Effective Masses of Carriers in the Degenerate Conduction Band: Interplay of Density of Electronic States Peculiarities and Magnetization

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For various DOS forms, it has been found that physically different regimes (of weak and strong magnetic field) can be realized in the concentration dependence of effective masses. In a weak field, despite the spin splitting occurrence due to translational mechanism of ferromagnetic order stabilization, a sharp change of the effective mass splitting exists for arbitrary electron concentrations, which can be utilized for tuning of the spin polarization by the external field. When the magnetic field is comparatively strong, the correlation band narrowing factor controls the critical concentration for the conduction type change. The DOS form governs the concentration dependence of transport characteristics, therefore the use of a realistic DOS for modeling of a spontaneous or magnetic field-induced ferromagnetic order is of importance.

Keywords: Mott-Hubbard ferromagnet, Degenerate conduction band, Effective masses of carriers, Density of electronic states.

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1. INTRODUCTION

In recent decades, a plethora of experimental data concerning the conductance of the nanoscopic systems has been accumulated [1, 2]. The correct interpretation of these results requires the development of theoretical models in which microscopic mechanisms of conductance can be identified. Strong intra-atomic Coulomb correlation described by parameter U appears to influence the electron hoppings between lattice sites or network nodes critically, which effect has been studied in detail in Hubbard-type models [3, 4]. If such a model, except the standard terms with interaction parameter U and inter-site hopping parameter t_{ij}, the correlated hopping processes are taken into account (see [5-8] and references therein) which make the observable physical characteristics dependent on the electron concentration n, then the electron-hole asymmetry of conductivity for narrow-band systems can be explained [6, 9]. Worth noting, the orbital degeneracy of electronic states is also responsible [10] for certain peculiarities of the system behavior with respect to the model of the non-degenerated band. In theoretical studies of conductance in strongly correlated system with orbital degeneracy, either the limiting cases are considered or a fixed electron concentration is assumed, which is not enough for a consistent theory of conductance for strongly correlated electron system with the orbital degeneracy. The effective Hamiltonians of the electron subsystem with doubly orbitally degenerate states have been formulated in papers [10-12]. In the paper [12], the form of unperturbed density of electronic states (DOS) has been shown to determine the critical concentrations at which a spontaneous ferromagnetic ordering occurs. These studies are to be continued for the model with orbital degeneracy of energy states. In this paper, we study the influence of the DOS form on the static conductivity and effective masses of current carriers by the modification of the kinetic energy and ferromagnetic order stabilization as well as an effect of the external magnetic field application on the transport properties of nanoscopic Mott-Hubbard material with partially filled orbitally degenerate narrow energy band.

2. CONDUCTANCE PECULIARITIES OF THE DOUBLY DEGENERATE BAND

In papers [12, 13], on the basis of Mott-Hubbard ferromagnet with doubly orbitally degenerate conduction band in the regime of strong Coulomb correlation and strong Hund's rule coupling, the quasiparticle energy spectra have been calculated. We shall use that for partially filled narrow band with $n < 1$:

$$E_{\vec{k}}^{\gamma s} = -\mu - z\mathrm{J}_{\mathrm{eff}} n_s + \alpha_{\gamma s} t_{\vec{k}}(n) + \beta_{\gamma s} - \eta_s h. \qquad (1)$$

Here the correlation band narrowing factor is

$$\alpha_{\gamma s} = 1 - n + n_s + (2n_{\bar{s}} n_s + n_s^2)/(1 - n + n_s), \qquad (2)$$

the correlation shift of the band center is determined by

$$\beta_{\gamma s} = -\frac{1}{1-n+n_s} \sum_{\vec{k}} t_{\vec{k}}(n) \begin{pmatrix} \left\langle X_i^{(\gamma\bar{s},0)} X_j^{(0,\gamma\bar{s})} \right\rangle_{\vec{k}} + \\ + \left\langle X_i^{(\bar{\gamma}\bar{s},0)} X_j^{(0,\bar{\gamma}\bar{s})} \right\rangle_{\vec{k}} + \\ + \left\langle X_i^{(\bar{\gamma}s,0)} X_j^{(0,\bar{\gamma}s)} \right\rangle_{\vec{k}} \end{pmatrix} \qquad (3)$$

