

**Vertex corrections to the electrical conductivity in models with elastically scattered electrons**

V. Janiš\* and V. Pokorný

*Institute of Physics, Academy of Sciences of the Czech Republic, Na Slovance 2, CZ-18221 Praha, Czech Republic*

(Received 21 January 2010; published 7 April 2010)

We study quantum coherence of elastically scattered lattice fermions. We calculate vertex corrections to the electrical conductivity of electrons scattered either on thermally equilibrated or statically distributed random impurities. We demonstrate that the sign of the vertex corrections to the Drude conductivity is in both cases negative. Quantum coherence due to elastic back scatterings always leads to diminution of diffusion.

DOI: [10.1103/PhysRevB.81.165103](https://doi.org/10.1103/PhysRevB.81.165103)

PACS number(s): 71.10.Fd, 71.28.+d, 72.10.Fk

**I. INTRODUCTION**

It is very difficult to describe full electron correlations due to a number of complex phenomena related to the quantum character of the electron. It is hence appropriate to approach the full description of electron correlations iteratively in several stages. The first one is the static mean-field approximation of the Hartree type. Such a mean-field theory completely neglects both charge and spin fluctuations and reduces the interacting system to a Fermi gas with renormalized, self-consistently determined, densities. Such a simplification may deliver reliable results only for macroscopic static quantities in the weak-coupling limit. Electron correlations in this approximation have no impact on dynamical and transport properties.

The next level in a comprehensive modeling of strong electron correlations are models and approximations allowing for charge fluctuations. In these models the spin of electrons does not play a significant role and electrons are subjected only to a potential scattering. It means that electrons are only scattered on fluctuations of the atomic potential in the lattice. The potential fluctuations are caused by impurities that may be distributed in the crystal either regularly or randomly. The paradigm for the former situation is the Falicov-Kimball model<sup>1</sup> (FKM) and for the latter the disordered Anderson model (DAM).<sup>2</sup> Unlike the static mean-field approximations, the models with a potential scattering lead to quantum dynamical effects and are applicable to the entire range of the interaction strength (variance of the potential fluctuations). The potential scattering does consequently affect spectral and transport properties of the system.

A common feature of the models with potential scatterings only is that energy is conserved during scattering events and need not be treated as a dynamical variable. Each energy, however, is renormalized in a different manner and hence the energy (frequency) is used as an external label. Conservation of energy in scattering events is a significant simplification in the description of electron correlations. It allows for an exact solution in the limit of infinite spatial dimensions (dynamical mean-field theory), where the effect of strong potential fluctuations may be studied without uncontrolled approximations.<sup>3-6</sup>

The two models, FKM and DAM, are standardly used for different purposes. The former one is aimed at a description of quantum fluctuations caused by electron correlations in thermally equilibrated states while the latter one was introduced so that a response of a disordered electron gas to weak-electromagnetic nonequilibrium perturbations can be

estimated in a controlled way. Both the models have served well their original purposes. The Falicov-Kimball model has been successfully applied to a simplified description of correlation-induced metal-insulator<sup>7,8</sup> and valence-change<sup>9</sup> transitions in rare-earth compounds or atoms in optical lattices.<sup>10,11</sup> The disordered Anderson model has been used to describe the spectral and transport properties of metallic alloys<sup>12</sup> and vanishing of diffusion, called Anderson localization.<sup>13</sup> There have been efforts to describe the combined effect of electron correlations and randomness in the disordered Falicov-Kimball model<sup>6</sup> or Anderson localization in FKM.<sup>14</sup> Only a few attempts have, however, been made in the calculation of the response of FKM to nonequilibrium perturbations beyond the mean-field approach.<sup>15</sup> In particular, it is little known about the electrical conductivity of FKM beyond the mean-field, Drude contribution.<sup>16</sup>

It is the aim of this paper to fill up this gap and to propose a systematic way how to calculate vertex corrections to the Drude (mean-field) electrical conductivity in models with elastic scatterings only, that is, FKM, DAM, or a disordered FKM. The method we use is an expansion around the mean-field solution obtained from the asymptotic limit to high spatial dimensions. We calculate the leading-order vertex correction in high spatial dimensions being of order  $1/d^2$  while the Drude conductivity is of order  $1/d$ . We demonstrate that the vertex corrections have a universal behavior for all models of elastically scattered electrons and are always negative, independent of whether they are caused by an external random potential (quenched randomness) or by static, thermally equilibrated electron correlations (annealed randomness).

**II. ELECTRICAL CONDUCTIVITY OF ELASTICALLY SCATTERED ELECTRONS**

Elastic scatterings of electrons are caused by either internal or external fluctuations of atomic potentials of frozen ions forming a crystalline lattice. That is, interactions of electrons of the same sort are excluded in models with elastic scatterings. They are actually forbidden in spinless models with locally interacting fermions. These models hence contain either more than one type of electrons or an externally governed distribution of atomic potentials. We consider only the elementary version of such models and take into account only two types of electrons, extended and localized ones. We further assume homogeneity in the distribution of the localized electrons and hence the noninteracting part of the Hamiltonian describing such a situation reads

$$\hat{H}_0 = \sum_{\mathbf{k}} \epsilon(\mathbf{k}) c^\dagger(\mathbf{k}) c(\mathbf{k}) + E_f \sum_i f_i^\dagger f_i. \quad (1a)$$

We are interested in dynamical properties of the delocalized electrons induced by fluctuations of the atomic potential the extended electrons feel. To this purpose we introduce an interacting term

$$\hat{H}_I = \sum_i [V_i + U f_i^\dagger f_i] c_i^\dagger c_i, \quad (1b)$$

where  $c_i = N^{-1} \sum_{\mathbf{k}} c(\mathbf{k}) \exp\{-i\mathbf{k} \cdot \mathbf{R}_i\}$ . We denoted  $V_i$  the atomic level of the ion situated in the elementary cell centered around the lattice vector  $\mathbf{R}_i$  and  $U$  is the interaction strength between the extended and localized electrons. We generally assume that the atomic potential  $V_i$  is a random variable with a static site-independent probability distribution of its values determined externally. If  $U=0$  the full Hamiltonian  $\hat{H} = \hat{H}_0 + \hat{H}_I$  is that of the Anderson model with disordered electrons and if  $V_i=0$ , the full Hamiltonian describes the Falicov-Kimball model. We hence see that the most general elementary Hamiltonian for elastically scattered electrons is just a disordered FKM. Actually, both the contributions to the interacting Hamiltonian from Eq. (1b) introduce randomness into the distribution of atomic potentials the extended electrons feel. Potential  $V_i$  represents a static (quenched) randomness and the interaction  $U$  a dynamical (annealed) one. Both contributions can be treated on the same footing.

