

Universal power-law behavior of local electron correlation functions in the Falicov–Kimball lattice model

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By studying the Falicov–Kimball lattice model, we demonstrate that the correlation functions of local electrons can be written directly in the form of the partition function of conduction electrons with a time dependent external potential. These general expressions of the correlation functions are equivalent to the exact ones obtained by the dynamical mean field theory in infinite dimension limit. Moreover, we also prove that the asymptotic power-law behavior of the local electron correlation functions is universal in any dimensions, as long as the conduction electron excitation spectrum is gapless, regardless whether they are Landau Fermi liquid or not. This conclusion is also valid for other quantum many-particle systems, if the coupling between the conduction and local electrons is on-site or short-range Coulomb interaction.

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I. INTRODUCTION

Local electron/fermion correlation effect in quantum many-particle systems has been extensively studied, such as the two local magnetic impurities scattering problem,¹ the Kondo lattice models² for heavy fermion systems, the periodic Anderson lattice model,³ the Falicov–Kimball lattice model,⁴ and quantum dot systems.⁵ All these systems have a common feature that there is no direct hybridization or Coulomb interaction among the local electrons. Instead, the local electron correlation is mediated by conduction electrons, resulting in low temperature physical behavior of these systems. It is well known that for a system with one local electron state, the time relaxation of an excited local electron is related to the Anderson orthogonal catastrophe,⁶ and the correlation functions of the local electrons are expected to have some universal behavior, even though the conduction electrons of each system may show completely different behavior.

The x-ray absorption and emission of two deep core electrons in metal is the simplest example for studying the local electron correlation, and its extension is the Falicov–Kimball lattice model, where the local electrons are randomly distributed on lattice sites. For the case of one local electron, it is the Mahan–Nozières–De Dominicis model, and the Green function of the local electron shows an edge singularity^{7,8} at zero temperature. When there are many local electrons, the behavior of the conduction electrons may be completely different from that for the single local electron case. What condition should we have in order for the edge singularity of the local electron correlation functions to survive?

In this paper, with the Falicov–Kimball lattice model, we study the local electron correlation effect, and give some exact asymptotic expressions of the local electron correlation functions. In Sec. II, we prove that the correlation functions of the local electrons can be written directly from the partition function of the conduction electrons under a time dependent external potential, which may be very useful for numerical simulations. In Sec. III, we show that in the infinite dimension limit these general expressions of the local elec-

tron correlation functions can be exactly calculated by the dynamical mean field theory (DMFT).^{4,9} In Sec. IV, by solving the Dyson equation of the conduction electron Green function, we demonstrate that if the spectrum of the conduction electrons is gapless, i.e., the density of states at the Fermi surface is finite, the asymptotic power-law (edge singularity) behavior of the local electron correlation functions is universal, no matter whether the conduction electrons show Landau Fermi liquid behavior or not. This conclusion is also valid for other quantum many-particle systems, if the coupling between the conduction and local electrons is on-site or short-range Coulomb interaction. We give our conclusions and discussions in Sec. V.

II. GENERAL FORMULAS OF CORRELATION FUNCTIONS

The Hamiltonian of the Falicov–Kimball model in a hypercubic lattice can be written as

$$H = -t \sum_{\langle ij \rangle} (\hat{c}_i^\dagger \hat{c}_j + \hat{c}_j^\dagger \hat{c}_i) + \sum_i \varepsilon_f \hat{f}_i^\dagger \hat{f}_i - \sum_i (\mu \hat{n}_{ci} + \mu_f \hat{n}_{fi}) + U \sum_i \hat{n}_{ci} \hat{n}_{fi}, \quad (1)$$

where $\langle ij \rangle$ represents the summation over the nearest neighbor sites, $\hat{c}_i^\dagger (\hat{c}_i)$ and $\hat{f}_i^\dagger (\hat{f}_i)$ are the creation (annihilation) operators of conduction and local electrons at lattice site \mathbf{x}_i , respectively, μ and μ_f are the corresponding chemical potentials of the conduction and local electrons, ε_f is the energy level of the local electrons, $\hat{n}_{ci} = \hat{c}_i^\dagger \hat{c}_i$ and $\hat{n}_{fi} = \hat{f}_i^\dagger \hat{f}_i$ are the density operators of the conduction and local electrons, respectively, and U is the Coulomb interaction between the conduction and local electrons, which controls the low temperature physical behavior of the system. At $U=0$, the conduction and local electrons are independent of each other. It would be noted that, for the Falicov–Kimball model, the local electron number on each lattice site is conserved, and the total number of local electrons is controlled by the chemical potential μ_f .

In general, the partition function of the system reads, $Z = \int D\psi^* D\psi D\varphi^* D\varphi e^{i\hbar S_0}$, and the action S_0 can be easily written down with the above Hamiltonian by standard path integral formulism, where $\psi_i(t)$ and $\varphi_i(t)$ are the conduction and local electron (Grassmann variables) fields, respectively. We introduce a Lagrange multiplier field (auxiliary field or Hubbard–Stratonovich field) $\phi(x_i, t)$ by taking $\hat{n}_{ci} = \hat{c}_i^\dagger \hat{c}_i$ as a constraint to add it to the system, then the partition function can be rewritten as

$$Z = \int D\psi^* D\psi D\varphi^* D\varphi Dn_c \delta(n_c - \psi^* \psi) e^{i\hbar S_0} \\ = \int D\psi^* D\psi D\varphi^* D\varphi Dn_c D\phi e^{i\hbar S_0 + i\sum_j \int dt \phi(x_j, t) [n_{c_j}(t) - \psi_j^*(t) \psi_j(t)]}.$$

