PHYSICAL REVIEW B **74**, 125119 (2006)

Correlation effect of local electrons in a one-dimensional Falicov-Kimball model

Qing-Wei Wang[1] and Yu-Liang Liu[2]
[1]*Center for Advance Study, Tsinghua University, Beijing 100084, People's Republic of China*
[2]*Department of Physics, Renmin University of China, Beijing 100872, People's Republic of China*
(Received 1 December 2005; revised manuscript received 20 May 2006; published 28 September 2006)

With the eigenfunctional theory, we give a general exact expression of the local electron Green function in the Falicov-Kimball model, and apply it to study the correlation effects of the local electrons in one dimension. For the two local electrons case, the correlation exponent of the local electron Green function has weak even-odd oscillation with the distance between these two local electrons, and it approaches zero in the strong coupling limit. While, at half filling of the local electrons, the ground-state phase is complicated. When the conduction electron is near 0.5, the ground state configuration is the chessboard phase for a considerable range of U/t^*, and the correlation exponent increases from zero to a finite value as U/t^* increases. When the conduction electron is far away from 0.5, the ground state configuration is the segregated phase, and the correlation exponent first increases and then jumps to zero when U/t^* is larger than a finite value which is a function of n_c. Our results are compared with previous numerical simulations.

DOI: 10.1103/PhysRevB.74.125119 PACS number(s): 71.27.+a, 72.15.Nj, 73.23.−b

I. INTRODUCTION

The local electron/fermion correlation effect in quantum many particle systems has been extensively studied, such as two local magnetic impurities scattering problem,[1] the Kondo lattice model[2] 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 conduct electrons, resulting in novel low temperature physical behavior of these systems.

One of the simplest examples for studying the local electron correlation is the x-ray absorption and emission of deep core-electrons in metals, and its extension is the Falicov-Kimball model, where the local electrons are randomly distributed on lattice sites. For the case of one local electron, we have the Mahan-Nozières-De Dominicis solution, and the Green function of local electrons shows an edge singularity at zero temperature. What about more than one local electron? In this paper, with a general Falicov-Kimball lattice model, we give an exact expression of the local electron Green function, and then apply it to study the correlation effects of the local electrons in one dimension. For the two local electrons case, the Green function of local electrons shows asymptotic power-law behavior, and we show the dependence of the correlation exponent of the local electron Green function on the coupling constant and the distance between these two local electrons. Furthermore, at the half filling of the local electrons, the ground-state phase diagram is complicated. We consider only the periodic configurations and the segregated phase, and give a restricted phase diagram. Then we calculated the correlation exponents for different local-electron configuration and different conduct-electron concentrations. In the periodic configurations, the coupling constant dependence of the correlation exponents is completely different from that for the two local electrons case, and in the strong coupling limit they approach finite values. While, in the segregated phase (which covers most of the phase diagram), the correlation exponents turn to zero when the coupling constant is larger than a certain value which is dependent on the concentration of the conduct electrons.

Our paper is arranged as follows: in Sec. II we give the general formalism and the exact expression of the local electron Green functions. We give further derivations of the Green function expression in Sec. III for the two local electron case, and we calculate its dependence on coupling constant. In Sec. IV we consider the half filling case of the local electrons. After a brief discussion of the ground-state phase diagram, we give the correlation exponent expression and show its dependence on coupling constant and local-electron configurations. We conclude in Sec. V with a summary of our main results and discussions.

II. GENERAL FORMALISMS

In order to give a general expression of the local electron Green function, we consider the Falicov-Kimball model in a hypercubic lattice,

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

where $\hat{n}_{ci}=\hat{c}_i^\dagger\hat{c}_i$, $\hat{n}_{fi}=\hat{f}_i^\dagger\hat{f}_i$, $\langle ij\rangle$ denotes 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 conduct and local electrons (local particles) at the lattice site $\mathbf{x}_i$, respectively, μ and μ_f are the corresponding chemical potentials of the conduct and local electrons, ε_f is the local electron energy level, and U is the Coulomb interaction potential between the conduct and local electrons. Chemical potentials μ and μ_f are employed to adjust the itinerant- and localized-electron concentrations, respectively. In the canonical ensemble, where the localized particle is fixed independently of the itinerant-electron concentration,[6] the localized-particle chemical potential μ_f can be absorbed into the site energy ε_f; in the grand canonical ensemble, where the localized particles are electrons and could be thermally mixed with the conduct electrons,[7] they share a common chemical potential with the conduct electrons $\mu = \mu_f$. We consider the first case in this paper. It should also be noted that, for the Falicov-Kimball model, the local electron number on each lattice site is conserved.

