The analytical description of a doped Mott insulator

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Abstract

With the hierarchical Green’s function approach, we study a doped Mott insulator described with the Hubbard model by analytically solving the equations of motion of an one-particle Green’s function and related multiple-point correlation functions, and find that the separation of the spin and charge degrees of freedom of the electrons is an intrinsic character of the doped Mott insulator. For enough of large on-site repulsive Coulomb interaction, we show that the spectral weight of the one-particle Green’s function is proportional to the hole doping concentration that is mainly produced by the charge fluctuation of electrons, while the excitation spectrum of the electrons is composed of two parts: one is contributed by the spin fluctuation of the electrons which is proportional to the hole doping concentration, and another one is coming from the coupling between the charge and spin fluctuations of the electrons that takes the maximum at undoping. All of these low energy/temperature physical properties originate from the strong on-site Coulomb interaction. The present results are consistent with the spectroscopy observations of the cuprate superconductors, and the numerical calculations in normal state above pseudogap regime.
I. INTRODUCTION

Since the discovery of the high \( T_c \) cuprate superconductive materials, 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. 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 originates from the strong correlation of electrons produced by the strong on-site 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.

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 on a square lattice, used to describe the basic characters of high \( T_c \) cuprate superconductivity, 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 strong on-site 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 strong on-site 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, and in the latter it is a fully polarized ferromagnetic metallic phase 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 $W = 8t_0$, $U \sim W$, and 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 calculation from microscopic theories. The 2D square lattice Hubbard model with intermediate coupling, likely cannot be treated using any fundamentally perturbation approach which starts with a non-interacting particle description because the strength of the interactions among electrons is comparable to or large than their kinetic energy. That is that there is not any controllable effectively small "interaction strength" as a perturbation expansion parameter in this system due to the strong correlation among electrons. 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.

The analytical description of a strongly correlated system is very successful only for one-dimensional case, such as the Bethe ansatz[15–17] and bosonization method[18] that cannot be extended for two or higher dimensions. However, any theory based on a perturbation expansion[19, 20] around the non-interacting limit is at least questionable, due to the non-perturbation nature of the strongly correlated system[21–24]. Beyond usual equation of motion of Green’s function approach[25–30], we use the hierarchic Green’s function approach[31] to study the intrinsic character of a doped Mott insulator with the Hubbard model under the strong on-site repulsive Coulomb interaction.

For a doped Mott insulator, the central issue is rigorous and/or effective treatment of the competition between the doped hole itineracy and the strong on-site repulsive Coulomb interaction to maintain local antiferromagnetic correlation of spins, that produces some new orders in the low energy/temperature region. This competition in fact is a many body effect of electrons and it cannot be effectively described by a perturbation parameter like that in usual weakly correlated systems, such as three-dimensional electron gas in high electron density limit. In this work, we make a step to this end. For simplicity, without introducing the pseudogap and other order parameters, we mainly study the influence of the doped holes on the one-particle Green’s function and the low-lying excitation spectrum under the large on-site Coulomb interaction $U$ which is of order the bandwidth $W$; Then we demonstrate that for the small hole doping concentration $\delta$, the spectral weight of the
electrons is proportional to $\delta$, that is mainly attributed to the charge fluctuation of electrons, while the excitation spectrum is composed of two parts: one is mainly contributed by the spin fluctuation of the electrons, which is proportional to $\delta$, and another one originates from the coupling between the charge and spin fluctuations of the electrons, which is proportional to $1 - \delta$. In fact, there takes place the separation of the charge and spin degrees of freedom of electrons. In Sec.II, with the hierarchic Green’s function approach, we give some key equations of motion of one-particle Green’s function and related multiple-point correlation functions. In Sec. III, under the soft cut-off approximation (see below), we solve these equations of motion, and give an analytic expression of the one-particle Green’s function. With these solutions, we demonstrate that the spectral weight of electrons is proportional to the hole doping concentration $\delta$, and the double occupation function of electrons goes to zero in the both regions around $\delta = 0$ and $\delta = 1$, respectively. We give our conclusion and discussion in Sec. IV, and more detail calculations in the Appendix.

II. THE EQUATION OF MOTION OF THE ONE-PARTICLE GREEN’S FUNCTION

With the hierarchic Green’s function approach, we can write out the equation of motion of the one-particle Green’s function (choosing $\hbar = 1$),

$$[i\partial_t + \mu] G_{iqa}(t) = \delta(t) \delta_{iq} + \sum_m \hat{h}_{im} G_{mq\sigma}(t) + \frac{U}{2} F^{(n)}_{iiq}(t) - \frac{\sigma U}{2} F^{(s)}_{iiq}(t) \quad (1)$$

where, $F^{(n)}_{ijq}(t) = -i < T\hat{n}_i(t) \hat{c}_{\sigma j}(t) \hat{c}^\dagger_{\sigma q}(0) >$, and $F^{(s)}_{ijq} = -i < T\hat{s}_i(t) \hat{c}_{\sigma j}(t) \hat{c}^\dagger_{\sigma q}(0) >$, they are produced by the on-site Coulomb interaction of electrons. Here $\hat{n}_i = \hat{n}_{i\uparrow} + \hat{n}_{i\downarrow}$ is the charge density operator, and $\hat{s}_i = \hat{n}_{i\uparrow} - \hat{n}_{i\downarrow}$ is the spin density operator. The related multiple-point correlation function $F^{(n)}_{ijq}(t)$ represents the contribution of the charge fluctuation of electrons to the one-particle Green’s function, while the related multiple-point correlation function $F^{(s)}_{ijq}(t)$ represents the contribution of the spin fluctuation of electrons to the one-particle Green’s function. This linear equation of motion of the one-particle Green’s function is rigorous, and the strong correlation effect of electrons is completely represented by the on-site correlation functions $F^{(n)}_{iiq}(t)$, and $F^{(s)}_{iiq}(t)$, thus these two correlation functions play a key role in solving the equation of motion of the one-particle Green’s function. Here, we do not consider the influence of the pseudogap of electrons on the low energy states, and the present
calculation is valid for a higher energy scale than the pseudogap $\Delta$ in the underdoping region.