After including these auxiliary fields $\phi(x_i, t)$ and $n_{ci}(t)$, the action of the Falicov–Kimball lattice model reads

$$S = \sum_{\langle ij \rangle} \int dt \psi_i^*(t) \hat{M}_{ij}(t) \psi_j(t) + \sum_i \int dt \varphi_i^* \hat{M}_i(t) \varphi_i(t) \\ + \sum_i \int dt \phi(x_i, t) n_{ci}(t), \quad (2)$$

where $\hat{M}_i(t) = i\hbar \partial_t - \varepsilon_f + \mu_f - Un_{ci}(t)$, and $\hat{M}_{ij}(t) = [i\hbar \partial_t + \mu - \phi(x_i, t)] \delta_{ij} + t^* (\hat{\gamma}_{ij} + \hat{\gamma}_{ji})$, $\hat{\gamma}_{ij} = 1$ for $\mathbf{x}_j = \mathbf{x}_i \pm a\mathbf{e}$, $\hat{\gamma}_{ij} = 0$ for $\mathbf{x}_j \neq \mathbf{x}_i \pm a\mathbf{e}$, where a is the lattice constant, and \mathbf{e} is a unit vector. In the present representation, the action of the system is only the quadratic form of the conduction and local electron fields $\psi_i(t)$ and $\varphi_i(t)$, respectively. Thus after integrating out them, the partition function can be written as

$$Z = \int Dn_c D\phi \text{Det}(\hat{M}_\psi) \text{Det}(\hat{M}_\varphi) e^{i\sum_j \int dt \phi(x_j, t) n_{c_j}(t)} \\ = \int Dn_c D\phi e^{Tr \ln(\hat{M}_\psi) + Tr \ln(\hat{M}_\varphi) + i\sum_j \int dt \phi(x_j, t) n_{c_j}(t)},$$

where $\hat{M}_\psi = \hat{M}_{ij}(t)$, $\hat{M}_\varphi = \hat{M}_i(t)$, and $-i \text{Tr} \ln(\hat{M}_\psi) - i \text{Tr} \ln(\hat{M}_\varphi)$ is a potential function. In standard perturbation theory, the potential function $-i \text{Tr} \ln(\hat{M}_\psi) - i \text{Tr} \ln(\hat{M}_\varphi)$ is taken as a series of perturbation expansions about the auxiliary fields $\phi(x_i, t)$ and $n_{ci}(t)$ in order to calculate the partition function, while for strong correlation of the conduction and local electrons, the results obtained in this way may be unreliable and invalid. However, the potential function $-i \text{Tr} \ln(\hat{M}_\psi) - \text{Tr} \ln(\hat{M}_\varphi)$ can be exactly calculated by solving the eigenvalue equations of the propagator operators \hat{M}_ψ and \hat{M}_φ of the conduction and local electrons. Then the second quantization representation of the conduction and local electron operators can be represented by the eigenfunctions of these two propagator operators, respectively. In terms of their second quantization representations, correlation functions of the conduction and local electrons can be calculated, which is the basic idea of the eigenfunctional theory (EFT).^{10,11} As shown above, the propagator operators \hat{M}_ψ and \hat{M}_φ act on functions of time and space coordinates t and \mathbf{x}_i , and the

calculation of the potential function $-i \text{Tr} \ln(\hat{M}_\psi) - i \text{Tr} \ln(\hat{M}_\varphi)$ are taken on the time and space. Therefore, the paramount difference between the EFT and Monte Carlo method is that in the latter case one reduces $\exp[\text{Tr} \ln(\hat{M}_\psi) + \text{Tr} \ln(\hat{M}_\varphi)]$ into a determinant of the operators {e.g., $1 + T \exp[-\int_0^\beta d\tau H(\tau)]$ } which acts on functions of \mathbf{x}_i only.¹²

In general, the eigenequation of the propagator operator is, $\hat{G}_{ij}(t) \Psi_m(x_j, t; [\chi]) = E_m[\chi] \Psi_m(x_i, t; [\chi])$, where $\hat{G}_{ij}(t) = \hat{M}_{ij}(t)$ or $\hat{M}_i(t)$, and m labels a set of quantum number which are good ones at $\chi(x_i, t) = 0$, and $\chi(x_i, t) = \phi(x_i, t)$ or $n_{ci}(t)$. By the Hellmann–Feynman theorem, the eigenvalue can be written as $E_m[\chi] = E_m - \Sigma_m[\chi]$, where E_m is the eigenvalue of the propagator operator $\hat{M}_{ij}(t)$ at $\chi(x_i, t) = 0$, and $\Sigma_m[\chi]$ is the self-energy which depends on the auxiliary field $\chi(x_i, t)$. According to this expression of the eigenvalue $E_m[\chi]$, the eigenfunctional $\Psi_m(x_i, t; [\chi])$ can be generally written as $\Psi_m(x_i, t; [\chi]) = \psi_m(x_i, t) \exp\{Q_m(x_i, t; [\chi])\}$, where $\psi_m(x_i, t)$ is the eigenfunction of the electrons at $\chi(x_i, t) = 0$, and $\exp\{Q_m(x_i, t; [\chi])\}$ represents the contribution by the electron interaction. The eigenfunctional $\Psi_m(x_i, t; [\chi])$ constitutes a set of orthogonal and complete basis, and the second quantization representation of the electron operators can be expressed in terms of them.¹¹

