Hamiltonian. Thus the correlation function $F_{\text{il}j\sigma}^{(n_\sigma)}(\omega)$ in fact represents the correlation effect of electrons from the mixture of both the kinetic energy and interaction potential parts of the system.

In the thermodynamic limit, this set of the hierarchical EOMs cannot be automatically closed. To solving this set of equations, for simplicity, we would cut off the EOMs at the level $L = 2$, thus we must take cut-off approximations for those multipe-site correlation functions belonging to the level $L = 3$ in these EOMs. According to the hierarchical character of the EOM of a multipe-site correlation function, we take the following cut-off approximations for the correlation functions belonging to the level $L = 3$ in the Eq.(10),

$$F_{\text{il}j\sigma}^{(n_\sigma X^\pm_\sigma)}(t_1, t_2) \simeq \langle \hat{n}_\sigma(t_1) \rangle F_{\text{il}j\sigma}^{(n_\sigma X^\pm_\sigma)}(t_1, t_2), \ j \neq i, l$$

$$+ \langle \hat{n}_l(t_1) \rangle F_{\text{il}j\sigma}^{(n_\sigma X^\pm_\sigma)}(t_1, t_2), \ n \neq l; \ j \neq n, l$$

Under these cut-off approximations, the subset of the EOMs of the correlation functions $F_{\text{il}j\sigma}^{(n_\sigma X^\pm_\sigma)}(t_1, t_2)$ is closed after taking, $F_{nm\text{il}j\sigma}^{(n_\sigma X^\pm_\sigma)}(t_1, t_2) \to 0$, where it is assumed that they have small contribution to the correlation functions $F_{\text{il}j\sigma}^{(n_\sigma X^\pm_\sigma)}(t_1, t_2)$. These cut-off approximations are consistent with the hierarchical character of the EOM of a multipe-site correlation function where any multipe-site correlation function with $L - 1$ does not appear in the subset of the EOMs of the multipe-site correlation functions with $L$. On the other hand, these cut-off approximations are qualitatively distinct from usual ones taken in perturbation theories, such as usual Hartree-Fock approximation and/or random-phase approximation (RPA), because before taking the above cut-off approximations, the on-site Coulomb interaction of electrons has been rigorously treated in the subset of the EOMs of the correlation functions with $L = 1$. That is, before taking any approximation, the Coulomb interaction of electrons has been effectively treated rather than taking the Coulomb interaction potential as a perturbative term like that doing in usual perturbation theories.

After taking the above approximations, the EOMs of the correlation functions $F_{il\sigma j\sigma}^{(X^\pm_\sigma)}(t_1, t_2)$ and $F_{n\text{il}j\sigma\sigma}^{(n_\sigma X^\pm_\sigma)}(t_1, t_2)$ can be further simplified by defining the following new functions,

$$F_{il\sigma j\sigma}^{(\pm X^\pm_\sigma)}(t_1, t_2) = \frac{1}{2} \left[ F_{il\sigma j\sigma}^{(X^\pm_\sigma)}(t_1, t_2) \pm F_{il\sigma j\sigma}^{(X^\pm_\sigma)}(t_1, t_2) \right]$$

$$F_{n\text{il}j\sigma\sigma}^{(\pm n_\sigma X^\pm_\sigma)}(t_1, t_2) = \frac{1}{2} \left[ F_{n\text{il}j\sigma\sigma}^{(n_\sigma X^\pm_\sigma)}(t_1, t_2) \pm F_{n\text{il}j\sigma\sigma}^{(n_\sigma X^\pm_\sigma)}(t_1, t_2) \right]$$

(12)
which can be used to decouple the EOMs of the correlation functions \( F_{n\ell jq\sigma}^{(X)\pm}(t_1, t_2) \) and \( F_{n\ell jq\sigma}^{(\sigma X)\pm}(t_1, t_2) \), respectively. With these new functions, the Eq. \((10)\) can be rewritten as that,

\[
[i\partial_{t_1} - U_{n\ell j}] F_{n\ell jq\sigma}^{(+n_\sigma X}\sigma))(t_1, t_2) = \delta(t_1 - t_2) < \hat{c}_{\ell \sigma}^\dagger \hat{c}_{\sigma} > n_\sigma \delta_{jq} - \hat{c}_{\sigma}^\dagger \hat{c}_{\sigma} \delta_{n\sigma}] > + \sum_m \left( \hat{h}_{jm} - \mu \delta_{jm} \right) F_{n\ell m\sigma q\sigma}(t_1, t_2)
- \sum_m \left[ \hat{h}_{im} F_{n\ell m\sigma q\sigma}(t_1, t_2) - \hat{h}_{lm} F_{n\ell m\sigma q\sigma}(t_1, t_2) \right]
\]

where \( U_{n\ell j} = \Delta_{n\ell j} + U (\delta_{ij} \pm \delta_{nl} \mp \delta_{ni}) \), and \( \Delta_{n\ell j} = U [(1 - \delta_{ij}) (1 - \delta_{lj}) n_\sigma \pm (\delta_{ni} - \delta_{nl}) n_\sigma] \) which is contributed by the correlation functions belonging to the level \( L = 3 \) under the cut-off approximations in Eq. \((11)\). The Eq. \((9)\) can be rewritten as that,

\[
[i\partial_{t_1} - U_{\ell ij}] F_{\ell jjq\sigma}^{(+X\sigma)}(t_1, t_2) = \delta(t_1 - t_2) < \hat{c}_{\sigma}^\dagger \hat{c}_{\sigma} > \delta_{jq} + U (\delta_{nl} - \delta_{ni}) F_{n\ell jq\sigma}^{(+n_\sigma X\sigma)}(t_1, t_2)
+ \sum_m \left( \hat{h}_{jm} - \mu \delta_{jm} \right) F_{n\ell m\sigma q\sigma}(t_1, t_2)
- \sum_m \left[ \hat{h}_{im} F_{n\ell m\sigma q\sigma}(t_1, t_2) - \hat{h}_{lm} F_{n\ell m\sigma q\sigma}(t_1, t_2) \right]
\]

