Effect of electron–lattice interaction on the phase separation in strongly correlated electron systems with two types of charge carriers

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Abstract
The effect of electron–lattice interaction is studied for a strongly correlated electron system described by the two-band Hubbard model. A two-fold effect of electron–lattice interaction is taken into account: in non-diagonal terms, it changes the effective bandwidth, whereas in diagonal terms, it shifts the positions of the bands and the chemical potential. It is shown that this interaction significantly affects the doping range corresponding to the electronic phase separation and can even lead to a jump-like transition between states with different values of strains.

1. Introduction
A typical feature of strongly correlated electron systems is the formation of inhomogeneous states [1, 2]. The nature of such inhomogeneities is based on the electron correlations. However, their specific manifestations can include the effects of different degrees of freedom existing in the solids: spin, charge, orbital, and lattice [3]. A strong electron–lattice coupling plays a fundamental role in such actively studied systems as high-temperature superconductors, manganites, cobaltites, and other related materials [4, 5]. An important characteristic of all these materials is a complicated electronic structure involving two or more conduction bands. The simplest model allowing an appropriate description of electron correlation effects is the Hubbard model and its multiband generalizations [6–8].

In [9], it was demonstrated that the existence of two bands in the Hubbard model gives rise to the existence of the electronic phase separation even in the absence of any type of additional factor (spin, charge, orbital, etc). However, these factors are necessary to give a realistic description of the particular physical system. For example, taking into account spin and orbital variables allows a detailed picture of the phase diagram for manganites [10, 11]. Including in the model the possibility of spin-state transitions gives an explanation of the phase separation in cobaltites [12, 13]. An important and vast field of research is the problem of the existence of inhomogeneities in high-temperature superconductors, especially in cuprates [5]. In this field, the multiband Hubbard model provides some insight into the properties of the cuprate superconductors.

Electron–lattice coupling has been incorporated in the multiband Hubbard model to describe the electronic structure of cuprates and manganites [14–18]. In these papers, the main emphasis was put on the polaron effects or the influence of the electron–phonon interaction on electron pairing. Here we use a similar type of electron–lattice coupling to analyse its effect on the formation of the inhomogeneous states within the two-band Hubbard model.
we limit ourselves to the case of small strains, $|\alpha| \ll 1$, when the theory of elasticity is applicable.

The Hamiltonian of such a system can be written as

$$H = H_{\text{el}} + H_U + H_{\text{cl-ph}} + H_{\text{ph}}.$$  \hspace{1cm} (1)

Here, $H_{\text{el}}$ corresponds to the energy of charge carriers without taking into account the interaction between them

$$H_{\text{el}} = - \sum_{\langle ij \rangle, \sigma} (t^a_{ij} a^+_i a_j + t^b_{ij} b^+_i b_j + \text{h.c.}) - \Delta E \sum_{k} n^b_k,$$  \hspace{1cm} (2)

where $a^+_i$ and $a_i$ ($b^+_i$ and $b_i$) are the creation and annihilation operators for $a$ $(b)$ electrons at site $i$ with spin projection $\sigma$, $\langle \cdots \rangle$ means the summation over the nearest neighbours, $t^a$ and $t^b$ are the corresponding hopping integrals, $\Delta E$ is the energy shift between $a$ and $b$ bands, and $n^a_k = a^+_k a_k$ and $n^b_k = b^+_k b_k$ are the number operators for $a$ and $b$ electrons, respectively.

The $H_U$ term corresponding to the on-site Coulomb repulsion of charge carriers has the form

$$H_U = \frac{1}{2} \sum_{l, \sigma} (U_a n^a_l n^a_l + U_b n^b_l n^b_l) + \frac{U_{ab}}{2} \sum_{l, \sigma, \sigma'} n^a_l n^b_{l \sigma}.$$  \hspace{1cm} (3)

where $U_a$, $U_b$, and $U_{ab}$ are the energies of Coulomb repulsion between two $a$, two $b$, and one $a$ and one $b$ electrons at one lattice site, respectively, and $\bar{\sigma}$ means the spin projection with sign opposite to that of $\sigma$. We assume that the on-site Coulomb repulsion is large, $U_a, U_b, U_{ab} \gg z t$ ($z$ is the number of nearest-neighbour sites, $z = 6$ for the simple cubic lattice considered in this paper) and $U_a \sim U_b \sim U_{ab} \sim U$. Here we do not analyse the magnetic properties of the system and therefore we do not include the Hund’s rule coupling term in the initial Hamiltonian.

