SUPERCONDUCTIVITY IN THE PSEUDOSPIN-ELECTRON MODEL

T.S. MYSAKOVYCH, I.V. STASYUK

Institute for Condensed Systems Physics, Nat. Acad. Sci. of Ukraine
(1, Sventsits'kogo Str., L'viv 79011, Ukraine, e-mail: mtaras@icmp.lviv.ua)

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The static susceptibility in the superconducting channel is investigated for the locally anharmonic crystalline systems with strong electron correlations within the framework of the pseudospin-electron model with the tunnel splitting of levels, in the limit of weak pseudospin-electron interaction. In the $\mu =$ const regime, when the chemical potential is located near the band center, the system undergoes a phase transition to the phase with a modulation of the lattice period. The transition to the superconducting state is revealed for a non-half filling of the band and for the case of the nonzero tunnel frequency Ω. The influence of the tunnel splitting on the phase transitions is investigated as well.

Introduction

Since the discovery of high temperature superconductivity (HTSC), this phenomenon has intensely been studied by means of various experimental techniques as well as theoretical simulations. In addition to the pure electron models, the "mixed" ones have also been employed to go beyond the limit of the former and consider additional degrees of freedom, such as phonons in the Holstein model, bosons in the boson-fermion model, and others. The Holstein model describes the interaction of fermions with bosons, thereby including phonons as a particular case. The phonons in the Holstein model are the Einsteinian ones, i.e. their frequencies are all equal. It has been shown for this model that, when the phonon frequency is nonzero and the electron band filling differs from a half, the application of the quantum Monte Carlo method in the infinite-dimensional limit on the one hand, and Migdal—-Eliashberg (ME) approximation (a neglect of vertex corrections in the susceptibility calculations) on the other hand, may give rise to the appearance of the superconducting state (SC) in the system [1–5]. Further, if the electron concentration is close to unit, a charge-density-wave state (CDW) appears. It has been revealed that the temperature of the transition to SC exhibits a maximum at a certain value of the constant of electron-phonon interaction, and that the maximum SC transition temperature is bounded from above by the maximum CDW transition temperature. A role which is played by both the vertex corrections [2] and the phonon oscillation anharmonicity [4] in the transitions to SC and CDW was also studied. The results obtained with the use of various approximations [1–5] were compared to the exact quantum Monte Carlo solution. It has been demonstrated that the ME approximation gives quite good results for the weak electron-oscillation interaction and low phonon frequencies.

One more theoretical model to describe superconductivity, namely the boson-fermion one, considers the interaction of itinerant electrons with the localized tightly bound electron pairs (bosons). The studies [6, 7] were aimed at the determination of the SC transition temperature, T_c, as well as a temperature T^*, at which a pseudogap in the electron density of states is opened up. It turned out that, depending on the doping level, T^* might be far greater than T_c.

To describe HTSC, the $t - J$ model has also been employed, which, for a two-sublattice antiferromagnet with a small level of the hole concentration, is reduced to the spin-polaron one [8]. It has been shown that the superconducting spin-polaron pairing may be one of the mechanisms of HTSC [8].

Furthermore, the anharmonic models of HTSC have been employed, and studies of the electron-phonon pairing caused by an interaction between charge carriers and highly anharmonic oscillations of the lattice atoms have been carried out [9, 10]. To describe such oscillations, a local double-well potential was utilized. Work [11] paid attention to a possibility of the increase of the SC transition temperature by means of a variation of the height of the barrier between the minima of this potential. The studies [12] revealed that, for an asymmetric double-well potential, the system is likely to turn into SC, and that the SC transition temperature achieves a maximum at a certain average atom position within this potential.