\[
[i\partial_{t_1} - U_{\ell ij}] F_{\ell jqq\sigma}^{(-X\sigma)}(t_1, t_2) = \delta(t_1 - t_2) < \hat{c}_{\sigma}^\dagger \hat{c}_{\sigma} > \delta_{jq} + U (\delta_{nl} - \delta_{ni}) F_{n\ell jq\sigma}^{(-n_\sigma X\sigma)}(t_1, t_2)
+ \sum_m \left( \hat{h}_{jm} - \mu \delta_{jm} \right) F_{n\ell m\sigma q\sigma}(t_1, t_2)
+ \sum_m \left[ \hat{h}_{im} F_{n\ell m\sigma q\sigma}(t_1, t_2) - \hat{h}_{lm} F_{n\ell m\sigma q\sigma}(t_1, t_2) \right]
\]

where the contribution from the correlation functions \((1 - \delta_{ij}) (1 - \delta_{lj}) F_{n\ell jq\sigma}^{(X)\pm \sigma\sigma}(t_1, t_2) \) has
been neglected, which is assumed to be small. While the Eq. (8) can be rewritten as that,

\[
[i\partial_{t_1} - U\delta_{ij}] F^{(n\sigma\sigma)}_{ij\sigma\sigma}(t_1, t_2) = \delta(t_1 - t_2) < \hat{n}_{i\sigma} > \delta_{jq} \\
+ \sum_m (\hat{h}_{jm} - \mu \delta_{jm}) F^{(n\sigma\sigma)}_{jm\sigma\sigma}(t_1, t_2) \\
+ \sum_m \hat{h}_{im} \left[ F^{(+X\sigma\sigma)}_{imj\sigma\sigma}(t_1, t_2) - F^{(-X\sigma\sigma)}_{imj\sigma\sigma}(t_1, t_2) \right]
\]

where we have neglected the contribution coming from the function \((1 - \delta_{ij}) F^{(n\sigma\sigma\sigma\sigma)}_{ij\sigma\sigma}(t_1, t_2)\).

As the correlation function \(F^{(n\sigma\sigma\sigma\sigma)}_{ij\sigma\sigma}(t_1, t_2)\) is a smoothly varying function in the lattice space, the contribution coming from the function \((1 - \delta_{ij}) F^{(n\sigma\sigma\sigma\sigma)}_{ij\sigma\sigma}(t_1, t_2)\) can be neglected as a simple approximation.

### III. SOLUTION OF THE EOM

The linear EOMs in Eqs. (13-17) can be solved after taking the Fourier representation of the multipe-site correlation functions, in which one needs more carefully as taking the Fourier transformation because these functions depend upon more than two lattice sites, i.e., they are the correlation functions defined by more than two operators residing at different sites. Moreover, the multipe-site functions \(F^{(n\sigma\sigma\sigma\sigma)}_{ij\sigma\sigma}(t_1, t_2)\), \(F^{(+X\sigma\sigma\sigma\sigma)}_{imj\sigma\sigma}(t_1, t_2)\) and \(F^{(\pm n_{\sigma\sigma}X\sigma\sigma\sigma)}_{imlj\sigma\sigma}(t_1, t_2)\) can be seen as "tensors" with different ranks, respectively, and the above linear EOMs in fact are the equations of the tensors.

With the help of the Fourier transformations of the electron operators,

\[
\hat{c}_{i\sigma}(t) = \frac{1}{\sqrt{N}} \sum_k \hat{c}_{k\sigma}(\omega) e^{i\omega t - ik \cdot x_i}
\]

\[
\hat{c}_{i\sigma}^\dagger(t) = \frac{1}{\sqrt{N}} \sum_k \hat{c}_{k\sigma}^\dagger(\omega) e^{ik \cdot x_i - i\omega t}
\]

where the site \(i\) is denoted by \(x_i\), we take the following Fourier representations of the
where the "Fourier functions" $G_{k\sigma}(\omega; iq)$, $F_{k'k'k'k'\sigma\sigma}(\omega; ijq)$, $F^{(\pm X_{\sigma\sigma})}_{k'k'k'k'\sigma\sigma}(\omega; niljq)$ and $F^{(\pm n_a X_{\sigma\sigma})}_{k'k'k'k'\sigma\sigma}(\omega; niljq)$ generally depend upon the lattice sites, because the corresponding correlation functions depend upon more than two lattice sites. However, the function $G_{k\sigma}(\omega; iq)$ depends upon the lattice site due to in its EOM there appears the function $F_{k'k'k'k'\sigma\sigma}(\omega; iiq)$.

Using the Fourier representations in Eq. (19), the EOMs in Eqs. (13-17) become a set of linear algebraic equations of the Fourier functions, in which the terms with the operator $\hat{h}_{im}$ in the right hand side of these EOMs make this set of algebraic equations be hardly solved because they depend upon the values of these functions on the nearest neighbour sites. If we assume that the Fourier functions $G_{k\sigma}(\omega; iq)$, $F_{k'k'k'k'\sigma\sigma}(\omega; ijq)$, $F^{(\pm X_{\sigma\sigma})}_{k'k'k'k'\sigma\sigma}(\omega; niljq)$ and $F^{(\pm n_a X_{\sigma\sigma})}_{k'k'k'k'\sigma\sigma}(\omega; niljq)$ are smoothly and slowly varying functions on the lattice sites, the difference of a Fourier function between two nearest neighbour sites would be a small quantity, and it can be safely neglected. Therefore, we can further take the following approximation as in solving these EOMs,

$$\sum_{m} \hat{h}_{jm}X_{(pk)\sigma\sigma}(\omega; \{imq\}) \simeq \sum_{m} \hat{h}_{jm}X_{(pk)\sigma\sigma}(\omega; \{ijq\})$$

(20)

where $X_{(pk)\sigma\sigma}(\omega; \{ijq\}) = G_{k\sigma}(\omega; iq)$, $F^{(\pm X_{\sigma\sigma})}_{k'k'k'k'\sigma\sigma}(\omega; ijq)$, $F^{(\pm n_a X_{\sigma\sigma})}_{k'k'k'k'\sigma\sigma}(\omega; niljq)$.