After introducing the Lagrange multiplier field $\phi(x_i,t)$ to decouple the interaction between the conduct and local electrons, the partition function of the system can be written as $Z = \int D\psi^* D\psi D\varphi^* D\varphi D\phi D n_c e^{(i/\hbar)S}$, where the action reads

$$S = \sum_{\langle ij\rangle} \int dt \psi_i^*(t)\left[\hat{M}_{0ij}(t) - \phi(x_i,t)\delta_{ij}\right]\psi_j(t) + \sum_i \int dt \varphi_i^*(t)\hat{M}_i(t)\varphi_i(t) + \sum_i \int dt \phi(x_i,t) n_{ci}(t), \tag{2}$$

where $\hat{M}_i(t) = i\hbar\partial_t - \varepsilon_f + \mu_f - U n_{ci}(t)$, and $\hat{M}_{0ij}(t) = (i\hbar\partial_t + \mu)\delta_{ij} + t^*(\hat{\gamma}_{ij} + \hat{\gamma}_{ji})$, $\hat{\gamma}_{ij} = 1$ for $\mathbf{x}_j = \mathbf{x}_i \pm a\mathbf{e}$, $\hat{\gamma}_{ij} = 0$ for $\mathbf{x}_j \neq \mathbf{x}_i \pm a\mathbf{e}$. Here $n_{ci}(t)$ and $\phi(x_i,t)$ are the auxiliary fields, a the lattice constant, and $\mathbf{e}$ a unit vector.

Using the eigenfunctional theory[8,9] to study the local electron correlation, we need to solve the eigenequation of the local electron propagator operator, $\hat{M}_i(t)\varphi_{i\omega}(t,[n]) = E_\omega[n]\varphi_{i\omega}(t,[n])$, then use the eigenfunctions $\varphi_{i\omega}(t,[n])$ to write down the second quantization representation of the local electron field operators $\hat{f}_j(t)$ and $\hat{f}_j^\dagger(t)$. With these expressions of the local electron operators, we obtain the Green function of the local electrons[9] $[G_{jj'}(t-t') = \langle T\hat{f}_j(t)\hat{f}_{j'}^\dagger(t')\rangle]$,

$$G_{jj'}(t-t') = \delta_{jj'} G_0(t-t')\langle T U_j(t) U_j^\dagger(t')\rangle,$$

where $U_j(t) = \exp[-iU/\hbar \int^t dt_1 n_{cj}(t_1)]$, and $G_0(t-t')$ is the Green function of local electrons without the Coulomb interaction. Furthermore, we could obtain the following expression:

$$G_{jj'}(t-t') = \frac{\delta_{jj'} e^{-i(\varepsilon_f - \mu_f)(t-t')}}{Z'} \times \left\{ \theta(t-t') \sum_{\{n_{fj}\}} Z'[n_{fj}] e^{-U\int_0^1 d\lambda \int_{t'}^t dt_1 G^\lambda(x_j,t_1;x_j,t_1)} - \theta(t'-t) \sum_{\{n'_{fj}\}} Z'[n_{fj'}] e^{-U\int_0^1 d\lambda \int_{t'}^t dt_1 G^\lambda(x_j,t_1;x_j,t_1)} \right\}, \tag{3}$$

where $\{n_{fj}\} \equiv \{n_{fl}, x_l \neq x_j, n_{fj} = 0\}$, $\{n'_{fj}\} \equiv \{n_{fl}, x_l \neq x_j, n_{fj} = 1\}$, $Z'[n_{fi}] = \exp[\mathrm{Tr}\ln(\hat{M}_{0il}(t_1) - U n_{fi}\delta_{il})]$, $Z' = \Sigma_{\{n_{fi}\}} Z'[n_{fi}]$, and $\theta(t)$ is usual step function. The Green function $G^\lambda(x_j,t_1;x_j,t_2)$ satisfies the Dyson equation

$$G^\lambda(x_j,t_1;x_j,t_2) = G(x_j,t_1;x_j,t_2) + \lambda U \int_{t'}^{t} dt_3 G(x_j,t_1;x_j,t_3) G^\lambda(x_j,t_3;x_j,t_2), \tag{4}$$

where $G(x_l,t_1;x_{l'},t_2)$ is the Green function of the conduct electrons at $\lambda = 0$, which can be written as

$$G(x_i,t;x_j,t') = \frac{1}{T_0}\sum_{k,\omega} \frac{\psi_k(x_i)\psi_k^*(x_j)}{\hbar\omega - E_k} e^{-i\omega(t-t')}, \tag{5}$$

where $\psi_k(x_i)$ is the eigen-wave function of the conduct electrons under the potential $U\Sigma_i n_{fi}$, and n_{fi} is the distribution of the local electrons.