For the Falicov–Kimball lattice model, the solution of the eigenequation of the propagator operator $\hat{M}_i(t)$ is^{10,11}

$$\hat{M}_i(t) \varphi_{i\omega}(t, [n]) = (\hbar\omega - \varepsilon - \Sigma[n]) \varphi_{i\omega}(t, [n]), \\ \varphi_{i\omega}(t, [n]) = \frac{1}{\sqrt{T_0}} e^{-i(\omega - \Sigma[n])t} e^{-(iU/\hbar) \int^t dt' n_{ci}(t')}, \quad (3)$$

where $\varepsilon = \varepsilon_f - \mu_f$, $\Sigma[n] = (1/T_0) \sum_j \int dt U n_{c_j}(t)$ is the self-energy, and $T_0 \rightarrow \infty$ is the time scale of the system. Here, the wave functions $\varphi_{i\omega}(t, [n])$ of the local electrons are the functional of the auxiliary field $n_{ci}(t)$. In terms of these wave functions $\varphi_{i\omega}(t, [n])$, the second quantization representation of the local electron field operators can be written as

$$\hat{f}_j(t) = \hat{f}_{0j}(t) e^{i\Sigma[n]t} U_j(t), \\ \hat{f}_j^\dagger(t) = \hat{f}_{0j}^\dagger(t) e^{-i\Sigma[n]t} U_j^\dagger(t), \\ U_j(t) = \exp\left[-\frac{iU}{\hbar} \int^t dt' n_{c_j}(t')\right], \quad (4)$$

where $\hat{f}_{0j}^\dagger(t) [\hat{f}_{0j}(t)]$ are the decoupled ($U=0$) local electron creation (annihilation) operators. Obviously, all influence of the conduction electrons on the local electrons is incorporated to the function $U_j(t)$, thus it is quite easy to calculate a variety of correlation functions of the local electrons by using the above relations.

With the above expressions, the Green function of the local electrons can be written as

$$G_{ji}(t - t') = \langle T \hat{f}_j(t) \hat{f}_i^\dagger(t') \rangle = \delta_{ji} G_0(t - t') \langle T U_j(t) U_j^\dagger(t') \rangle$$

$$\begin{aligned} \langle TU_j(t)U_j^\dagger(t') \rangle \\ = \frac{1}{Z} \int D\psi^* D\psi D\varphi^* D\varphi D\phi Dn_c U_j(t)U_j^\dagger(t') e^{(i\hbar)S}, \end{aligned} \quad (5)$$

where $G_0(t) = \theta(t)e^{-i\epsilon_f t} - \theta(-t)e^{-i\epsilon_f t}$, $\theta(t)$ is usual step function, and ϵ_f is the effective energy level of the local electrons. Since the number of local electrons on each lattice site is conserved, we have assumed that the lattice site \mathbf{x}_j is unoccupied by the local electrons. In order to calculate the linear response to external electrical fields, and/or the absorption/emission of the x ray, we define a type of composite density operators, $\hat{n}_{jfc}(t) = \hat{f}_j^\dagger(t)\hat{c}_j(t)$, and $\hat{n}_{jcf}(t) = \hat{c}_j^\dagger(t)\hat{f}_j(t)$, where $\hat{c}_j(t)$ are the conduction electron operators. Then their correlation functions can be written as

$$\begin{aligned} F_{jcf}(t-t') &= \langle T\hat{n}_{jfc}(t)\hat{n}_{jcf}(t') \rangle \\ &= -G_0(t'-t) \langle T\hat{c}_j(t)\hat{c}_j^\dagger(t')U_j^\dagger(t)U_j(t') \rangle, \end{aligned} \quad (6)$$

where we have used the fact that the lattice site \mathbf{x}_j is occupied by the local electrons. These two correlation functions in Eqs. (5) and (6) are rather simplified. They could be represented by the correlation function of $U_j(t)$ which is the functional of the auxiliary field $n_{ci}(t)$. Notice that the correlation function $F_{jcf}(t-t')$ only represents the linear response to the external field, and we do not consider a static spontaneous hybridization term which does not exist in the Falicov–Kimball lattice model.¹³ However, if we consider a hybridization term with a small but finite amplitude between the conduction and local electrons, the asymptotic power-law behavior of the local electron correlation functions (see below) will be strongly suppressed.¹⁴

According to Eq. (4), the function $U_j^\dagger(t)U_j(t')$ is

$$U_j^\dagger(t)U_j(t') = e^{iU\hbar \int dt_1 \Theta(t_1; t, t') n_{cj}(t_1)}, \quad (7)$$

where $\Theta(t_1; t, t') = \theta(t-t_1) - \theta(t'-t_1)$. Substituting Eq. (7) into Eqs. (5) and (6), the factor $U \int dt_1 \Theta(t_1; t, t') n_{cj}(t_1)$ contributed by $U_j^\dagger(t)U_j(t')$ can be incorporated to the last term of the action (2). After integrating out the auxiliary fields $\phi(x_i, t)$ and $n_{ci}(t)$, the correlation functions $\langle TU_j^\dagger(t)U_j(t') \rangle$ and $\langle T\hat{c}_j(t)\hat{c}_j^\dagger(t')U_j^\dagger(t)U_j(t') \rangle$ can be written as the following forms:

$$\begin{aligned} \langle TU_j^\dagger(t)U_j(t') \rangle &= \frac{1}{Z} \int D\psi^* D\psi D\varphi^* D\varphi e^{(i\hbar)S[\Phi_j(t, t')]}, \\ \langle T\hat{c}_j(t)\hat{c}_j^\dagger(t')U_j^\dagger(t)U_j(t') \rangle \\ &= \frac{1}{Z} \int D\psi^* D\psi D\varphi^* D\varphi \psi_j(t)\psi_j^*(t') e^{(i\hbar)S[\Phi_j(t, t')]}, \end{aligned} \quad (8)$$

where $S[\Phi_j(t, t')] = \sum_i \int dt_1 \varphi_i^*(t_1) \hat{M}_{0i}(t_1) \varphi_i(t_1) + \sum_{\langle ij \rangle} \int dt_1 \psi_i^*(t_1) \hat{M}_{il}[t_1, \Phi_j(t, t')] \psi_l(t_1)$, $\hat{M}_{0i}(t_1) = i\hbar \partial_{t_1} - \epsilon_f + \mu_f$, $\hat{M}_{il}[t_1, \Phi_j(t, t')] = [i\hbar \partial_{t_1} + \mu - U n_{fi}(t_1) + \Phi_{i,j}(t, t')] \delta_{il} + t^* (\hat{\gamma}_{il} + \hat{\gamma}_{li})$, $n_{fi}(t_1) = \varphi_i^*(t_1) \varphi_i(t_1)$, and $\Phi_{i,j}(t, t') = U \Theta(t_1; t, t') \delta_{ij}$. Obviously, the physical meaning of these expressions of the correlation functions in Eq. (8) is that the function $U_j^\dagger(t)U_j(t')$ provides the on-site time dependent external po-

tential $\Phi_{i,j}(t, t')$ to the conduction electrons. Thus, the correlation functions of the local electrons can be written down directly by some kinds of partition functions similar to that of Eq. (8), which may be very useful for numerical simulations. These expressions are valid regardless of dimensionality and lattice type. They are also valid whether they include the Coulomb interaction of the conduction electrons or not.