Under the approximation in Eq. (20), the EOMs in Eqs. (13-17) can be analytically solved. For simplicity, the one-particle Green function $G_{k\sigma}(\omega)$ can be written as following three parts,

$$G_{k\sigma}(\omega) = G_{k\sigma}^{S}(\omega) + G_{k\sigma}^{LC}(\omega) + G_{k\sigma}^{NLC}(\omega)$$

(21)
where the Green function $G_{k\sigma}^{S}(\omega)$ is contributed by the functions $F_{k'k\sigma\sigma}^{(n\pm X)}(\omega;ijq)$ and $F_{k'k'\sigma\sigma}^{(+X\pm)}(\omega;iljq)$ without considering the functions $F_{p'k'k\sigma\sigma}^{(\pm n\mp X)}(\omega;niljq)$, and the Green function $G_{k\sigma}^{LC}(\omega)$ and $G_{k\sigma}^{NLIC}(\omega)$ are contributed by the functions $F_{p'k'k\sigma\sigma}^{(\pm n\mp X)}(\omega;niljq)$, in which there naturally emerge the static correlation functions $N_{k_1k'} = \langle \hat{n}_{k_1\sigma} \hat{c}_{k'\sigma} \rangle$ and $C_{pkk'k} = \langle \hat{c}_{k+p\sigma} \hat{c}_{k+1-k'\sigma} \hat{c}_{k'\sigma} \rangle$. The appearance of the static correlation functions $N_{k_1k'}$ and $C_{pkk'k}$ in the one-particle Green function means that the possible intertwined orders in low temperature regime derived by the strong Coulomb interaction would drastically influence the spectral density function of elecrons. On the other hand, it is also shown that the HGFA can uncover the intrinsic relation between the one-particle Green function and a variety of inhomogeneous states in highly correlated systems.

The Green function $G_{k\sigma}^{S}(\omega)$ can be written as that,

$$
G_{k\sigma}^{S}(\omega) = \left[ 1 - n_{\sigma} + \frac{1}{N} \sum_{k_1} \left( \frac{\xi_{k_1} n_{k_1\sigma}}{\epsilon_{k_1}} - \frac{\xi_{k_1} n_{k_1\sigma}}{\epsilon_{k_1} + U} \right) \right] \frac{1}{\omega - \epsilon_k} + \left[ n_{\sigma} - \frac{1}{N} \sum_{k_1} \left( \frac{\xi_{k_1} n_{k_1\sigma}}{\epsilon_{k_1}} + \frac{\xi_{k_1} n_{k_1\sigma}}{\epsilon_{k_1} - U} \right) \right] \frac{1}{\omega - \epsilon_k - U} - \frac{1}{N} \sum_{k_1} \left( \frac{\xi_{k_1} n_{k_1\sigma}}{\epsilon_{k_1}} + \frac{\xi_{k_1} n_{k_1\sigma}}{\epsilon_{k_1} - U} \right) \frac{1}{\omega - \epsilon_k - \epsilon_{k_1}} - \frac{1}{N} \sum_{k_1} \left( \frac{\xi_{k_1} n_{k_1\sigma}}{\epsilon_{k_1}} - \frac{\xi_{k_1} n_{k_1\sigma}}{\epsilon_{k_1} + U} \right) \frac{1}{\omega - \epsilon_k - \epsilon_{k_1} - U} (22)
$$

where $n_{\sigma} = \langle \hat{n}_{\sigma} \rangle$, $n_{k\sigma} = \langle \hat{c}_{k\sigma} \hat{c}_{k\sigma} \rangle$, $\epsilon_k = \xi_k - \mu$, $\epsilon_k = 4t_0 + \xi_k$, and $\xi_k = 2t_0 \cos (ak_x) + \cos (ak_y)$, here $a$ is the lattice constant. Notice that the Green function $G_{k\sigma}^{S}(\omega)$ has a similar expression like that for an one site Hubbard model, in which as taking, $t_0 = 0$, it is reduced to a two level structure form of the one-particle Green function for one site Hubbard model. There is a gap between the lower and upper Hubbard bands, which is proportional to $U$ in the large $U$ limit. However, the appearence of the third term in the right hand side reveals that there emerge new states within this gap because the function $\epsilon_k$ is positive, $\epsilon_k \geq 0$. 
The Green function $G_{k\sigma}^{LC}(\omega)$ reads that,

$$
G_{k\sigma}^{LC}(\omega) = -\frac{1}{N^2} \sum_{k'k} A_{k'_k \sigma} N_{k_k} \frac{1}{1-n_\sigma} \frac{1}{\omega - \varepsilon_k - U} + \frac{1}{N^2} \sum_{k'k} B_{k'_k \sigma} N_{k_k} \frac{1}{1-n_\sigma} \frac{1}{\omega - \varepsilon_k - U}
- \frac{1}{N^2} \sum_{k'k} \left( \frac{\xi_{k+k'}'}{\eta_{k_k'}} - \frac{\xi_{k+k'}}{\eta_{k_k'}} \right) \frac{N_{k_k'} (1-n_\sigma)^{-1}}{\omega - E_k (k_1, k')}
+ \frac{1}{N^2} \sum_{k'k} \left( \frac{\xi_{k+k'}}{\eta_{k_k}} - \frac{\xi_{k+k'}}{\eta_{k_k}} \right) \frac{N_{k_k'} (1-n_\sigma)^{-1}}{\omega - E_k (k_1, k') - (1-n_\sigma) U}
+ \frac{1}{N^2} \sum_{k'k} \left( \frac{\xi_{k'}}{\eta_{k_k}} - \frac{\xi_{k'}}{\eta_{k_k}} + (1-n_\sigma) U \right) \frac{N_{k_k'} (1-n_\sigma)^{-1}}{\omega - E_k (k_1, k') - n_\sigma U}
$$