The electron–lattice interaction can be chosen in the following form

$$H_{\text{cl-ph}} = \sum_{\langle ij \rangle, \sigma} (\lambda a^+_i a_j u_j + \lambda' b^+_i b_j u_j + \text{h.c.)} + \sum_{l, \sigma} (\lambda_{\alpha} a^+_l a_{l \sigma} + \lambda_{\beta} b^+_l b_{l \sigma}),$$  \hspace{1cm} (4)

where $\lambda$, $\lambda'$, and $\lambda_{\alpha,\beta}$ are corresponding constants of the electron–phonon interaction and $u_l$ are the local distortions of the unit cell containing site $i$. The first sum in this equation describes the change of the hopping probabilities due to lattice distortions affecting both intersite distance and the form of electron wavefunctions. The second sum corresponds to the change in the electron–ion interaction induced by strain. Thus, we take into account the effect of lattice strains both on the on-site electron energy and intersite charge transfer.

We approximate the phonon self-energy term $H_{\text{ph}}$ as an elastic energy of the system depending on distortions at different sites

$$\mathcal{F}_{\text{elast}} = \frac{K}{2} \sum_{l} u^2_l,$$  \hspace{1cm} (5)

where $K$ is the elastic modulus.

We study the problem in the adiabatic approximation considering phonons as a classical static elastic field, neglecting the dynamic effects which could be important, for example, for the analysis of mechanisms of superconductivity. Here our main aim is to demonstrate the possibility of phase separation in the static limit, then the effects of lattice dynamics should be considered on the background of the phase-separated state.

To find a self-consistent solution to the problem, we first perform averaging of the Hamiltonian over the electronic degrees of freedom. From the condition of the energy minimum with respect to strains, $\partial (H(u_l))/\partial u_l = 0$, we obtain

$$\bar{u}_l = -\frac{\lambda z (a^+_l a_j) + \lambda' z (b^+_l b_j) + \lambda_{\alpha} (n^a_l) + \lambda_{\beta} (n^b_l)}{K}.$$  \hspace{1cm} (6)

where $i$ and $j$ are the nearest-neighbour sites.

Using (6), we can present the effective electron Hamiltonian as

$$H_{\text{eff}} = -\sum_{\langle ij \rangle, \sigma} [(t^a - \lambda \bar{u}_i) a^+_i a_j + (t^b - \lambda' \bar{u}_i) b^+_i b_j + \text{h.c.}]$$

$$- \sum_{k} \left[ \Delta E + (\lambda_{\alpha} + \lambda_{\beta}) \bar{u}_i \right] n^b_k + H_U$$

$$- \sum_{l, \sigma} (\mu - \lambda_{\alpha} \bar{u}_i) (n^a_l + n^b_l) + \frac{K}{2} \sum_{l} \bar{u}^2_l,$$  \hspace{1cm} (7)

where $\mu$ is the chemical potential.

Hamiltonian (7) clearly demonstrates that the effect of electron–lattice interaction is two-fold. This interaction in non-diagonal terms changes the effective bandwidth whereas in diagonal terms, it shifts the positions of the bands and the chemical potential. In the earlier analysis [9, 19], we have shown that the qualitative features of the phase diagram for the two-band Hubbard model are mainly determined by two dimensionless parameters: the ratio of the bandwidths and the relative positions of the bands. Thus, to construct a minimal model capturing the main physical effects of electron–lattice interaction, it is sufficient to keep only $\lambda$ and $\lambda_{\beta}$. In addition, we put $\Delta E = 0$ to emphasize the effect of band shift related only to the electron–lattice interaction. As a result, we get