We are not interested in this paper in equilibrium thermodynamic properties of FKM but rather in its dynamical behavior and particularly in the static, optical conductivity. The electrical conductivity, although static, is nevertheless a dynamical property since we need at least two different energies (small imaginary parts) to determine it. The Kubo formula for the diagonal part of the electrical conductivity in models with only elastically scattered electrons can be written as<sup>17</sup>

$$\begin{aligned} \sigma_{\alpha\alpha} = & -\frac{e^2}{N^2} \sum_{\mathbf{k}\mathbf{k}'} v_\alpha(\mathbf{k}) v_\alpha(\mathbf{k}') \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} \left\{ \frac{df(\omega)}{d\omega} [G_{\mathbf{k}\mathbf{k}'}^{AR}(\omega, \omega; \mathbf{0}) \right. \\ & - G_{\mathbf{k}\mathbf{k}'}^{AA}(\omega, \omega; \mathbf{0})] + \frac{1}{2} f(\omega) \frac{\partial}{\partial \omega} [G_{\mathbf{k}\mathbf{k}'}^{RR}(\omega, \omega; \mathbf{0}) \\ & \left. - G_{\mathbf{k}\mathbf{k}'}^{AA}(\omega, \omega; \mathbf{0})] \right\} \\ = & -\frac{e^2}{N^2} \sum_{\mathbf{k}\mathbf{k}'} v_\alpha(\mathbf{k}) v_\alpha(\mathbf{k}') \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} \frac{df(\omega)}{d\omega} [G_{\mathbf{k}\mathbf{k}'}^{AR}(\omega, \omega; \mathbf{0}) \\ & - \Re G_{\mathbf{k}\mathbf{k}'}^{RR}(\omega, \omega; \mathbf{0})], \quad (2) \end{aligned}$$

where  $v_\alpha(\mathbf{k}) = \partial \epsilon(\mathbf{k}) / \partial k_\alpha$  is the group velocity in the direction  $\alpha$  and the averaged (translationally invariant) two-particle Green's functions are defined as

$$G_{\mathbf{k}\mathbf{k}'}^{AR}(\omega, \omega'; \mathbf{q}) = G_{\mathbf{k}\mathbf{k}'}^{(2)}(\omega - i0^+, \omega' + i0^+; \mathbf{q}),$$

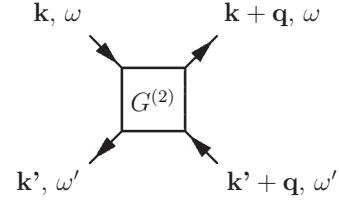


FIG. 1. Translationally invariant (averaged) two-particle Green's function in momentum space in the notation used in the Kubo formula for electrical conductivity.

$$G_{\mathbf{k}\mathbf{k}'}^{RR}(\omega, \omega'; \mathbf{q}) = G_{\mathbf{k}\mathbf{k}'}^{(2)}(\omega + i0^+, \omega' + i0^+; \mathbf{q}).$$

We denoted  $\omega = E - \mu$  the energy measured from the Fermi level and  $f(E) = 1 / (1 + e^{\beta(E - \mu)})$  is the Fermi function. See Fig. 1 for the way the variables in the two-particle Green's function are used in this paper. We utilized integration per parts to derive the second equality in Eq. (2). We use throughout the paper symbols  $\Re$  and  $\Im$  for the real and imaginary parts of complex quantities.

The expression for the electrical conductivity simplifies if we resort to zero temperature. Then the integrals over frequencies can be performed explicitly and we obtain a simple formula

$$\sigma_{\alpha\alpha} = \frac{e^2}{2\pi N^2} \sum_{\mathbf{k}\mathbf{k}'} v_\alpha(\mathbf{k}) v_\alpha(\mathbf{k}') [G_{\mathbf{k}\mathbf{k}'}^{AR} - \Re G_{\mathbf{k}\mathbf{k}'}^{RR}] \quad (3)$$

with the values of the two-particle Green's functions at the Fermi energy. We used an abbreviation  $G_{\mathbf{k}\mathbf{k}'}^{AR} = G_{\mathbf{k}\mathbf{k}'}^{AR}(0, 0; \mathbf{0})$ .

The two-particle Green's function  $G^{(2)}$  carries information on both the uncorrelated and correlated motion of two electrons. Only the latter one is the genuine two-particle quantity. It is our task to identify this contribution to the electrical conductivity. To do so, we introduce the two-particle vertex  $\Gamma$  defined from an equation

$$G_{\mathbf{k}\mathbf{k}'}^{AR} = G_{\mathbf{k}\mathbf{k}'}^A G_{\mathbf{k}\mathbf{k}'}^R [\delta(\mathbf{k} - \mathbf{k}') + \Gamma_{\mathbf{k}\mathbf{k}'}^{AR} G_{\mathbf{k}\mathbf{k}'}^A G_{\mathbf{k}\mathbf{k}'}^R], \quad (4)$$

where we again used a notation  $G_{\mathbf{k}\mathbf{k}'}^R = G_{\mathbf{k}\mathbf{k}'}^R(0)$ . With the aid of the vertex function we can decompose the conductivity tensor into two parts

$$\sigma_{\alpha\alpha} = \sigma_{\alpha\alpha}^{(0)} + \Delta\sigma_{\alpha\alpha}, \quad (5)$$

where

$$\sigma_{\alpha\alpha}^{(0)} = \frac{e^2}{\pi N} \sum_{\mathbf{k}} |v_\alpha(\mathbf{k})|^2 |\Im G^R(\mathbf{k})|^2 \quad (6)$$

is the standard one-electron or Drude conductivity at zero temperature. The genuine two-particle contribution is called a vertex correction and is proportional to the appropriate matrix element of the two-particle vertex that at zero temperature reads

$$\begin{aligned} \Delta\sigma_{\alpha\alpha} = & \frac{e^2}{2\pi N^2} \sum_{\mathbf{k}\mathbf{k}'} v_\alpha(\mathbf{k}) v_\alpha(\mathbf{k}') \{ |G_{\mathbf{k}\mathbf{k}'}^R|^2 \Delta \Gamma_{\mathbf{k}\mathbf{k}'}^{AR} |G_{\mathbf{k}\mathbf{k}'}^R|^2 \\ & - \Re [(G_{\mathbf{k}\mathbf{k}'}^R)^2 \Delta \Gamma_{\mathbf{k}\mathbf{k}'}^{RR} (G_{\mathbf{k}\mathbf{k}'}^R)^2] \}. \quad (7) \end{aligned}$$

It is not the full two-particle vertex  $\Gamma$  that is important for the

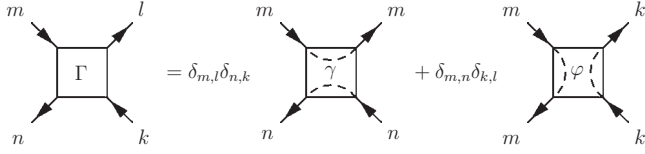


FIG. 2. Graphical representation of Eq. (12). The dashed lines within the boxes indicate charge propagation from the incoming to the corresponding outgoing line.

electrical conductivity but only its odd part  $\Delta\Gamma$ . That is, only the part of the vertex function being on bipartite lattices an odd function in fermionic momenta  $\mathbf{k}$  and  $\mathbf{k}'$ , contributes to the electrical conductivity.