The equations of motion of the multiple-point correlation function $F_{ijq}^{(n)}(t)$ and $F_{ijq}^{(s)}(t)$ can be written as that,

$$
[i\partial_t + \mu]F_{ilq}^{(n)}(t) = \langle \hat{n}_i \rangle \delta(t)\delta_{ilq} + \frac{U}{2} F_{ilq}^{(nn)}(t) - \frac{\sigma U}{2} F_{ilq}^{(ns)}(t)
+ \sum_m \left[ \hat{h}_{im} F_{imq}^{(n)}(t) + \hat{h}_{im} F_{imlq}^{(P(-))}(t) \right]
\tag{2}
$$

$$
[i\partial_t + \mu]F_{ilq}^{(s)}(t) = \langle \hat{s}_i \rangle \delta(t)\delta_{ilq} + \frac{U}{2} F_{ilq}^{(sn)}(t) - \frac{\sigma U}{2} F_{ilq}^{(ss)}(t)
+ \sum_m \left[ \hat{h}_{im} F_{imq}^{(s)}(t) + \hat{h}_{im} F_{imlq}^{(Q(-))}(t) \right]
\tag{3}
$$

where the definition of the high order related multiple-point correlation functions appearing in the above equations is given in the Appendix. With the same procedures, we can write out the equations of motion of these correlation functions in which there will appear more high order new correlation functions, and this set of equations of motion is not closed. In order to calculate the one-particle Green’s function, we need to cut-off this set of equations of motion at some level. According to the above equations, it is clear that the correlation functions $F_{ilq}^{(n)}(t)$ and $F_{ilq}^{(s)}(t)$ are directly coupled by the high order correlation function $F_{ijql}^{(sn)}(t)$, while they are independent of each other as without completely considering the contribution of these high order correlation functions. In the large on-site repulsive Coulomb interaction region, the coupling between both the charge and spin fluctuation plays important role in studying of the low energy behavior of the one-particle Green’s function, and the following approximation taken would effectively incorporate in the contribution of the correlation function $F_{ijql}^{(sn)}(t)$. Here the correlation functions $F_{ijql}^{(P(-))}(t)$ and $F_{ijql}^{(Q(-))}(t)$ represent high order charge and spin fluctuations, and their contribution to the correlation functions $F_{ilq}^{(n)}(t)$ and $F_{ilq}^{(s)}(t)$ is to mainly modify the chemical potential.

The Eqs. (1-3) are the key ones that we use them to calculate the one-particle Green’s function in the large $U$ region, where the spin and charge fluctuations are separated obviously that are represented by the multiple-point correlation functions $F_{ilq}^{(n)}(t)$ and $F_{ilq}^{(s)}(t)$, respectively. Next we write out the equations of motion of the high order multiple-point correlation functions appearing in Eqs. (1-3),

$$
[\omega + \mu] F_{ijql}^{(nn)}(\omega) = \langle \hat{n}_i \rangle \hat{n}_l \delta_{ijq} + \frac{U}{2} F_{ijql}^{(nnn)}(\omega) - \frac{\sigma U}{2} F_{ijql}^{(nns)}(\omega)
+ \sum_m \left[ \hat{h}_{jm} F_{jlmq}^{(nn)}(\omega) + \hat{h}_{im} F_{ilmjq}^{(P(-))}(\omega) + \hat{h}_{im} F_{ilmjq}^{(nP(-))}(\omega) \right]
\tag{4}
$$
\[
[\omega + \mu] F^{(sn)}_{illq}(\omega) = < \hat{s}_i \hat{n}_l > \delta_{jq} + \frac{U}{2} F^{(snm)}_{illjq}(\omega) - \frac{\sigma U}{2} F^{(sns)}_{illjq}(\omega) \\
+ \sum_m \left[ \hat{h}_{jm} F^{(sn)}_{ilmq}(\omega) + \hat{h}_{im} F^{(Q(-)n)}_{ilmjq}(\omega) + \hat{h}_{im} F^{(sP(-))}_{ilmjq}(\omega) \right]
\]
(5)

\[
[\omega + \mu] F^{(ss)}_{illq}(\omega) = < \hat{s}_i \hat{s}_l > \delta_{jq} + \frac{U}{2} F^{(ssn)}_{illjq}(\omega) - \frac{\sigma U}{2} F^{(sss)}_{illjq}(\omega) \\
+ \sum_m \left[ \hat{h}_{jm} F^{(ss)}_{ilmq}(\omega) + \hat{h}_{im} F^{(Q(-)s)}_{ilmjq}(\omega) + \hat{h}_{im} F^{(sQ(-))}_{ilmjq}(\omega) \right]
\]
(6)

where there emerge new more higher order multiple-point correlation functions, and there appear the static spin-spin and density-density correlation functions that can be self-consistently determined by calculating spin-spin and density-density correlation functions under equal-time limit in the above equations. In order to effectively including the coupling between the spin and charge fluctuation of electrons induced by the large on-site repulsive Coulomb interaction, we only take some approximations in the Eqs. (1-6). For simplicity, we neglect all the static quantities appearing in these equations.

In the equation of motion of the one-particle Green’s function Eq. (1), there only appears the correlation functions \( F^{(n)}_{iiq}(t) \) and \( F^{(s)}_{iiq}(t) \), while in their equations of motion Eq. (2,3) (taking \( l = i \)) there emerge the correlation functions \( F^{(nn)}_{iiq}(t) = -i < T [\hat{n}_i(t)]^2 \hat{c}_{\sigma i}(t)\hat{c}_{\sigma q}^\dagger(0) > \) and \( F^{(ss)}_{iiq}(t) = -i < T [\hat{s}_i(t)]^2 \hat{c}_{\sigma i}(t)\hat{c}_{\sigma q}^\dagger(0) > \). On the other hand, the correlation functions \( F^{(n)}_{iiq}(t)/F^{(s)}_{iiq}(t) \) and \( F^{(nn)}_{illq}(t)/F^{(ss)}_{illq}(t) \) are connected by the Eq.(2)/(3), in which there emerge the correlation functions \( F^{(nn)}_{illq}(t) \), \( F^{(sn)}_{illq}(t) \), \( F^{(ss)}_{illq}(t) \), and others. As taking \( l = j \) or \( i = j \) in the Eqs.(1-6), there will be a lot of the correlation functions that in their definitions there appear the charge operator \( [\hat{n}_i(t)]^2 \) or the spin operator \( [\hat{s}_i(t)]^2 \), for example, \( F^{(nnn)}_{ijjjq}(t) = -i < T\hat{n}_i(t) [\hat{n}_j(t)]^2 \hat{c}_{\sigma j}(t)\hat{c}_{\sigma q}^\dagger(0) > \), and \( F^{(sss)}_{ijjjq}(t) = -i < T\hat{s}_i(t) [\hat{s}_j(t)]^2 \hat{c}_{\sigma j}(t)\hat{c}_{\sigma q}^\dagger(0) > \), et al. It is a key point how to effectively treat these correlation functions that have the charge operator \( [\hat{n}_i(t)]^2 \) or the spin operator \( [\hat{s}_i(t)]^2 \) appearing in the Eqs. (2-6). In the following we use a special relation between the charge operator \( \hat{n}_i \) and spin operator \( \hat{s}_i \) to approximately treat these correlation functions.