$$\bar{u}_l = -\frac{\lambda z (a^+_l a_j) + \lambda' z (b^+_l b_j)}{K}.$$  \hspace{1cm} (8)

and

$$H_{\text{eff}} = -\sum_{\langle ij \rangle, \sigma} [(t^a - \lambda \bar{u}_i) a^+_i a_j + t^b b^+_i b_j + \text{h.c.}] + H_U$$

$$+ \sum_{k} \lambda_{\beta} \bar{u}_i n^b_k - \sum_{l, \sigma} \mu (n^a_l + n^b_l) + \frac{K}{2} \sum_{l} \bar{u}^2_l.$$  \hspace{1cm} (9)

Starting from Hamiltonian (9), we can point out the main qualitative effects of the electron–lattice interaction in the two-band model. In the absence of doping, $n = 0$, bands $a$ and $b$ are empty and their centres coincide. With the growth of $n$ the wider band $a$ begins to be filled up from the bottom. The band filling is accompanied by the strain $\bar{u}_i = -\lambda z (a^+_l a_j)/K$. The average $(a^+_l a_j)$ is proportional to the hopping probability and thus is positive. The strain $\bar{u}_i$ is positive if $\lambda < 0$ and negative if $\lambda > 0$. From (9), it is easy to see that at any sign of $\lambda$ the bandwidth increases with the strain. At a certain doping level, the chemical potential attains the bottom of the narrower band.
b and this second band starts to be filled up. In this range of
doping, we have two types of electrons and the energy of the
system depends on n in a rather complicated manner due to
electron–electron correlations. As we have shown earlier [9],
such a situation is favourable for phase separation even in the
absence of the electron–lattice interaction.

However, the characteristic feature of the system under
study is the dependence of the effective band shift \( \Delta E_{\text{eff}} = -\lambda_b \bar{u}_i \) on the strain and, hence, on the doping, according to (8). The
sign of the shift depends on the signs of \( \lambda_b \) and \( \lambda_b \).
A simple analysis of (8) and (9) shows that for the same signs of \( \lambda_b \) and
\( \lambda_b \), the value of \( \Delta E_{\text{eff}} \) is negative and the sign of \( \bar{u}_i \) remains
the same at any n. If the signs of \( \lambda_b \) and \( \lambda_b \) are different, the
strain can change its sign at some doping level. The change
of the sign of the strain results in the sign of the change of the
sign of the effective band shift \( \Delta E_{\text{eff}} \).

The dependence of \( \Delta E_{\text{eff}} \) on doping can give rise to a
more sophisticated behaviour of the system. If at some doping
level \( n^* \), the narrower band crosses the bottom of the wider
band, that is \( \lambda_b n^*/K \gg \bar{u}_i \), then it could be favourable to
have almost all electrons in the b band. So, a competition
appears between two states with different values of the strain.
It suggests the possibility of a transition between these two states,
which can have a jump-like form.

In section 3, we present a quantitative analysis of the possible
situations.

3. Mean-field approach

In the limit of strong electron correlations, \( U \to \infty \), we can
describe the evolution of the band structure with the change of
n following the method presented in [9]. We introduce one-
particle Green functions for a and b electrons. For band \( a \), we have

\[
G_{a\alpha}(1 - j, t) = -i\langle \hat{T} a_{\alpha}(t) a_{\alpha}^+(0) \rangle.
\]

(10)

where \( \hat{T} \) is the time-ordering operator. The similar expression
can be written for band \( b \). The equation of motion for the one-
particle Green function with Hamiltonian (9) includes two-
particle Green functions of the form

\[
G_{a\alpha, b\beta}(1 - j, t) = -i\langle \hat{T} a_{\alpha}(t) n_{b\beta}(t) a_{\beta}^+(0) \rangle.
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In the considered limit of strong on-site Coulomb repulsion, the
presence of two electrons at the same site is unfavourable, and
the two-particle Green function is of the order of \( 1/U \). The
equation of motion for two-particle Green functions includes the
three-particle terms coming from the commutator of \( a_{\alpha}(t) \) or
\( b_{\beta}(t) \) with the \( U \) terms of Hamiltonian (9), which are of
the order of \( 1/U^2 \) and so on. In these equations, following the
Hubbard I approach [20], we neglect the terms of the order of
\( 1/U^2 \) and use the following decoupling in the Green functions

\[
\langle \hat{T} a_{\alpha+\mu}(t) n_{b\beta}(t) a_{\beta}^+(0) \rangle \rightarrow \langle n_{b\beta}(t) \rangle \langle \hat{T} a_{\alpha+\mu}(t) a_{\beta}^+(0) \rangle.
\]