### III. EQUILIBRIUM MEAN-FIELD THERMODYNAMICS

The Kubo formula for the electrical conductivity, Eq. (2), was derived within the linear-response theory and hence the Green's functions entering this formula are the equilibrium ones. To estimate quantitatively the vertex corrections to the electrical conductivity we need to know the equilibrium thermodynamics of FKM. To reduce the impact of uncontrolled approximations we should at best know the exact equilibrium grand potential. An exact solution to FKM is known in the limit of infinite spatial dimensions (mean-field limit) with which we start up. The equilibrium thermodynamics of the disordered FKM in  $d=\infty$  was analyzed in Ref. 6. The functional of the averaged grand potential was found to be represented via a set of complex variational parameters  $G_n$  and  $\Sigma_n$ , where the index  $n$  corresponds to the  $n$ th fermionic Matsubara frequency

$$\beta\langle\Omega\rangle_{av} = - \sum_{n=-\infty}^{\infty} \left\{ \int_{-\infty}^{\infty} dE \rho(E) \ln[i\omega_n + \mu - E - \Sigma_n] + \langle \ln[1 + G_n(\Sigma_n - V)] \rangle_{av} \right\} - \langle \ln[1 + \exp\{\beta(\mu - E_f - \mathcal{E}_V)\}] \rangle_{av}. \quad (8)$$

Symbol  $\langle \rangle_{av}$  stands for averaging over the distribution of the random potential  $V_i$ . The shift of the  $f$ -electron atomic level  $\mathcal{E}_V$  is determined via the same complex numbers  $G_n$  and  $\Sigma_n$

$$\mathcal{E}_V = -T \sum_{n=-\infty}^{\infty} \ln \left[ 1 - \frac{UG_n}{1 + G_n(\Sigma_n - V)} \right] \quad (9)$$

and depends on the configuration of the random atomic potential  $V$ .

The equilibrium thermodynamics is obtained as a stationarity point with respect to small variations in complex numbers  $\Sigma_n$  and  $G_n$  of the averaged grand potential  $\langle\Omega\rangle_{av}$  from Eq. (8). Vanishing of variations in the former and the latter parameters lead to a couple of equations for each Matsubara frequency  $i\omega_n$

$$G_n = \int_{-\infty}^{\infty} \frac{d\epsilon \rho(\epsilon)}{i\omega_n + \mu - \epsilon - \Sigma_n}, \quad (10a)$$

$$1 = \left\langle \frac{1 - f(E_f + \mathcal{E}_V)}{1 + G_n(\Sigma_n - V)} + \frac{f(E_f + \mathcal{E}_V)}{1 + G_n(\Sigma_n - V - U)} \right\rangle_{av}. \quad (10b)$$

The first equation states that in equilibrium  $G_n$  is the local element of the one-electron thermal Green's function with a self-energy  $\Sigma_n$ . The second equation determines the value of the equilibrium self-energy. These equations of thermal equilibrium must be completed with an equation determining the chemical potential  $\mu$  from the total electron density  $n$ . This equation then is

$$n = \langle f(E_f + \mathcal{E}_V) \rangle_{av} + \sum_{n=-\infty}^{\infty} G_n e^{i\omega_n 0^+} = \langle f(E_f + \mathcal{E}_V) \rangle_{av} - \int_{-\infty}^{\infty} \frac{d\omega}{\pi} f(\omega) \Im G^R[\omega - \Sigma^R(\omega)], \quad (11)$$

where  $G^R(z) = N^{-1} \sum_{\mathbf{k}} G^R(\mathbf{k}, z)$ . Equations (9), (10a), (10b), and (11) fully determine the equilibrium thermodynamics for a given temperature  $T$  and a total particle density  $n$ .

Only one-particle equilibrium functions can be directly calculated from the grand potential  $\langle\Omega\rangle_{av}$ . To derive higher-order correlation functions we have to slightly perturb equilibrium and look at the corresponding response functions. For the electrical conductivity we need to know two-particle vertex within the mean-field theory is to keep the nonequilibrium perturbation local.<sup>18</sup> The resulting vertex remains local and is only frequency (energy) dependent.

The equilibrium two-particle vertex has generally three independent (Matsubara) frequencies. In the case of FKM investigated here, the resulting two-particle vertex can have maximally two independent frequencies. The two frequencies can, however, be placed in two different ways. The full local two-particle vertex for FKM can be represented as

$$\Gamma_{mn,kl}^{MF} = \delta_{m,l} \delta_{n,k} \gamma_{m,n} + \delta_{m,n} \delta_{k,l} \varphi_{m,k}. \quad (12)$$

The two contributions to the full vertex correspond to two ways the electron lines go through the vertex. The electron line entering into the vertex at the upper left corner goes out either via the upper right corner (vertex  $\gamma$ ) or via the lower left corner (vertex  $\varphi$ ). See Fig. 2 for a graphical representation and notation used in Eq. (12). Due to energy conservation in this model the incoming and outgoing frequencies must equal. Notice that the two vertices  $\gamma$  and  $\varphi$  never mix up and are completely detached in the solution. The former vertex is relevant for the transport while the latter one for the thermodynamics. It is hence sufficient to take into account only vertex  $\gamma$  for the calculation of the electrical conductivity.

We can represent vertex  $\gamma$  via a local Bethe-Salpeter equation with a local irreducible vertex  $\Lambda_{m,n}$ . We have

$$\Gamma_{m,n} = \frac{\Lambda_{m,n}}{1 - \Lambda_{m,n} G_m G_n}. \quad (13)$$

Charge conservation leads to a generalized Ward identity that matches a nonequilibrium variation in the self-energy  $\delta\Sigma_{m,n}$  with the equilibrium irreducible vertex  $\Lambda_{m,n}$

$$\Lambda_{m,n} = \frac{\delta \Sigma_{m,n}}{\delta G_{m,n}} = \frac{1}{G_m G_n} [1 - \lambda_{m,n}^{-1}], \quad (14)$$

where we abbreviated

$$\lambda_{m,n} = \left\langle \frac{1 - f(E_f + \mathcal{E}_V)}{[1 + G_m(\Sigma_m - V)][1 + G_n(\Sigma_n - V)]} + \frac{f(E_f + \mathcal{E}_V)}{[1 + G_m(\Sigma_m - V - U)][1 + G_n(\Sigma_n - V - U)]} \right\rangle_{av}. \quad (15)$$

The latter representation was derived with the aid of stationarity equations, Eqs. (10a) and (10b).

We have derived all the necessary equilibrium quantities needed for the calculation of the electrical conductivity. We must, however, go beyond the local, mean-field limit in order to calculate transport properties. That is, we have to perturb the equilibrium with time-dependent nonlocal excitations. To do it in a controlled manner we use a perturbation expansion around a mean field. This can be consistently achieved within an asymptotic expansion in high spatial dimensions.

#### IV. EXPANSION AROUND MEAN FIELD—VERTEX CORRECTIONS TO THE ELECTRICAL CONDUCTIVITY

An asymptotic expansion around a mean-field solution in  $d = \infty$  for noninteracting disordered electrons was recently derived by one of us in Ref. 19. The only ingredients of such an expansion are the local mean-field vertex  $\gamma$  and the nonlocal one-electron propagator. The relevance and applicability of this expansion goes beyond the model of disordered electrons. It can be applied to any model where energy is conserved in scattering events (elastic scatterings) and where only spatial fluctuations matter. The disordered FKM studied here falls into this category and we can hence use the expansion concept of Ref. 19 for it. It is a considerable advantage to expand around a mean-field solution since all the effects of scatterings on impurities are included already in the local vertex  $\gamma$ . The variance of the potential fluctuations is not a small parameter and the expansion terms do not depend on whether the scatterings are due to thermally equilibrated or randomly distributed static impurities, that is, whether the disorder is annealed or quenched.