Accordingly, we may also define a composite density operator $\hat{n}_{ij}(t) = \hat{f}_i^\dagger(t)\hat{f}_j(t)$, which at $i=j$ becomes the usual density operator of the local electrons. Following the procedures described above, the correlation function of $\hat{n}_{ij}(t)$ ($i \neq j$) can be represented as

$$\langle Tn_{ij}(t)n_{ji}(t') \rangle = \frac{1}{Z} \int D\psi^* D\psi D\varphi^* D\varphi e^{(i\hbar)S[\Phi_{ij}(t, t')]}, \quad (9)$$

where the external potential $\Phi_{i,j}(t, t') = U \Theta(t_1; t, t') [\delta_{il} - \delta_{jl}]$ is dependent on the lattice sites \mathbf{x}_i and \mathbf{x}_j , and we have used the condition that the lattice site \mathbf{x}_i is occupied by the local electrons while the site \mathbf{x}_j is empty. In the same way, we can calculate other correlation functions of interest. Here we only consider those three types of correlation functions of the local electrons. When calculating these correlation functions, the local electron number on each lattice site must be conserved.

The expressions in Eqs. (8) and (9) can be easily generalized to the finite temperature case by replacing time t with imaginary time $\tau = it$, where the external potentials $\Phi_{i,j}(t, t')$ and $\Phi_{l,i}(t, t')$ are replaced by $\Phi_{i,j}(\tau, \tau') = U \Theta(\tau_1; \tau, \tau') \delta_{ij}$ and $\Phi_{l,i}(\tau, \tau') = U \Theta(\tau_1; \tau, \tau') [\delta_{il} - \delta_{jl}]$, respectively, and the action becomes $S[\Phi_j(\tau, \tau')] = \sum_i \int_0^\beta d\tau_1 \varphi_i^* \hat{M}_{0i}(\tau_1) \varphi_i + \sum_{\langle ij \rangle} \int_0^\beta d\tau_1 \psi_i^* \hat{M}_{il}[\tau_1, \Phi_j(\tau, \tau')] \psi_l$, where $\beta = 1/k_B T$, $\Theta(\tau_1; \tau, \tau') = \theta(\tau - \tau_1) - \theta(\tau' - \tau_1)$, and T is the temperature of the system. On the other hand, according to the definition of the partition function, it can also be written as,

$$Z = \text{Tr}(e^{-\beta H})$$

thus the correlation function $\langle TU_j^\dagger(\tau)U_j(\tau') \rangle$ can be represented as⁴

$$\langle TU_j^\dagger(\tau)U_j(\tau') \rangle = \frac{1}{Z} \text{Tr} \left\{ e^{-\beta H_f} \int D\psi^* D\psi e^{-S_\psi[\Phi_j(\tau, \tau')]} \right\}, \quad (10)$$

where $S_\psi[\Phi_j(\tau, \tau')] = \sum_{\langle ij \rangle} \int_0^\beta d\tau_1 \psi_i^*(\tau_1) \{ [\partial_{\tau_1} - \mu + U \hat{n}_{fi} - \Phi_{i,j}(\tau, \tau')] \delta_{il} - t^* (\hat{\gamma}_{il} + \hat{\gamma}_{li}) \} \psi_l(\tau_1)$, and $H_f = \sum_i \epsilon_{fi} \hat{f}_i^\dagger \hat{f}_i - \mu_f \sum_i \hat{n}_{fi}$. The correlation functions $\langle T\hat{c}_j(\tau)\hat{c}_j^\dagger(\tau')U_j^\dagger(\tau)U_j(\tau') \rangle$ and $\langle Tn_{ij}(\tau)n_{ji}(\tau') \rangle$ have the expressions similar to that in Eq. (10). In fact, the expression of the correlation function $\langle TU_j^\dagger(\tau)U_j(\tau') \rangle$ is useful only for the case of single or low density of local electrons. However, this expression can be used to make connections with the exact solution of the DMFT in the infinite dimension limit.^{4,9,15,16}

III. EXACT EXPRESSIONS OF CORRELATION FUNCTIONS IN THE INFINITE DIMENSION LIMIT

In this section, in the infinite dimension limit, we give the general expressions of the correlation functions in Eq. (8) at finite temperatures, and compare them with exact solutions of the DMFT.