(23)

where $\eta_{q_\sigma} = \sum_{k} \xi_{k+k'} \eta_{k_k'}, E_k (k, k') = \varepsilon_k - \eta_{k_k'}, \eta_{k_k'} = \varepsilon_{k_1} - \xi_{k_1} + \xi_{k_1}', A_{k'_k \sigma} = -\frac{\xi_{k+k'}'}{\eta_{k_k'}} + \frac{\xi_{k+k'}}{\eta_{k_k'}}$ and $B_{k'_k \sigma} = -\frac{\xi_{k+k'}'}{\eta_{k_k'}} + \frac{\xi_{k+k'}}{\eta_{k_k'}} + \xi_{k+k'} + \frac{\xi_{k+k'}}{\eta_{k_k'}} - \frac{\xi_{k+k'}}{\eta_{k_k'}}$.

The Green function $G_{k\sigma}^{LC}(\omega)$ is contributed by the static correlation function $N_{k_k'} = \langle \hat{c}_{k+k'} \hat{c}_{k+k'}^\dagger \rangle$, which is mainly related to the density-density correlation effect of electrons. In contrast with the Green function $G_{k\sigma}^S(\omega)$, there emerge new terms with poles residing around in the middle of the gap between the lower and upper Hubbard bands in the large $U$ limit, and it clearly reveals that there emerge new states in this regime. As taking a simple Hartree-Fock approximation to the function $N_{k_k'}$, $N_{k_k'} \Rightarrow N_{n_\sigma n_{k-k'\sigma}}^2 \delta_{0k_1}$, the Green function $G_{k\sigma}^{LC}(\omega)$ can be incorporated into the Green function $G_{k\sigma}^S(\omega)$ to more clearly show the emerged states in this gap.

The Green function $G_{k\sigma}^{NL}(\omega)$ can be written as that,

$$
G_{k\sigma}^{NL}(\omega) = \frac{1}{N^2} \sum_{pk'k} A_{k'_k \sigma} (p) C_{pk'k} \frac{1}{1-n_\sigma} \frac{1}{\omega - \varepsilon_k - p - U} + \frac{1}{N^2} \sum_{pk'k} B_{k'_k \sigma} (p) C_{pk'k} \frac{1}{1-n_\sigma} \frac{1}{\omega - \varepsilon_k - p - U}
+ \frac{1}{N^2} \sum_{pk'k} \left( \frac{\xi_{-k'-k'}}{\eta_{k_k'}} - \frac{\xi_{-k'-k'}}{\eta_{k_k'}} + U \right) \frac{C_{pk'k} (1-n_\sigma)^{-1}}{\omega - E_{k+p} (k_1, k')}
+ \frac{1}{N^2} \sum_{pk'k} \left( \frac{\xi_{-k'+k'}}{\eta_{k_k}} - \frac{\xi_{-k'-k'}}{\eta_{k_k}} \right) \frac{C_{pk'k} (1-n_\sigma)^{-1}}{\omega - E_{k+p} (k_1, k') - (1-n_\sigma) U}
+ \frac{1}{N^2} \sum_{pk'k} \left( \frac{\xi_{-k-k'+k'}}{\eta_{k_k}} - \frac{\xi_{-k-k'+k'}}{\eta_{k_k}} \right) \frac{C_{pk'k} (1-n_\sigma)^{-1}}{\omega - E_{k+p} (k_1, k') - n_\sigma U}
$$

(24)
where \( A_{NL}^{k_1k'} (p) = \frac{-\xi_{p-k'}}{\eta_{k_1k'} + n_{\sigma} U} + \frac{\xi_{p-k'}}{\eta_{k_1k'-(1-n_{\sigma}) U}} + \frac{\xi_{p+k_1}}{\eta_{k_1k'-n_{\sigma} U}} \) and \( B_{NL}^{k_1k'} (p) = -\frac{-\xi_{p-k'}}{\eta_{k_1k'+U}} + \frac{\xi_{p+k_1}}{\eta_{k_1k'+(1-n_{\sigma}) U}} \). The Green function \( G_{k\sigma}^{{NL}} (\omega) \) is contributed by the static correlation function \( C_{pk1k'k} = \langle \hat{c}_{k+p,\sigma}^\dagger \hat{c}_{k+p+k_1-k',\sigma}^\dagger \hat{c}_{k_1,\sigma} \hat{c}_{k',\sigma} \rangle \), and it is mainly related to the spin-spin correlation effect of electrons and possible electronic pairing density correlation. On the other hand, the function \( C_{pk1k'k} \) makes the Fourier function \( G_{k\sigma} (\omega; iq) \) depend upon the lattice coordinate \( x_i - x_q \), meanwhile it also produces new terms with poles residing around in the middle of the gap between the lower and upper Hubbard bands in the large \( U \) limit, which shows that there emerge new states in this regime.