This is an exact expression of the local electron Green function completely represented by the Green function of the conduct electrons, which is valid for any filling factor of the local electrons and a general type of lattice. For one local electron case, the system is reduced to usual x-ray absorption and emission of a deep hole in metal,[10,11] which can be exactly solved.[11] On the other hand, in the infinite dimension limit, the Falicov-Kimball lattice model can be exactly solved,[12] and the correlation effects of the local electrons has been extensively studied.[13,14] Hereafter, to analytically study the correlation effect of the local electrons, we focus on two special distributions of the local electrons in one dimension: one is only two local electrons on two different lattice sites, and another one is a half filling distribution of the local electrons.

III. TWO LOCAL ELECTRONS CASE

In the case of two local electrons, the distribution of the local electrons is $n_{fi} = \delta_{ii_1} + \delta_{ii_2}$, and the local electron Green function can be rewritten as

$$G_{jj'}(t-t') = \delta_{jj'} e^{-i(\varepsilon_f - \mu_f)(t-t')}\theta(t-t') e^{-U\int_0^1 d\lambda \int_{t'}^t dt_1 G^\lambda(x_j,t_1;x_j,t_1)}. \tag{6}$$

While, in the present situation, the eigenequation of the conduct electrons reads

$$[-t^*(\hat{\gamma}_{ij} + \hat{\gamma}_{ji}) + (U n_{fi} - \mu)\delta_{ij}]\psi_k(x_j) = \varepsilon_k \psi_k(x_i). \tag{7}$$

This equation can be exactly solved, and the eigenwave function of the conduct electrons can be written as $(k > 0)$

$$\psi_k(x_i) = \frac{1}{\sqrt{2L}}\begin{cases} e^{ikx_i} + a_k(R)e^{-ikx_i}, & x_i \leq -R \\ b_k(R)e^{ikx_i} + c_k(R)e^{-ikx_i}, & -R < x_i < R \\ d_k(R)e^{ikx_i}, & R \leq x_i. \end{cases} \tag{8}$$

For $k < 0$, it reads

$$\psi_k(x_i) = \frac{1}{\sqrt{2L}}\begin{cases} e^{ikx_i} + \bar{a}_k(R)e^{-ikx_i}, & R \leq x_i \\ \bar{b}_k(R)e^{ikx_i} + \bar{c}_k(R)e^{-ikx_i}, & -R < x_i < R \\ \bar{d}_k(R)e^{ikx_i}, & x_i \leq -R, \end{cases} \tag{9}$$

where $\varepsilon_k = -2t^*\cos(ak) - \mu$. With the boundary conditions at the local electron sites, we obtain the following expressions of the coefficients:

$$a_k(R) = \bar{a}_{-k}(R) = -\frac{iU}{2t^*}\frac{L_k(U)e^{-2ikR} + L_k^*(U)e^{2ikR}}{B_k(U,R)[B_k(-U,R) + iU]},$$

$$b_k(R) = \bar{b}_{-k}(R) = \frac{t^*}{2}\left[\frac{\sin ka}{B_k(U,R)} + \frac{\sin ka}{B_k(-U,R) + iU}\right],$$

$$c_k(R) = \bar{c}_{-k}(R) = \frac{t^*}{2}\left[\frac{\sin ka}{B_k(U,R)} - \frac{\sin ka}{B_k(-U,R) + iU}\right],$$

$$d_k(R) = \bar{d}_{-k}(R) = (t^*)^2\frac{\sin ka}{B_k(U,R)}\frac{\sin ka}{B_k(-U,R) + iU},$$

where $L_k(U) \equiv t^* \sin ka + \frac{iU}{2}$, and $B_k(U,R) \equiv t^* \sin ka + \frac{iU}{2}(1 + e^{2ikR})$. Furthermore, it is straightforward to verify the relations $|a_k|^2 + |d_k|^2 = 1$ and $|c_k|^2 + |d_k|^2 = |b_k|^2$.

Substituting Eqs. (8) and (9) into Eq. (5), we obtain the conduct electron Green function at the site x_{i_0},

$$G(x_{i_0},t;x_{i_0},t') = i\theta(t-t')\int_0^{\xi_0} d\varepsilon N(\varepsilon,U,R)e^{-i\varepsilon(t-t')} - i\theta(t'-t)\int_{-\xi_0}^{0} d\varepsilon N(\varepsilon,U,R)e^{-i\varepsilon(t-t')}, \tag{10}$$

where

$$N(\varepsilon,U,R) = \frac{1}{2}N(\varepsilon)[\theta(-k)|d_{-k}(R)|^2 + \theta(k)(1 + |a_k(R)|^2 + a_k(R)e^{i2kR} + a_k^*(R)e^{-i2kR})]$$

is the spectral density of conduct electron at site $x_{i_0}=R$, and $\varepsilon=-2t^* \cos(ak)-\mu$, with μ the chemical potential of the conduct electron which is determined by the filling factor ν of the conduct electron. It is easy to see that the Green function of the conduct electrons at site $x_{i_0'}$ is the same as that at site x_{i_0}, i.e., $G(x_{i_0'},t;x_{i_0'},t')=G(x_{i_0},t;x_{i_0},t')$.