where n_s stands for the concentration of electrons with spin projection s in orbital γ, for the equivalent orbitals we have

$$n_{\uparrow} = \frac{n+m}{4}; \; n_{\downarrow} = \frac{n-m}{4}. \qquad (4)$$

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Let us generalize the approach for the calculation of conductivity developed in papers [6, 9, 14, 15] on the case of the model with doubly orbitally degenerate energy states:

$$\sigma = -\frac{e^2 \tau z}{3Na} \sum_{\gamma s} \beta_{\gamma s} \left(1 - n + n_s\right) = -\frac{\sigma_0}{3} \sum_{\gamma s} \beta_{\gamma s} \left(1 - n + n_s\right). \quad (5)$$

Solving the equation for the system magnetization numerically by the ground state energy minimization, from Eq. (5) the concentration dependence of static conductivity can be found and the influence of the external magnetic field on the conductance of the orbitally degenerate system can be investigated. Fig. 1-Fig. 5 illustrate the peculiarities of the conductance in the external field characteristic for the system under consideration at different types of the model DOS. In distinction from the non-degenerate band, the effective inter-site exchange is but an additional factor in the spontaneous magnetic ordering stabilization, therefore we may limit ourselves to the case of no direct effective exchange and negligible correlated hopping, to emphasize the effects caused by the DOS form variations. The neglected factors can be easily incorporated into the above expressions, their role will be studied elsewhere.

There is an essential difference between the concentration dependence for different DOS forms, which is shown in Fig. 1. For the model rectangular DOS in the considered model only the saturated ferromagnetic state is realized, therefore, the concentration dependence calculated with the rectangular DOS completely reproduces the corresponding result for the non-degenerate model [16]. For semi-elliptical DOS which corresponds to a hypercubic lattice, at some critical value n_1 of the electron concentration (see [10] for details) the transition to the saturated ferromagnet state occurs and the increase of $\sigma(n)$ is damped till the value n_2, at which the ferromagnetic ordering saturates. Even more pronounced effect is observed for the DOS of a simple cubic lattice – in the region of concentration from n_1 to n_2 the conductivity decreases with rising n, which is caused by the competition between the electric field increasing the kinetic energy and ferromagnetic ordering processes which cause the electron localization. This concentration interval of the conductivity anomaly can be used for developing sensitive sensors of light and magnetic field.

One can see from Fig. 2 that the external magnetic field application smears out the sharp changes of $\sigma(n)$, similarly to the non-degenerate model [6, 9]. However, the characteristic values of the magnetic field in this case are substantially lower, which may be interpreted as greater comparative effectiveness of the translational mechanism of the ferromagnetic ordering in the model with orbital degeneracy. This conclusion is supported by the fact that the saturated ferromagnetism in the degenerate model is realized at lower concentrations than in the non-degenerate band. The applied magnetic field suppresses conductance through magnetic ordering. The concentration region $0 < n < 1$ can be split up in three distinct parts, namely the paramagnetic type of conductance, partial ferromagnetic ordering and saturated ferromagnetism. Both paramagnetic and saturated ferromagnetic regions are characterized by monotonic increase of σ at small electron concentrations and monotonic decrease of σ in more-than-half-filled lower subband.