A specific feature of superconductors of the YBaCuO type is that the electron transfer mainly occurs within the CuO planes. One more peculiarity of such crystals

is the existence of strongly anharmonic elements of the structure. For YBaCuO, this manifests itself in the local anharmonic oscillations of the oxygen atoms both within the CuO chains and of the apex O atoms in the direction of the CuO planes' normal. On the application of the pseudospin formalism for a case where the variable S_i^z takes on two values, $S_i^z = \pm 1/2$, two oscillation states lowest in energy should be taken into account. The standard formulation of the corresponding model [10, 13—16] implies that the electron subsystem is described by the Hubbard Hamiltonian, and the interaction of electrons with the anharmonic subsystem is included in the external field which depends on a pseudospin orientation. Thus, the Hamiltonian of the pseudospin-electron model (PEM) is:

$$H = \sum_i \Big(U n_{i,\uparrow} n_{i,\downarrow} - \mu (n_{i,\uparrow} + n_{i,\downarrow}) +$$

$$+ g S_i^z (n_{i,\uparrow} + n_{i,\downarrow}) - h S_i^z - \Omega S_i^x \Big) + \sum_{i,j,\sigma} t_{ij} c_{i,\sigma}^{\dagger} c_{j,\sigma}. \quad (1)$$

Here, t_{ij}-term describes the hopping of the electron with a spin σ from a site i to a site j, U-term — the Coulomb repulsion, g-term — the pseudospin-electron interaction, Ω-term — the tunnel splitting of levels, and h-term — the asymmetry of the local anharmonic potential. In work [15], employing quantum Monte Carlo simulations to the PEM, the conditions under which the system underwent a transition to SC were studied in detail. For a fixed electron concentration and both the s- and d-symmetries, a relationship was determined between the Ω, g, U theory parameters, which gave rise to the appearance of SC. In particular, for a weak pseudospin-electron coupling, SC with the s-symmetry was shown to be likely to appear.

It should be noted that the PEM is similar to the known Falicov—Kimball (FK) model [17] which describes a system whose characteristic feature is the interaction between itinerant and localized particles (electrons). The solutions obtained upon application of the dynamic mean field theory DMFT to this model contain a homogeneous phase, phases with either double or incommensurate lattice period modulation, as well as a phase separation state [18–22]. What differs the FK model from the PEM one is the absence of the term, which in the latter is responsible for the tunnel splitting of the levels. In addition, the former is usually treated in the regime of a constancy of the concentration of localized particles (for the PEM, this corresponds to a fixation of an average pseudospin value), whereas for the latter, the regimes of the fixation of either the chemical potential or the concentration of itinerant particles are used.

The previous studies of the PEM have been devoted to the analysis of the electron spectrum [23], investigation of the behavior of dielectric susceptibility, examination of phase transitions and appearance of the phase separation [24–30]. In particular, it was shown in [25], that the first-order transition between homogeneous phases and the phase separation are likely to occur in the PEM with a direct pseudospins interaction, provided that $\Omega, t = 0$. Similar results were obtained for $\Omega, t \neq 0$ and large g, either in the $U \to \infty$ limit for the two-sublattice PEM [26], or for a case where $U = 0$ [27,28]. In [28], basing on a thermodynamically consistent scheme of a generalized random phase approximation (RPA), the phase with a double lattice period modulation was revealed to be likely to appear when $U = 0$ and $\Omega = 0$.

When the pseudospin-electron interaction is weak ($g < W$, where W is a half-width of the band which is not split in a case of the weak interaction) and $U = 0, \Omega \neq 0$, the application of mean field approximation (MFA) and RPA has been shown to may lead to the appearance of CDW. Depending on the chemical potential value, the system has been found to undergo the transition to the phase with the double lattice period modulation (the chemical potential is near the band center), to the homogeneous phase (the chemical potential is close to the band edges), or to the phase with the incommensurate lattice period modulation (at intermediate values of the chemical potential). Appearance of the phase separation phenomenon has also been examined. For the $n = \text{const}$ regime, with n being the electron concentration, the system may separate either into homogeneous phases with different values of the average pseudospin and electron concentrations, or into the homogeneous and modulated phases [29–31]. However, when the tunnel frequency Ω is nonzero, the effective interaction between electrons becomes dynamical, and, as a set of the theory parameters meets the specific requirements, the system may go into SC (Anderson theorem [32]). Thus, under these conditions, the transition to CDW will compete with that to SC. Among others, the close attention to this problem was paid in [33]. It was shown that, when there is no electron correlation, the transition temperature to CDW, T_p, is higher than that to SC, T_c. The authors, however, considered only the case where the local potential is symmetric and the electron filling is close to a half. The question concerning the appearance of the superconductivity for a wider range of the model

parameters and electron concentrations has not been examined yet. Just this point is the subject of the given work.

