Anomalous resistivity and the electron-polaron effect in the two-band Hubbard model with one narrow band

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Abstract. We search for anomalous normal and superconductive behavior in the two-band Hubbard model with one narrow band. We analyze the influence of electron-polaron effect and Altshuler-Aronov effect on effective mass enhancement and scattering times of heavy and light components in the clean case. We find anomalous behavior of resistivity at high temperatures $T > W^*_h$ both in 3D and 2D situation. The SC instability in the model is governed by enhanced Kohn-Luttinger effect for p-wave pairing of heavy electrons via polarization of light electrons.

Key words: electron-polaron effect, two-band Hubbard model, marginality, anomalous resistivity

1. Introduction.

The two-band model plays an important role both in the physics of conventional multiband s-wave superconductors like Nb [1,2] and in the physics of high-$T_c$ materials [3]. It can be useful also for the description of anomalous normal and superconducting properties in different unconventional superconductors such as ruthenates Sr$_2$RuO$_4$, MgB$_2$, new superconductors (SC) based on FeAs layers such as BaFe$_2$(As$_{1-x}$P$_x$)$_2$ [4,5], layered semimetals, dichalcogenites and superlattices, organic superconductors et al. [6-8]. At the recent conference on stripes and high Tc superconductivity in Rome the fermion-boson multiband SC and Bose-BCS crossover was also analyzed in [9,10]. In this context we could mention as well [11,12]. In the present paper we consider two-band fermionic Hubbard model with one narrow band [13,14]. This model is a very rich one. It describes adequately mixed valence systems such as uranium-based HF and possibly also some other novel superconductors and transition-metal systems with orbital degeneracy such as complex magnetic oxides in optimally doped case. Moreover it contains such highly nontrivial effect as Electron Polaron Effect [15,16] in the homogeneous state. Let us verify this model with respect to marginality [17-19] and anomalous resistivity characteristics.

2. Two-band Hubbard model.

In real space the Hamiltonian of the two-band Hubbard model reads:

$$\hat{H} = -t_1 \sum_{\langle i,j \rangle \sigma} c^\dagger_{i\sigma} c_{j\sigma} - t_2 \sum_{\langle i,j \rangle \sigma} b^\dagger_{i\sigma} b_{j\sigma} - \epsilon_i \sum_{\sigma} n_{i\sigma} - \mu \sum_{\sigma} (n_{i\sigma}^c + n_{i\sigma}^v) + U_{aa} \sum_{i} n_{i\sigma}^c n_{i\sigma}^c + U_{bb} \sum_{i} n_{i\sigma}^v n_{i\sigma}^v + \frac{U_{ab}}{2} \sum_{i} n_{i\sigma}^c n_{i\sigma}^v \quad (1)$$
2.1 Electron-polaron effect.

We call the electron-polaron effect (EPE) the non-adiabatical part of many-particle wave function which describes the heavy particle dressed in a cloud of virtual electron-hole pairs of light particles. Nonadiabaticity of the cloud in some energy interval manifests itself when the heavy particle moves from one elementary cell to a neighboring one. Formally EPE is connected with interband Hubbard interaction $U_{hL}$. In the second order of perturbation theory

$$
\frac{m_h^*}{m_h} = Z_h^{-1} = 1 + b \ln \frac{m_h}{m_L},
$$

(2)

where $b = 2 f_0^2$, $Z_h^{-1} = 1 - \frac{\partial \Sigma_{hh}(\omega, \epsilon_q)}{\partial \omega} \bigg|_{\omega \to 0}$. 

In more general case of low density and strong Hubbard interaction $U_{L}$, in the unitary limit the polaron exponent $b$ can reach the value of $\frac{1}{2}$ and thus

$$
\frac{m_h^*}{m_h} \sim \left( \frac{m_h}{m_L} \right)^{b/(1-b)}.
$$

In the unitary limit the polaron exponent $b$ can reach the value of $\frac{1}{2}$ and thus

$$
\frac{m_h^*}{m_h} \sim \left( \frac{m_h}{m_L} \right)^{2}.
$$

And if we start with $\frac{m_h}{m_L} \sim 10$ in LD approximation for example we can finish with $\frac{m_h^*}{m_L} \sim 100$ due to many-body effects. Thus EPE can possibly explain the origin of a heavy mass in uranium-based HF.

