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Vertex Corrections to the Electrical Conductivity of the Disordered Falicov–Kimball Model

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Quantum coherence of elastically scattered lattice fermions is studied. We calculate vertex corrections to the electrical conductivity of electrons scattered either on thermally equilibrated or statically distributed random impurities and we demonstrate that the sign of the vertex corrections to the Drude conductivity is in both cases negative.

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1. Model

The Coulomb interactions and disorder can individually result in a metal–insulator transitions (MIT). It is not much known how this transition is modified when both forces act simultaneously. It is the aim of this contribution to investigate such a situation when only elastic scatterings are taken into account.

We consider the disordered Falicov–Kimball model (FKM) described by the following Hamiltonian:

$$\mathcal{H} = t\sum_{\langle ij\rangle} c_i^\dagger c_j + U\sum_i c_i^\dagger c_i f_i^\dagger f_i + \sum_i V_i c_i^\dagger c_i, \qquad (1)$$

where $c_i^\dagger$ (c_i) represents a creation (annihilation) operator of an itinerant electron on site i and $f_i^\dagger$ (f_i) represents a creation (annihilation) operator for an electron localised on site i. We denoted by t the nearest-neighbor hopping amplitude for itinerant electrons, U is the interaction strength between the itinerant and localised electrons and finally V_i is the on-site random atomic potential with a static site-independent probability distribution $\mathcal{P}(V)$. For $U = 0$ the Hamiltonian (1) reduces to the disordered Anderson model. For $V_i = 0$ we recover the pure Falicov–Kimball model that can be interpreted as a model of electrons scattered on thermally equilibrated impurities where U represents the strength of a dynamic (annealed) disorder.

The exact solution for the FKM is known in $d = \infty$ limit and the equilibrium thermodynamics as well as transport properties were reviewed in [1]. There have been also efforts to describe the effect of randomness on the MIT in FKM by using a geometric mean of the local density of states [2, 3]. However, little is known about the electrical conductivity of FKM beyond the mean-field Drude contribution.

The method for calculating vertex corrections to the one-electron Drude conductivity for models with elastically scattered electrons was recently developed by us [4]. It is based on a systematic expansion around the $d = \infty$ mean-field solution via the asymptotic limit to high spatial dimensions [5]. We use the formulae for the averaged mean-field (Drude) conductivity σ_0 and the vertex correction to it $\Delta\sigma$ from Ref. [4].

2. Results and discussion

We evaluated numerically only the leading $1/d$-order vertex correction to the Drude zero-temperature conductivity from Ref. [4]. Its important feature is that it carries information about the sign of the correction. That is, whether elastic scatterings lead to increase or decrease of the mean-field conductivity. We set $t = 1$ as the energy unit. We resort here only to half-filling with a symmetric binary-alloy distribution of the random atomic potential $\mathcal{P}(V) = \frac{1}{2}[\delta(V - \Delta/2) + \delta(V + \Delta/2)]$, where Δ is the measure of disorder strength. For explicit calculations we use a semi-elliptic density of states $\rho(\varepsilon) = 2/\pi\sqrt{1-\varepsilon^2}$ and set the spatial dimension $d = 3$. We neglect the chess-board long-range order of the pure model, since the ground state is then insulating.

The Drude conductivity σ_0, total conductivity $\sigma_0 + \Delta\sigma$ and the density of states at the Fermi energy ρ_{F} for $U = 0.5$ are plotted in Fig. 1 as functions of disorder strength Δ. Disorder decreases both the density of states and the Drude conductivity down to the MIT which takes place at $\Delta_{\mathrm{c}} \approx 1.27$. The total conductivity vanishes at $\Delta \approx 1.2$ and becomes negative for larger Δ. This unphysical behavior indicates breakdown of the decomposition of the total conductivity into a mean-field and vertex corrections in regions close to the MIT. Another approach utilizing gauge invariance and the Einstein relation between the conductivity and diffusion from the density response function should be used to avoid negative sign of the conductivity [6].

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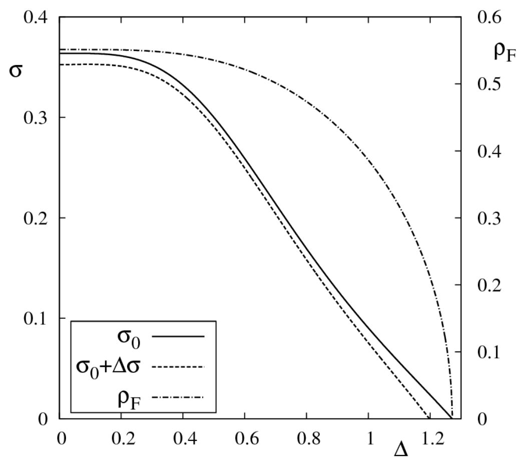

Fig. 1. Drude conductivity (solid line, left scale), total conductivity (dashed line, left scale) and the density of states at the Fermi energy (dashed-dotted line, right scale) for $U = 0.5$.

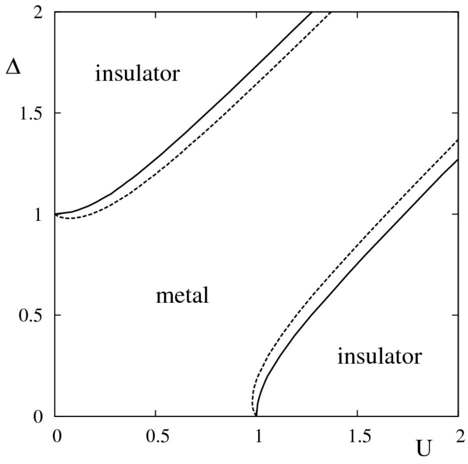

Fig. 2. Ground state phase diagram for the disordered FKM at half-filling. The dashed line indicates the border at which the vertex correction compensates the Drude term. The mean-field conductivity between the dashed and solid lines becomes unreliable.

The ground state phase diagram for the half-filled disordered FKM is shown in Fig. 2. Solid lines represent the metal–insulator transition lines. The dashed lines indicate vanishing of the total conductivity where $|\Delta\sigma| = \sigma_0$. We cannot rely on the mean-field conductivity and an unrenormalized perturbation theory beyond these lines.

3. Conclusions

Vertex corrections to the zero-temperature one--electron Drude conductivity of the disordered FKM were calculated. Numerical calculations prove that the vertex correction $\Delta\sigma$ is always negative as shown in [4] and almost everywhere at least one order smaller than the Drude term. Only close to MIT the vertex correction is of order of the Drude one and for $\varDelta > 0$ its absolute value can even become larger, leading to a negative total conductivity $\sigma_0 + \Delta\sigma$. This indicates that one needs to consider the full representation of the vertex correction with a two-particle self-consistency to describe energy regions close to MIT.

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