1. Susceptibility in a Superconducting Channel

To examine the possibility of the appearance of CDW, the previous papers [30, 31] were aimed at studying the PEM dielectric susceptibility

$$\chi^{\rm CDW}(\vec{q},\omega_n) =$$

$$= \int\limits_0^\beta \langle T_\tau M(0)M(\tau)\rangle_{\vec{q}} e^{i\omega_n\tau}d\tau - \beta\langle M\rangle^2\delta(\omega_n) \qquad (2)$$

in the weak interaction limit ($g < W$). Here, $M_i = d_e n_i + d_s S_i^z$ is a cell's dipole moment, and, for the layered structures like YBaCuO, it includes only a transverse component. Within the frames of the RPA, which accounts for the contributions having a structure of the serial loop connections in a diagram representation (this will be discussed in more details below), the static dielectric susceptibility was shown to diverge (this means that the system undergoes the transition to CDW) under the following conditions:

$$\lambda^2 + g^2\sin^2\theta\lambda\langle\sigma^z\rangle_0\Pi_q(0) + \lambda^2 g^2\beta b'\cos^2\theta\Pi_q(0) = 0, \qquad (3)$$

where

$$\Pi_q(\omega) = \frac{2}{N}\sum_k \frac{n(t_k) - n(t_{k-q})}{\omega + t_k - t_{k-q}},$$

$$b' = (\frac{1}{4} - \langle\sigma^z\rangle_0^2), \quad \sin\theta = \frac{\Omega}{\lambda},$$

$$\lambda = \sqrt{(gn-h)^2 + \Omega^2}, \quad \langle\sigma^z\rangle_0 = \frac{1}{2}\tanh\left(\frac{\beta\lambda}{2}\right). \qquad (4)$$

For the homogeneous ordering and s-symmetry, the static susceptibility in a superconducting (Cooper) channel can be expressed as

$$\chi^{\rm SC} = \frac{T}{N}\sum_{k,q}\int\limits_0^\beta \langle T_\tau c_{\downarrow k}(\tau)c_{\uparrow -k}(\tau)c^\dagger_{\uparrow -q}c^\dagger_{\downarrow q}\rangle e^{i\omega_n\tau}d\tau, \qquad (5)$$

with operators being in the Heisenberg representation: $A(\tau) = e^{\tau H}Ae^{-\tau H}$. Consider the $U = 0$ case and, similarly to [30], rewrite the Hamiltonian as

$$H = H_0 + H_{\rm int},$$

$$H_0 = -\lambda\sum_i \sigma_i^z - gNn\eta + \sum_{k,\sigma}(g\eta - \mu + t_k)n_{k\sigma},$$

$$H_{\rm int} = g\sum_i (\frac{1}{N}\sum_{\sigma k k'} e^{i(k-k')R_i}c^+_{k\sigma}c_{k'\sigma} - n)(S_i^z - \eta). \qquad (6)$$

Here, a rotational transformation [30],

$$S_i^z = \sigma_i^z\cos\theta + \sigma_i^x\sin\theta,$$

$$S_i^x = \sigma_i^x\cos\theta - \sigma_i^z\sin\theta,$$

$$\sin\theta = \frac{\Omega}{\lambda}, \qquad (7)$$

has been used. Further, to build a zero-approximation Hamiltonian, we carry out the MFA as follows:

$$gn_iS_i^z \to gn_i\langle S_i^z\rangle + g\langle n_i\rangle S_i^z - g\langle n_i\rangle\langle S_i^z\rangle. \qquad (8)$$

Application of the similar schema to the Hubbard model in the limit of a weak electron correlation, U, makes it possible to describe its magnetic properties, when there is no correlation splitting of the electron band. It was shown in [27] that, for the PEM in the DMFT, the band is also not split when the pseudospin-electron interaction, g, which is an analog of the Coulomb repulsion U in the Hubbard model, is sufficiently weak ($g < W$). Thus, a choice of the MFA as a zero approximation is well grounded for the weak interaction limit.