In the infinite dimension limit, this model could be exactly solved by the DMFT method^{9,16} by scaling the hopping matrix element $\bar{t}=t^*/2\sqrt{D}$, where D is the spatial dimension, and introducing a dynamical mean field $\lambda_i(\tau)$ which is determined self-consistently.^{4,16,17} In the infinite dimension limit, $D \rightarrow \infty$, the hopping matrix element can be taken as a reasonable perturbation parameter and the system is reduced to the single impurity-type problem in which the local particles are interacting with an environment produced by the particles residing in other lattice sites. This environment can be represented by the dynamical mean field $\lambda_i(t)$. Thus, in the infinite dimension limit the correlation functions in Eq. (8) can be easily written as

$$\begin{aligned} \langle TU_j^\dagger(t)U_j(t') \rangle &= \frac{1}{Z_j} \int D\psi_j^* D\psi_j D\varphi_j^* D\varphi_j e^{(i\hbar)S_j[\Phi_j(t,t')]}, \\ \langle T\hat{c}_j(t)\hat{c}_j^\dagger(t')U_j^\dagger(t)U_j(t') \rangle &= \frac{1}{Z_j} \int D\psi_j^* D\psi_j D\varphi_j^* D\varphi_j \psi_j(t)\psi_j^*(t') e^{(i\hbar)S_j[\Phi_j(t,t')]}, \end{aligned} \quad (11)$$

where $S_j[\Phi_j(t,t')] = \int dt_1 \psi_j^*(t_1)[i\hbar\partial_{t_1} + \mu - Un_{fj}(t_1) + \Phi_{j,j}(t,t') - \lambda_j(t_1)]\psi_j(t_1) + \int dt_1 \varphi_j^*(t_1)\hat{M}_{0j}(t_1)\varphi_j(t_1)$, and $Z_j = \int D\psi_j^* D\psi_j D\varphi_j^* D\varphi_j e^{(i\hbar)S_j[0]}$. At finite temperatures, by using the imaginary time $\tau=it$ and the conservation of the local electron number on each lattice site, the above expressions can be rewritten as

$$\begin{aligned} \langle TU_j^\dagger(\tau)U_j(\tau') \rangle &= \frac{e^{-\beta(\epsilon_{jj}-\mu)}}{Z_j} \int D\psi_j^* D\psi_j e^{-S_{\psi j}[\Phi_j(\tau,\tau')]}, \\ \langle T\hat{c}_j(\tau)\hat{c}_j^\dagger(\tau')U_j^\dagger(\tau)U_j(\tau') \rangle &= \frac{e^{-\beta(\epsilon_{jj}-\mu)}}{Z_j} \int D\psi_j^* D\psi_j \psi_j(\tau)\psi_j^*(\tau') e^{-S_{\psi j}[\Phi_j(\tau,\tau')]}, \end{aligned} \quad (12)$$

where $S_{\psi j}[\Phi_j(\tau,\tau')] = \int_0^\beta d\tau_1 \psi_j^*(\tau_1)[\partial_{\tau_1} - \mu + U - \Phi_{j,j}(\tau,\tau') + \lambda_j(\tau_1)]\psi_j(\tau_1)$ is the action on the lattice site \mathbf{x}_j of the conduction electrons under the external potential $-\Phi_{j,j}(\tau,\tau')$. The dynamical mean field $\lambda_j(\tau_1)$ is determined by the DMFT self-consistency condition for the conduction electron Green function.^{4,16,17} After including the unoccupied state of the local electron at site \mathbf{x}_j , the last expression of Eq. (12) is equivalent to the on-site (\mathbf{x}_j) Green function of the conduction electrons under the external potential $-\Phi_{j,j}(\tau,\tau')$. However, the correlation function in Eq. (9) involves two different lattice sites \mathbf{x}_i and \mathbf{x}_j . If the distance between these two sites is much larger than the lattice constant a , we can also use the DMFT method to calculate it. In the infinite dimen-

sion limit, the correlation function in Eq. (9) is reduced to a simple form ($|\mathbf{x}_i - \mathbf{x}_j| \gg a$)

$$\langle Tn_{ij}(\tau)n_{ji}(\tau') \rangle = \frac{e^{-\beta(\epsilon_{ji}-\mu)}}{Z_{ij}} \int D\psi^* D\psi e^{-S_{\psi ij}[\Phi_{ij}(\tau,\tau')]}, \quad (13)$$

where $S_{\psi ij}[\Phi_{ij}(\tau,\tau')] = \sum_{l=i,j} \int_0^\beta d\tau_1 \psi_l^*(\tau_1)[\partial_{\tau_1} - \mu + U\delta_{li} - \Phi_{l,ij}(\tau,\tau') + \lambda_l(\tau_1)]\psi_l(\tau_1)$ is the action of two coupling conduction electrons residing on different sites by the external field $-\Phi_{l,ij}(\tau,\tau')$, and $Z_{ij} = \int \prod_{l=i,j} D\psi_l^* D\psi_l D\varphi_l^* D\varphi_l e^{-S_{ij}[0]}$. Here we have introduced two independent dynamical mean fields $\lambda_i(\tau_1)$ and $\lambda_j(\tau_1)$. Obviously, the expressions of the correlation functions of the local electrons are much more simplified in the infinite dimension limit.

After integrating out the conduction electron fields, we obtain the following relations:

$$\begin{aligned} \int D\psi_j^* D\psi_j e^{-S_{\psi j}[\Phi_j(\tau,\tau')]} &= e^{\text{Tr} \ln[\hat{G}_0^{-1}[U,\Phi(\tau,\tau')] + \lambda]} \\ &= Z_0[U,\Phi] \text{Det}\{1 + \hat{G}_0[U,\Phi(\tau,\tau')] \lambda\} \\ \int D\psi^* D\psi e^{-S_{\psi ij}[\Phi_{ij}(\tau,\tau')]} &= Z_0[U,\Phi] Z_0[0,-\Phi] \\ &\quad \times \text{Det}\{1 + \hat{G}_0[U,\Phi(\tau,\tau')] \lambda\} \\ &\quad \times \text{Det}\{1 + \hat{G}_0[0,-\Phi(\tau,\tau')] \lambda\}, \end{aligned} \quad (14)$$

where $\hat{G}_0^{-1}[U,\Phi(\tau,\tau')] = \partial_{\tau_1} - \mu + U - \Phi_{j,j}(\tau,\tau')$, and $Z_0[U,\Phi] = e^{-\text{Tr} \ln[\hat{G}_0[U,\Phi(\tau,\tau')]]}$. Substituting the first expression of Eq. (14) into Eqs. (12) and (5), we have¹⁸

$$\begin{aligned} G_{jl}(\tau - \tau') &= \frac{1}{Z_j} \delta_{jl} G_0(\tau - \tau') Z_0[0,-\Phi] \\ &\quad \times \text{Det}\{1 + \hat{G}_0[0,-\Phi(\tau,\tau')] \lambda\} \end{aligned} \quad (15)$$

which is exactly the same Green function of the local electrons as obtained by the DMFT method.^{9,15} Using these expressions of the correlation functions of the local electrons, we can study the local electron correlation. However, the dynamical mean field $\lambda_j(\tau_1)$ need to be determined by the DMFT self-consistency condition for the conduction electron Green function, and it strongly influences the density of states of the conduction electrons near the Fermi surface. These expressions should be very useful for numerical simulations.