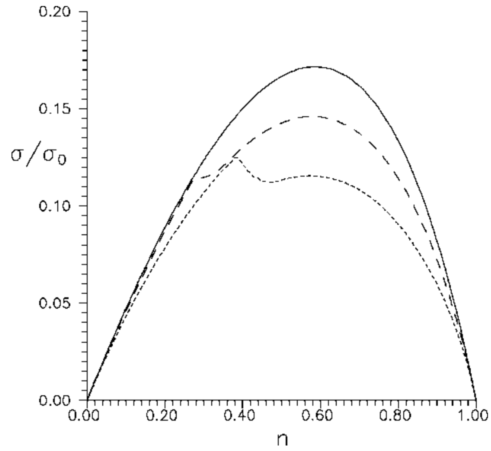

Fig. 1 – Influence of the DOS form on the magnitude of the static conductivity at change of band filling. Solid curve corresponds to rectangular DOS, long-dashed curve corresponds to semi-elliptic DOS, short-dashed curve corresponds to DOS for sc-lattice

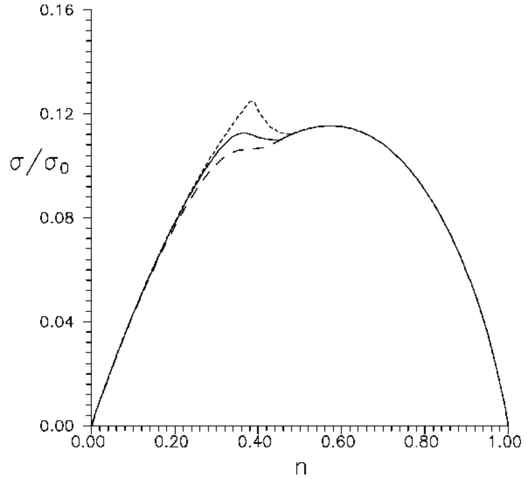

Fig. 2 – Influence of magnetic field on concentration dependence of conductivity at DOS of sc-lattice. Short-dashed curve corresponds to $h/w = 0$; solid curve – $h/w = 0.03$; long-dashed curve – $h/w = 0.06$

The peculiarities of concentration dependence are caused by the ferromagnetic ordering (see papers [1, 2], where corresponding analysis for non-degenerate case has been done). In the paramagnetic regime, the external magnetic field leads to an insignificant decrease of conductivity without a change of the $\sigma(n)$ dependence type. In the partial ordering regime $\sigma(n)$ decreases with the electron concentration increase due to the increase of magnetization, what makes the energy cost of the hopping through spin states $\lambda\downarrow\downarrow$ much greater, thus the corresponding processes become unfavorable. When this mechanism is exhausted (in the point of full spin polarization), the conductivity becomes a typical one for the saturated ferromagnet.

One can see from Fig. 3 that changes of conductivity in the degenerate model are smooth, the jumps of $\sigma(n)$ observed in non-degenerate case [1, 2] do not occur due to the absence of sharp changes of the system magnetization. The upper curve in Fig. 3 corresponds to fully polarized ferromagnetic system, so the external magnetic field has no effect. At parameters corresponding to the middle curve, the system in the absence of the external field is in the partial polarization regime. With increase of the applied field, the magnetization tends to its maximum value and the conductivity reaches a plateau corresponding to ferromagnetic state. The same effect could be obtained by setting non-zero value of J_{eff}. For the lowest curve in Fig. 3 one has a paramagnetic state before application of the magnetic field and the field itself is an origin of the system magnetization. The lower is the electron concentration, the higher value of magnetic field is needed to reach a plateau of $\sigma(n)$ dependence, which indicates the saturated ferromagnetic order stabilization.

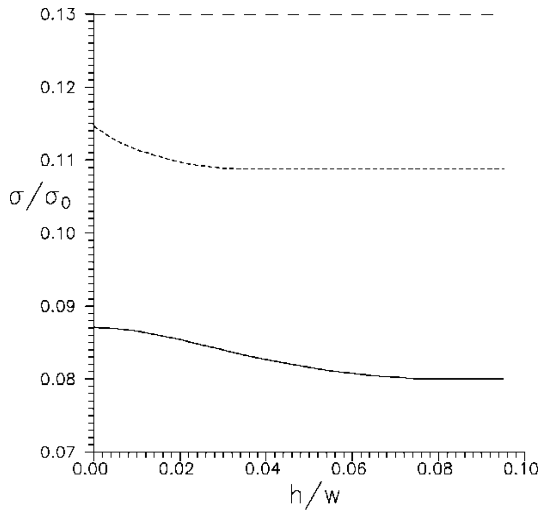

Fig. 3 – Magnetic field dependences of conductivity for fixed values of band filling (semi-elliptic DOS, $zJ_{\rm eff}/w = 0$). The upper curve corresponds to $n = 0.4$; middle curve $n = 0.3$; the lower curve $n = 0.2$