We construct the expansion around a mean field as an asymptotic series on a hypercubic lattice in high spatial dimensions. The expansion parameter is the off-diagonal one-electron propagator from the mean-field theory. We define

$$\bar{G}(\mathbf{k}, \zeta) = \frac{1}{\zeta - \epsilon(\mathbf{k})} - \int \frac{d\epsilon \rho(\epsilon)}{\zeta - \epsilon}, \quad (16)$$

where we denoted  $\zeta = z - \Sigma(z)$  and the local self-energy  $\Sigma(z)$  is that of the mean-field solution. The off-diagonal two-particle bubble is a convolution of the off-diagonal one-electron propagators. We hence define

$$\bar{\chi}(\zeta, \zeta'; \mathbf{q}) = \frac{1}{N} \sum_{\mathbf{k}} \bar{G}(\mathbf{k}, \zeta) \bar{G}(\mathbf{k} + \mathbf{q}, \zeta'). \quad (17)$$

The frequency indices are external parameters and we suppress them when they are not necessary to specify a particular type of the one- or two-electron propagators.

The asymptotic limit of the full two-particle vertex in high spatial dimensions contains beyond the local mean-field vertex  $\gamma$  also nonlocal contributions from the electron-hole and electron-electron ladders.<sup>19</sup> It can be represented as follows:

$$\Gamma_{\mathbf{k}\mathbf{k}'}(\mathbf{q}) = \gamma \left\{ 1 + \gamma \left[ \frac{\bar{\chi}(\mathbf{q})}{1 - \gamma \bar{\chi}(\mathbf{q})} + \frac{\bar{\chi}(\mathbf{Q})}{1 - \gamma \bar{\chi}(\mathbf{Q})} \right] \right\}, \quad (18)$$

where we denoted  $\mathbf{Q} = \mathbf{q} + \mathbf{k} + \mathbf{k}'$  the momentum conserved in the electron-electron channel. Notice that the contribution from the electron-hole channel with  $\bar{\chi}(\mathbf{q})$  is part of the two-particle vertex from the coherent potential approximation (CPA) and can be derived from a Velický-Ward identity.<sup>20</sup> The two-particle vertex from CPA does not carry the full  $1/d$  correction to the local vertex and moreover it is not electron-hole symmetric on the two-particle level.<sup>19</sup> A consistent extension of the local mean-field two-particle vertex must contain both nonlocal contributions from the electron-hole and the electron-electron channels as given in Eq. (18).

The contribution from multiple scatterings in the electron-electron channel to the asymptotic two-particle vertex is important, in particular, in the calculation of the vertex corrections to the mean-field electrical conductivity. The CPA vertex, as notoriously known, does not generate vertex corrections, unless we introduce odd dispersion relations in multiorbital models. It is only the second term in the parentheses on the right-hand side of Eq. (18) that contributes to the averaged conductivity and the we can identify

$$\Delta \Gamma_{\mathbf{k}\mathbf{k}'}(\mathbf{q}) = \gamma^2 \frac{\bar{\chi}(\mathbf{k} + \mathbf{k}' + \mathbf{q})}{1 - \gamma \bar{\chi}(\mathbf{k} + \mathbf{k}' + \mathbf{q})} \quad (19)$$

from the formula for the vertex corrections to the electrical conductivity, Eq. (7). Inserting representation from Eq. (19) into Eq. (7) we obtain

$$\Delta \sigma_{\alpha\alpha}^{MF} = \frac{e^2}{2\pi N^2} \sum_{\mathbf{k}\mathbf{k}'} \left\{ (\gamma^{RA})^2 |G_{\mathbf{k}}^R|^2 \frac{v_{\alpha}(\mathbf{k}) \bar{\chi}^{RA}(\mathbf{k} + \mathbf{k}') v_{\alpha}(\mathbf{k}')}{1 - \gamma^{RA} \bar{\chi}^{RA}(\mathbf{k} + \mathbf{k}')} |G_{\mathbf{k}'}^R|^2 - \Re \left[ (\gamma^{RR})^2 (G_{\mathbf{k}}^R)^2 \frac{v_{\alpha}(\mathbf{k}) \bar{\chi}^{RR}(\mathbf{k} + \mathbf{k}') v_{\alpha}(\mathbf{k}')}{1 - \gamma^{RR} \bar{\chi}^{RR}(\mathbf{k} + \mathbf{k}')} (G_{\mathbf{k}'}^R)^2 \right] \right\}. \quad (20)$$

It is a general formula for the leading-order corrections to the mean-field (Drude) conductivity and can be applied in any

dimension. Vertex  $\Delta \Gamma$  contains the so-called Cooper pole being the image of the diffusion pole contained in the CPA

vertex after an appropriate electron-hole transformation. The Cooper pole is responsible for the so-called weak-localization corrections in the Anderson model of disordered electrons.<sup>21</sup> These corrections are here identical with those determined by Eq. (20). They are negative and diverge in spatial dimensions  $d \leq 2$ . The mean-field corrections to the electrical conductivity from Eq. (20) can effectively be applied only in dimensions  $d \geq 3$  and not too close to the band edges.

We can further simplify Eq. (20) in that we get rid of the local mean-field vertex  $\gamma$ . We utilize the Ward identity from Eq. (14) connecting the one-electron self-energy  $\Sigma$  and the two-particle irreducible vertex  $\Lambda$ . Using the stationarity equation, Eq. (10a), we easily obtain

$$\Lambda_{+-} = \frac{\Im \Sigma_+}{\Im G_+} = \frac{1}{\chi_{+-}(\mathbf{0})}, \quad (21a)$$

$$\Lambda_{++} = \frac{\Sigma'_+}{G'_+} = \frac{Z_+}{\chi_{++}(\mathbf{0})}, \quad (21b)$$

where we denoted  $\Sigma'_+ = \partial \Sigma_+(\omega) / \partial \omega|_{\omega=0}$ ,  $G'_+ = \partial G_+(\omega) / \partial \omega|_{\omega=0}$ , and  $Z_+ = \Sigma'_+ / (\Sigma'_+ - 1)$ . With these relations and the local Bethe-Salpeter equation, Eq. (13), we can rewrite Eq. (20) to