Substituting Eq. (10) into Eq. (4), the equation of the Green function $G^\lambda(x_j,t_1;x_j,t_2)$ is reduced to the Muskhelishvili equation.[15] Following the same procedures as that in Refs. 9 and 17, the general solution of $G^\lambda(x_j,t_1;x_j,t_2)$ can be written down by the Green function $G(x_{i_0},t;x_{i_0},t')$, then with this solution of $G^\lambda(x_j,t_1;x_j,t_2)$, we obtain the Green function of the local electrons in the long time limit $\xi_0|t-t'|\gg 1$,

$$G_{jj'}(t-t') = -\delta_{jj'}e^{-i(\varepsilon_f-\mu_f)(t-t')}\theta(t'-t) \times \left(\frac{1}{|\xi_0(t-t')|}\right)^{(\delta(U,R)/\pi)^2}, \tag{11}$$

where $\delta(U,R)=\arctan(-U \operatorname{Im} G(x_{i_0'},0)/[1-U \operatorname{Re} G(x_{i_0'},0)])$, $G(x_{i_0'},\omega)$ is the Fourier transformation of the conduct electron Green function $G(x_{i_0'},t;x_{i_0'},t')$, and $\xi_0 \sim 4t^*$ is the bandwidth of the conduct electrons.

In Fig. 1, we show the dependence of the phase shift $\delta(U,R)$ on the coupling constant U/t^* and the distance parameter $2R$ at different filling factors of the conduct electrons.[16] For a definite U/t^*, the phase shift $\delta(U,R)$ shows a weak even-odd oscillation with $2R$, which originates from the dependence of the density of states on the phase factors $e^{\pm 2ikR}$. While in the strong coupling limit $U/t^* \gg 1$, the phase shift $\delta(U,R)$ goes to zero. It can be easily understood from the above expression of the wave functions in Eq. (8), where in the strong coupling limit $U/t^* \gg 1$, the conduct electrons are completely reflected by the local electrons, which results in that the density of states of the conduct electrons approach zero at the local electron sites x_{i_0} and $x_{i_0'}$.

IV. HALF FILLING OF LOCAL ELECTRONS

Similarly to the two local electrons case, we can have

$$\langle TU_j(t)U_j^\dagger(t')\rangle = \exp\left(-U\int_0^1 d\lambda \int_{t'}^{t} dt_1 G_c^\lambda(x_j,t_1;x_j,t_1)\right), \tag{12}$$

where $G_c^\lambda(x_j,t_1;x_j,t_2)$ is the local Green function of the conduct electrons at site x_j under the external potential $\lambda\Phi(t_1;t,t')=\lambda U[\theta(t_1-t')-\theta(t_1-t)]$, and it satisfies the Dyson equation:

$$G_c^\lambda(x_j,t_1;x_j,t_2) = G_c^0(t_1-t_2) - \lambda U\int_{t'}^{t} dt_3 G_c^0 \times (t_1-t_3)G_c^\lambda(x_j,t_3;x_j,t_2), \tag{13}$$

where $G_c^0(t_1-t_2)$ is the local Green function of the conduct electrons at x_j when $\lambda=0$.

In previous work,[17] the case of $t' \to -\infty$ and $t=0$ was considered, and the author obtained the result which is consistent with that by solving the Muskhelishvili equation for the noninteracting conduct electrons. In the present case, the situation becomes a little more complex, where the integral interval $[t', t]$ of t_3 is larger $\Delta t=t-t' \to \infty$, but $t' \neq -\infty$ and/or $t \neq \infty$. In order to solve Eq. (13) under the condition $\Delta t \to \infty$, we consider two limiting cases: one is $\int_{t'}^{t} dt_3 \Rightarrow \int_{t'}^{t'+\Delta t} dt_3$ for finite t', and another one is $\int_{t'}^{t} dt_3 \Rightarrow \int_{t-\Delta t}^{t} dt_3$ for finite t. In the first case, after making the Fourier transformation, Eq. (13) can be rewritten as

$$G_c^\lambda(\omega,t_2) = G_c^0(\omega)e^{i\omega t_2} - \frac{i\lambda U}{2\pi}G_c^0(\omega)\int d\omega' \frac{G_c^\lambda(\omega',t_2)}{\omega'-\omega-i\eta}e^{-i(\omega-\omega')t'}. \tag{14}$$

This is a Muskhelishvili equation and we can obtain its solution:

$$G_c^\lambda(\omega,t_2) = \frac{(-1)}{2\pi i}\int d\omega' \frac{G_c^0(\omega')}{X^{(+)}(\omega')}e^{i\omega'(t_2'-t')+i\omega t'} \times \left(\frac{X^{(+)}(\omega)}{\omega'-\omega+i\eta} - \frac{X^{(-)}(\omega)}{\omega'-\omega-i\eta}\right), \tag{15}$$