3. EFFECTIVE MASSES OF CURRENT CARRIERS AT VARIOUS DOS FORMS

For calculation of the effective masses we use the energy spectrum of the lower quasiparticle subband obtained in the previous works [12, 13], which describes the lower quasiparticle subband for the case of double orbital degeneracy, and use a generalization of the approach [9]:

$$m_{\rm eff}^{s} = \left(\frac{\partial^2 E^{\gamma s}\left(t_{\vec{k}}\right)}{\partial k^2} \right)^{-1} \tag{6}$$

where $E^{\gamma s}\left(t_{\vec{k}}\right)$ is the quasiparticle energy spectrum for $n < 1$.

For the lattice of simple cubic symmetry, the dependence of the hopping integral on momentum is determined by the expression

$$\left|t_{\vec{k}}\right| = 2t\left(\cos\left(k_x b\right) + \cos\left(k_y b\right) + \cos\left(k_z b\right)\right). \tag{7}$$

Using the formula for the correlation band narrowing factor $\alpha_{\gamma s}$ and expression (6), one has for the effective mass

$$m_{\rm eff}^{s} = \frac{m_0}{\left(1 - \tau_1 n\right)\alpha_{\gamma s}}, \tag{8}$$

where b stands for the lattice constant, m_0 denotes the effective mass of current carriers in the absence of intra-atomic Coulomb correlation and correlated hopping.

Renormalization of effective mass in the considered system is determined by two factors, namely the correlated hopping of electrons and band narrowing factor. From the obtained formula one concludes that the effective masses are spin-dependent, as prompted by the changes of conductivity in magnetic field. The realization of spontaneous (or field-induced) ferromagnetic ordering in the system at conditions, determined mainly by the form of unperturbed DOS, substantially modifies the behavior of effective masses. From the obtained expressions one can see that the effective masses appear to be spin-dependent which drives the conductivity changes in the external magnetic fields. The realization of spontaneous ferromagnetic ordering, for which the DOS form is responsible in the degenerate case, modifies the behavior of the effective masses substantially.

Spin-projection dependence of the mass enhancement has been analyzed for the case of non-degenerate Hubbard model [16-19], the orbitally doubly degenerate version of the Hubbard model [20], and has been confirmed experimentally recently [21, 22] for the case of 5*f*-electron systems.

We will focus on more realistic DOS forms in the case of electron concentration $n << 1$ (for $n > 1$ the absolute value of the effective mass will be renormalized substantially by the correlated hopping processes and the peculiarities of translational processes in doubly degenerate case).

In Fig. 4, the behavior of the effective mass at the change of the band filling is shown for the system with semi-elliptic DOS. It is worth to note that for rectangular DOS in the doubly degenerate model only saturated ferromagnetism is realized for arbitrary electron concentration. For this reason, the case of model rectangular DOS provides lower and upper bounds for effective masses of spin up and spin down current carriers. At concentration $n_1 = 0.28$, an onset of ferromagnetic order and spin-splitting of effective masses occur, and at $n_2 = 0.34$, the magnetic moment reaches saturation. In this point, $m_{\rm eff}^{\downarrow}$ increases sharply and $m_{\rm eff}^{\uparrow}$ takes the value characteristic to full spin polarization.