$$\Delta \sigma_{\alpha\alpha}^{MF} = \frac{e^2}{2\pi N^2} \sum_{\mathbf{k}\mathbf{k}'} \left\{ \frac{|G_{\mathbf{k}}^R|^2 v_{\alpha}(\mathbf{k}) \bar{\chi}_{+-}(\mathbf{k} + \mathbf{k}') v_{\alpha}(\mathbf{k}') |G_{\mathbf{k}'}^R|^2}{[\chi_{+-}(\mathbf{0}) - \langle G_+ \rangle]^2 [\chi_{+-}(\mathbf{0}) - \chi_{+-}(\mathbf{k} + \mathbf{k}')]}} - \Re \left\{ \frac{Z_+^2 (G_{\mathbf{k}}^R)^2 v_{\alpha}(\mathbf{k}) \bar{\chi}_{++}(\mathbf{k} + \mathbf{k}') v_{\alpha}(\mathbf{k}') (G_{\mathbf{k}'}^R)^2}{(\chi_{++}(\mathbf{0}) - Z_+ \langle G_+ \rangle^2) [\chi_{++}(\mathbf{0}) - Z_+ \chi_{++}(\mathbf{k} + \mathbf{k}')]}} \right\} \right\}, \quad (22)$$

where we used an abbreviated notation

$$\langle G_{\pm} \rangle = \int_{-\infty}^{\infty} \frac{d\epsilon \rho(\epsilon)}{[E_F - \epsilon - \Sigma_{\pm} \pm i0^+]}, \quad (23a)$$

$$\langle G_{\pm}^2 \rangle = \int_{-\infty}^{\infty} \frac{d\epsilon \rho(\epsilon)}{[E_F - \epsilon - \Sigma_{\pm} \pm i0^+]^2}. \quad (23b)$$

Representation [Eq. (22)] of the vertex corrections to the electrical conductivity does not explicitly contain the

strength of elastic scatterings in the model. This strength is beyond the self-energy of the one-electron propagators implicitly comprised in the spatial fluctuations of the two-particle bubble  $\chi(\mathbf{q})$ . A singular structure of the integrand in momentum representation of the vertex corrections to the Drude conductivity becomes transparent in Eq. (22).

## V. VERTEX CORRECTIONS TO THE ELECTRICAL CONDUCTIVITY FROM HIGH SPATIAL DIMENSIONS

To evaluate the vertex corrections to the mean-field electrical conductivity, Eq. (20), we resort to high spatial dimensions where we can explicitly perform the convolutions over momenta. We are interested only in the leading-order contributions in the inverse spatial dimension  $1/d$ . The conductivity vanishes in the mean-field limit,  $d \rightarrow \infty$ , where only local quantities survive. The actual mean-field conductivity is due to the velocity in a particular direction proportional to  $1/d$  and hence can be treated only asymptotically for  $d \rightarrow \infty$ . On a hypercubic lattice we have  $v_{\alpha}(\mathbf{k}) = \partial \epsilon(\mathbf{k}) / \partial k_{\alpha} = t d^{-1/2} \sin k_{\alpha}$ . Inserting this result in the mean-field conductivity, Eq. (6), we obtain the Drude conductivity on a hypercubic  $d$ -dimensional lattice to be

$$\sigma_0 = \frac{e^2 t^2}{4\pi d} [\langle |G_+|^2 \rangle - \Re \langle G_+^2 \rangle] = \frac{e^2 t^2}{2\pi d} \Im \Sigma^2 \langle |G_+ G_-|^2 \rangle. \quad (24)$$

To evaluate the vertex corrections we represent the one- and two-particle propagators so that we can separate the Cartesian components of momenta. We use the following integral representation for the one-electron propagator:

$$G(\mathbf{k}, \zeta_{\pm}) = -i \int_0^{\infty} du e^{\pm iu\zeta_{\pm}} \prod_{\nu=1}^d \exp\left\{ \pm \frac{itu}{\sqrt{d}} \cos k_{\nu} \right\}, \quad (25)$$

where we assumed that  $\Im \zeta_+ > 0$  and  $\Im \zeta_- < 0$  in order to keep the integrals convergent. Here  $k_{\nu}$  is the  $\nu$ th Cartesian component of momentum  $\mathbf{k}$  on a  $d$ -dimensional hypercubic lattice.

The two-particle bubble can be represented in a similar way. Performing the integration over momenta we obtain in the leading asymptotic order for  $d \rightarrow \infty$

$$\chi(\mathbf{q}; \zeta, \zeta') = - \int_0^{\infty} du \int_0^{\infty} dv e^{iu\zeta} e^{iv\zeta'} \exp\left\{ \frac{t^2(u^2 + v^2)}{4} \right\} \prod_{\nu=1}^d \exp\left\{ - \frac{uv t^2}{2d} \cos q_{\nu} \right\}. \quad (26)$$

For simplicity we assumed that both complex energies  $\zeta$  and  $\zeta'$  have positive imaginary parts. A generalization to different imaginary parts is straightforward.

The above integral representations suffice to evaluate the leading order of the vertex corrections. We realize that the denominator in the representation of the vertex corrections, Eq. (20), does not contribute in the leading order for  $d \rightarrow \infty$ . We denote

$$J_{\alpha\alpha}^{RR} = \frac{1}{N^2} \sum_{\mathbf{k}\mathbf{k}'} (G_{\mathbf{k}}^R)^2 v_{\alpha}(\mathbf{k}) \bar{\chi}^{RR}(\mathbf{k} + \mathbf{k}') v_{\alpha}(\mathbf{k}') (G_{\mathbf{k}'}^R)^2. \quad (27)$$

We use the integral representation separating the Cartesian components of momenta. We then have

$$J_{\alpha\alpha}^{RR} = \frac{t^2}{d} \int_0^\infty da \int_0^\infty db \int_0^\infty da' \int_0^\infty db' \int_0^\infty du \int_0^\infty dv e^{i(a+b+a'+b'+u+v)\zeta_+} \exp\left\{-\frac{t^2(u^2+v^2)}{4}\right\} \sin k_\alpha \sin k'_\alpha \prod_{\nu=1}^d \exp\left\{\frac{i(a+b)t}{\sqrt{d}} \cos k_\nu + \frac{i(a'+b')t}{\sqrt{d}} \cos k'_\nu - \frac{uv t^2}{2d} \cos(k_\nu + k'_\nu)\right\}.$$

The leading nonvanishing contribution from the summation over momenta is proportional to  $1/d$ . Performing the calculation we obtain

$$J_{\alpha\alpha}^{RR} = \frac{t^4}{8d^2} \int_0^\infty da \int_0^\infty db \int_0^\infty da' \int_0^\infty db' \int_0^\infty du \int_0^\infty dv e^{i(a+b)\zeta_+} \exp\left\{-\frac{(a+b)^2 t^2}{4}\right\} e^{i(a'+b')\zeta_+} \exp\left\{-\frac{(a'+b')^2 t^2}{4}\right\} e^{iu\zeta_+} \exp\left\{\frac{u^2 t^2}{4}\right\} \times e^{iv\zeta_+} \exp\left\{\frac{v^2 t^2}{4}\right\} uv. \quad (28)$$

Using representation [Eq. (23)] we can rewrite  $J_{\alpha\alpha}^{RR}$  in a simple form

$$J_{\alpha\alpha}^{RR} = -\frac{t^4}{8d^2} \langle G_+ G_+ \rangle^2 \langle G_+^2 \rangle \langle G_+^2 \rangle, \quad (29a)$$

where each Green's function  $G_+$  stands for the selection of the imaginary part of the propagator, the retarded one. In the case of the retarded and advanced propagators we then have

$$J_{\alpha\alpha}^{RA} = -\frac{t^4}{8d^2} \langle G_+ G_- \rangle^2 \langle G_+^2 \rangle \langle G_-^2 \rangle. \quad (29b)$$