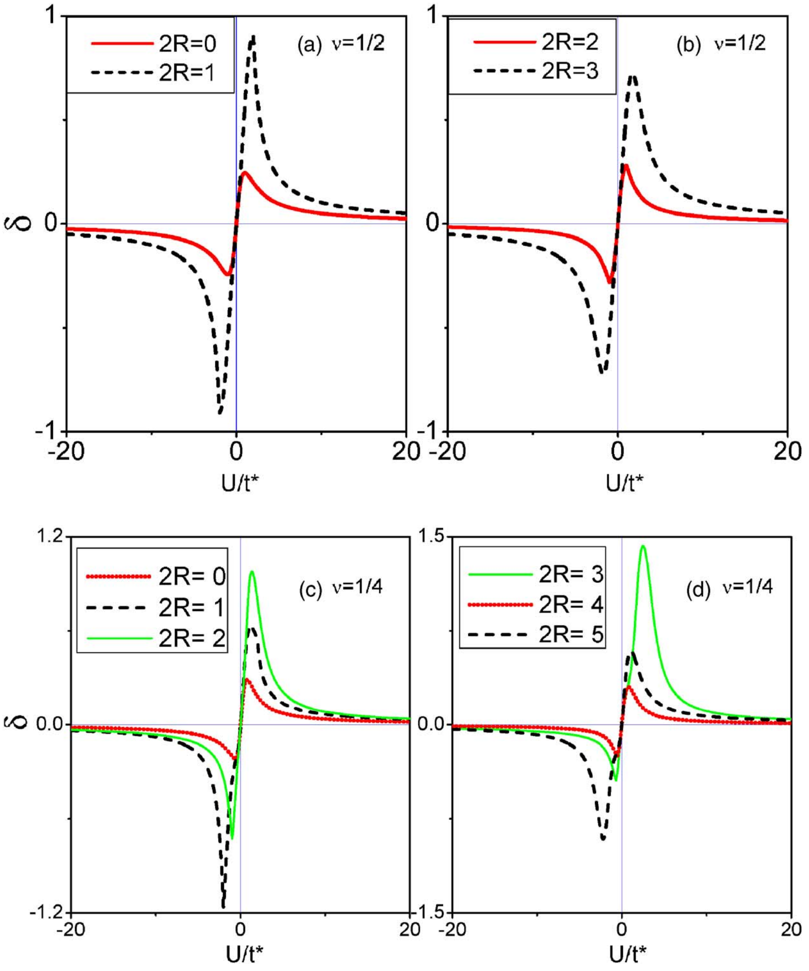

FIG. 1. (Color online) Dependence of phase shift δ on U/t^* and $2R$ in the two local electron case. Here ν is the filling factor of conduction electron, and $2R$ is the distance between the two local electrons (measured with the lattice constant a).

$$X^{(\pm)}(\omega)=\exp\left(\frac{1}{2\pi i}\int d\omega'\frac{\ln[1-\lambda U G_c^0(\omega')]}{\omega'-\omega\pm i\eta}\right). \qquad (16)$$

Similarly, in the case of $\int_{t'}^{t}dt_3 \Rightarrow \int_{t-\Delta t}^{t}dt_3$, the Green function $G_c^{\lambda}(\omega,t_2)$ has a similar expression. Using these expressions, we obtain the following relation:

$$-U\int_0^1 d\lambda\int_{t'}^{t'+\Delta t}dt_1 G_c^{\lambda}(t_1,t_1)=-U\int_0^1 d\lambda\int_{t-\Delta t}^{t}dt_1 G_c^{\lambda}(t_1,t_1) = \frac{1}{2}\left(\frac{\delta}{\pi}\right)^2\ln\left(\frac{\Delta}{\xi_0}\right) + \text{imaginary part}, \qquad (17)$$

$$\delta=\arctan\left(\frac{-U\,\mathrm{Im}\,G_c^0(\omega=\mu)}{1-U\,\mathrm{Re}\,G_c^0(\omega=\mu)}\right), \qquad (18)$$

where μ is the chemical level, and $\Delta \ll \xi_0$ is an infrared energy cutoff constant. According to the uncertainty relation, we can take $\Delta \sim \hbar/|t-t'|$.