In investigations of translational ferromagnetism, asymmetric DOS, which reproduces the semi-elliptical DOS at $a = 0$ and has a peak on the band edge at $a = 1$, is widely used. In our opinion, for a nanoscopic system such a tunable DOS can be applied to model transport properties. In Fig. 5 and Fig. 6, the influence of the asymmetry parameter a on effective masses of carriers with different spin projections is shown. From these figures we conclude that shifting the maximum of DOS towards the bottom of conductivity band leads to essential change of electron concentration at which spin splitting arises. Occurrence of the concentration region with partial polarization at increasing a explains the smooth change of m_{eff} (decrease for spin-up electrons and increase for spin-down electrons).

In systems with large DOS asymmetries ($a > 0.5$), the behavior of $m_{eff}(n)$ does not differ, because the saturated ferromagnetism is realized in whole concentration interval. Our calculations show that in doubly degenerate model of the system with asymmetrical DOS, sharp changes of effective masses with small changes of electron concentration can be observed. Contrary to semi-elliptical DOS, we obtain that the spin splitting is not pronounced in the vicinity of critical concentration.

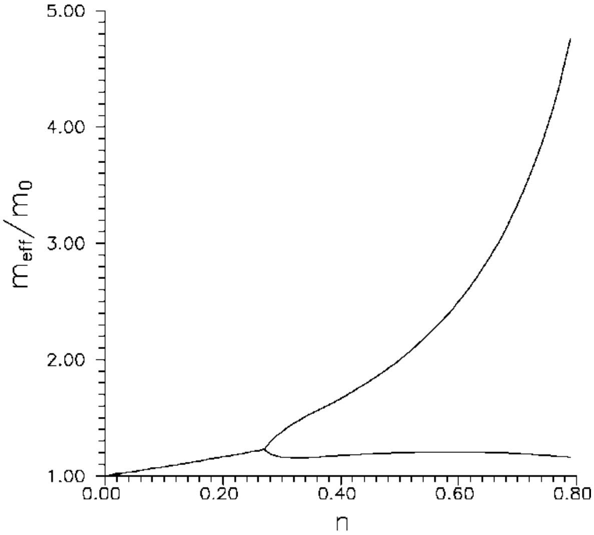

Fig. 4 – Concentration dependence of the effective masses of current carriers with spin ↓↓ (upper curve) and ↑↑ (lower curve) at $J_{eff}/w = 0$ in the absence of the correlated hopping for semi-elliptic DOS

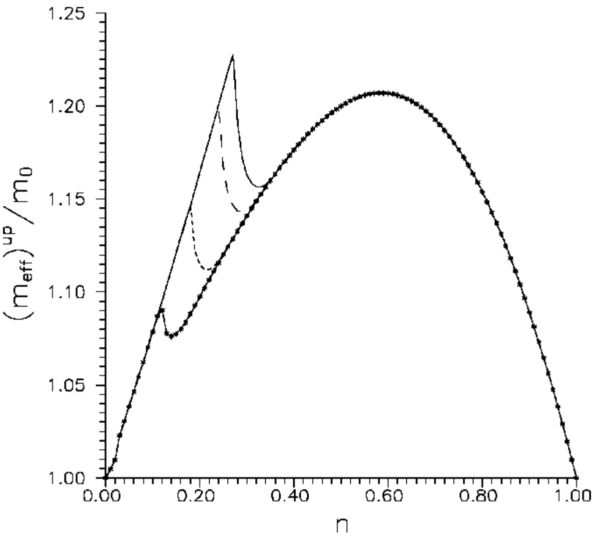

Fig. 5 – Concentration dependence of the effective masses of current carriers with spin ↓↓ (upper curve) and ↑↑ (lower curve) at $J_{eff}/w = 0$ in the absence of the correlated hopping for semi-elliptic DOS