With the use of the representation

$$e^{-\beta H} = e^{-\beta H_0}\sigma(\beta), \quad \sigma(\beta) = T\exp(-\int\limits_0^\beta H_{\rm int}(\tau)d\tau), \qquad (9)$$

we may write the mean value of the expression:

$$\langle T_\tau c_{\downarrow k}(\tau)c_{\uparrow -k}(\tau)c^\dagger_{\uparrow -q}c^\dagger_{\downarrow q}\rangle =$$

$$= \frac{1}{\langle\sigma(\beta)\rangle_0}\langle T_\tau c_{\downarrow k}(\tau)c_{\uparrow -k}(\tau)c^\dagger_{\uparrow -q}c^\dagger_{\downarrow q}\sigma(\beta)\rangle_0 =$$

$$= \langle T_\tau c_{\downarrow k}(\tau)c_{\uparrow -k}(\tau)c^\dagger_{\uparrow -q}c^\dagger_{\downarrow q}\sigma(\beta)\rangle_0^c, \qquad (10)$$

where the operators are in the interaction representation $A(\tau) = e^{\tau H_0}Ae^{-\tau H_0}$, and the symbol $\langle ...\rangle_0^c$ implies accounting for the coupled diagrams when averaging over the H_0 distribution.

Employ the perturbation theory to calculate the average value of the above expression:

$$\langle T_\tau c_{\downarrow k}(\tau)c_{\uparrow -k}(\tau)c^\dagger_{\uparrow -q}c^\dagger_{\downarrow q}\sigma(\beta)\rangle_0^c =$$

$$= \langle T_\tau c_{\downarrow k}(\tau)c_{\uparrow -k}(\tau)c^\dagger_{\uparrow -q}c^\dagger_{\downarrow q}\rangle_0^c -$$

$$-\int_0^\beta d\tau_1 \langle T_\tau c_{\downarrow k}(\tau) c_{\uparrow -k}(\tau) c^\dagger_{\uparrow -q} c^\dagger_{\downarrow q} H_{\rm int}(\tau_1)\rangle_0^c + \frac{1}{2!}\int_0^\beta d\tau_1 \times$$

$$\times \int_0^\beta d\tau_2 \langle T_\tau c_{\downarrow k}(\tau) c_{\uparrow -k}(\tau) c^\dagger_{\uparrow -q} c^\dagger_{\downarrow q} H_{\rm int}(\tau_1) H_{\rm int}(\tau_2)\rangle_0^c - \ldots \quad (11)$$

To calculate the average values of the T-products, we utilize the diagram technique and Wick's theorem for both the spin- and fermi-operators (see, for example, [34]), performing, at the same time, a cumulant expansion to calculate the average of the product of operators σ^z. We introduce the designations for the unperturbed Green functions,

$$\langle T_\tau \sigma^+_l(\tau)\sigma^-_{l'}(\tau')\rangle_0 = -2\langle\sigma^z\rangle_0 K^0_{ll'}(\tau-\tau'),$$

$$\langle T_\tau c_{k\sigma}(\tau) c^+_{k'\sigma}(\tau')\rangle_0 = \delta_{kk'} G^0_{k\sigma}(\tau-\tau'), \quad (12)$$

and cumulants

$$\langle T_\tau \sigma^z_l(\tau)\sigma^z_{l'}(\tau')\rangle_0 = b^2 + b'\delta_{ll'},$$

$$b = b(\beta\lambda) = \langle\sigma^z_l\rangle_0 = \frac{1}{2}{\rm tg}\frac{\beta\lambda}{2}; \quad b' = \frac{\partial b}{\partial(\beta\lambda)}. \quad (13)$$

After proceeding to the ω, k-presentations in the form

$$\frac{1}{\beta}\sum_n e^{-i\omega_n(\tau_1-\tau_2)}\frac{1}{N}\sum_k e^{ik(R_l-R_i)} K^0_k(\omega_n) =$$

$$= K^0_{li}(\tau_1-\tau_2), \quad (14)$$

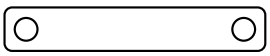
the unperturbed Green functions become:

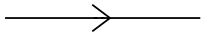
$$G^0_{k\sigma}(\omega_n) = \frac{1}{i\omega_n - t_k - g\eta + \mu},$$

$$K^0_q(\omega_n) = \frac{1}{i\omega_n - \lambda}. \quad (15)$$

It is worth noting that the diagrams containing the "single-tail" inclusions in both the Green functions and cumulants are compensated, because it is the MFA that is chosen as a zero-approximation and, thus, the zero-field corrections are already included in the unperturbed Green functions and cumulants.