Instead of taking a simple cut-off approximation for high order multiple-point correlation functions, we use the character of the charge operator \( \hat{n}_i \) and spin operator \( \hat{s}_i \) to simplify these equations, where they have the following relation,

\[
(\hat{n}_i)^2 + (\hat{s}_i)^2 = 2\hat{n}_i
\]
(7)
which is independent of whether the system is doped by holes, and it shows that the spin and charge degrees of electrons are intimately intertwined on each lattice site, which is very important in the large $U$ limit for the Hubbard model. For a Mott insulator described by the Hubbard model, we have the relation, $(\hat{n}_i)^2 = (\hat{s}_i)^2 = 1$; while for a doped Mott insulator with small hole doping concentration $\delta$, we can take the approximation, called soft cut-off approximation (SCA), in which we use the parameters $n^2 = \langle (\hat{n}_i)^2 \rangle$ and $s^2 = \langle (\hat{s}_i)^2 \rangle$ to replace the charge and spin operators $(\hat{n}_i)^2$ and $(\hat{s}_i)^2$, respectively, in the Eqs. (2-6). These two parameters $n^2$ and $s^2$ have the relation with the hole doping concentration $\delta$,

$$n^2 + s^2 = 2(1 - \delta) \quad (8)$$

which is rigorous due to the Eq. (7). On the other hand, for enough of large $U$ where the double occupied states are completely depleted, we can take the relation, $n^2 = s^2 = 1 - \delta$.

Under the SCA, the equations of motion in Eqs. (1-3) can be significantly simplified, but there are still some other high order ($L = 3$) multiple-point correlation functions. Fortunately, under the SCA, in these equations there may appear the terms including the one-particle Green’s function. As a zeroth order approximation, we neglect all these high order ($L = 3$) correlation functions appearing in the Eqs. (1-3), and we only remain ones that are the lower order ($L \leq 2$) correlation functions. Under this approximation, the set of the equations of motion of the one-particle Green’s function and the related correlation functions Eqs. (1-3) is closed. In fact, this approximation is similar to a “self-consistent field theory” that the multiple-point correlation functions $F^{(nn)}_{iljq}(\omega)$, $F^{(sn)}_{iljq}(\omega)$, $F^{(ss)}_{iljq}(\omega)$, $F^{(P(-))}_{ijlq}(t)$ and $F^{(Q(-))}_{ijlq}(t)$ can be seen as some “external fields” that are the functions of the one-particle Green’s function and the correlation functions $F^{(n)}_{ilq}(t)$ as well as $F^{(s)}_{ilq}(t)$, then the set of equations of motion in Eqs. (1-3) can be self-consistently solved.

Obviously, the present approach is completely distinct from previous perturbation expansion and/or cut-off approximations, and it has the advantages that: (1) it can effectively treat the local spin and charge fluctuations induced by the on-site repulsive Coulomb interaction with Eqs. (1-3); (2) it effectively incorporate in the coupling between the spin and charge fluctuations in Eqs. (2-3); (3) it does not need any ”perturbation term” as a parameter to be expanded, like usual perturbation expansion approach; (4) the basic equations of motion in Eqs. (1-3) are rigorous, and the spin and charge fluctuations are represented by the correlation functions $F^{(n)}_{ilq}(t)$ and $F^{(s)}_{ilq}(t)$, respectively, where they satisfy different equation...
of motion. It is helpful in future to introducing different order parameters in the low energy limit.

III. SOLUTION OF THE ONE-PARTICLE GREEN’S FUNCTION

The related multiple-point correlation functions \( F^{(n)}_{ijq}(t) \) and \( F^{(s)}_{ijq}(t) \) appearing in the equation of the one-particle Green’s function are playing different roles, and they both have significant contribution to the self-energy of electrons. Under the SCA, their analytical expressions are given in the Appendix \((38,39)\). The multiple-point correlation function \( F^{(n)}_{ijq}(t) \) represents the contribution of the charge fluctuation of electrons to the electronic correlation effect. It has three significant contributions: (1) it modifies the chemical potential by a factor, \(-n^2J_U\); (2) it strongly suppresses the spectral weight of the electrons by contributing a factor, \(-\langle \hat{n}_i \rangle \delta_{iq}\) to the one-particle Green’s function \( G_{iq\sigma}(\omega) \), that makes the spectral weight of the electrons be proportional to the doping concentration \( \delta \); (3) it contributes a term to the excitation spectrum proportional to \( 1 - \delta \), that originates from the coupling between the spin and charge fluctuations in the large \( U \) limit. The multiple-point correlation function \( F^{(s)}_{ijq}(t) \) represents the contribution of the spin fluctuation of electrons to the electron correlation effect. It significantly suppresses the itineracy of the electrons, which makes the effective hopping amplitude of the electrons be proportional to the hole doping concentration \( \delta \). It means that the strong spin fluctuation induced by the large on-site Coulomb interaction \( U \) significantly suppresses the itineracy of the doping holes, and it tends to localize the electrons.

With the help of the analytical expressions of the correlation functions \( F^{(n)}_{ijq}(t) \) and \( F^{(s)}_{ijq}(t) \), and after taking the Fourier transformation of time, we can obtain the following equation of the one-particle Green’s function which is reliable in the low energy region \((\Delta < |\omega| \ll t_0)\),

\[
[\omega + \mu_{eff}] G_{iq\sigma}(\omega) = [1 - \langle \hat{n}_i \rangle + \sigma \langle \hat{s}_i \rangle] \delta_{iq} + \sum_m h_{im}^{eff} G_{mq\sigma}(\omega)
\]

(9)

where \( \mu_{eff} = \mu - n^2J_U \), \( J_U = \frac{4t^2}{U} \), and \( h_{ij}^{eff} = \left( \delta + \frac{n^2U}{2J_U} \right) \hat{h}_{ij} \). If we take an average over the spin degrees of the one-particle Green’s function, \( G_{iq\sigma}(\omega) = \frac{1}{2} [G_{iq\uparrow}(\omega) + G_{iq\downarrow}(\omega)] \), the factor \( \sigma \langle \hat{s}_i \rangle \delta_{iq} \) appearing in the Eq.\((9)\) has no contribution to the spectral weight of electrons. Thus, in the strong on-site repulsive Coulomb interaction limit, \( t_0 \ll U \), the effective spectral weight of electrons is that, \( 1 - \langle \hat{n}_i \rangle = \delta \). Moreover, the equation of
motion of the one-particle Green’s function in Eqs. (9) is valid for a general lattice Hubbard model, for example, a chain, a square lattice, et al. On the other hand, as considering the next nearest neighbor hoping of the electrons, \( t'_{ij} \), we should add a term \( \delta t'_{in}G_{mq\sigma}(\omega) \) in the right side of Eq. (9), where the parameter \( t'_{ij} \) is renormalized to \( \delta t'_{ij} \) due the strong on-site repulsive Coulomb interaction.