It becomes more clear that the emerged states in the gap between the lower and upper Hubbard bands in the large \( U \) limit are coming from two aspects: one is contributed by the static quantities \( \langle \hat{X}_{i\sigma}^{(z)} \rangle \), and another one is contributed by the static correlation functions \( \{ \hat{n}_{\sigma} \hat{c}_{j\sigma}, \hat{c}_{i\sigma}^\dagger \} \hat{X}_{i\sigma}^{(z)} \), that are represented by the functions \( N_{k_1k'} \) and \( C_{pk1k'k} \) in the phase space. However, the more high order static correlation functions emerged in the series of the hierarchical EOMs have expectantly small contribution, and they cannot drastically alter the present calculations.

According to the expression of the one-particle Green function \( G_{k\sigma} (\omega) \) in Eq. (21), we can demonstrate that the spectral density function, \( A_\sigma (\omega, k) = -2 \text{Im} G_\sigma (\omega + 0^+, k) \), satisfies the following sum rule,

\[
\frac{1}{2\pi} \int_{-\infty}^{\infty} d\omega A_\sigma (\omega, k) = 1 \tag{25}
\]

which is independent of the approximations taken in solving the EOMs of the multiplets correlation functions. It is resulting in that the EOMs of the multiplets correlation functions are linear.

In order to show a more clear analytical expression of the spectral density function \( A_\sigma (\omega, k) \), we need to take some approximations for the static correlation functions \( N_{k_1k'} \) and \( C_{pk1k'k} \) that emerge in the expressions of the Green functions \( G_{k\sigma}^{L} (\omega) \) and \( G_{k\sigma}^{NL} (\omega) \) in the Eqs. (23) and (24), respectively. For example, we can rewrite them as the following forms,

\[
N_{k_1k'} = \langle \hat{n}_{k_1\sigma} \hat{c}_{k'\sigma}^\dagger \hat{c}_{k'\sigma} \rangle_o + N n_{\sigma} n_{\sigma} \delta_{0k_1} \\
C_{pk1k'k} = \langle \hat{c}_{k+p,\sigma}^\dagger \hat{c}_{k+p+k_1-k',\sigma}^\dagger \hat{c}_{k_1,\sigma} \hat{c}_{k',\sigma} \rangle_o + \Delta_{k_1}^* \Delta_{k'}^* \delta_{k_1+k+p} - S_{k'}^+ S_{k_1}^+ \delta_{k+k+p} \tag{26}
\]

where \( \Delta_{k'} = \langle \hat{c}_{k',\sigma} \hat{c}_{-k',\sigma} \rangle \) is an uniform electronic pairing order parameter, \( S_{k'}^+ = \langle \hat{c}_{k'\sigma}^\dagger \hat{c}_{k'\sigma} \rangle \)
and $S_{k_1} = \langle \hat{c}_{k_1\sigma}^\dagger \hat{c}_{k_1\sigma} \rangle$ are spin order parameters. The fluctuation parts $\langle \hat{n}_{k_1\sigma} \hat{c}_{k_1\sigma}^{\dagger} + \hat{c}_{k_1\sigma} \hat{c}_{k_1\sigma}^{\dagger} \rangle_o$ and $\langle \hat{c}_{k_1\sigma} \hat{c}_{k_1\sigma}^{\dagger} \rangle_o$ can be corresponded to the static correlation functions of the charge/spin density wave and the electronic pairing density wave orders, respectively. For simplicity, hereafter we do not consider these fluctuation parts. It would be pointed out that the present approach only shows the influence of possible order parameters, such as $\Delta_{k'}$ and $S_{k'}^\pm$, etc., on the one-particle Green function, and it cannot answer how to fix these order parameters. For example, the uniform electronic pairing parameter $\Delta_{k'}$ and the spin order parameters $S_{k'}^\pm$ can be self-consistently determined by taking the minimum of the ground state energy which can be calculated by the spectral density function $A_{\sigma}(\omega, k)$ and the correlation function $F_{\sigma\sigma}(t_1, t_1 + 0^+)$. 

IV. THE SPECTRAL DENSITY FUNCTION

With the help of the expressions of the Green functions $G_{k\sigma}^S(\omega)$, $G_{k\sigma}^{LC}(\omega)$ and $G_{k\sigma}^{NLC}(\omega)$ in Eqs. (22-24), under the approximations taken in Eqs. (26), we can write out the analytical expression of the spectral density function of electrons $A_{\sigma}(\omega, k)$, in which there exist two characteristic main peaks with the corresponding factors $\delta(\omega - \varepsilon_k)$ and $\delta(\omega - \varepsilon_k - U)$, respectively, that come from the lower and upper Hubbard bands. The gap between these two main peaks is proportional to $U$ in the large $U$ limit. On the other hand, as the hole doping, there emerge new states within this gap, and for enough large of the hole doping, these emerged states would fill in this gap. It may be the origins of a variety of novel low temperature behavior shown by the 2D square lattice Hubbard model at the intermediate coupling $U$.

Under the approximations of the Eqs. (26), and after discarding the contributions from the fluctuation parts of the static correlation functions $N_{k_1k'}$ and $C_{pk_1k'k}$, we can write out the spectral density function $A_{\sigma}(\omega, k)$ as the following three parts,

$$A_{\sigma}(\omega, k) = A_{\sigma}^{L-U}(\omega, k) + A_{\sigma}^{Em}(\omega, k) + A_{\sigma}^{Con}(\omega, k) \tag{27}$$

where the spectral density function $A_{\sigma}^{L-U}(\omega, k)$ is the contribution coming from the lower and upper Hubbard bands, the spectral density function $A_{\sigma}^{Em}(\omega, k)$ is contributed by the emerged states of electrons due to the doped holes, and the spectral density function $A_{\sigma}^{Con}(\omega, k)$ is related to the pairing order parameter $\Delta_k$ and spin order parameters $S_{k}^\pm$, which is contributed
by the emerged collective modes.