Obviously, the above results show that as the spectrum of the conduct electrons is gapless, the Green function of the local electrons has asymptotic power-law behavior:

$$G_{jj'}(t-t') \propto \delta_{jj'}G_0(t-t')\left(\frac{1}{|\xi_0(t-t')|}\right)^{(\delta(U,R)/\pi)^2}. \qquad (19)$$

In order to show the coupling constant dependence of the correlation exponents, we need to calculate the spectrum of the conduct electrons $\rho(x_j,\omega)$:

$$\rho(x_j,\omega)=-\frac{1}{\pi}\,\mathrm{Im}\,G_c^0(x_j,\omega), \qquad (20)$$

which could be calculated as in the two local electron case, or use the formulas given by Lyzwa for periodic configurations of local electrons.[18] Furthermore, the phase shift δ can be expressed as

$$\delta=\arctan\left(\frac{\pi U\rho(x_j,\omega=\mu)}{1-U\int d\omega\rho(x_j,\omega)/(\omega-\mu)}\right). \qquad (21)$$

For half filling of the local electrons (n_f=0.5), the spectrum of conduct electrons is strongly dependent on the configuration, denoted by Γ, of the local electrons and the conduct electron concentration n_c. Given a Γ and n_c, we can calculate the phase shift and therefore the correlation exponent. To this purpose, we first obtain the energy bands E_k^l and the corresponding wave functions $\Psi_k^l(x_i)$. Second, we can obtain the density of states (DOS) $D^{\Gamma}(\omega)=\Sigma_{l,k}\delta(\omega-E_k^l)$ and the spectrum $\rho(x_j,\omega)=\Sigma_{l,k}\delta(\omega-E_k^l)|\Psi_k^l(x_j)|^2$. The chemical level μ can be obtained according to the relation: $n_c=\int_{-\infty}^{\mu}D^{\Gamma}(\omega)d\omega$. Finally, using Eq. (21), we can calculate the phase shift $\delta^{\Gamma}(U;n_c)$.

In the following we would first give a brief discussion of the ground-state configuration Γ_g, and then calculate the phase shift $\delta^{\Gamma}(U;n_c)$ for some special Γ and n_c.

A. Ground-state phase diagram

For the half filling of the local electrons, the configuration may be a periodic one with period $2n(n=1,2,3,\ldots)$, which would be denoted by P_{2n}. If there is more than one distinct configuration with the same period (it is usually the case) we can add an additional index α to distinguish them: P_{2n}^{α}. The simplest periodic configuration is $P_2=[\cdots XOXO\cdots]$ (or, chessboard phase), where X represents a site occupied by a local electron, and O represents an empty site. Furthermore, we have $P_4=[\cdots XXOO\cdots], P_6^{\alpha}=[\cdots XXXOOO\cdots], P_6^{\beta}=[\cdots XXOOXO\cdots],\ldots$, and so on.

In addition to the one-phase periodic configurations, a physically relevant two-phase configuration called the segregated phase should be considered. The segregated phase is an incoherent mixture of the full and empty domains with weights n_f and $(1-n_f)$, respectively. The DOS is a linear combination:

$$D^{seg}(\epsilon)=n_fD^{full}(\epsilon)+(1-n_f)D^{empty}(\epsilon)$$

of the DOS for the empty and full domains. The segregated phase is important since it is expected to be the ground state in the large-interaction limit $|U/t^*|\to\infty$, except for some special cases ($n_c+n_f=1$ for $U\to+\infty$ and $n_c=n_f$ for $U\to-\infty$). The physical idea is the following.[19] In the large-interaction limit the itinerate electrons are trapped between boundaries of full-empty domains. The dominant contribution to the ground-state energy is the kinetic energy of the electrons, which is minimized by making the box as large as possible. This favors the segregated phase to be the ground state. However, at the point where the electrons completely fill the box ($n_c+n_f=1$ for $U\to+\infty$ and $n_c=n_f$ for $U\to-\infty$) the Pauli exclusion principle requires the additional electrons to be placed above a large potential barrier. At this point a periodic arrangement of the f electrons may actually lower the ground-state energy. These physical ideas are summarized in the so-called *segregation principle*: In the large-interaction limit the segregated phase is the ground state for all values of the electron concentration except the specific values $n_c+n_f=1$ for $U\to+\infty$ and $n_c=n_f$ for $U\to-\infty$. This is proved to be true.[20]

Since there are so many different configurations and any one may be the ground-state configuration for appropriate U and n_c, the ground-state phase diagram is complicated. In Fig. 2, we show a rather restricted phase diagram, in which we only consider four distinct configurations: P_2, P_4, P_6^{α}, and the segregated phase (SP). It does reflect some basic features of behavior (segregated/periodic phases) although it is quite approximate. One can find more precise diagrams in the literature.[21]