After taking the Fourier transformation, we have the following analytical expression of the one-particle Green’s function in a square lattice

\[
\bar{G}_{k}(\omega) = \frac{\delta}{\omega + \mu_{\text{eff}} - \varepsilon_{k}^{\text{eff}}} \tag{10}
\]

where \( \varepsilon_{k}^{\text{eff}} = \left( \delta + \frac{n^{2}J_{t}}{2U} \right) \varepsilon_{k}^{0} \), and \( \varepsilon_{k}^{0} = -2t_{0}\left[ \cos(ak_{x}) + \cos(ak_{y}) \right] \), where \( a \) is the lattice constant. This dispersion \( \varepsilon_{k}^{\text{eff}} \) is very similar to that of the slave boson mean field theory with the complete condensed of holons in the t-J model, and the term with the coefficient \( \frac{n^{2}J_{t}}{2U} \) in the excitation spectrum may be corresponding to the excitation spectrum of spinons\(^{32}\).

This analytical expression of the one-particle Green’s function is reliable in the low energy region, \( |\omega| \ll t_{0} \), as calculating the contribution of the high order multiple-point correlation functions we have used the conditions, \( |\omega| \ll t_{0} \ll U, \mu \simeq U/2 \), and neglected the static quantities appearing in the equations of motion of high order multiple-point correlation functions. That is, the expression of the one-particle Green’s function in the high energy region, such as \( |\omega| \gg t_{0} \), is different from the above one.

According to the Eq. (10), the spectral function of electrons can be written as that in the lower Hubbard band,

\[
A_{k}^{L}(\omega) = 2\pi\delta \times \delta \left( \omega + \mu_{\text{eff}} - \varepsilon_{k}^{\text{eff}} \right) \tag{11}
\]

and the most of spectral weight is transferred to the upper Hubbard band in the under-doping region. On the other hand, according to the related multiple-point correlation functions \( F_{ijq}^{(n)}(t) \) and \( F_{ijq}^{(s)}(t) \), we can calculate the double occupation function of electrons,

\[
< \hat{n}_{i\uparrow}\hat{n}_{i\downarrow} > = -\frac{i}{2} \left[ F_{ii}^{(n)}(t) - \sigma F_{ii}^{(s)}(t) \right]_{t \to 0+}, \text{which is that in the lower Hubbard band,}
\]

\[
< \hat{n}_{i\uparrow}\hat{n}_{i\downarrow} > \propto \frac{\delta (1 - \delta) t_{0}}{U} + O \left( \frac{1 - \delta}{U^{2}} \right) \tag{12}
\]

Obviously, this quantity goes to zero in the both regions around \( \delta = 0 \) and \( \delta = 1 \), respectively. The former is the result of the strong on-site repulsive Coulomb interaction, in which the double occupied state on each site is highly prohibited in the large \( U \) limit, and the latter
is trivial due to no electron in the sites. Note that it is valid in the $U >> t_0$ limit due to we used the solutions of the correlation functions $F_{ijq}^{(n)}(t)$ and $F_{ijq}^{(s)}(t)$ in this limit.

At undoping $\delta = 0$, where the system is at the half-filling of electrons, the spectral weight of the electrons goes to zero, and the system is a Mott insulator. Moreover, the excitation energy spectrum of electrons is composed of two parts: one is proportional to the hole doping concentration $\delta$, which goes to zero in the underdoping limit, and another one is proportional to $1 - \delta$, that take the maximum value at undoping. Now it becomes more clear that the significantly suppressed of the spectral weight (proportional to $\delta$) of electrons is mainly produced by the charge fluctuation described by the correlation function $F_{ijq}^{(n)}(t)$; while the localization effect of electrons showing in the low energy excitation spectrum (the part of it proportional to $\delta$) is mainly produced by the spin fluctuation represented by the correlation function $F_{ijq}^{(s)}(t)$, and another part of the excitation spectrum proportional to $1 - \delta$ is coming from the coupling between the charge and spin fluctuations induced by the strong on-site repulsive Coulomb interaction. Physically, it means that the charge and spin freedoms of electrons are separated due to the strong on-site repulsive Coulomb interaction. This phenomenon takes place not only in one dimension but also in two and three dimensional lattices. The Mott insulator is a special case in which the charge degrees of electrons is completely suppressed, and the low energy excitation spectrum coming from the charge degrees of electrons is gapful.

The separation of the charge and spin degrees of freedom of the electrons may be a common phenomenon in doped Mott insulators in which there exists the strong correlation effect among electrons, and its origin is the strong on-site repulsive Coulomb interaction of electrons. This is different from that one for an one-dimensional weakly interacting electron gas where two separated Fermi levels of the system play the key role in the charge-spin separation of electrons, and even for very weak repulsive interaction, the one-particle Green’s function would show a power-law asymptotic behavior. The present calculations are completely consistent with previous conjecture that there takes place the charge and spin separation in strongly correlated electronic systems which can be represented by the resonant valence bond (RVB) states and/or slave-fermion/boson representations. In the doped Mott insulators, the parameter of the hole doping concentration $\delta$ plays a central role in understanding of the physical quantities observed in experiments that are related to the one-particle Green’s function, such as the Drude weight, the Hall coefficient and the
spectral function of electrons, et al. For example, the present calculations show that the spectral function of electrons around the Fermi surface is proportional to $A_k^L(\omega)$, and the Drude weight\cite{34} is proportional to $\delta$.

IV. CONCLUSION AND DISCUSSION

With the hierarchical Green’s function approach, we have studied a doped Mott insulator described by the Hubbard model by analytically solving the equations of motion of the one-particle Green’s function and related multiple-point correlation functions, and found that the separation of the spin and charge degrees of freedom of the electrons is an intrinsic character of the doped Mott insulator. For enough of large on-site repulsive Coulomb interaction, we have shown that the spectral weight of the one-particle Green’s function is proportional to the hole doping concentration that is mainly produced by the charge fluctuation of the electrons, while the excitation spectrum of the electrons is composed of two parts: one is mainly contributed by the spin fluctuation of the electrons, and its coefficient is proportional to the hole doping concentration that is zero at the half-filling of the electrons; another one is coming from the coupling between the charge and spin fluctuations of the electrons, which can be seen as the spinon excitations, and its coefficient would decrease as the hole doping concentration increasing. However, all these intrinsic low energy properties of the system originate from the strong on-site repulsive Coulomb interaction of electrons, that induces the strongly correlation effect among electrons, and it may produce a variety of low energy intertwined orders in different energy scales, such as spin density order, charge density order, pre-pairing of electrons order and others.

The present results are consistent with the spectroscopy observations of the cuprate superconductors in normal states\cite{35,37}, and the numerical calculations\cite{38,39} based on the Anderson’s RVB theory with a Gutzwiller projected BCS wave function. Moreover, this exotic excitation spectrum of the electrons shows that only the doped holes take part in the low energy/temperature transport behavior, and the electrons are nearly localized in the underdoped regime, in which the spin fluctuation of the electrons would play the important role in explaining the novel behavior of the normal states in the underdoped and optimal doped regimes of the cuprate superconductors.