2.2 Tendency towards phase separation.

Let us consider other mechanisms of mass-enhancement. The EPE is connected with Z-factor of heavy particle

$$
\frac{\partial \Sigma_{hh}(\omega, \epsilon_q)}{\partial \omega} \bigg|_{\omega \to 0}.
$$

However in 3D-case momentum dependence of heavy-light self energy

$$\frac{\partial \Sigma_{hl}(\omega, \mathcal{E}_q)}{\partial \mathcal{E}_q} \bigg|_{q \rightarrow q_F}$$  \hspace{1cm} (6)

also becomes very important. Hence as it is shown in [13,14] the full expression for $m^*/m_h$ in the second order of perturbation theory reads

$$\frac{m^*_h}{m_h} = 1 + b \ln \frac{m_h}{m_L} + \frac{b}{18} \frac{m_h n_h}{m_L n_L}$$  \hspace{1cm} (7)

and possess the additional term which is linear in the bare mass-ration $m_h/m_L$. If in LD approximation $m_h \sim 10m_L$, then this term becomes dominant over EPE contribution $\sim \ln \frac{m_h}{m_L}$ for large density mismatch $n_h \geq 5n_L$. It is very interesting that in 3D the same parameter $b \frac{m_h n_h}{m_L n_L} \geq 1$ governs the tendency towards phase-separation in the two-band model yielding negative partial compressibility

$$\chi_{hh}^1 \sim c_h^2 \sim (n_h / m_h) \left( \frac{\partial \mu_h}{\partial n_h} \right)$$  \hspace{1cm} (8)

where $\mu_h$ is chemical potential of the heavy particle. This result is in qualitative agreement with predictions of mean-field type variational analysis [20]. Note that in 2D case the contribution to $m^*$ from $\frac{\partial \Sigma_{hl}}{\partial \mathcal{E}_q}$ and the tendency towards phase-separation are absent due to specific form of polarization operator [13,14].

### 3. Transport properties

#### 3.1 Resistivity in the homogeneous case in 3D.

Exact solution of coupled kinetic equations with an account of umklapp processes yields for $p_{Fh} \sim p_{FL} \sim p_F \sim 1/d$ and low temperature $T < W_h^* < W_L$ for the inverse scattering times:

$$1/\tau_L \sim 1/\tau_{lh} \sim f_0 \frac{T^2}{W_h^* m_L}, \quad 1/\tau_h \sim 1/\tau_{hl} \sim f_0 \frac{T^2}{W_h^*}.$$  \hspace{1cm} This behavior corresponds to Landau Fermi-liquid picture. Accordingly for the conductivities we have: $\sigma_h \sim \sigma_{hl} \sim \sigma_L \sim \sigma_{lh} \sim \frac{\sigma_{\text{min}}}{b} \left( \frac{W_h^*}{T} \right)^2$ at low temperatures $T < W_h^*$. Thus the resistivity

$$R \sim \frac{1}{(\sigma_h + \sigma_L)} \sim \frac{b}{\sigma_{\text{min}}} \left( \frac{T}{W_h^*} \right)^2,$$  \hspace{1cm} (9)

where $\sigma_{\text{min}} = e^2 p_F / \hbar$ is minimal Mott-Regel conductivity in 3D. At high temperatures $T > W_h^*$ the inverse scattering times read: $1/\tau_L \sim 1/\tau_{lh} \sim b W_L, \quad 1/\tau_h \sim 1/\tau_{lh} \sim bT$. 

Thus heavy component is marginal – heavy electrons more diffusively in the surrounding of light electrons. However, light electrons scatter on the heavy ones as if on a static impurity and thus light component is non-marginal. Correspondingly for the conductivities:

\[
\sigma_L - \sigma_{Lh} \sim \frac{n_L e^2}{m_L} \tau_{Lh} \sim \frac{n_L e^2}{m_L b W_L} \sim \frac{\sigma_{\text{min}}^2}{b},
\]

(10)

\[
\sigma_h - \sigma_{hl} \sim \frac{\sigma_{\text{min}}^2}{b} \left( \frac{W_h^*}{T} \right)^2.
\]

(11)

with an account for Einstein relation \( \frac{\partial n_h}{\partial \varepsilon} \sim \frac{W_h^*}{T} \) at high temperatures \( T > W_h^* \). Hence the resistivity

\[
R \sim \frac{1}{(\sigma_{Lh} + \sigma_{hl})} \sim \frac{b}{\sigma_{\text{min}} \left[ 1 + \left( \frac{W_h^*}{T} \right)^2 \right]}.
\]

(12)

goes on saturation in 3D case (see Fig.2). This behavior of \( R(T) \) is typical for some uranium-based HF-compounds like UNi₂Al₃.