We use these results to represent the vertex correction to the electrical conductivity in high spatial dimensions. We obtain

$$\Delta_d \sigma = -\frac{e^2 t^4}{16\pi d^2} \{ \langle |G_+|^2 \rangle^2 \langle G_+^2 \rangle^2 \gamma_{+-}^2 - \Re[\langle G_+^2 \rangle^4 \gamma_{++}^2] \}. \quad (30)$$

With the aid of the Ward identity, Eq. (21), we can further simplify the expression for the leading contribution to the electrical conductivity beyond the Drude formula in  $d$  spatial dimensions

$$\Delta_d \sigma = -\frac{e^2 t^4}{16\pi d^2} \left\{ \frac{\langle |G_+|^2 \rangle^2 \langle G_+^2 \rangle^2}{[\langle |G_+|^2 \rangle - \langle G_+ \rangle^2]^2} - \Re \left[ \frac{Z_+^2 \langle G_+^2 \rangle^4}{[\langle G_+^2 \rangle - Z_+ \langle G_+ \rangle^2]^2} \right] \right\}. \quad (31)$$

The sign of the vertex correction is negative. Although it is only the leading asymptotic term, it determines the overall sign of the vertex correction. The neglected higher-order terms must be summed to infinite order so that the denominators on the right-hand side of Eq. (22) are recovered. The higher-order terms then do not change the sign of the leading-order vertex correction to the electrical conductivity.

## VI. RESULTS

To reach numerical values for the vertex corrections to the electrical conductivity we need the stationarity equation for

the self-energy, Eq. (10b). This equation significantly simplifies in the pure model at half filling with a symmetry between  $c$  and  $f$  electrons, it means if  $n_c = 1/2$ ,  $n_f = 1/2$ ,  $E_f = 0$ , and  $E_c = U/2$ . We then obtain  $\Re \Sigma(0) = U/2$  and the solution for the local functions can be expressed in terms of a single parameter

$$x = \langle |G_+|^2 \rangle = \int_{-\infty}^{\infty} \frac{d\epsilon \rho(\epsilon)}{\epsilon^2 + \Im \Sigma_+^2} > 0.$$

It is easy to find from Eq. (10b) that

$$\Im \Sigma_+ = -\sqrt{\frac{1}{x} - \frac{U^2}{4}}, \quad (32a)$$

$$\Im G_+ = -\sqrt{x \left(1 - \frac{U^2}{4}x\right)}, \quad (32b)$$

$$\gamma_{+-} = \frac{4}{U^2 x^2} = \gamma_{++}. \quad (32c)$$

The stationarity equation for the parameter  $x$  reads

$$1 = \int_{-\infty}^{\infty} \frac{d\epsilon \rho(\epsilon)}{x \left(\epsilon^2 - \frac{U^2}{4}\right) + 1} \equiv \left\langle \frac{1}{x \left(\epsilon^2 - \frac{U^2}{4}\right) + 1} \right\rangle, \quad (33)$$

where we again abbreviated the integral over energy weighted by the density of energy states by angular brackets.

The two-electron bubble for zero momentum can be represented as follows:

$$\langle G_+^2 \rangle = -x \left[ 1 - \frac{U^2}{2}x + 2 \left(1 - \frac{U^2}{4}x\right)x_2 \right], \quad (34a)$$

where we introduced variance of nonlocal fluctuations

$$x_2 = \frac{1}{x^2} \left[ \int_{-\infty}^{\infty} \frac{d\epsilon \rho(\epsilon)}{[\epsilon^2 + \Im \Sigma_+^2]^2} - x^2 \right]. \quad (34b)$$

The Drude conductivity then is

$$\sigma_0 = \frac{e^2}{2\pi d} x \left(1 - \frac{U^2}{4} x\right) (1 + x_2) \quad (35)$$

and the vertex correction reads

$$\Delta_d \sigma = -\frac{e^2}{\pi d^2} \frac{1 - \frac{U^2}{4} x}{U^4} \left[1 - \frac{U^2}{2} x + 2 \left(1 - \frac{U^2}{4} x\right) x_2\right]^2 \times \left\{ U^2 x - 4x_2 \left[1 - \frac{U^2}{2} x + \left(1 - \frac{U^2}{4} x\right) x_2\right] \right\}. \quad (36)$$

We set the energy scale  $t=1$ . Note that  $0 \leq x \leq 4/U^2$  for  $U^2 \leq 4\langle\epsilon^2\rangle$ . The upper limit on the interaction strength  $U$  in the above equations is imposed by the metal-insulator transition at which  $x=0$  and the density of the extended electrons at the Fermi level vanishes.

The Drude conductivity in the weak-coupling limit ( $U \rightarrow 0$ ) diverges, that is, the resistivity vanishes as it should be for the Fermi gas without impurity scatterings. The two parameters  $x$  and  $x_2$  behave in the weak-coupling limit  $x \sim 4/U^2 - \pi^2 \rho(0)^2$  and  $x_2 \sim 2/U^2 \pi^2 \rho(0)^2 - 1$  and hence

$$\sigma_0 = \frac{e^2}{\pi d} \frac{1}{U^2}. \quad (37)$$

The vertex correction from Eq. (36) remains finite in the limit  $U \rightarrow 0$  even without external randomness in the atomic energy levels. This fact is a consequence of the singular structure of the two-particle bubbles  $x$  and  $x_2$  diverging as  $U^{-2}$  in the weak-coupling limit, hence the same reason why the Drude conductivity diverges for the Fermi gas. To derive an explicit expression for the weak-coupling vertex correction, we had to expand the asymptotic solution for the parameters  $x$  and  $x_2$  up to the third order in  $d^{-1}$ .

For the explicit calculation we used the semielliptic density of states (DOS)  $\rho(\omega) = 2/\pi\sqrt{1-\omega^2}$ . We choose the dimensionality parameter  $d=3$  in our calculations. The Drude conductivity is plotted in Fig. 3. It is compared to the DOS of the mobile electrons at the Fermi energy. Coulomb interaction decreases both the DOS and the conductivity down to the metal-insulator transition, where the self-energy diverges. The vertex correction  $\Delta\sigma$  from Eq. (36) is plotted in Fig. 4. The modulus of the vertex correction is not a monotonic function and it reaches maximum at about  $U_m \approx 0.82$ . The vertex correction is negative but is much smaller than the Drude conductivity. Their ratio is plotted in Fig. 5. Only close to the metal-insulator transition the vertex correction is of order of the mean-field conductivity.