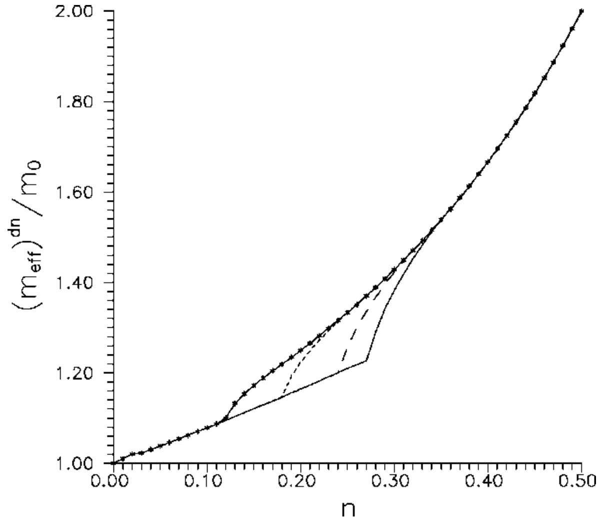

Fig. 6 – Concentration dependence of the effective mass for current carriers of spin ↓↓ at different values of parameter a in asymmetric DOS. Solid curve – $a = 0$; long-dashed curve – $a = 0.1$; short-dashed curve – $a = 0.3$; solid curve with dots – $a = 0.5$ at $zJ_{\text{eff}}/w = 0$ without the correlated hopping

For real systems, cubic symmetry is common. Let us consider a simple cubic (sc) lattice, for which concentration dependence of the effective mass is given in Fig. 7. In distinction from semi-elliptic DOS, the splitting is less pronounced in the region of the critical concentration. Notably, a spontaneous magnetic ordering in sc-lattice stabilizes at greater concentrations than in all the cases considered above. From Fig. 8 one can see that the absolute values of the effective mass for spin-up carriers in a region of critical band filling in the case of sc-lattice are a bit greater than for the lattice with asymmetry and its partial case, the semi-elliptic DOS. This is related to the fact that the saturated ferromagnetic state in this case stabilizes at higher electron concentrations in the conduction band, therefore the peculiarities of the concentration dependence of kinetic energy of electrons manifest themselves.

The external magnetic field application causes the occurrence of the induced magnetic moment and changes the concentration dependence of the effective masses qualitatively. In Fig. 9 for a case of semi-elliptic DOS, dependences of the effective masses on electron concentration in the absence of the external field (with characteristic step-wise spin splitting) and in the applied field are shown. One can clearly see qualitative distinctions which allow us to distinguish two different regimes, namely of weak and strong field.

In a weak field, despite the occurrence of spin splitting for arbitrary electron concentrations the sharp change of the effective mass difference due to translational mechanism of the ferromagnetic ordering stabilization is observed. This situation can have an experimental application, for example, for an enhancement of the spin polarization of a current by a weak magnetic field. In the strong field regime, the main effect is the qualitative change of the concentration dependence of the correlation band narrowing factor which can drive the shift of the critical value of concentration at which the conductivity type changes. As the band filling increases, the rise of spin-up electron effective masses is changed to a decrease (see Fig. 10) due to the correlation band narrowing factor change as a function of the magnetization.

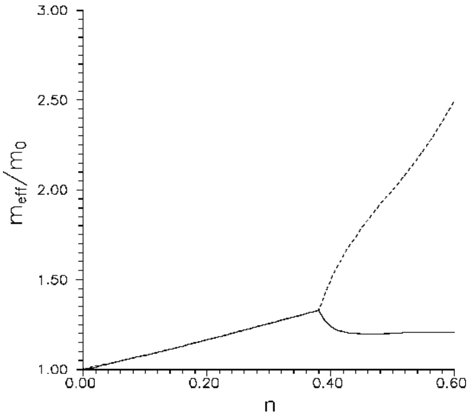

Fig. 7 – Concentration dependence of the effective mass for current carriers of spin ↓↓ (upper curve) and ↑↑ (lower curve) at $zJ_{eff}/w = 0$ in absence of the correlated hopping for DOS of sc-lattice

