

SUSCEPTIBILITY AND PHASE TRANSITIONS IN THE PSEUDOSPIN-ELECTRON MODEL AT WEAK COUPLING*

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The pseudospin-electron model (PEM) is considered in the case of the weak pseudospin-electron coupling. It is shown that the transition to uniform and chess-board phases occurs when the chemical potential is situated near the electron band edges and near the band centre, respectively. The incommensurate phase is realized at the intermediate values of the chemical potential.

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1. Introduction

To investigate the role of the interaction of electrons with a local anharmonic mode of lattice vibrations in the high temperature superconductors (HTSC) the pseudospin-electron model (PEM) [1, 2] was proposed. The model Hamiltonian includes the electron transfer (t -term), electron correlation (U -term), pseudospin-electron interaction (g -term); energy of the local (tunneling-like) level splitting (Ω -term) and asymmetry of the local anharmonic potential (h -term) are taken into account also:

$$\begin{aligned}
 H = & \sum_i (U n_{i,\uparrow} n_{i,\downarrow} - \mu (n_{i,\uparrow} + n_{i,\downarrow}) + g S_i^z (n_{i,\uparrow} + n_{i,\downarrow}) - h S_i^z - \Omega S_i^x) \\
 & + \sum_{\langle i,j \rangle, \sigma} t_{ij} c_{i,\sigma}^\dagger c_{j,\sigma}.
 \end{aligned} \tag{1}$$

The possibility of the first order phase transitions between uniform states as well as the phase separation was established in the case $\Omega = 0$ at the large values of the interaction constant g both in the limit $U \rightarrow \infty$ [3] and

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at $U = 0$ [4]. The presence of the chess-board phase was established in the case of the strong coupling at $U = 0$, $\Omega = 0$ [4].

The PEM has a similarity to the Falicov–Kimball (FK) model with the interaction between localized and moving electrons. Recent investigations [5–7] revealed the presence of homogeneous or modulated phases and transitions between them as well as the possibility of the phase separations. However, in comparison with PEM there exists a difference in the regime of thermodynamical averaging; the term with the transverse field Ω is absent in the FK model. Besides, in contradiction to the PEM, localized and moving particles in the FK model possess usually the common chemical potential [5]. The aim of this work is the investigation of the stable states of the simplified ($U = 0$) PEM in the case of the weak coupling (the band does not split in this case); the behaviour of the dielectric susceptibility and the role of the transverse field Ω are analysed.

2. Susceptibility and thermodynamical instabilities

We will calculate the dielectric susceptibility using the Matsubara Green's functions method. The dielectric susceptibility in the dipole approximation is determined by the Green's function constructed of the operators of the electric dipole momentum. In the case of isothermal response

$$\chi_T(\vec{q}, \omega_n) = \int_0^\beta \langle T_\tau M(0)M(\tau) \rangle_{\vec{q}} e^{i\omega_n \tau} d\tau - \beta \langle M \rangle^2 \delta(\omega_n). \quad (2)$$

The dipole momentum of the unit cell is as follows [2]:

$$M_i = d_e n_i + d_s S_i^z. \quad (3)$$

Consideration of the model in the weak coupling approximation will be carried out analogously to the traditional scheme of the investigation of the weak one-site correlation U in the Hubbard model. Constructing the zero-order Hamiltonian, we use the mean field approximation (MFA)

$$g n_i S_i^z \rightarrow g n_i \langle S_i^z \rangle + g \langle n_i \rangle S_i^z - g \langle n_i \rangle \langle S_i^z \rangle. \quad (4)$$

The unperturbed Hamiltonian H_0 has a diagonal form after an appropriate transformation

$$\begin{aligned} H_0 &= -\lambda \sum_i \sigma_i^z - g N n \eta + \sum_{k, \sigma} (g\eta - \mu + t_k) n_{k\sigma}, \\ H_{\text{int}} &= g \sum_i \left(\frac{1}{N} \sum_{\sigma k k'} e^{i(k-k')R_i} c_{k\sigma}^+ c_{k'\sigma} - n \right) (S_i^z - \eta). \end{aligned} \quad (5)$$