As a result, we derive a closed system for the one- and two-particle
Green functions [9, 20]. This system can be solved in a
conventional manner by passing from the time–space \( (t, r) \)
to the frequency–momentum \( (\omega, \mathbf{k}) \) representation. We limit
ourselves to consideration of the case when the total number of
electrons per site does not exceed unity, \( n = n^a + n^b \leq 1 \). The
upper Hubbard sub-bands are empty, and we can proceed to the
limit \( U \to \infty \). In this case, the one-particle Green functions are
independent of \( U \) and can be written in the frequency–
momentum representation as [9]

\[
G_{a\alpha}(\mathbf{k}, \omega) = \frac{g_{ab}}{\omega + \mu - g_{a\alpha} w_{a}(1 - \lambda_b \bar{u}/t_b) \zeta(\mathbf{k})},
\]

(12)

\[
G_{b\alpha}(\mathbf{k}, \omega) = \frac{g_{ba}}{\omega + \mu + \lambda_b \bar{u} - g_{b\alpha} w_b \zeta(\mathbf{k})},
\]

where we put \( \bar{u} = \bar{u} \) assuming a homogeneous strain and introduce the following notation:

\[
w_a = z t_a, \alpha = a, b,
\]

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g_{\alpha\alpha} = 1 - \sum_{\sigma} n_{\alpha\sigma}^a - n_{\alpha\sigma}^b = \langle n_{\alpha\sigma}^a \rangle = \langle n_{\alpha\sigma}^b \rangle = \langle n_{\alpha\sigma} \rangle.
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\]

(12)

\[
G_{b\alpha}(\mathbf{k}, \omega) = \frac{g_{ba}}{\omega + \mu + \lambda_b \bar{u} - g_{b\alpha} w_b \zeta(\mathbf{k})},
\]

where we put \( \bar{u} = \bar{u} \) assuming a homogeneous strain and introduce the following notation:

\[
w_a = z t_a, \alpha = a, b,
\]

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g_{\alpha\alpha} = 1 - \sum_{\sigma} n_{\alpha\sigma}^a - n_{\alpha\sigma}^b = \langle n_{\alpha\sigma}^a \rangle = \langle n_{\alpha\sigma}^b \rangle = \langle n_{\alpha\sigma} \rangle.
\]

As a simple structure of the phase-separated state

The filling of the bands gives rise to a non-zero strain $\bar{u}$, see (8), and hence to the band shift $\Delta E_{\text{eff}}$. The plots $\bar{u}(n)$ and $\Delta E_{\text{eff}}(n)$ are shown in figure 2. When $\lambda$ and $\lambda_b$ have the same signs the band $b$ shifts downward ($\Delta E_{\text{eff}} > 0$). Thus, with the increase of $n$, the chemical potential crosses the bottom of the $b$ band and $b$ electrons appear in the system. Due to electron–electron correlations, the effective width of the $a$ band starts to decrease. This band narrowing and increase of $\Delta E_{\text{eff}}$ leads to decreasing of the number of $b$ electrons, and at some doping level the charge carriers of type $a$ disappear in the system, see figure 1.