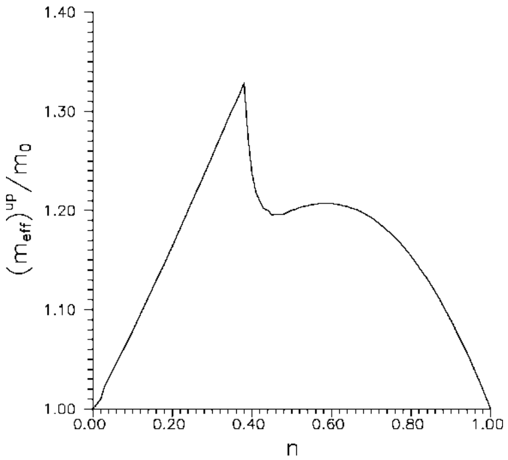

Fig. 8 – Concentration dependence the effective mass for current carriers of spin ↑↑ for band filling interval $n < 1$ at $zJ_{eff}/w = 0$ in the absence of the correlated hopping for DOS of sc-lattice

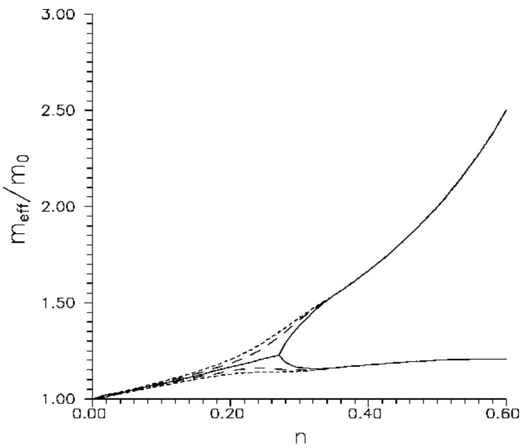

Fig. 9 – Concentration dependence of the effective mass for current carriers of spin ↑↑ for band filling interval $n < 1$ at $zJ_{eff}/w = 0$ in the absence of the correlated hopping for DOS of sc-lattice

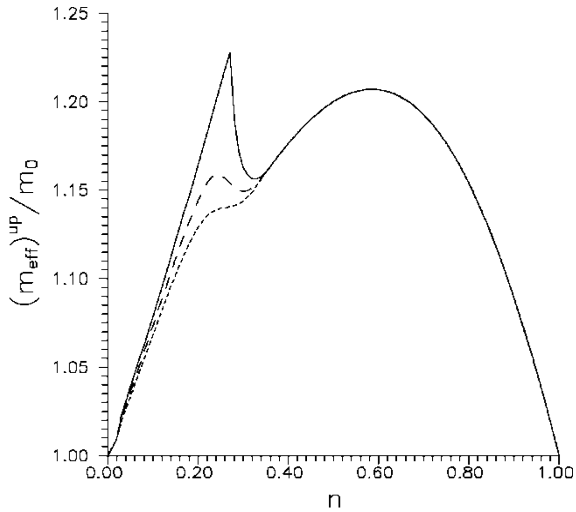

Fig. 10 – Comparison of concentration dependences of effective masses of current carriers with spin in the absence (solid curve) or presence (long-dashed curve – $h/w = 0.01$, short-dashed curve – $h/w = 0.02$) of magnetic field (semi-elliptic DOS, $zJ_{eff}/w = 0$, $\tau_1 = 0$)