Let us introduce the following diagram designations:

$\Sigma(\omega)$:  ;

$G^0_k(\omega)$:  ,

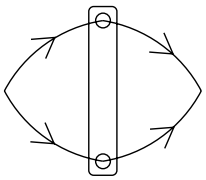
where

$$\Sigma(\omega) = \sin^2\theta\frac{K^0(\omega)+K^0(-\omega)}{2} - b'\beta\cos^2\theta\delta(\omega). \quad (16)$$

For the susceptibility $\chi^{\rm CDW}$, in a zeroth-order of perturbation theory, we obtain the expression

$$\frac{1}{N}\sum_{k,n} G^0_k(\omega_n) G^0_{-k}(-\omega_n). \quad (17)$$

First-order contributions are mutually canceled. To each inner diagram vertex, we assign a multiplier g. In the second order in g, we have the diagram

 ,

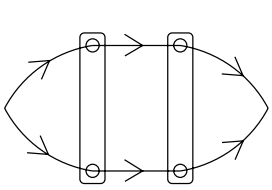
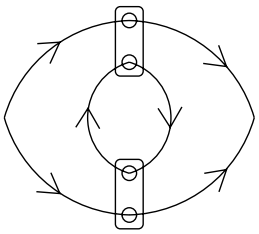
or, in the analytical form,

$$-\frac{g^2 T}{N^2}\sum_{k_1,k_2,n_1,n_2} G^0_{k_1}(\omega_{n_1}) G^0_{-k_1}(-\omega_{n_1})\times$$

$$\times\Sigma(\omega_{n_1}-\omega_{n_2}) G^0_{k_2}(\omega_{n_2}) G^0_{-k_2}(-\omega_{n_2}). \quad (18)$$

In the higher orders, we should take account of the diagrams, which correspond to a ladder approximation for an "anomalous" scattering channel (with the parallel directions of the arrows of the Green Fermi-functions) and to a chain one for a "normal" scattering channel (with the antiparallel directions of the arrows of the Green Fermi-functions in loops), the latter approximation dealing with a summation of the series of the loop diagrams.

In particular, in the fourth-order of perturbation theory, these are the diagrams


and


with the analytical contributions

$$\frac{g^4T^2}{N^3}\sum_{k_1,k_2,k_3,n_1,n_2,n_3} G^0_{k_1}(\omega_{n_1})G^0_{-k_1}(-\omega_{n_1})\times$$

$$\times\Sigma(\omega_{n_1}-\omega_{n_3})G^0_{k_3}(\omega_{n_3})G^0_{-k_3}(-\omega_{n_3})\times$$

$$\times\Sigma(\omega_{n_3}-\omega_{n_2})G^0_{k_2}(\omega_{n_2})G^0_{-k_2}(-\omega_{n_2}) \qquad (19)$$

and

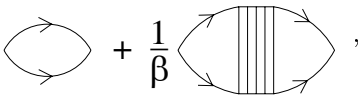
$$\frac{g^4T}{N^2}\sum_{k_1,k_2,n_1,n_2} G^0_{k_1}(\omega_{n_1})G^0_{+-k_1}(-\omega_{n_1})\times$$

$$\times\Sigma(\omega_{n_1}-\omega_{n_2})\Pi_{k_2-k_1}(\omega_{n_1}-\omega_{n_2})\times$$

$$\times\Sigma(\omega_{n_1}-\omega_{n_2})G^0_{k_2}(\omega_{n_2})G^0_{-k_2}(-\omega_{n_2}), \qquad (20)$$

correspondingly.

Accounting for the above scattering channels, we can express the susceptibility $\chi^{\rm SC}$ either in the diagram form



or in the analytical form

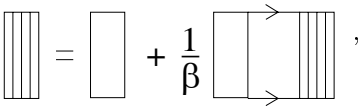
$$\chi^{\rm SC}=\sum_{\omega,k}\chi^0_\omega(k)+T\times$$

$$\times\sum_{k_1,k_2,\omega_1,\omega_2}\chi^0_{\omega_1}(k_1)\Gamma_{\omega_1,\omega_2}(k_1,k_2)\chi^0_{\omega_2}(k_2), \qquad (21)$$

where

$$\chi^0_{\omega_1}(k_1)=\frac{1}{N}G^0_{k_1}(\omega_1)G^0_{-k_1}(-\omega_1). \qquad (22)$$