The energy of the system in the homogeneous state,

$$E_{\text{hom}} = \sum_a \int \rho_a(E') \delta E' \, dE',$$

is the sum of electron energies in all filled bands. After straightforward calculations, we can write $E_{\text{hom}}$ in the form

$$E_{\text{hom}} = 2g_a^2 w_a \left( \frac{1 - \lambda_a}{t_a} \right) \varepsilon_0 \left[ \frac{\mu}{g_a w_a (1 - \lambda_a/t_a)} + 2g_b^2 w_b \left( \frac{\mu - \lambda_b \bar{u}}{g_b w_b} \right) + \lambda_b n_b + \frac{K \bar{u}^2}{2} \right], \quad (18)$$

where

$$\varepsilon_0(\mu') = \int_{-1}^{\mu'} \delta E' \rho_b(E'). \quad (19)$$

The dependence of $E_{\text{hom}}(n)$ is shown in figure 3 by the solid line. We see that within a certain $n$ range the system can have a negative compressibility, $\delta^2 E_{\text{hom}}/\delta n^2 < 0$, which means a possibility for the charge carriers to form two phases with different electron concentrations [9].

The values of parameters chosen to plot figures 1–3 correspond to a continuous evolution of the strain with doping. However, as was mentioned in section 2, one could also expect a jump-like transition between states with different values of the strains at certain values of parameters. Such a situation is illustrated in figures 4 and 5. In figure 4, we can see that at some $n = n^*$ the strain $\bar{u}$ exhibits a stepwise transition with the change of the sign. In the vicinity of $n^*$, there exist two
The existence of two competing states in some range of parameters can be illustrated in the following way. Let us study Hamiltonian (9) where the strain $\bar{u}$ is considered as an independent parameter. We analyse this Hamiltonian in a way similar to that described above. Namely, at each given $\bar{u}$, we solve the system of equations (14) and (16) for $n^a$, $n^b$, and $\mu$, and then find the system energy per lattice site $E_{\text{hom}}(\bar{u})$. The optimum value $\bar{u}$ is then determined by minimization of $E_{\text{hom}}(\bar{u})$. The numerical analysis shows that the function $E_{\text{hom}}(\bar{u})$ has one or two minima depending on the model parameters. The functions $E_{\text{hom}}(\bar{u})$ calculated for two sets of parameters $\lambda$, $\lambda_b$, $K$ and $w_b$ at different doping levels $n$ are shown in figure 6. At $u = \bar{u}$ corresponding to the minimum of $E_{\text{hom}}(\bar{u})$, we have

$$\frac{\partial E_{\text{hom}}}{\partial u} = \frac{1}{N} \left( \frac{\partial H_{\text{eff}}}{\partial u} \right) = \lambda z (\sigma_{\mu j}^a a_{\mu j}^a) + \lambda_b n^b + K \bar{u} = 0, \quad (20)$$

and we come back to (8) for $\bar{u}$.

In the general case, it is difficult to find explicit conditions for the existence of the jump-like transition. Here, we analyse the important particular case of $\lambda = 0$. Let us consider the function $E'(u) = \partial E_{\text{hom}}/\partial u$, which now has a form $E'(u) = Ku + \lambda_b n^b(u)$. The $E'(u)$ curves calculated at different values of doping are illustrated in figure 7. For large negative strain,
the $b$ band lies far below the $a$ band, and we have $n^a = 0$ and $n^b = n$. Thus, $E'(u) = K a + \lambda_b n$ linearly grows with $u$ up to the point $u = u_1$, when the chemical potential $\mu$ reaches the bottom of the effective $a$ band $-g_a w_a = -(1-n)w_a$, and $a$ electrons appear in the system. Using the second equation in the system (14) with $n_0 = n$, and $\mu = -(1-n)w_a$, we obtain the following expression for $u_1$:

$$u_1 = -\frac{1}{\lambda_b} \left[ (1-n)w_a + \left(1 - \frac{n}{2}\right) w_b \mu_0 \left(\frac{n}{2-n}\right) \right],$$  \hspace{1cm} (21)

where $-1 < \mu_0(n) < 1$ is the function inverse to $n_0(\mu)$, (15). This function is shown in the inset in figure 7. For large positive $u$, when band $b$ lies above band $a$, we have $n^a = n$ and $n^b = 0$, and consequently $E'(u) = K a$ linearly decreases with $u$ until the point $u_2 > u_1$, where $b$ electrons appear. Acting in a similar way, we find

$$u_2 = \frac{1}{\lambda_b} \left[ (1-n)w_b + \left(1 - \frac{n}{2}\right) w_a \mu_0 \left(\frac{n}{2-n}\right) \right].$$  \hspace{1cm} (22)

