J Supercond Nov Magn (2012) 25:1379–1382
DOI 10.1007/s10948-012-1523-3

ORIGINAL PAPER

# Anomalous Resistivity and the Electron–Polaron Effect in the Two-Band Hubbard Model with One Narrow Band

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Published online: 30 March 2012


**Abstract** We search for anomalous normal and superconductive behavior in the two-band Hubbard model with one narrow band. We analyze the influence of the electron–polaron effect and the 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 situations. The SC instability in the model is governed by an enhanced Kohn–Luttinger effect for p-wave pairing of heavy electrons via polarization of light electrons.

**Keywords** 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 $Sr_2RuO_4$, $MgB_2$, 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, etc. [6–8].

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At the 2011 conference on stripes and high $T_c$ superconductivity in Rome, the fermion-boson multiband SC and Bose-BCS crossover was analyzed [9, 10]. In this context, we will also mention [11, 12] as well. In the present paper, we consider the 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 an optimally doped case. Moreover, it contains such highly nontrivial effects as the 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:

$$\begin{aligned}\hat{H}' = &-t_h \sum_{\langle ij\rangle\sigma} a_{i\sigma}^+ a_{j\sigma} - t_L \sum_{\langle ij\rangle\sigma} b_{i\sigma}^+ b_{j\sigma} - \varepsilon_0 \sum_{i\sigma} n_{ih}^{\sigma} \\ &- \mu \sum_{i\sigma} \left(n_{i\sigma}^L + n_{i\sigma}^h\right) + U_{hh} \sum_i n_{ih}^{\uparrow} n_{ih}^{\downarrow} \\ &+ U_{LL} \sum_i n_{iL}^{\uparrow} n_{iL}^{\downarrow} + \frac{U_{hL}}{2} \sum_i n_{iL} n_{ih}\end{aligned}$$

We consider low density $(n_h + n_L)d^D \ll 1$ and strong-coupling limit $U_{hh} \sim U_{hL} \sim U_{LL} \gg W_L \gg W_h$ of this model; $\mu$ is a chemical potential. The band structure is presented in Fig. 1.

### 2.1 Electron–Polaron Effect

We call the electron–polaron effect (EPE) the nonadiabatical part of the many-particle wave function which describes

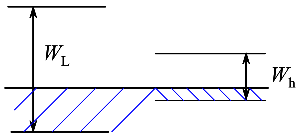


**Fig. 1** The band structure in the two-band model with one narrow band. $W_h$ and $W_L$ are the bandwidths of heavy and light electrons

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,

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

where $b = 2f_0^2$, $Z_h^{-1} = 1 - \frac{\partial \Sigma_{hL}(\omega,\varepsilon_q)}{\partial\omega}|_{\omega\to 0}$; $Z_h$ is $Z$-factor of heavy particle. In Born approximation, $f_0 = U_{hL}\nu_L(\varepsilon_F)$. In a more general case of low density and strong Hubbard interaction,

$$U_{hL} > W_L: \qquad f_0 = \frac{2dp_F}{\pi}.$$

is Galitskii gas parameter in 3D, $d$ is intersite distance. In 2D

$$f_0 = \frac{1}{2\ln\frac{1}{dp_F}}$$

is gas-parameter of Bloom. Generally (after collecting of the polaron exponent), the effective mass reads $\frac{m_h^*}{m_h} \sim (\frac{m_h}{m_L})^{b/(1-b)}$ [15, 16]. In the unitary limit, the polaron exponent $b$ can reach the value of $\frac{1}{2}$, and thus $\frac{m_h^*}{m_h} \sim \frac{m_h}{m_L}$. Accordingly, $\frac{m_h^*}{m_L} \sim (\frac{m_h}{m_L})^2$ 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 Toward Phase Separation

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

$$\left(\text{with } \frac{\partial\Sigma_{hL}(\omega,\varepsilon_{\vec q})}{\partial\omega}\bigg|_{\omega\to 0}\right).$$

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

$$\frac{\partial\Sigma_{hL}(\omega,\varepsilon_{\vec q})}{\partial\varepsilon_{\vec q}}\bigg|_{q\to p_F}$$

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

$$\frac{m_h^*}{m_h} = 1 + b\ln\frac{m_h}{m_L} + \frac{b}{18}\frac{m_h n_h}{m_L n_L}$$

and possesses the additional term which is linear in the bare mass-ration $m_h/m_L$. If in LD approximation $m_h \sim 10 m_L$, 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 toward phase-separation in the two-band model yielding negative partial compressibility

$$\chi_{hh}^{-1} \sim c_h^2 \sim (n_h/m_h)(\partial\mu_h/\partial n_h)$$

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 the 2D case the contribution to $m_h^*$ from $\frac{\partial\Sigma_{hL}}{\partial\varepsilon_{\vec q}}$ and the tendency toward phase-separation are absent due to specific form of the 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:

$$1/\tau_L \sim 1/\tau_{Lh} \sim f_0^2\frac{T^2}{W_h^*}\frac{m_h}{m_L}; \qquad 1/\tau_h \sim 1/\tau_{hL} \sim f_0^2\frac{T^2}{W_h^*}.$$