To calculate the susceptibility we use an approximation which is analogous to the random phase approximation (RPA), that is usually applied in the case of pseudospin systems with the direct interaction between pseudospins, or to the generalized random phase approximation (GRPA) elaborated at the consideration of the strongly correlated electron systems. The contributions from the pseudospin "boson" excitations, the band electron polarization and pseudospin one-site correlations are taken into account. Finally, the correlator $\langle TS^z S^z \rangle_q$ has a form:

$$\begin{aligned} \langle TS^z S^z \rangle_{q\omega_n} &= -\frac{\Sigma}{1 - g^2 \Sigma \Pi_q}, \\ \Pi_q &= \frac{1}{N} \sum_k \frac{n(t_k) - n(t_{k-q})}{\omega + t_k - t_{k-q}}, \quad b' = \frac{1}{4} - \langle \sigma^z \rangle_0^2, \\ \Sigma &= \sin^2 \theta \frac{\lambda \langle \sigma^z \rangle_0}{\omega^2 - \lambda^2} - \beta b' \cos^2 \theta \delta(\omega). \end{aligned}$$

Let us investigate when the static susceptibility diverges. The numerical calculations were used to calculate Π_q (square lattice is considered, direct momentum summation is used; we put $W = 1, g = 0.5$). At the fixed values of the chemical potential the critical point can be defined as an upper point of spinodal (on the (T, h) plane) with the highest temperature depending on the wave vector \vec{q} value. Fig.1 shows the dependences of the critical temperature and the corresponding wave vector on the chemical potential. We can see that the case $\vec{q} = (\pi, \pi)$ is realized when $|\mu| \lesssim 0.25$, that means

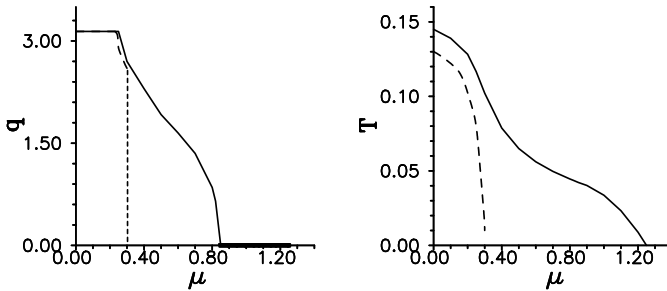


Fig. 1. The dependences of the modulation wave vector $\vec{q} = (q, q)$ and the temperature of absolute instability of high-temperature phase on the chemical potential, $\Omega = 0$ (solid lines); $\Omega = 0.2$ (dashed lines). Dotted line denotes the boundary of the instability region at $\Omega = 0.2$.

that the system can pass into the chess-board phase. The case $\vec{q} = 0$ (the transition into the uniform phase) is realized when $0.85 \lesssim |\mu| \leq 1.25$ ($1.25 = W + g/2$; this value corresponds to the upper edge of the band when $\langle S^z \rangle = \frac{1}{2}$). The system undergoes the transition to the incommensurate phase at

intermediate values of the chemical potential. The presence of the tunneling splitting leads to the decrease of the temperature of the transitions and to the narrowing the interval of values of μ at which the mentioned transitions take place; at high enough values of Ω the transition into the chess-board phase occurs only [8]. The cases $q = 0$ and $q = \pi$ were considered more detaily in [8]. Analysing the behaviour of the grand canonical potential it was shown that the system undergoes the first order phase transition between two uniform phases with jumps of the electron concentration and the pseudospin mean values. In the case $q = \pi$ the possibility of the first or second order phase transition from the uniform to the chess-board phase was revealed. In the regime $n = \text{const.}$ the presence of phase separation was established.

The obtained here results agree with the ones obtained for the Falicov–Kimball model at the small values of the coupling constant describing the interaction between the moving and localized particles (electrons). In addition to this we show that the tunneling-like splitting leads to the decrease of the phase transition temperatures and narrowing of the interval of the μ values at which the transitions occur. We consider in this work the two dimensional lattice. This gives an advantage at the interpretation of the dielectric susceptibility divergences due to the explicit dependence of the $\chi_T(\vec{q}, 0)$ function on the wave vector. In the $d \rightarrow \infty$ limit such dependence enters only through the function $X(q) = \frac{1}{d} \sum_j^d \cos q_j$ [5]; it leads to some difficulties at the consideration of incommensurate ordering. The phase transitions to the incommensurate phase in the PEM are present only at the weak coupling; in the case of the strong interaction [4] the transitions to the uniform or chess-board phase take place only.

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