It is clearly seen from figure 7, that if

$$E'(u_1) = K a u_1 + \lambda_b n u_1 \geq 0, \hspace{1cm} E'(u_2) = K a u_2 \leq 0,$$  \hspace{1cm} (23)

then the function $E'(u)$ has three zeros, and the energy $E(u)$, in turn, has two minima. Using (21) and (22), and taking the equality signs in relations (23), we get the estimate for the minimum value of $\lambda_b$, at which the jump-like transition can occur

$$\frac{(\lambda_b^*)^2}{K} = \frac{1 - n_2}{n_2} w_a \left(1 - \frac{w_2^*}{w_a^*}\right),$$  \hspace{1cm} (24)

where $n_2$ is found from the equation

$$\mu_0 \left(\frac{n_2}{2-n_2}\right) = \frac{1 - n_2}{1 - n_2/2} \frac{w_b}{w_a}.$$  \hspace{1cm} (25)

The value of $\lambda_b^*$ decreases with $w_b$. For very small ratio $w_b/w_a \ll 1$, we have $\mu_0[n_2/(2 - n_2)] \approx 0$, that is, $n_2 \approx 2/3$, and

$$\lambda_b^* \approx \sqrt{\frac{w_b K}{2}}.$$  \hspace{1cm} (26)

Note that the function $E(u)$ can still have two minima when conditions (23) are not met, since the derivative $E'(u)$ can continue to grow (decrease) above (below) $u_1$ ($u_2$), and, consequently, $\lambda_b^*$ found from these conditions overestimates its value.

For $\lambda = 0$ the jump-like transition occurs for relatively large values of $\lambda_b$. For example, at $K = 16 w_a$ and $w_b = 0.25 w_a$, from (24) one obtains $\lambda_b^* \approx 3.6 w_a$. The numerical analysis shows, however, that even small negative (if $\lambda_b > 0$) $\lambda$ sufficiently reduces the threshold value of $\lambda_b^*$. For example, at $\lambda = -0.4 w_a$, the jump-like behaviour arises starting from $\lambda_b^* \approx 2.0 w_a$ ($K = 16 w_a$ and $w_b = 0.25 w_a$). Thus, different signs of $\lambda$ and $\lambda_b$ favour the existence of such a transition.

5. Conclusions

The electron–lattice interaction plays an important role in systems with strongly correlated electrons affecting their behaviour with doping. The interaction of electrons with the lattice distortions results, first, in the hopping probability and, second, in the relative shifts of the electronic bands. We analysed the problem in the framework of the two-band Hubbard model. We demonstrated that if the electron–lattice interaction is strong enough, a competition appears between states with different values of strains and the transition between these states can occur in a jump-like manner. We also showed that the electron–lattice interaction produces a pronounced effect on the conditions of the electronic phase separation since it influences the value of the bandwidth ratio and the relative positions of the bands. The results obtained in this paper should be important for systems with strong electron–lattice interaction, especially those containing Jahn–Teller ions, such as manganites and cuprates. In these compounds, electron–lattice coupling could be the main driving force of the phase separation determining the structure of the phase-separated state and characteristic scales of inhomogeneities.

In our analysis, we neglected the dynamical nature of the phonons. Nevertheless, the phonon dynamics can affect the phase separation phenomena. Indeed, the renormalization of the electron hopping integrals is a well-known effect of such a dynamics, which usually leads to an additional narrowing of the energy bands. As a result, the ratio of the widths of the narrow and wider bands becomes smaller, which favours phase separation. In addition, an interaction of the electrons with the Jahn–Teller-active modes can give rise to an anisotropy of the hopping integrals and hence to a more complicated type of phase separation. This interaction can also lead to a charge disproportionalization and even to charge ordering [24]. Note that the phonon dynamics can be especially important near the onset of phase separation, where we can have a crossover from positive to negative compressibility (see figure 3) and strong fluctuations are expected.
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