### 3.2. Altshuler-Aronov effect in 2D.

In 2D case we should take into account weak-localization corrections due to quantum-mechanical backward scattering to classical Drude formulae for conductivity of the light band[21,22]:

\[
\Delta \sigma_L / \sigma_{0L} \sim b \ln \frac{\tau_{\varphi}}{\tau}, \text{where } \sigma_{0L} = \frac{\sigma_{\text{min}}}{b} \text{ is classical Drude conductivity of light band, } \sigma_{\text{min}} = \frac{e^2}{\hbar}.
\]

Mott-Regel minimal conductivity in 2D, \( \tau_{\varphi} = \tau_{ee} = \tau_{LL} \) - is decoherence time for light electrons, \( \tau = \tau_{el} = \tau_{Lh} \) and \( l_{el} = v_{FL} \tau_{Lh} \) are elastic time and length, \( L_{\varphi} = \sqrt{D \tau_{\varphi}} = v_{FL} \sqrt{\tau_{Lh} \tau_{LL}} \) - is diffusive length, and \( 1/\tau_{Lh} \sim b W_L \) as in 3D. Correspondingly \( 1/\tau_{\varphi} = b^2 T \) - Altshuler-Aronov effect in "dirty" metal in 2D (electron-electron scattering time becomes marginal in dirty limit when between two subsequent scattering events for light electrons, a light electron scatters a lot of time on heavy electrons as if on almost elastic impurities, see Fig.3). Hence the conductivity of the light band:

\[
\sigma_L = \frac{\sigma_{\text{min}}}{b} \left( 1 - b \ln \frac{W_L}{b T} \right).
\]

Thus in 2D case light component has a tendency towards localization for \( b T \geq W_h^* \). Moreover the additional narrowing of the heavy band and additional localization of the light band are governed for \( b T \sim W_h^* \) by the same parameter \( b \ln \left( m_h / m_L \right) \geq 1 \).

### 3.3 Resistivity in homogeneous case in 2D.

Thus instead of desired marginal Fermi-liquid behavior at high-temperatures \( T > W_h^* \) in 2D we have even more interesting behavior of resistivity \( R \sim \frac{1}{(\sigma_L + \sigma_h)} \), where \( \sigma_h = \frac{\sigma_{\text{min}}}{b} \left( \frac{W_h^*}{T} \right)^2 \) as in the 3D
case. Namely $R(T)$ in 2D has a maximum and then a localization tail at higher temperatures (see Fig.4). Such resistivity characteristics resembles the curve for $R(T)$ in optimally doped layered CMR-systems.

3.4 Superconductivity in the two-band model with one narrow band.
In the homogeneous state the leading instability in the two band model at low electron densities corresponds to p-wave pairing via enhanced Kohn-Luttinger mechanism of SC [23-27]. Namely SC critical temperature is mostly governed by the pairing of heavy electrons via polarization of light electrons. P-wave critical temperature $T_{CJ}$ is strongly dependent upon relative fillings of the two bands $n_h/n_L$ and has a large and broad maximum for $n_h/n_L\sim 4$ in 2D [13,14,26,27]. For $\varepsilon_{Fh}\sim (30-50)K$ – typical for HF-compounds or semimetals (superlattices, heterostructures in 2D) $T_{CJ}$ can reach (1-5)K which is quite nice [13,14]. The two SC gaps for heavy and light electrons are opened simultaneously below this temperature [6].

Conclusions.
We have analyzed EPE and other mechanisms of mass-enhancement for the heavy electrons in the framework of the two-band Hubbard model with one narrow band. These mechanisms can produce the effective heavy masses $m_h^* \sim 100m_e$ which are typical for uranium-based HF-compounds. For a large mismatch between the densities of heavy and light bands $n_h >> n_L$ we also found a tendency towards phase-separation in 3D. We evaluate scattering times and resistivities in the homogeneous case in 3D and in 2D. Both in 3D and 2D cases at low temperatures $T < W_h^*$ the resistivity behaves in Landau Fermi-liquid fashion. At high temperatures $T > W_h^*$ the resistivity in 3D goes on saturation as in UNi$_2$Al$_3$. In 2D case due to weak-localization corrections of Altshuler-Aronov type the resistivity has a maximum and then a localization tail at higher temperatures. We analyzed the possibility of SC-transition in this model. The leading instability is towards triplet p-wave pairing and is governed by enhanced KL-mechanism of SC for pairing of heavy electrons via polarization of light electrons.

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Figure Captions

Fig. 1 The band structure in the two-band model with one narrow band. \( \text{Wh and WL} \) are the bandwidths of heavy and light electrons.

Fig. 2 The resistivity characteristics \( R(T) \) in the two-band model in 3D.

Fig. 3 Multiple scattering of light particle on the heavy ones in between of the scattering of light particle on another light particle. \( L\varphi \) is a diffusive length, \( l \) is elastic length.

Fig. 4 Resistivity \( R(T) \) in a 2D case for the two-band model with one narrow band.
FIGURES

Fig. 1

Fig. 2

Fig. 3

Fig. 4