According to the one-particle Green function in Eq.(21), the spectral density function $A_{\sigma}^{L-U}(\omega, k)$ can be written as that,

$$A_{\sigma}^{L-U}(\omega, k) = 2\pi \left[ 1 - n_{\sigma} - Z^L \right] \delta (\omega - \varepsilon_k) + 2\pi \left[ n_{\sigma} - Z^U \right] \delta (\omega - \varepsilon_k - U) \tag{28}$$

where the constants $Z^L$ and $Z^U$ are that,

$$Z^L = -\frac{1}{N} \frac{1 - 2n_{\sigma}}{1 - n_{\sigma}} \sum_{k_1} \left( \frac{\xi_{k_1} n_{\sigma}}{\epsilon_{k_1}} - \frac{\xi_{k_1} n_{\sigma}}{\epsilon_{k_1} + U} \right)$$

$$+ \frac{1}{N} \frac{n_{\sigma}}{1 - n_{\sigma}} \sum_{k_1} \left( \frac{\xi_{k_1} n_{\sigma}}{n_{\sigma}U + \epsilon_{k_1}} - \frac{\xi_{k_1} n_{\sigma}}{\epsilon_{k_1} + (1 - n_{\sigma})U} \right) \tag{29}$$

$$Z^U = -\frac{1}{N} \frac{1 - 2n_{\sigma}}{1 - n_{\sigma}} \sum_{k_1} \left( \frac{\xi_{k_1} n_{\sigma}}{U - \epsilon_{k_1}} + \frac{\xi_{k_1} n_{\sigma}}{\epsilon_{k_1}} \right)$$

$$- \frac{1}{N} \frac{n_{\sigma}}{1 - n_{\sigma}} \sum_{k_1} \left( \frac{\xi_{k_1} n_{\sigma}}{n_{\sigma}U - \epsilon_{k_1}} - \frac{\xi_{k_1} n_{\sigma}}{(1 - n_{\sigma})U - \epsilon_{k_1}} \right) \tag{30}$$

This expression of the spectral density function $A_{\sigma}^{L-U}(\omega, k)$ is obviously similar to that for one site case, and the two peaks denoted respectively by the functions $\delta (\omega - \varepsilon_k)$ and $\delta (\omega - \varepsilon_k - U)$, corresponding to the lower and upper Hubbard bands, is separated by $U$.

At half filling, $n_{\sigma} = \frac{1}{2}$, $\sigma = \uparrow, \downarrow$, the constants $Z^L$ and $Z^U$ both are equal to zero, and the spectral weight constants of electrons in both the lower and upper Hubbard bands are the same, and equal $\frac{1}{2}$. Thus the system is a Mott insulator with the gap proportional to $U$ in the large $U$ limit, in which there exist some collective excitation modes (i.e., $A_{\sigma}^{Em}(\omega, k) = 0$, $A_{\sigma}^{Con}(\omega, k) \neq 0$, see below). While, as the hole doping, $n_{\sigma} = \frac{1}{2} - \delta$, the constants $Z^L$ and $Z^U$ are positive, and proportional to the hole doping concentration $\delta$ in the large $U$ limit. This means that as the hole doping, the spectral weight of electrons in both the lower and upper Hubbard bands is reduced, and the part of them is transferred into the gap where there emerge new states.
The spectral density function $A_{\sigma}^{Em}(\omega, k)$ can be written as that,

$$A_{\sigma}^{Em}(\omega, k) = \frac{-2\pi}{N} \frac{1 - 2n_{\sigma}}{1 - n_{\sigma}} \sum_{k_1} \frac{U\xi_{k_1} n_{k_1 \sigma}}{\epsilon_{k_1}(U - \epsilon_{k_1})} \delta(\omega - \epsilon_k - \epsilon_{k_1}) - \frac{2\pi}{N} \frac{U n_{\sigma}}{1 - n_{\sigma}} \sum_{k_1} \frac{\xi_{k_1} n_{k_1 \sigma}}{n_{\sigma} U - \epsilon_{k_1}}(\epsilon_{k_1} + (1 - n_{\sigma})U) \delta(\omega - \epsilon_k - \epsilon_{k_1} - (1 - n_{\sigma})U) + \frac{2\pi}{N} \frac{U n_{\sigma}}{1 - n_{\sigma}} \sum_{k_{1'}} \frac{\xi_{k_{1'}} n_{k_{1'} \sigma}}{(\epsilon_{k_{1'}} + n_{\sigma} U)[(1 - n_{\sigma}) U - \epsilon_{k_1}]} \delta(\omega - \epsilon_k - \epsilon_{k_{1'}} - U) - \frac{2\pi}{N} \frac{1 - 2n_{\sigma}}{1 - n_{\sigma}} \sum_{k_1} \frac{U\xi_{k_1} n_{k_1 \sigma}}{\epsilon_{k_1}(\epsilon_{k_1} + U)} \delta(\omega - \epsilon_k - \epsilon_{k_1} - U) \tag{31}$$

It is noticeable that at the half filling $n_{\sigma} = \frac{1}{2}$, the spectral density function $A_{\sigma}^{Em}(\omega, k)$ is zero, $A_{\sigma}^{Em}(\omega, k) = 0$. After the hole doping, $n_{\sigma} = \frac{1}{2} - \delta$, there emerge new states that reside in the gap and at the top of the upper Hubbard bands, respectively. In the above expression of the spectral density function $A_{\sigma}^{Em}(\omega, k)$, the first three terms in the right hand side are contributed by the emerged states in the gap, where the first term resides at the top of the upper Hubbard band, which is also proportional to the hole doping concentration $\delta$. The second and third terms residing around in the middle of the gap take converse values, and they are proportional to $\frac{1}{U}$ for large $U$. In the underdoped regime, after considering $A_{\sigma}^{Con}(\omega, k)$, the total spectral density function of electrons $A_{\sigma}(\omega, k)$ may show a dip around in the middle of the gap. The last term in the right hand side is contributed by the emerged states residing at the top of the upper Hubbard band, which is also proportional to the hole doping concentration $\delta$. In the low temperature limit, the first term of the spectral density function $A_{\sigma}^{Em}(\omega, k)$ is mainly responsible for the infrared reflectivity spectrum in the gap, where the effective carrier density grows in proportion to the hole doping concentration $\delta$, consistent with the experimental observations.