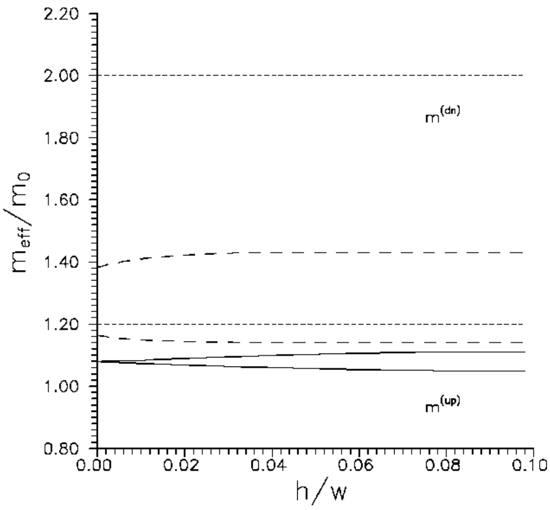

Fig. 11 – Comparison of concentration dependences of effective masses of current carriers with spin ↑↑ in the absence (solid curve) or presence (long-dashed curve – $h/w = 0.01$, short-dashed curve – $h/w = 0.02$) of magnetic field (semi-elliptic DOS, $zJ_{eff}/w = 0$, $\tau_1 = 0$)

One can see from Fig. 11 that substantial differences in the spin splitting character are possible, depending on the electron concentration values. At small concentrations, the effective masses difference is small as the magnetic moment cannot reach a substantially large value even at saturation.

On the opposite side of the concentration interval the ferromagnetic spin ordering is stable even in the absence of the external field, so the field application has no effect on the effective masses of current carriers. At intermediate concentrations, in almost quarter-filled band, sharp changes of the effective masses and conductivity are possible due to the competition of different factors. At fixed electron concentration, the closer the system is to the region of maximum conductance, the greater is the spin-splitting value. This applies also to the results obtained with the use of more realistic DOS forms, for example, the DOS with asymmetry. In the case of double orbital degeneracy for those DOS forms, the sharp changes of the effective masses are not observed as the magnetic transitions are smooth, with unsaturated magnetic moment in an extended region of parameters.

The external magnetic field influence on the concentration dependence of the effective mass is the most pronounced for the semi-elliptic DOS and asymmetrical DOS for small values of the asymmetry parameter.

4. CONCLUSIONS

In the doubly degenerate model of strongly correlated electron system, the external magnetic field suppresses conductance through the effect of magnetic ordering. As a natural consequence of similarity between the expressions for conductivity, on the one hand, and kinetic energy of electrons, on the other hand, the concentration dependences of conductivity and effective masses are determined mainly by the form of unperturbed DOS. It proves the importance of using the realistic DOSs for investigations of transport properties of prospective narrow-band systems of Mott-Hubbard materials. The realization of a spontaneous (or field-induced) magnetic ordering in the system, for which stability criteria are determined mainly by the DOS form, modifies substantially the effective masses behavior. In a weak magnetic field, despite the spin splitting for arbitrary electron concentrations, a jump in effective mass splitting is still of notable value, due to the translational mechanism of ferromagnetic ordering. In the strong field regime, the principal effect is the qualitative change of concentration dependence for correlation band narrowing factor, which can lead to the shift of concentration value for conductivity type change. At intermediate concentrations, in almost quarter-filled band, sharp changes of effective masses (and conductivity) are possible because at these concentrations the competition between the factors studied in the present work is realized.

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Ефективні маси носіїв у виродженій зоні провідності: взаємодія особливостей густини електронних станів та намагніченості

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Для різних форм густини електронних станів (ГЕС) було встановлено, що фізично різні режими (слабкого і сильного магнітного поля) можуть бути реалізовані в концентраційній залежності ефективних мас. У слабкому полі, незважаючи на виникнення спінового розщеплення внаслідок трансляційного механізму стабілізації феромагнітного порядку, існує різка зміна розщеплення ефективних мас для довільних концентрацій електронів, які можна використовувати для налаштування спінової поляризації зовнішнім полем. Коли магнітне поле порівняно сильне, коефіцієнт кореляційного звуження контролює критичну концентрацію для зміни типу провідності. Форма ГЕС регулює концентраційну залежність транспортних характеристик, тому використання реалістичної ГЕС для моделювання феромагнітного порядку індукованого спонтанним або магнітним полем має важливе значення.

Ключові слова: Феромагнетик Мотта-Хаббарда, Вироджена зона провідності, Ефективні маси носіїв, Густина електронних станів.