The separation of the spin and charge degrees of freedom of the electrons in a doped
Mott insulator is derived from the competition between the tendency to maintain local antiferromagnetic correlations originated from the strong on-site repulsive Coulomb interaction and the doped hole itineracy, and this strong correlation effect of the electrons would induce some intertwined orders in the low energy region. To deeply understanding of the low energy property of a doped Mott insulator, we need to introduce these possible orders, and to judge which one of them can survive and be robust in the strong on-site repulsive Coulomb interaction. The recent calculations of the spin susceptibility for a spin 1/2 Heisenberg model on a square lattice show that the low-lying excitations of the spins can be divided as two parts: one is the spin wave excitations that residing in the lowest boundary of the low-lying excitations around the momentum $\mathbf{k} = (\pi, \pi)$; another one is the nearly deconfined spinon excitations that mainly residing in the high energy region around the momentum $\mathbf{k} = (\pi, \pi)$ and other momentum regions, such as, $\mathbf{k} = (\pi, 0)$ and $\mathbf{k} = (\frac{\pi}{2}, \frac{\pi}{2})$, et al., where the spin wave excitations become very weak. This phenomenon is observed in a recent neutron scattering experiment[40], and numerical calculations[41]. The influence of these two distinct low-lying excitations of the spins on the intertwined orders observed in the normal state of the cuprate superconductors deserves to be further carefully studied in the future.

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VI. APPENDIX

The Hamiltonian of the Hubbard model is that,

$$\hat{H}_H = -t_0 \sum_{ij,\sigma} \gamma_{ij} \left( \hat{c}^{\dagger}_{\sigma i} \hat{c}_{\sigma j} + \hat{c}^{\dagger}_{\sigma j} \hat{c}_{\sigma i} \right) + U \sum_i \hat{n}_{\uparrow i} \hat{n}_{\downarrow i} - \mu \sum_{\sigma i} \hat{n}_{\sigma i}$$  \hspace{1cm} (13)

where $\hat{c}^{\dagger}_{\sigma i}$/$\hat{c}_{\sigma i}$ creates/annihilates an electron with spin $\sigma = \uparrow$, $\downarrow$ on site $\mathbf{x}_i$, $\hat{n}_{\sigma i} = \hat{c}^{\dagger}_{\sigma i} \hat{c}_{\sigma i}$ 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. Here we take the on-site repulsive Coulomb interaction $U$ as one of the largest energy scale of the system, which is of order the bandwidth $W(= 8t_0), t_0 \ll U \sim W$.

### A. The basic commutation relations

According to the definitions of the one-particle Green’s function, $G_{ij}(t) = -i < T\hat{c}_{\sigma i}(t)\hat{c}_{\sigma j}^\dagger(0) >$, in order to write out its equation of motion with the hierarchic Green’s function approach, we need the commutation relations of the electron operators $\hat{c}_{\sigma i}$ and other operators with the Hamiltonian, here we write out some of them as that,

$$[\hat{c}_{\sigma i}, H] = \hat{h}_{im}\hat{c}_{\sigma m} + \frac{U}{2} [\hat{n}_i - \sigma \hat{s}_i] \hat{c}_{\sigma i}$$ \hspace{1cm} (14)

$$[\hat{n}_i, \hat{H}] = \hat{h}_{im}\hat{P}^{(-)}_{im}$$

$$[\hat{s}_i, \hat{H}] = \hat{h}_{im}\hat{Q}^{(-)}_{im}$$ \hspace{1cm} (15)

where $\hat{h}_{il} = -t_0 (\hat{\gamma}_{il} + \hat{\gamma}_{li})$, $\hat{n}_i = \hat{n}_{i\uparrow} + \hat{n}_{i\downarrow}$, $\hat{s}_i = \hat{n}_{i\uparrow} - \hat{n}_{i\downarrow}$, $\hat{P}^{(\pm)}_{ij} = \hat{N}_{ij} \pm \hat{S}_{ij}$, and $\hat{Q}^{(\pm)}_{ij} = \hat{S}_{ij} \pm \hat{S}_{ji}$, where $\hat{N}_{ij} = \hat{c}_{i\uparrow}\hat{c}_{j\uparrow} + \hat{c}_{i\downarrow}\hat{c}_{j\downarrow}$, and $\hat{S}_{ij} = \hat{c}_{i\uparrow}\hat{c}_{j\downarrow} - \hat{c}_{i\downarrow}\hat{c}_{j\uparrow}$. These commutation relations are the elementary ingredients as writing out the equations of motion of related multiple-point correlation functions that directly or indirectly appearing in the equation of motion of the one-particle Green’s function. Here we separate the charge and spin degrees of freedom of electrons by writing out, $\hat{n}_{\sigma i} = \frac{1}{2} [\hat{n}_i - \sigma \hat{s}_i]$, that is produced by the on-site Coulomb interaction in the above commutation relations. In this way, we can separately define the charge and spin fluctuations of electrons by different correlation functions.

### B. Definition of multiple-point correlation functions

In order to tersely represent multiple-point correlation functions, we introduce new composite multiple-point operators $\hat{F}^{(A_1\ldots A_L)}_{\{\alpha_1\ldots \alpha_L\}}$.
\[
\hat{F}^{(A_1 \cdots A_L)}_{\{\alpha_1 \cdots \alpha_L\}} = \prod_{k=1}^L \hat{A}_\alpha
\]

where \(\hat{A}_\alpha = \{\hat{n}_i, \hat{s}_i, \hat{P}_{ij}^{(\pm)}, \hat{Q}_{ij}^{(\pm)}\}\), and \(L\) is the number of the operator \(\hat{A}_\alpha\) appearing in the composite operators \(\hat{F}^{(A_1 \cdots A_L)}_{\{\alpha_1 \cdots \alpha_L\}}\). With the help of these composite operators \(\hat{F}^{(A_1 \cdots A_L)}_{\{\alpha_1 \cdots \alpha_L\}}\), we define the corresponding multiple-point correlation functions \(F^{(A_1 \cdots A_L)}_{\{\alpha_1 \cdots \alpha_L\}mq}(t_1, t_2)\),

\[
F^{(A_1 \cdots A_L)}_{\{\alpha_1 \cdots \alpha_L\}mq}(t) = -i < T \hat{F}^{(A_1 \cdots A_L)}_{\{\alpha_1 \cdots \alpha_L\}}(t) \hat{c}_{m\sigma}(t) \hat{c}_{q\sigma}^\dagger(0) >
\]

Some of these multiple-point correlation functions \(F^{(A_1 \cdots A_L)}_{\{\alpha_1 \cdots \alpha_L\}mq}(t)\) will enter into the series of hierarchical equations of motion originated from the equation of motion of the one-particle Green’s function Eqs. (1), such as \(F^{(a)}_{ijq}(t)\) and \(F^{(s)}_{ijq}(t)\), et al., and they will construct a set of linear equations of motion with the one-particle Green’s function \(G_{iq\sigma}(t)\). The physics meaning, for example, of the operator \(\hat{F}^{(A_1 \cdots A_L)}_{\{\alpha_1 \cdots \alpha_L\}}\hat{c}_{m\sigma}\) in the correlation function \(F^{(A_1 \cdots A_L)}_{\{\alpha_1 \cdots \alpha_L\}mq}(t)\) is that an electron \(\hat{c}_{m\sigma}\) with spin \(\sigma\) at site \(x_m\) attached other electrons represented by the operator \(\hat{F}^{(A_1 \cdots A_L)}_{\{\alpha_1 \cdots \alpha_L\}}\) 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 \(\hat{c}_{m\sigma}\). Thus the correlation function \(F^{(A_1 \cdots A_L)}_{\{\alpha_1 \cdots \alpha_L\}mq}(t)\) in fact represents the evolution process of an electron from the initial state incorporated the influence of a definite distribution of other electrons around it to final state.