The spectral density function $A_{\sigma}^{Con}(\omega, k)$ can be directly obtained by the Green function $G_{k\sigma}^{NLC}(\omega)$ which originates from the static correlation function $<\hat{c}_{k+p\sigma}^{\dagger} \hat{c}_{k+p+k_{1}-k' \sigma}^{\dagger} \hat{c}_{k' \sigma} \hat{c}_{k \sigma}>$. Under the approximations in Eqs. (26), it can be written as two parts,

$$A_{\sigma}^{Con}(\omega, k) = A_{\sigma}^{spin}(\omega, k) + A_{\sigma}^{pair}(\omega, k) \tag{32}$$

where the spectral density function $A_{\sigma}^{spin}(\omega, k)$ is related to the spin parameters $S_{k'_{1}}^{+}$,

$$A_{\sigma}^{spin}(\omega, k) = -\frac{2\pi}{(1 - n_{\sigma}) N^2} \sum_{k'_{1}} \Gamma_{k_{1}k_{1'}}(\omega) S_{k_{1}}^{+} S_{k_{1}}^{+} \tag{33}$$
At the half filling, the spectral density function $A_{k'k} (\omega) = A_{k'k}^{NL} (k' - k) \delta (\omega - \varepsilon_{k'}) - B_{k'k}^{NL} (k' - k) \delta (\omega - \varepsilon_{k'} - U)
+ \frac{U \xi_{-k} \delta (\omega + \eta_{k'k} - \varepsilon_{k'})}{\eta_{k'k} (\eta_{k'k} + U)} - \frac{U \xi_{-k} \delta (\omega + \eta_{k'k} - \varepsilon_{k'} - (1 - n_{\sigma}) U)}{(\eta_{k'k} - (1 - n_{\sigma}) U) (\eta_{k'k} + n_{\sigma} U)}$
+ \frac{U \xi_{-k} \delta (\omega + \eta_{k'k} - \varepsilon_{k'} - n_{\sigma} U)}{(\eta_{k'k} - n_{\sigma} U) (\eta_{k'k} + (1 - n_{\sigma}) U)}
+ \frac{U \xi_{-k} \delta (\omega + \eta_{k'k} - \varepsilon_{k'} - n_{\sigma} U)}{(\eta_{k'k} - n_{\sigma} U) (\eta_{k'k} + (1 - n_{\sigma}) U)}$ (34)

And the spectral density function $A_{\sigma}^{pair} (\omega, k)$ is contributed by the electronic pairing parameters $\Delta_{k}$,

$A_{\sigma}^{pair} (\omega, k) = \frac{2\pi}{(1 - n_{\sigma}) N^{2}} \sum_{k'k} \Lambda_{k'k} (\omega) \Delta_{k}^{*} \Delta_{k'}$ (35)

$\Lambda_{k'k} (\omega) = A_{k'k}^{NL} (-k - k) \delta (\omega - \varepsilon_{-k}) - B_{k'k}^{NL} (-k - k) \delta (\omega - \varepsilon_{-k} - U)
+ \frac{U \xi_{-k'k} \delta (\omega + \eta_{k'k} - \varepsilon_{k'})}{\eta_{k'k} (\eta_{k'k} + U)} + \frac{U \xi_{-k} \delta (\omega + \eta_{k'k} - \varepsilon_{k'} - (1 - n_{\sigma}) U)}{(\eta_{k'k} + n_{\sigma} U) (\eta_{k'k} - (1 - n_{\sigma}) U)}$
+ \frac{U \xi_{-k'k} \delta (\omega + \eta_{k'k} - \varepsilon_{k'} - n_{\sigma} U)}{(\eta_{k'k} - n_{\sigma} U) (\eta_{k'k} + (1 - n_{\sigma}) U)} (36)

At the half filling, the spectral density function $A_{\sigma}^{Com} (\omega, k)$ does not be zero, while the spectral density function $A_{\sigma}^{Em} (\omega, k)$ is zero. This means that at the half filling there only emerge the collective modes corresponding to the electronic spin density wave, and the uniform electronic pairing parameter $\Delta_{k}$ is expectedly zero in the large $U$ limit.

At the half filling, the last two terms residing around in the middle of the gap in the expressions of the functions $\Gamma_{k'k} (\omega)$ and $\Lambda_{k'k} (\omega)$ are small quantities because they are inverse proportion to $U$ in the large $U$ limit, and the contribution of the collective modes to the spectral density function is not zero mainly around the lower and upper Hubbard bands. Of course, for any electron density, the total spectral density function $A_{\sigma} (\omega, k)$ must be positive, meanwhile it also satisfy the sum rule in Eq.(25).

The above properties of the spectral density function $A_{\sigma} (\omega, k)$ is based on the cut-off approximations in Eq.(11). However, to high order approximations, if we solve the EOMs of the correlation functions $F_{n\sigma}^{X_{\sigma}} (t_1, t_2)$, under taking the cut-off approximations similar to that in the Eq.(11) for the correlation functions belonging to the level $L = 4$ that emerge in the EOMs of the correlation functions $F_{n\sigma}^{X_{\sigma}} (t_1, t_2)$, we will find that the basic behavior of
the spectral density function $A_{\sigma}(\omega, k)$ is unchanged, in which the total spectral weight of the emerged states of electrons in the gap is also proportional to the hole doping concentration $\delta$ in the large $U$ limit, that is independent of the cut-off approximations in Eq.(11).