IV. DYSON EQUATION SOLUTION

In this section, we consider only the zero temperature case. By solving the Dyson equation of the conduction electron Green function, we calculate analytically the correlation functions of the local electrons and show that, if the density of states of the conduction electrons at the Fermi surface is finite, the asymptotic power-law behavior of the correlation

functions of the local electrons is universal in any dimension.

In the finite dimension case, for simplicity, we only calculate the correlation functions of the local electrons at zero temperature. Due to the conservation of the local electron number on each lattice site, the action $S[\Phi_j(t, t')=0] \times \{=S[\Phi_{ij}(t, t')=0]\}$ in fact describes the motion of conduction electrons influenced by randomly distributed potential produced by the local electrons. As done in the DMFT, this effect can be incorporated to the Green function of the conduction electrons by adding a suitable self-energy term. Thus, after integrating out the conduction and local electron fields, for example, the first expression in Eq. (8) can be written as

$$\langle TU_j^\dagger(t)U_j(t') \rangle = \exp\{\text{Tr} \ln[\hat{G}^{-1} + \Phi_j(t, t')] - \text{Tr} \ln(\hat{G}^{-1})\}. \quad (16)$$

Using the formula, $\text{Tr} \ln(\hat{A} + \hat{B}) = \text{Tr} \ln(\hat{A}) + \text{Tr} \int_0^1 d\lambda \hat{B}[\hat{A} + \lambda \hat{B}]^{-1}$, the above expression can be rewritten as

$$\langle TU_j^\dagger(t)U_j(t') \rangle = \exp \left[U \sum_{q, q'} \int_0^1 d\lambda \int_{t'}^t dt_1 G_{qq'}^\lambda(t_1, t_1; t, t') \right], \quad (17)$$

where $G_{qq'}^\lambda(t_1, t_1'; t, t')$ is the local Green function of the conduction electrons under the external potential $\lambda \Phi_{ij}(t, t')$, and it satisfies the following equation:

$$G^\lambda(t_1, t_1'; t, t') = G(t_1 - t_1') - \lambda U \int_{t'}^t dt_2 G(t_1 - t_2) G^\lambda(t_2, t_1'; t, t'), \quad (18)$$

where $G^\lambda(t_1, t_1'; t, t') = \sum_{q, q'} G_{qq'}^\lambda(t_1, t_1'; t, t')$, and $G(t_1 - t_1') = \sum_{q, q'} G_{qq'}(t_1 - t_1')$ is the local Green function of the conduction electrons at site \mathbf{x}_j , in which the contribution of the local electrons is incorporated by taking a suitable self-energy term, and \mathbf{q} is the wave vector of the conduction electrons. These two equations, (17) and (18), are universal for the on-site Coulomb interaction between the conduction and local electrons. Therefore they are valid for both finite-dimensional and infinite-dimensional Falicov–Kimball lattice model and other similar models. In the infinite dimension limit, the Green function $G(t_1 - t_1')$ can be written by taking the dynamical mean field $\lambda_j(\tau_1)$ which plays the role of the self-energy produced by the local electron potential (U term) and the hopping hybridization with other conduction electrons around the site \mathbf{x}_j . Obviously, the correlation of the local electrons strongly depends on the behavior of the conduction electrons which mediates the correlation among the local electrons. In general, the low energy physical property of the Falicov–Kimball lattice model also depends upon the filling factor of the conduction and local electrons and lattice type. Here we only consider square and/or hypercubic lattice, and assume that the filling factor of the local electrons is less than half-filling. In the following calculation, we do not need to know the concrete expression of the Green function $G(t)$ of the conduction electrons, and we only concern whether the spectrum of the conduction electrons is gapless at zero

temperature, i.e., whether the density of states of the conduction electrons at the Fermi surface is finite.

A. Two local electrons case

As a simple example, we apply the above general formulas for the case of two local electrons. In this situation, the modification of the local electron potential to the conduction electron Green function is small, and it can be effectively incorporated to the density of states of the conduction electrons at the Fermi surface. Thus the Green function of the conduction electrons can be generally represented as, $G(t) = \theta(t) \int_{-\xi_0}^{\xi_0} d\epsilon N(\epsilon) e^{-i\epsilon t} - \theta(-t) \int_{-\xi_0}^{\mu} d\epsilon N(\epsilon) e^{-i\epsilon t}$, where $N(\epsilon)$ is the density of states, and ξ_0 is the bandwidth of the conduction electrons. When t is large, $G(t)$ is controlled by the discontinuity at $\epsilon = \mu$, and its limiting behavior for both signs of t is $G(t) \rightarrow (N(0)/it) e^{-i\mu t}$. Therefore, as $\xi_0 |t| \gg 1$, that is for t larger than a typical atomic time, it can be written as, $G(t) = -N(0)/[t - i(1/\xi_0) \text{sgn}(t)]$, where $N(0)$ is the density of states of the conduction electrons at the Fermi surface. Substituting this expression of the conduction electrons into Eq. (18), the integral equation of the Green function $G^\lambda(t_1, t_1'; t, t')$ is reduced to the Muskhelishvili equation¹⁹ which can be exactly solved.⁸ In this case, we obtain the following asymptotic behavior of the local electron correlation functions ($\xi_0 |t - t'| \gg 1$),

$$\begin{aligned} \langle TU_j^\dagger(t)U_j(t') \rangle &= \left(\frac{1}{\xi_0 |t - t'|} \right)^{2(\bar{\delta}/\pi)^2}, \\ \langle Tn_{ij}(t)n_{ji}(t') \rangle &= \left(\frac{1}{\xi_0 |t - t'|} \right)^{2(\bar{\delta}/\pi)^2}, \\ \langle T\hat{c}_j(t)\hat{c}_j^\dagger(t')U_j^\dagger(t)U_j(t') \rangle &= \left(\frac{1}{\xi_0 |t - t'|} \right)^{1-2\bar{\delta}/\pi+2(\bar{\delta}/\pi)^2}. \end{aligned} \quad (19)$$