In contrast with usual correlation functions defined in the momentum space, the present multiple-point correlation functions can more effectively describe the correlation effect of electrons derived from the on-site Coulomb interaction, and the parameter \(L\) appearing in the composite operators \(\hat{F}^{(A_1 \cdots A_L)}_{\{\alpha_1 \cdots \alpha_L\}}\) can be used to classify the correlation functions \(F^{(A_1 \cdots A_L)}_{\{\alpha_1 \cdots \alpha_L\}mq}(t)\) into different levels, where the correlation functions \(F^{(A_1 \cdots A_L)}_{\{\alpha_1 \cdots \alpha_L\}mq}(t)\) in the same level \(L\) can constitute one or more subset of equations of motion.
C. Solutions of the high order related multiple-point correlation functions

Based on the basic commutation relations in the Eqs. (14,15), we can write out equations of motion of the high order related multiple-point correlation functions,\

\[ [\omega + \mu] F_{iljq}^{(n)}(\omega) = <\hat{n}_i \hat{n}_l > \delta_{jq} + \frac{U}{2} F_{iljq}^{(mn)}(\omega) - \frac{\sigma U}{2} F_{iljq}^{(ns)}(\omega) + \sum_m \left[ \hat{n}_m F_{ilmjq}^{(n)}(\omega) + \hat{n}_m F_{ilmjq}^{(P(-)_n)}(\omega) \right] \]

(18)

\[ [\omega + \mu] F_{iljq}^{(s)}(\omega) = <\hat{s}_i \hat{s}_l > \delta_{jq} + \frac{U}{2} F_{iljq}^{(sn)}(\omega) - \frac{\sigma U}{2} F_{iljq}^{(ss)}(\omega) + \sum_m \left[ \hat{n}_m F_{ilmjq}^{(s)}(\omega) + \hat{n}_m F_{ilmjq}^{(Q(-)_s)}(\omega) \right] \]

(19)

\[ [\omega + \mu] F_{iljq}^{(nn)}(\omega) = <\hat{n}_i \hat{n}_l > \delta_{jq} + \frac{U}{2} F_{iljq}^{(nn)}(\omega) - \frac{\sigma U}{2} F_{iljq}^{(ns)}(\omega) + \sum_m \left[ \hat{n}_m F_{ilmjq}^{(nn)}(\omega) + \hat{n}_m F_{ilmjq}^{(P(-)_n)}(\omega) \right] \]

(20)

\[ [\omega + \mu] F_{iljq}^{(sn)}(\omega) = <\hat{s}_i \hat{n}_l > \delta_{jq} + \frac{U}{2} F_{iljq}^{(sn)}(\omega) - \frac{\sigma U}{2} F_{iljq}^{(ss)}(\omega) + \sum_m \left[ \hat{n}_m F_{ilmjq}^{(sn)}(\omega) + \hat{n}_m F_{ilmjq}^{(Q(-)_n)}(\omega) \right] \]

(21)

\[ [\omega + \mu] F_{iljq}^{(ns)}(\omega) = <\hat{n}_i \hat{s}_l > \delta_{jq} + \frac{U}{2} F_{iljq}^{(ns)}(\omega) - \frac{\sigma U}{2} F_{iljq}^{(ss)}(\omega) + \sum_m \left[ \hat{n}_m F_{ilmjq}^{(ns)}(\omega) + \hat{n}_m F_{ilmjq}^{(P(-)_s)}(\omega) \right] \]

(22)

\[ [\omega + \mu] F_{iljq}^{(ss)}(\omega) = <\hat{s}_i \hat{s}_l > \delta_{jq} + \frac{U}{2} F_{iljq}^{(ss)}(\omega) - \frac{\sigma U}{2} F_{iljq}^{(ss)}(\omega) + \sum_m \left[ \hat{n}_m F_{ilmjq}^{(ss)}(\omega) + \hat{n}_m F_{ilmjq}^{(Q(-)_s)}(\omega) \right] \]

(23)

where we have written out the equations of motion of the related multiple-point correlation functions $F_{iljq}^{(sn)}(\omega)$ and $F_{iljq}^{(ns)}(\omega)$, respectively, that would be different under the SCA approximation due to the different order of the operators $\hat{s}_i$ and $\hat{n}_i$ appearing in these correlation functions. With the same procedures, we can also write out the equations of motion of the correlation functions $F_{ijlq}^{(P(-)_n)}(\omega)$ and $F_{ijlq}^{(Q(-)_s)}(\omega)$ where their contributions are mainly to
modify the chemical potential of electrons. Here we do not further to write out the equations of motion of the multiple-point correlation functions belonging to the $L = 3$ level, such as $F_{iijj}^{(n)}(\omega)$, $F_{ijjj}^{(ns)}(\omega)$, and $F_{ijjj}^{(ss)}(\omega)$, et al., and we take a cut-off approximation, that is under the SCA approximation we simply discard those multiple-point correlation functions belonging to the $L = 3$ level.