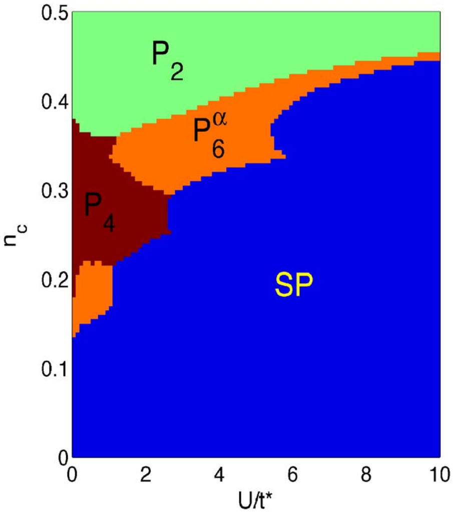

FIG. 2. (Color online) A numerically calculated restricted phase-diagram at half filling of the local electrons, i.e., $n_f=0.5$. Four distinct configurations: P_2, P_4, P_6^{α}, and the segregated phase (SP) are considered, which are represented by different colors.

We see that the numerically calculated phase diagram is consistent with the segregation principle. The SP phase takes up most of the region, whereas the periodic configurations, except P_2, take up rather finite pieces in the small coupling region.

B. Correlation exponents

We see that when $n_c\sim0.5$, the ground-state configuration is P_2 for a large range of the coupling constant U/t^*, and when n_c is far away from 0.5, the ground-state configuration is SP except for a very small region at $U/t^*\sim0$. In Figs. 3 and 4, we show the phase shift for the P_2 and SP configurations, respectively. Of course, we should not take every curve too seriously in the two figures. For example, in Fig. 3, we should only take the curves for $n_c\sim0.5$ seriously, and the other curves are just for comparison.

When the local electrons configuration is the simplest periodic one, P_2, the phase shift is shown in Fig. 3. At half

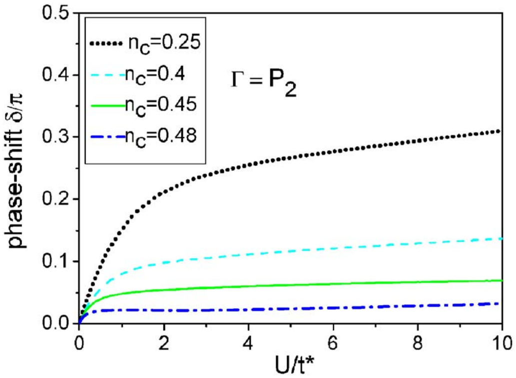

FIG. 3. (Color online) Dependence of phase shift δ on U/t^* and n_c for the local electrons configuration Γ being P_2. Here only the curves for $n_c\sim0.5$ (i.e., $n_c=0.48$ and 0.45) should be taken seriously, and the other curves are just for comparison.

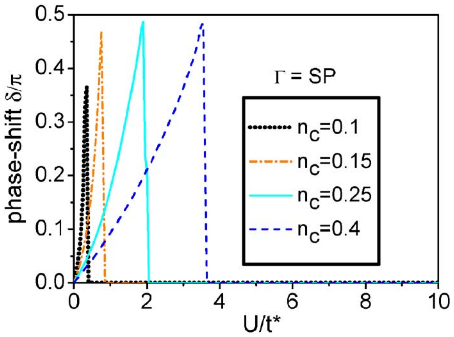

FIG. 4. (Color online) Dependence of phase shift δ on U/t^* and n_c for the local electrons configuration Γ being a segregated phase (SP). Here only the curves for n_c far away from 0.5 (i.e., $n_c=0.1$ and 0.15) should be taken seriously, and the other curves are just for comparison.

filling of the conduct electrons, i.e., when $n_c=0.5$, the P_2 is the ground-state configuration, and the chemical level is resided in the energy gap, therefore the phase shift and the correlation exponents are zero. When the conduct electron concentration n_c departs from 0.5 a little, the ground-state configuration Γ_g is still P_2 for a finite range of the coupling constant U/t^*, as shown in Fig. 2, and the phase shift increases from zero when $U/t^* \sim 0$ to a finite value when U/t^* is large. However, if the conduct electron concentration n_c is far away from 0.5, P_2 is not the ground-state configuration, and we should consider the segregated phase (SP).

In Fig. 4 we see that when the local electrons configuration is SP, the phase shift first increases as U/t^* increases from zero to finite value, and then jumps to zero when U/t^* is larger than a finite value which is a function of n_c. This is consistent with previous numerical simulations.[22] This case is similar to the two local electron case, where the phase shift first increases and then decreases to zero *smoothly* as U/t^* increases. While, in the case of $n_f=0.5$, the phase shift goes to zero *suddenly*.

When the conduct electron concentration is intermediately large, the ground-state configuration Γ_g is a complicated function of U/t^* and n_c, i.e., $\Gamma_g(U/t^*,n_c)$. And the phase shift $\delta^{\Gamma_g}(U/t^*,n_c)$ can be also calculated in this formalism if one knows a general expression of the density of states of the conduct electrons.