The Falicov-Kimball model away from half filling is more complicated. First, we need two parameters to describe the local quantities. They are

$$x = \langle |G_+|^2 \rangle = \int_{-\infty}^{\infty} \frac{d\epsilon \rho(\epsilon)}{(E_F - \Re \Sigma - \epsilon)^2 + \Im \Sigma_+^2}$$

and

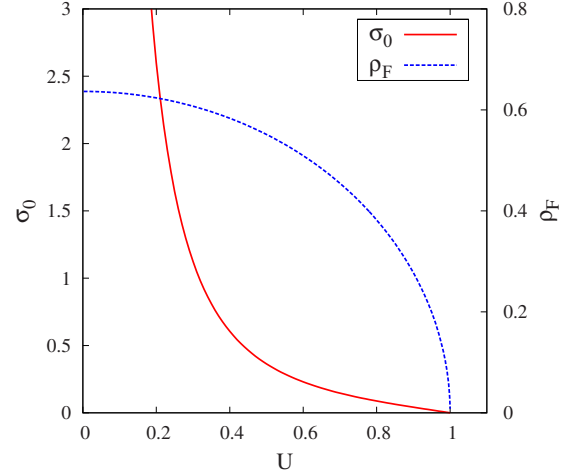


FIG. 3. (Color online) Drude conductivity  $\sigma_0$  (left scale) and density of states at the Fermi energy  $\rho_F$  (right scale) for the electron-hole symmetric Falicov-Kimball model with semielliptic density of states and  $d=3$ .

$$y = \int_{-\infty}^{\infty} \frac{d\epsilon \rho(\epsilon) \epsilon}{(E_F - \Re \Sigma - \epsilon)^2 + \Im \Sigma_+^2},$$

where we subtract the Fermi energy and the self-energy from their values in the electron-hole symmetric case  $n_f = 1/2$ ,  $n_c = 1/2$ . Explicit formulas are more involved and we do not present them here. Second, as discussed in Ref. 22, a nontrivial solution at zero temperature exists only for  $1/2 < n < 3/2$ . Outside this region the  $f$ -electron energy level is either empty ( $n \leq 1/2$ ) or fully filled ( $n \geq 3/2$ ). We plotted the Drude conductivity and DOS in Fig. 6 for a total filling  $n=0.7$ . The density of states at the Fermi energy is almost constant within the interval  $0 \leq U \leq 0.82$ , within which the extended electrons scatter on  $f$  electrons. The extended electrons go over to a Fermi gas in both limiting values of interaction, hence the Drude conductivity diverges at both ends. The asymptotics is, however, different at the two ends. The

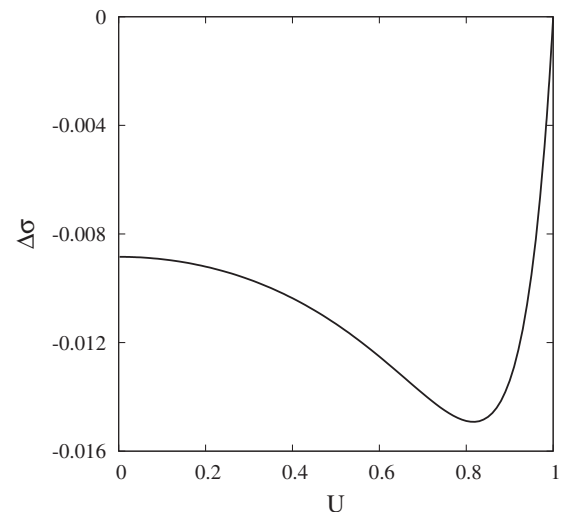


FIG. 4. Vertex correction to the conductivity for the electron-hole symmetric case.

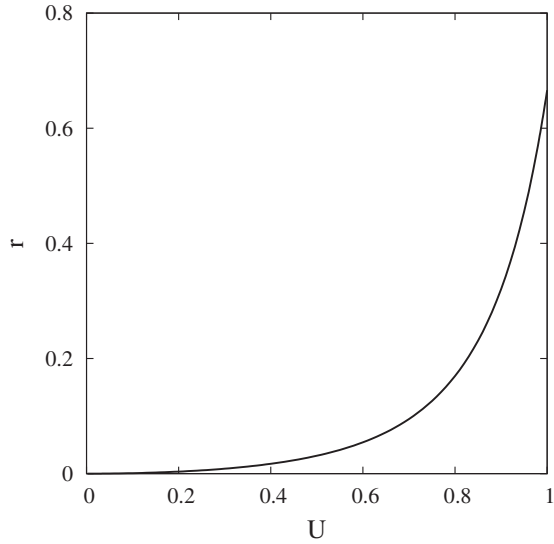


FIG. 5. Ratio  $r=|\Delta\sigma|/\sigma_0$  for the electron-hole symmetric case.

asymmetry between the two limiting interaction strengths is demonstrated in Fig. 7, where we plotted the vertex correction to the Drude conductivity. It is two orders smaller than the mean-field one. This is clearly seen from their ratio plotted in Fig. 8. The ratio is no longer a monotonically increasing function as in the electron-hole symmetric case but reaches maximum at  $U_m \approx 0.48$ .

VII. CONCLUSIONS

We studied effects of elastic scatterings of mobile electrons on either thermally equilibrated or frozen, randomly distributed static impurities. We concentrated on quantum coherence effects due to correlated back scatterings and its impact on the electrical conductivity. We calculated vertex corrections to the mean-field (Drude) conductivity. We used a systematic expansion around the mean-field solution via the asymptotic limit to high spatial dimensions. Our principal

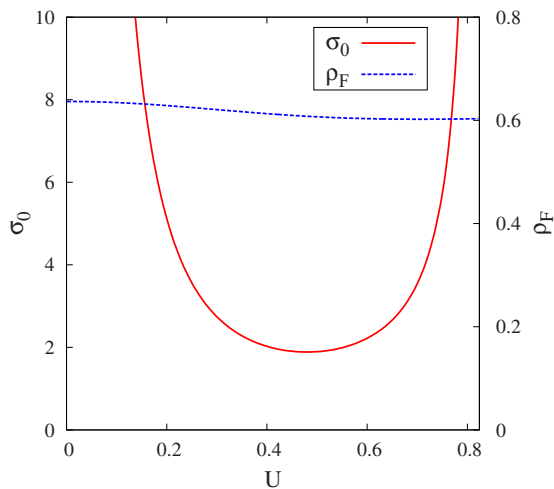


FIG. 6. (Color online) Drude conductivity (left scale) and density of states (right scale) for filling  $n=0.7$ .

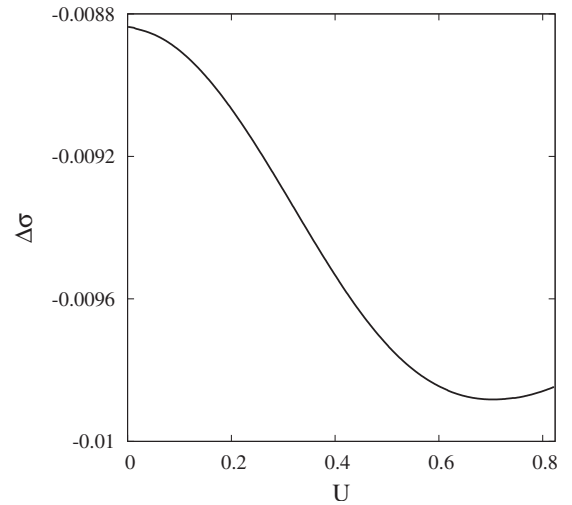


FIG. 7. Vertex correction to the conductivity for filling  $n=0.7$ .

finding is that elastic scatterings always lead to diminution of the Drude conductivity. That is, vertex corrections due to elastic scatterings have negative sign. The sign of the vertex correction is determined by its leading high-dimensional term, that is, by the numerators in Eq. (22). The sign of the vertex correction is not affected by the type of randomness in the distribution of the scattering impurities. Coulomb interaction in the pure Falicov-Kimball model has the same (qualitative) effect on the electrical conductivity as variance of fluctuations of the atomic potential in the disordered Anderson model, it hinders diffusion.