After taking the SCA approximation, and only keeping the lowest order terms, we can write out the equations of motion of the correlation functions $F_{iijq}^{(n)}(\omega)$ and $F_{iijq}^{(s)}(\omega)$ as that taking $\mu = U/2$,

\[
[\Omega - \eta(\omega)] F_{iijq}^{(n)}(\omega) = \langle \hat{\eta}_i > \delta_{iq} - \frac{Us^2}{2} G_{iq\sigma}(\omega) + \sum_m \hat{h}_{im}F_{iimq}^{(n)}(\omega) - \frac{\sigma U}{2} F_{iijq}^{(s)}(\omega) \] (24)

\[
[\omega - \eta(\omega)] F_{iijq}^{(s)}(\omega) = \langle \hat{\eta}_i > \delta_{iq} - \frac{Us^2}{2} G_{iq\sigma}(\omega) + \sum_m \hat{h}_{im}F_{iimq}^{(s)}(\omega) \] (25)

\[
[\omega + \frac{U}{2}] F_{iijq}^{(n)}(\omega) = \langle \hat{\eta}_i > \delta_{ij} + \frac{U}{2} F_{ijjj}^{(nn)}(\omega) - \frac{\sigma U}{2} F_{ijjj}^{(ns)}(\omega) \] (26)

\[
[\omega + \frac{U}{2}] F_{iijq}^{(s)}(\omega) = \langle \hat{\eta}_i > \delta_{ij} + \frac{U}{2} F_{ijjj}^{(sn)}(\omega) - \frac{\sigma U}{2} F_{ijjj}^{(ss)}(\omega) \] (27)

where $\eta(\omega) = \frac{2}{\omega + \frac{U}{2}} \sum_m \left( \hat{h}_{im} \right)^2$, it is contributed by the correlation functions $F_{ijlj}^{(p(-))}(\omega)$ or $F_{ijlj}^{(q(-))}(\omega)$. The other equations of motion of the high order related multiple-point correlation functions can be reduced as that after neglecting high order terms,

\[
[\omega - \frac{U}{2}] F_{ijjj}^{(nn)}(\omega) = \langle \hat{\eta}_i \hat{\eta}_j > \delta_{ij} + \hat{h}_{ij} F_{ijjj}^{(nn)}(\omega) - \frac{s^2 U}{2} F_{ijjj}^{(n)}(\omega) \]

\[
-\frac{1}{2} \hat{h}_{ij} \left[ F_{ijij}^{(n)}(\omega) - n^2 G_{ij\sigma}(\omega) \right] \] (28)

\[
\omega F_{ijjj}^{(ns)}(\omega) = \langle \hat{\eta}_i \hat{\eta}_j > \delta_{ij} + \frac{\sigma}{2} \hat{h}_{ij} \left[ F_{ijij}^{(n)}(\omega) - n^2 G_{ij\sigma}(\omega) \right] + \hat{h}_{ij} F_{ijjj}^{(ns)}(\omega) - \frac{\sigma s^2 U}{2} F_{ijjj}^{(n)}(\omega) \]

\[
[\omega - \frac{U}{2}] F_{ijjj}^{(ns)}(\omega) = \langle \hat{\eta}_i \hat{\eta}_j > \delta_{ij} + \hat{h}_{ij} F_{ijjj}^{(ns)}(\omega) - \frac{s^2 U}{2} F_{ijjj}^{(s)}(\omega) \]

\[
+ \frac{\sigma}{2} \hat{h}_{ij} \left[ n^2 G_{ij\sigma}(\omega) + \sigma F_{ijjj}^{(s)}(\omega) \right] \] (29)

\[
[\omega - \frac{U}{2}] F_{ijjj}^{(ss)}(\omega) = \langle \hat{\eta}_i \hat{\eta}_j > \delta_{ij} + \hat{h}_{ij} F_{ijjj}^{(ss)}(\omega) - \frac{s^2 U}{2} F_{ijjj}^{(s)}(\omega) \]

\[
+ \frac{\sigma}{2} \hat{h}_{ij} \left[ n^2 G_{ij\sigma}(\omega) + \sigma F_{ijjj}^{(s)}(\omega) \right] \] (30)
\[
\left[ \omega - \frac{U}{2} \right] F_{ijjq}^{(sn)}(\omega) = < \hat{s}_i \hat{n}_j > \delta_{jq} + \hat{h}_{ij} F_{ijjq}^{(sn)}(\omega) - \frac{s^2 U}{2} F_{ijjq}^{(s)}(\omega) - \frac{1}{2} \hat{h}_{ij} \left[ F_{ijjq}^{(n)}(\omega) - n^2 G_{iq\sigma}(\omega) \right]
\]

where under the present approximation the difference between \( F_{ijjq}^{(ns)}(\omega) \) and \( F_{ijjq}^{(sn)}(\omega) \), as well as between \( F_{ijjq}^{(ns)}(\omega) \) and \( F_{ijjq}^{(sn)}(\omega) \) originates from the different order of the operators \( \hat{s}_i \) and \( \hat{n}_i \) appearing in these correlation functions. In the above calculations, we approximately take the chemical potential, \( \mu = U/2 \), that is rigorous at undoping, and reasonable in the underdoped region.

These equations in Eqs.\( \text{(28-33)} \) are some simple sets of equations, and they can be analytically solved as that,

\[
F_{ijjq}^{(ns)}(\omega) = \frac{\Omega}{D_{ns}(\omega)} \left\{ \begin{aligned}
&< \hat{n}_i \hat{n}_j > \delta_{jq} - \frac{s^2 U}{2} F_{ijjq}^{(n)}(\omega) - \frac{1}{2} \hat{h}_{ij} \left[ F_{ijjq}^{(n)}(\omega) - n^2 G_{iq\sigma}(\omega) \right] \\
+ \frac{\hat{h}_{ij}}{D_{ns}(\omega)} \left< \hat{n}_i \hat{n}_j > \delta_{jq} - \frac{s^2 U}{2} F_{ijjq}^{(n)}(\omega) - \frac{1}{2} \hat{h}_{ij} \left[ F_{ijjq}^{(n)}(\omega) - n^2 G_{iq\sigma}(\omega) \right] \right. 
\end{aligned} \right. \]

(31)

\[
\omega F_{ijjq}^{(sn)}(\omega) = < \hat{s}_i \hat{n}_j > \delta_{jq} + \hat{h}_{ij} F_{ijjq}^{(sn)}(\omega) - \frac{s^2 U}{2} F_{ijjq}^{(s)}(\omega) + \frac{1}{2} \hat{h}_{ij} \left[ \sigma s^2 G_{jq\sigma}(\omega) + F_{ijjq}^{(s)}(\omega) \right]
\]

(32)

\[
\omega F_{ijjq}^{(ss)}(\omega) = < \hat{s}_i \hat{s}_j > \delta_{jq} + \frac{1}{2} \hat{h}_{ij} \left[ F_{ijjq}^{(n)}(\omega) - n^2 G_{iq\sigma}(\omega) \right] + \frac{\hat{h}_{ij}}{D_{ss}(\omega)} \left\{ \begin{aligned}
&< \hat{n}_i \hat{n}_j > \delta_{jq} - \frac{s^2 U}{2} F_{ijjq}^{(n)}(\omega) - \frac{1}{2} \hat{h}_{ij} \left[ F_{ijjq}^{(n)}(\omega) - n^2 G_{iq\sigma}(\omega) \right] \\
+ \frac{\hat{h}_{ij}}{D_{ss}(\omega)} \left< \hat{n}_i \hat{n}_j > \delta_{jq} - \frac{s^2 U}{2} F_{ijjq}^{(n)}(\omega) - \frac{1}{2} \hat{h}_{ij} \left[ F_{ijjq}^{(n)}(\omega) - n^2 G_{iq\sigma}(\omega) \right] \right. 
\end{aligned} \right. \]

(33)
where $\Omega = \omega - \frac{U}{2}$, $D_{nn} (\omega) = \Omega^2 - i_0^2$, $D_{ns} (\omega) = \omega \Omega - i_0^2$, and $D_{ss} (\omega) = \omega^2 - i_0^2$. Obviously, under the present approximation, these high order correlation functions are the functional of the one-particle Green’s function and the correlation functions $F_{ijq}^{(n)} (\omega)$ and $F_{ijq}^{(s)} (\omega)$ that represent the charge and spin fluctuations, respectively. While they can be seen as some “effective external fields” that appear in the equations of motion of the correlation functions $F_{ijq}^{(n)} (\omega)$ and $F_{ijq}^{(s)} (\omega)$ in the Eqs. (26,27).