Under usual s -wave scattering approximation, the phase shift of the conduction electrons at Fermi surface $\bar{\delta} = \arctan\{-U \text{Im} G(0)/[1 - U \text{Re} G(0)]\}$ is exact, because the first and third correlation functions in Eq. (19) only involve the single local electron where the spherical symmetry is kept. While the phase shift $\bar{\delta}$ can be approximately written as, $\bar{\delta} = \arctan\{[-2U \sin(2|\mathbf{x}_i - \mathbf{x}_j|k_F) \text{Im} G(0)]/[1 - 2U \sin(2|\mathbf{x}_i - \mathbf{x}_j|k_F) \text{Re} G(0)]\}$, because the spherical symmetry is broken in the second correlation function of Eq. (19), and we have used the approximation $e^{i\mathbf{k} \cdot (\mathbf{x}_i - \mathbf{x}_j)} \rightarrow e^{ik_F |\mathbf{x}_i - \mathbf{x}_j|}$ in calculating $\bar{\delta}$. In fact, for the correlation function involving two local electrons on different sites \mathbf{x}_i and \mathbf{x}_j , such as the second correlation function in Eq. (19), the potential $\Phi_{l,ij}(\tau, \tau')$ depends on the sites \mathbf{x}_i and \mathbf{x}_j , and in this situation, large angular momentum channels of the conduction electrons may also contribute to the correlation exponent. Thus, after considering large angular momentum channel scattering, the correlation exponent $2(\bar{\delta}/\pi)^2$ in second expression of Eq. (19) can be replaced by $2\sum_l (2l+1)(\bar{\delta}_l/\pi)^2$, i.e., $(\bar{\delta}/\pi)^2 \rightarrow \sum_l (2l+1)$

$\times (\bar{\delta}_l/\pi)^2$, where $\bar{\delta}_l$ is determined by the effective potential in the l th angular momentum channel. These results are valid for any dimension D and consistent with previous calculations.^{8,20,21}

B. The general case

For a finite density of the local electrons, the randomly distributed potential produced by the local electrons can make the conduction electrons behave as non-Fermi liquid, insulator, or localized for low-dimensional case. Thus in general the Green function $G(t)$ does not have the form $G(t) = -N(0)/[t - i(1/\xi_0)\text{sgn}(t)]$, and Eq. (18) cannot be reduced to the Muskhelishvili equation. Now we use another method²² to solve Eq. (18).

In previous work,²³ the case of $t' \rightarrow -\infty$ and $t=0$ was considered, and the author obtained the result which is consistent with that by solving the Muskhelishvili equation for the noninteracting conduction electrons. In the present case, the situation becomes a little more complex, where the integral interval $[t', t]$ of t_2 is larger $\Delta t = t - t' \rightarrow \infty$, but $t' \neq -\infty$ and/or $t \neq \infty$. In order to solve Eq. (18) under the condition $\Delta t \rightarrow \infty$, we consider two limiting cases: one is $\int_{t'}^t dt_2 \Rightarrow \int_{t'}^{t'+\Delta t} dt_2$ for finite t' , and another one is $\int_{t'}^t dt_2 \Rightarrow \int_{t-\Delta t}^t dt_2$ for finite t . In the latter case, after making the Fourier transformation, Eq. (18) can be rewritten as

$$G^\lambda(\omega, t'_1; t, t') = G(\omega) e^{i\omega t'_1} + \frac{i\lambda U}{2\pi} G(\omega) \int d\omega' \frac{G^\lambda(\omega', t'_1; t, t')}{\omega' - \omega + i\eta} e^{-i(\omega' - \omega)t} \quad (20)$$

which has a general solution

$$G^\lambda(\omega, t'_1; t, t') = \frac{1}{2\pi i} \int d\omega' \frac{G(\omega')}{X^{(+)}(\omega')} e^{i\omega'(t'_1 - t) + i\omega t} \cdot \left(\frac{X^{(+)}(\omega)}{\omega' - \omega - i\eta} - \frac{X^{(-)}(\omega)}{\omega' - \omega + i\eta} \right), \quad (21)$$

where $X^{(\pm)}(\omega) = \exp((1/2\pi i) \int d\omega' \{\ln[1 - \lambda U G(\omega')]/\omega' - \omega \mp i\eta\})$. Similarly, in the case of $\int_{t'}^t dt_2 \Rightarrow \int_{t'}^{t'+\Delta t} dt_2$, the Green function $G^\lambda(\omega, t'_1; t, t')$ has a similar expression. Using these expressions, we obtain the following relation:

$$\begin{aligned} & -U \int_0^1 d\lambda \int_{t'}^{t'+\Delta t} dt_1 G^\lambda(t_1, t_1; t, t') = \\ & -U \int_0^1 d\lambda \int_{t-\Delta t}^t dt_1 G^\lambda(t_1, t_1; t, t') \\ & = \frac{1}{2} \left(\frac{\delta}{\pi} \right)^2 \ln \left(\frac{\Delta}{\xi_0} \right) + \text{imaginary part}, \end{aligned} \quad (22)$$