This behavior corresponds to Landau Fermi-liquid picture. Accordingly, for the conductivities, we have $\sigma_h \sim \sigma_{hL} \sim \sigma_L \sim \sigma_{Lh} \sim \frac{\sigma_{\min}}{b}(\frac{W_h^*}{T})^2$ at low temperatures $T < W_h^*$. Thus, the resistivity

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

where $\sigma_{\min} = \frac{e^2 p_F}{\hbar}$ is minimal Mott–Regel conductivity in 3D. At high temperatures $T > W_h^*$, the inverse scattering times read:

$$1/\tau_L \sim 1/\tau_{Lh} \sim bW_L, \qquad 1/\tau_h \sim 1/\tau_{hL} \sim bT.$$

Thus, the heavy component is marginal; heavy electrons are 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 nonmarginal. Correspondingly, for the conductivities,

$$\sigma_L \sim \sigma_{Lh} \sim \frac{n_L e^2}{m_L}\tau_{Lh} \sim \frac{n_L e^2}{m_L b W_L} \sim \frac{\sigma_{\min}}{b},$$

$$\sigma_h \sim \sigma_{hL} \sim \frac{\sigma_{\min}}{b}\left(\frac{W_h^*}{T}\right)^2$$

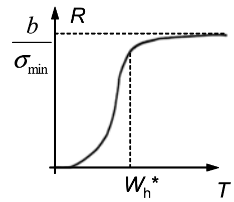


**Fig. 2** The resistivity characteristics $R(T)$ in the two-band model in 3D

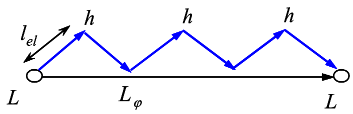


**Fig. 3** Multiple scattering of the light particle on the heavy ones in between the scattering of the light particle on another light particle. $L\varphi$ is a diffusive length, l is elastic length

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

$$R \sim \frac{1}{(\sigma_{Lh} + \sigma_{hL})} \sim \frac{b}{\sigma_{\min}[1 + (\frac{W_h^*}{T})^2]}$$

goes on saturation in 3D case (see Fig. 2). This behavior of $R(T)$ is typical for some uranium-based HF-compounds like $UNi_2Al_3$.

### 3.2 Altshuler–Aronov Effect in 2D

In the 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]: $\Delta\sigma_L/\sigma_{0L} \sim b \ln \frac{\tau_\varphi}{\tau}$, where $\sigma_{0L} = \frac{\sigma_{\min}}{b}$ is classical Drude conductivity of light band, $\sigma_{\min} = \frac{e^2}{\hbar}$—Mott–Regel minimal conductivity in 2D, $\tau_\varphi = \tau_{ee} = \tilde{\tau}_{LL}$—is decoherence time for light electrons, $\tau = \tau_{ei} = \tau_{Lh}$ and $l_{el} = v_{FL}\tau_{Lh}$ are elastic time and length, $L_\phi = \sqrt{D\tau_\varphi} = v_{FL}\sqrt{\tau_{Lh}\tilde{\tau}_{LL}}$ is diffusive length, and $1/\tau_{Lh} \sim bW_L$ as in 3D. Correspondingly, $1/\tilde{\tau}_{LL} = b^2 T$—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: $\sigma_L = \frac{\sigma_{\min}}{b}(1 - b \ln \frac{W_L}{bT})$. Thus, in the 2D case, the light component has a tendency toward localization for $bT \geq W_h^*$. Moreover, the additional narrowing of the heavy band and additional localization of the light band are governed for $bT \sim W_h^*$ by the same parameter $b \ln(m_h/m_L) \geq 1$.

### 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 $\sigma_h \sim \frac{\sigma_{\min}}{b}(\frac{W_h^*}{T})^2$ 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 resemble the curve for $R(T)$ in optimally doped layered CMR-systems.

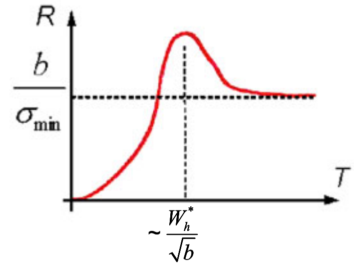


**Fig. 4** Resistivity $R(T)$ in a 2D case for the two-band model with one narrow band

### 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 $T_{C1}$ 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) $T_{C1}$ 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].

## 4 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 $m_h^* \sim 100 m_e$ which are typical for uranium-based HF-compounds. For a large mismatch between the densities of heavy and light bands $n_h \gg n_L$, we also found a tendency toward 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 $UNi_2Al_3$. In the 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 toward triplet p-wave pairing and is governed by enhanced KL-mechanism of SC for pairing of heavy electrons via polarization of light electrons.

**Acknowledgements** We are grateful to P. Fulde, Yu. Kagan, K.I. Kugel, N.V. Prokof'ev, P. Nozieres, and C.M. Varma for the numerous stimulating discussions. We acknowledge financial support of the RFBR Grant No. 11-02-00741.

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