We explicitly calculated only the leading high-dimensional vertex correction to the Drude zero-temperature conductivity in the disordered phase of the Falicov-Kimball model without static randomness in atomic levels. We disregarded possible thermodynamic phases with a long-range order in the static  $f$  electrons (chessboard structure at half filling) since there the model is insulating. We found that the vertex correction in the metallic phase is quantitatively al-

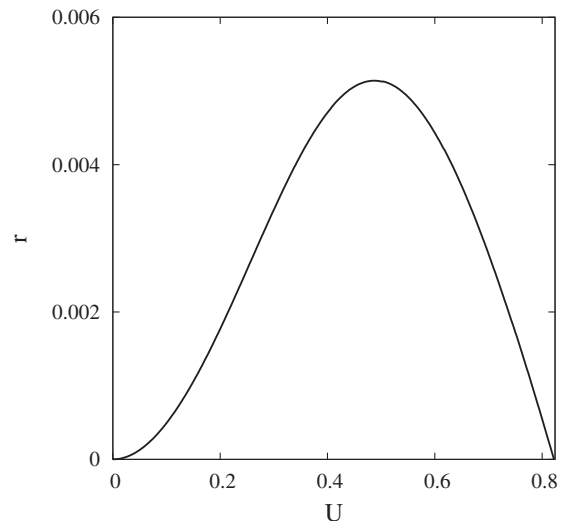


FIG. 8. Ratio  $r=|\Delta\sigma|/\sigma_0$  for filling  $n=0.7$ .



most everywhere two orders smaller than the Drude term. It is due to the fact that the Drude conductivity diverges in the limit of the Fermi gas while the vertex correction asymptotically approaches a finite value when the interaction is switched off. Only close to the metal-insulator transition in the electron-hole symmetric case the vertex correction is of order of the Drude one, however, they both vanish at the transition point. The leading high-dimensional contribution to the vertex correction of the mean-field conductivity is quantitatively negligible. It is important only for determining the sign of the vertex correction. To obtain a more realistic values of the vertex corrections in low-dimensional systems, one has to consider the full representation of the vertex correction from Eq. (22) containing the Cooper pole. Only then we are able to include a sizable impact of spatial dimensionality.

Extension of our calculation of the electrical conductivity to finite temperatures is straightforward via Eq. (2). This general representation is suitable for application of the Sommerfeld expansion. The thermal corrections to the zero-temperature conductivity in the metallic phase of the Falicov-Kimball model would be of order  $T^2$  provided the Sommerfeld expansion be regular. This seems, however, not to be the case of the electrical conductivity. The regular asymptotics can be modified by singularities in the derivatives

of the integrand (electron-hole Green's function) on the right-hand side of Eq. (2). Explicit calculations of the temperature dependence of the electrical conductivity and its vertex corrections in the metallic phase of the Falicov-Kimball will be performed elsewhere.

The method for evaluating vertex corrections to the mean-field electrical conductivity via an asymptotic expansion in high spatial dimensions is universal and is suitable for any model with elastically scattered electrons. We can hence use it to investigate whether the Coulomb interaction in FKM can lead to suppression of diffusion in low-dimensional systems as well as to study an interplay between the Anderson localization and Mott-Hubbard metal-insulator transition in the disordered Falicov-Kimball model.

#### ACKNOWLEDGMENTS

Research on this problem was carried out within Project No. AV0Z10100520 of the Academy of Sciences of the Czech Republic and supported in part by Grant No. 202/07/0644 of the Grant Agency of the Czech Republic. We thank M. Žonda for illuminating discussions on the numerical solution of the Falicov-Kimball model and J. Kolorenč for discussions on behavior of the Drude conductivity in the weak scattering limit.

\*janis@fzu.cz

- <sup>1</sup>L. M. Falicov and J. C. Kimball, *Phys. Rev. Lett.* **22**, 997 (1969).
- <sup>2</sup>P. W. Anderson, *Phys. Rev.* **109**, 1492 (1958).
- <sup>3</sup>V. Janiš, *Phys. Rev. B* **40**, 11331 (1989).
- <sup>4</sup>U. Brandt and C. Mielsch, *Z. Phys. B: Condens. Matter* **75**, 365 (1989).
- <sup>5</sup>V. Janiš, *Z. Phys. B: Condens. Matter* **83**, 227 (1991).
- <sup>6</sup>V. Janiš and D. Vollhardt, *Phys. Rev. B* **46**, 15712 (1992).
- <sup>7</sup>R. Ramirez, L. M. Falicov, and J. C. Kimball, *Phys. Rev. B* **2**, 3383 (1970).
- <sup>8</sup>J. K. Freericks and L. M. Falicov, *Phys. Rev. B* **45**, 1896 (1992).
- <sup>9</sup>I. Felner and I. Nowik, *Phys. Rev. B* **33**, 617 (1986).
- <sup>10</sup>C. Ates and K. Ziegler, *Phys. Rev. A* **71**, 063610 (2005).
- <sup>11</sup>P. Farkašovský, *Europhys. Lett.* **84**, 37010 (2008).
- <sup>12</sup>A. Gonis, *Green Functions for Ordered and Disordered Systems* (North-Holland, Amsterdam, 1992).
- <sup>13</sup>B. Kramer and A. MacKinnon, *Rep. Prog. Phys.* **56**, 1469 (1993).
- <sup>14</sup>K. Byczuk, *Phys. Rev. B* **71**, 205105 (2005).
- <sup>15</sup>J. K. Freericks and V. Zlatić, *Rev. Mod. Phys.* **75**, 1333 (2003).
- <sup>16</sup>P. de Vries, K. Michielsen, and H. de Raedt, *Z. Phys. B: Condens. Matter* **92**, 353 (1993); **95**, 475 (1994).
- <sup>17</sup>V. Janiš, J. Kolorenč, and V. Špička, *Eur. Phys. J. B* **35**, 77 (2003).
- <sup>18</sup>V. Janiš, *Phys. Rev. Lett.* **83**, 2781 (1999).
- <sup>19</sup>V. Janiš and J. Kolorenč, *Phys. Rev. B* **71**, 245106 (2005).
- <sup>20</sup>B. Velický, *Phys. Rev.* **184**, 614 (1969).
- <sup>21</sup>E. Akkermans and G. Montambaux, *Mesoscopic Physics of Electrons and Photons* (Cambridge University Press, Cambridge, 2007).
- <sup>22</sup>Q. Si, G. Kotliar, and A. Georges, *Phys. Rev. B* **46**, 1261 (1992).