where $\Delta \ll \xi_0$ is an infrared energy cutoff constant. At zero temperature, no matter whether the conduction electrons show Landau Fermi liquid behavior, if only the spectrum of the conduction electrons is gapless, i.e., the density of states

of the conduction electrons at the Fermi surface is finite, according to the uncertainty relation the cutoff constant Δ can be taken as $\Delta \sim \hbar/|t - t'|$ which is the smallest effective energy scale of the frequency in thermodynamic limit. As $\Delta t \rightarrow \infty$, we replace the integral $\int_{t'}^t dt_1 G^\lambda(t_1, t_1; t, t')$ in Eq. (17) by $\int_{t'}^{t'+\Delta t} dt_1 G^\lambda(t_1, t_1; t, t') + \int_{t-\Delta t}^t dt_1 G^\lambda(t_1, t_1; t, t')$ which includes two possible contours of integral, then we obtain the same asymptotic expressions of the correlation functions $\langle TU_j^\dagger(t) U_j(t') \rangle$ and $\langle T n_{ij}(t) n_{ji}(t') \rangle$ as that in Eq. (19). However, it is hard to calculate the asymptotic expression of the correlation function $\langle T \hat{c}_j(t) \hat{c}_j^\dagger(t') U_j^\dagger(t) U_j(t') \rangle$ by Eq. (21), which depends on the asymptotic behavior of the Green function $G(t)$, but it can be generally represented as⁸ ($\xi_0 |t - t'| \gg 1$),

$$\langle T \hat{c}_j(t) \hat{c}_j^\dagger(t') U_j^\dagger(t) U_j(t') \rangle \propto \tilde{G}(t - t') \left(\frac{1}{\xi_0 |t - t'|} \right)^{2(\delta/\pi)^2}, \quad (23)$$

where $\tilde{G}(t - t')$ is the Green function of the conduction electrons under the external potential $\Phi_{j,j}(t, t')$.

If the spectrum of the conduction electrons is gapful, the infrared cutoff constant Δ will be replaced by the energy gap Δ_0 . In this case, the phase shifts go to zero, $\delta, \bar{\delta} \rightarrow 0$, and the correlation among the local electrons disappears in low energy limit, which is consistent with the common consensus.

The above expression of the correlation function $\langle TU_j^\dagger(t) U_j(t') \rangle$ is consistent with previous works^{21,24,25} for the infinite-dimensional Falicov–Kimball lattice model. On the other hand, for the case of finite dimensions and small Coulomb interaction U , the conduction electrons show the Landau Fermi liquid behavior, and the local electron Green function has the power-law asymptotic behavior, just as shown in the first expression of Eq. (19), where the correlation exponent is $2(\delta/\pi)^2 = 2((1/\pi) \arctan\{-U \text{Im} G(0)\}/[1 - U \text{Re} G(0)])^2$. For the single local electron case, this correlation exponent is exact and proportional to $[UN(0)]^2$ as $UN(0) \ll 1$. While, in the half-filling of the local electrons, the numerical simulation shows that the correlation exponent of the local electron Green function has a linear dependence on the dimensionless coupling constant²⁶ $UN_{eff}(0)$ for $UN_{eff}(0) \ll 1$. This variation of the correlation exponent with the filling factor of the local electrons needs to be clarified in the future.

The above results clearly show that as the spectrum of the conduction electrons is gapless, the correlation functions of the local electrons have the asymptotic behavior similar to that of x-ray absorption/emission of a deep core electron in metal, and show the asymptotic power-law behavior. This phenomenon can be easily explained by referring to Eq.(8). In the present representation, all correlation functions of the local electrons can be written down directly by the partition function of the conduction electrons under the time dependent external potential $\Phi_{i,j}(t, t')$ [or $\Phi_{l,ij}(t, t')$]. At lattice site \mathbf{x}_j , the potential $\Phi_{j,j}(t, t')$ is equal to a constant in time interval $[t', t]$, and it is zero otherwise. This property of the potential is similar to that of the x-ray absorption and emis-

sion of the deep core electron in metal, which leads to that they both show similar asymptotic behavior. However, it does not mean that the local electrons are independent of each other, just as shown in Eq. (9), there in fact also exists correlation among them. On the other hand, this asymptotic power-law behavior can be survived as including the Coulomb interaction of the conduction electrons, if it does not open a gap in the spectrum of the conduction electrons. For high dimensions, the main effect of the Coulomb interaction is just to modify the density of states of the conduction electrons. For the one-dimensional case, the Coulomb interaction not only modifies the density of states, but also contributes to the correlation exponents of the local electron correlation functions.

V. CONCLUSIONS AND DISCUSSIONS

By studying the Falicov–Kimball lattice model, we derived general expressions of the correlation functions of the local electrons which return to the exact ones obtained by the DMFT method in the infinite dimension limit. We demonstrated that at zero temperature, the asymptotic power-law behavior of the local electron correlation functions is universal for any dimensions, no matter whether the conduction electrons show Landau Fermi liquid behavior or not, if only

their spectrum is gapless, i.e., the density of states of the conduction electrons at the Fermi surface is finite. Moreover, such asymptotic power-law behavior of the local electron correlation functions also exists in other quantum many-particle systems, if the coupling between conduction and local electrons is on-site or short-range Coulomb interaction, and the spectrum of the conduction electrons is gapless. Therefore, this phenomenon can be observed in experiments and numerical simulations, which manifests the edge singularity of x-ray absorption/emission under certain conditions, as shown in Eq. (23), where the response function of the x-ray absorption/emission is proportional to the correlation function $\langle T\hat{c}_j(t)\hat{c}_j^\dagger(t')U_j^\dagger(t)U_j(t') \rangle$. However, for a realistic system, there are a lot of factors that can smear or destroy this edge singularity. For example, energy level distribution of the local electrons, small hybridization between the conduction and local electrons, and small hopping of the local electrons between different lattice sites.

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