V. CONCLUSION AND DISCUSSIONS

In summary, with the Falicov-Kimball model, we have given the general exact expression of the local electron Green function, then applied it to study the correlation effects of the local electrons in one dimension. For the two local electrons case, the correlation exponent of the local electron Green function has weak even-odd oscillation with the distance between these two local electrons, and it approaches zero in the strong coupling limit. While, at half filling of the local electrons, the ground-state phase is complicated. When the conduct electron concentration is near 0.5, the ground-state configuration is the chessboard phase (P_2) for a considerable range of U/t^*, and the correlation exponent increases from zero to a finite value as U/t^* increases. When the conduct electron concentration is far away from 0.5, the ground-state configuration is the segregated phase, and the correlation exponent first increases and then jumps to zero when U/t^* is larger than a finite value which is a function of n_c.

ACKNOWLEDGMENTS

Y. L. Liu thanks the hospitality of the Max-Plank Institute for Physics of Complex Systems where some of this work was carried out. This work was supported by the NSF of China, Grant No. 90403015.

---

[1] B. A. Jones and C. M. Varma, Phys. Rev. Lett. **58**, 843 (1987); B. A. Jones, C. M. Varma, and J. W. Wilkins, *ibid.* **61**, 125 (1988); R. M. Fye, *ibid.* **72**, 916 (1994); I. Affleck, A. W. W. Ludwig, and B. A. Jones, Phys. Rev. B **52**, 9528 (1995).

[2] A. C. Hewson, *The Kondo Problem to Heavy Fermions* (Cambridge Univ. Press, Cambridge, 1993).

[3] H. Q. Lin, H. Y. Shik, Y. Q. Wang, C. D. Batista, and J. E. Gubernatis, J. Magn. Magn. Mater. **281**, 240 (2004); H. Y. Shik, Y. Q. Wang, J. E. Gubernatis, and H. Q. Lin, J. Appl. Phys. **95**, 7195 (2004).

[4] J. K. Freericks and V. Zlatić, Rev. Mod. Phys. **75**, 1333 (2003); A. Georges, G. Kotliar, W. Krauth, and M. J. Rozenberg, *ibid.* **68**, 13 (1996).

[5] H. Jeong, A. M. Chang, and M. R. Melloch, Science **293**, 2221 (2001); J. C. Chen, A. M. Chang, and M. R. Melloch, Phys. Rev. Lett. **92**, 176801 (2004).

[6] J. K. Freericks, C. Gruber, and N. Macris, Phys. Rev. B **60**, 1617 (1999).

[7] W. Chung and J. K. Freericks, Phys. Rev. Lett. **84**, 2461 (2000).

[8] Y. L. Liu, Int. J. Mod. Phys. B **16**, 4127 (2002); Phys. Rev. B **71**, 014404 (2005).

[9] Y. L. Liu, Phys. Rev. B **72**, 045123 (2005).

[10] G. D. Mahan, Phys. Rev. **163**, 612 (1967).

[11] P. Nozières and C. T. De Dominicis, Phys. Rev. **178**, 1097 (1969).

[12] U. Brandt and C. Mielsch, Z. Phys. B: Condens. Matter **75**, 365 (1989); **79**, 295 (1990); **82**, 37 (1991).

[13] W. Metzner and D. Vollhardt, Phys. Rev. Lett. **62**, 324 (1989); U. Brandt and M. P. Urbanek, Z. Phys. B: Condens. Matter **89**, 297 (1992); J. K. Freericks, V. M. Turkowski, and V. Zlatić, Phys. Rev. B **71**, 115111 (2005).

[14] P. Farkasovšký, Z. Phys. B: Condens. Matter **104**, 553 (1997); Phys. Rev. B **65**, 081102(R) (2002); G. Czycholl, *ibid.* **59**, 2642 (1999); L. G. Sarasua and M. A. Continentino, *ibid.* **65**, 233107 (2002); Q. Si, G. Kotliar, and A. Georges, *ibid.* **46**, 1261 (1992).

[15] N. I. Muskhelishvili, *Singular Integral Equations* (P. Noordhoff Ltd., Groningen, The Netherlands, 1953).

[16] It is reduced to the single impurity scattering problem at $2R=0$.

[17] D. R. Hamann, Phys. Rev. Lett. **26**, 1030 (1971).
[18] R. Lyzwa, Physica A **192**, 231 (1993).
[19] J. K. Freericks and L. M. Falicov, Phys. Rev. B **41**, 2163 (1990).
[20] J. K. Freericks, E. H. Lieb, and D. Ueltschi, Phys. Rev. Lett. **88**, 106401 (2002).
[21] Z. Gajek, J. Jedrzejewski, and R. Lemanski, Physica A **223**, 175 (1996).
[22] F. B. Anders and G. Czycholl, Phys. Rev. B **71**, 125101 (2005).