Substituting these solutions in Eqs. (34,37) into the Eqs. (26,27), we have the following expressions of the correlation functions $F_{ijq}^{(n)} (\omega)$ and $F_{ijq}^{(s)} (\omega)$,

\[
F_{ijq}^{(n)} (\omega) = \frac{\langle \hat{n}_i > \delta_{jq} \rangle}{\Gamma_n (\omega)} + \frac{U}{2 \Gamma_n (\omega)} \frac{1}{D_{nn} (\omega)} \langle \hat{n}_i \hat{n}_j \rangle + \frac{n^2 \Omega U}{4 \Gamma_n (\omega)} \left( \frac{1}{D_{nn} (\omega)} + \frac{1}{D_{ns} (\omega)} \right) \hat{h}_{ij} G_{iqr} (\omega)
\]

\[
F_{ijq}^{(s)} (\omega) = \frac{\langle \hat{s}_i > \delta_{jq} \rangle}{\Gamma_s (\omega)} - \frac{U}{2 \Gamma_s (\omega)} \frac{1}{D_{ss} (\omega)} \langle \hat{s}_i \hat{s}_j \rangle + \frac{\sigma n^2 \omega U}{4 \Gamma_s (\omega)} \left( \frac{1}{D_{ss} (\omega)} - \frac{1}{D_{ns} (\omega)} \right) \hat{h}_{ij} G_{iqr} (\omega)
\]

where $\Gamma_n (\omega) = \omega + \frac{U}{2} \left( 1 - \frac{\omega^2 \Omega U}{2D_{ns} (\omega)} \right)$ and $\Gamma_s (\omega) = \omega + \frac{U}{2} \left( 1 - \frac{s^2 \omega U}{2D_{ss} (\omega)} \right)$. With the above expressions and the Eqs. (24,25), we finally obtain the following analytical expression of the correlation function $F_{iq}^{(n)} (\omega) - \sigma F_{iq}^{(s)} (\omega)$ by the one-particle Green’s function,

\[
F_{iq}^{(n)} (\omega) - \sigma F_{iq}^{(s)} (\omega) = \frac{\langle \hat{n}_i > \delta_{iq} + P_{iq}^{(n)} (\omega) \rangle}{\Omega - \eta (\omega)} - \sigma \left( \frac{\langle \hat{s}_i > \delta_{iq} + P_{iq}^{(s)} (\omega) \rangle}{\Omega - \eta (\omega)} \right)
\]

\[
+ \alpha (\omega) G_{iqr} (\omega) + \sum_m \zeta_{im} (\omega) G_{mqr} (\omega)
\]

where the coefficients $\alpha (\omega)$, $\zeta_{im} (\omega)$, $P_{iq}^{(n)} (\omega)$ and $P_{iq}^{(s)} (\omega)$ read that,

\[
\alpha (\omega) = \frac{n^2 \Omega U}{4 \Gamma_n (\omega) [\Omega - \eta (\omega)]} \left( \frac{1}{D_{nn} (\omega)} + \frac{1}{D_{ns} (\omega)} \right) \sum_m \left( \hat{h}_{im} \right)^2
\]

\[
- \frac{n^2 \omega U}{4 \Gamma_s (\omega) [\Omega - \eta (\omega)]} \left( \frac{1}{D_{ss} (\omega)} - \frac{1}{D_{ns} (\omega)} \right) \sum_m \left( \hat{h}_{im} \right)^2
\]

\[
(41)
\]
\[ \zeta_{im}(\omega) = \frac{n^2 t_0^2 U}{4 \Gamma_n(\omega) [\Omega - \eta(\omega)]} \left( \frac{1}{D_{nn}(\omega)} - \frac{1}{D_{ns}(\omega)} \right) \tilde{h}_{im} \]

\[ - \frac{t_0^2 U}{4 \Gamma_s(\omega) [\Omega - \eta(\omega)]} \left( \frac{n^2}{D_{ss}(\omega)} + \frac{s^2}{D_{ns}(\omega)} \right) \tilde{h}_{im} \]

(42)

\[ P_{iq}^{(n)}(\omega) = \sum_m \left( \frac{\langle \tilde{n}_i \rangle \tilde{h}_{im} \delta_{mq} \Gamma_n(\omega)}{\Gamma_n(\omega)} + \frac{U}{2 \Gamma_n(\omega)} \frac{\langle \tilde{n}_i \rangle \tilde{n}_m \rangle \tilde{h}_{im} \left[ \Omega \delta_{mq} + \tilde{h}_{im} \delta_{iq} \right]}{D_{nn}(\omega)} \right) \]

(43)

\[ P_{iq\sigma}^{(s)}(\omega) = \sum_m \left( \frac{\langle \tilde{s}_i \rangle \tilde{h}_{im} \delta_{mq} \Gamma_s(\omega)}{\Gamma_s(\omega)} - \frac{U}{2 \Gamma_s(\omega)} \frac{\sigma \langle \tilde{s}_i \rangle \tilde{s}_m \rangle \tilde{h}_{im} \left[ \omega \delta_{mq} + \tilde{h}_{im} \delta_{iq} \right]}{D_{ss}(\omega)} \right) \]

(44)

In the low energy limit, \( \omega \to 0 \), the coefficients \( \alpha(\omega) \) and \( \zeta_{im}(\omega) \) are reduced as that,

\[ \zeta_{im}(\omega) \xrightarrow{\omega \to 0} \left[ \frac{4n^2 t_0^2}{\Omega^3} - \frac{n^2 + s^2}{U} \right] \tilde{h}_{im} \]

(45)

\[ \alpha(\omega) \xrightarrow{\omega \to 0} \frac{n^2}{8} \left( \frac{W_{2D}}{U} \right)^2 \]

(46)

where \( W_{2D} = 8t_0 \). With the Eq.(40), and neglecting the functions \( P_{iq}^{(n)}(\omega) \) and \( P_{iq\sigma}^{(s)}(\omega) \), we can obtain the equation of motion of the one-particle Green’s function in Eq.(9) under the large \( U \) limit, \( |\omega| \ll t_0 \ll U \sim W \).

VII.

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