V. CONCLUSIONS

By introducing multipe-site correlation functions, we have proposed a hierarchical Green function approach, and applied it to study a 2D square lattice Hubbard model by solving the EOMs of one-particle Green function and related multipe-site correlation functions. Under a cut-off approximation for the correlation functions belonging to the level $L = 3$ that emerge in the EOMs of the multipe-site correlation functions $F_{nij\sigma}(t_1, t_2)$. Then by using the Fourier representation of these correlation functions, we have solved this set of closed EOMs, and obtained an analytical expression of one-particle Green function with possible order parameters emerging in the ground state. With this one-particle Green function, we have calculated the spectral density function of electrons, and found that besides usual two main peaks corresponding to the lower and upper Hubbard bands in the spectral density function, there emerge some novel states between these two main peaks, and the total spectral weight of these emerged states is proportional to the hole doping concentration $\delta$ for large $U$, that is distinct from that one in a metal. Meanwhile, there also emerge some collective modes related to possible charge/spin density wave and/or electronic pairing density wave ordering states. However, at the half filling, it is a Mott insulator with a gap that is in proportion to $U$ in the large $U$ limit. The present results are completely consistent with the spectroscopy observations of the cuprate superconductors in normal states[11–13]. On the other hand, the appearance of the static correlation functions in the one-particle Green function can be used to describe the intertwined orders observed in the normal state of the cuprate superconductors. Moreover, the present approach can also be used to study other quantum many particle systems, such as Anderson impurity model and Heisenberg model.

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[1] J. G. Bednorz and K. A. Müller, Z. Phys. B64, 189 (1986).
[2] P. W. Anderson, Science 235, 1196 (1987).
[3] F. C. Zhang and T. M. Rice, Phys. Rev. B37, 3759 (1988).
[4] G. Baskaran, Z. Zou and P. W. Anderson, Solid State Commun. 63, 973 (1987); I. Affleck and J. B. Marston, Phys. Rev. B37, 3774 (1988); G. Kotliar and J. Liu, Phys. Rev. B38, 5142 (1988).
[5] G. Baskaran and P. W. Anderson, Phys. Rev. B37, 580 (1988); L. Ioffe and A. Larkin, Phys. Rev. B39, 8988 (1989); P. A. Lee and N. Nagaosa, Phys. Rev. B45, 966 (1992).
[6] P. W. Anderson, P. A. Lee, M. Renderia, T. M. Rice, N. Trivedi and F. C. Zhang, J. Phys.: Condens. Matter 24, R755 (2004).
[7] P. A. Lee, N. Nagaosa and X. G. Wen, Rev. Mod. Phys. 78, 17 (2006).
[8] P. W. Anderson, The Theory of Superconductivity in the High-Tc Cuprates (Princeton Univ. Press, Princeton, NJ, 1997).
[9] J. Hubbard, Proc. Roy. Soc. (London) A276, 238 (1963); A281, 401 (1964).
[10] C. M. Varma, P. B. Littlewood, S. Schmitt-Rink, E. Abrahams, and A. E. Ruckenstein, Phys. Rev. Lett. 63, 1996 (1989).
[11] S. L. Cooper, G. A. Thoma, J. Orenstein, D. H. Rapkine, A. J. Millis, S.-W. Cheong, A. S. Cooper, and Z. Fisk, Phys. Rev. B41, 11605 (1990).
[12] S. Uchida, T. Ido, H. Takagi, T. Arima, and Y. Tokura, Phys. Rev. B43, 7942 (1991).
[13] W. J. Padilla, Y. S. Lee, M. Dummm, G. Blumberg, S. Ono, K. Segawa, S. Komiya, Y. Ando, and D. N. Basov, Phys. Rev. B72, 060511(R) (2005).
[14] D. L. Feng, D. H. Lu, K. M. Shen, C. Kim, H. Eisaki, A. Damascelli, R. Yoshizaki, J. I. Shimoyama, K. Kishio, G. D. Gu, S. Oh, A. Andrus, J. O’Donnell, J. N. Echstein, and Z. X. Shen, Science 289, 277 (2000).
[15] E. Fradkin, and S. A. Kivelson, Nat. Phys. 8, 864 (2012).
[16] E. Fradkin, S. A. Kivelson and J. M. Tranquada, Rev. Mod. Phys. 87, 457 (2015).
[17] B. Keimer, S. A. Kivelson, M. R. Norman, S. Uchida, and J. Zaanen, Nature 518, 179 (2015).
[18] S. Raghu, S. A. Kivelson, and D. J. Scalapino, Phys. Rev. B81, 224505 (2010).
[19] L. Liu, H. Yao, E. Berg, S. R. White, and S. A. Kivelson, Phys. Rev. Lett. 108, 126406 (2012).
[20] L. Hedin, Phys. Rev. 139, A796 (1965); L. Hedin and S. Lundqvist, Solid State Physics, Vol. 23 (Ehrenreich, H. and Seitz, F. and Turnbull, D. Academic Press, New York, 1969).
[21] P. Romaniello, F. Bechstedt and L. Reining, Phys. Rev. B85, 155131 (2012).
[22] R. Zwanzig, In Lectures in Theoretical Physics, Vol. 3 (Interscience, New York, 1961); H. Mori, Prog. Teor. Phys. 33, 423 (1965).
[23] P. Fulde, Electron Correlations in Molecules and Solids (Springer-Verlag, 1991).
[24] G. D. Mahan, Many Particle Physics (Plenum, New York, 1981).
[25] D. P. Arovas, A. Auerbach, Phys. Rev. B38, 316 (1988).
[26] S. Chakravarty, B. I. Halperin, and D. R. Nelson, Phys. Rev. B39, 2344 (1989).
[27] H. Q. Lin and J. E. Hirsch, Phys. Rev. B35, 3359 (1987).