For the $\Gamma_{\omega_1,\omega_2}(k_1,k_2)$ vertex part, to which a shaded rectangle in the diagram corresponds, we obtain the Bethe–Salpeter equation:

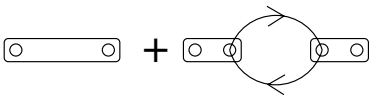


or, in the analytical form

$$\Gamma_{\omega_1,\omega_2}(k_1,k_2)=\Gamma^0_{\omega_1,\omega_2}(k_1,k_2)+$$

$$+T\sum_{k_3,\omega_3}\Gamma^0_{\omega_1,\omega_3}(k_1,k_3)\chi^0_{\omega_3}(k_3)\Gamma_{\omega_3,\omega_2}(k_3,k_2). \qquad (23)$$

Here, within the approximation accepted, the $\Gamma^0_{\omega_1,\omega_3}(k_1,k_3)$ unperturbed vertex is formed by the "normal" scattering channel. In the diagram representation, it corresponds to the series



or, in the analytical form,

$$\Gamma^0_{\omega_1,\omega_2}(k_1,k_2)=$$

$$=-\frac{g^2\Sigma(\omega_1-\omega_2)}{1-g^2\Pi_{k_2-k_1}(\omega_1-\omega_2)\Sigma(\omega_1-\omega_2)}. \qquad (25)$$

Series (24) is similar to what has been obtained in the limits of the generalized RPA at the calculation of the paired "normal" correlation functions (susceptibilities) for the highly correlated electron systems, making use of the basis account for direct interactions, in particular, magnetic susceptibility of the $t-J$ model [35], dielectric susceptibility of the PEM for both the strong [24] and weak [30, 31] interactions. In our case, provided that $U=0$, a connection between the loops is accomplished with the help of the cumulants and Green Bose-functions. In this case, expression (25) for the "zeroth" $\Gamma^0_{\omega_1,\omega_2}(k_1,k_2)$ vertex part has a structure similar to that obtained for the Holstein model in the ME approximation employed in [1], although this model contains no cumulant contributions, only the phonon propagators (analog of the Green Bose-functions $K^0(\omega)$ in our model).

Introducing a variable $\tilde\chi^{\rm SC}_{\omega_1,\omega_2}(k_1,k_2)$ associated with $\chi^{\rm SC}$ as

$$\chi^{\rm SC}=\sum_{\omega_1,\omega_2,k_1,k_2}\tilde\chi^{\rm SC}_{\omega_1,\omega_2}(k_1,k_2), \qquad (26)$$

we can write the equation which is equivalent to the Larkin equation for the systems with direct interactions:

$$\tilde\chi^{\rm SC}_{\omega_1,\omega_2}(k_1,k_2)=\chi^0_{\omega_1}(k_1)\delta_{k_1,k_2}\delta_{\omega_1,\omega_2}+T\chi^0_{\omega_1}(k_1)\times$$

$$\times\sum_{k_3,\omega_3}\Gamma^0_{\omega_1,\omega_3}(k_1,k_3)\tilde\chi^{\rm SC}_{\omega_3,\omega_2}(k_3,k_2). \qquad (27)$$

It should be noted that the structure of Eq. (27) is similar to that obtained in the Holstein model [1–4].

The use of both the approximations, the ladder one for the $\Gamma_{\omega_1,\omega_2}(k_1,k_2)$ vertex construction and the chain one for the construction of $\Gamma^0_{\omega_1,\omega_2}(k_1,k_2)$, was employed by analogy with what was done in the $t-J$ model for the SC description [36]. The approximations mentioned correspond to the known ME one, which is usually used for the consideration of electron-phonon

systems, particularly in the Holstein model. As was shown in [2], when, in the latter model, the limit was taken where the phonon frequencies were small enough in comparison with the transfer integral, such an approximation made it possible to achieve the results, which were in qualitative resemblance to those obtained on the basis of quantum Monte Carlo simulations. In addition, in the aforementioned paper, the effect of the corrections to the vertex part, which were neglected in the ME approximation, on the SC transition temperature was studied. It was shown that, for a case of non-half filling, this means that if the electron or hole concentration is sufficiently small, the role of such corrections is negligible at small phonon frequencies. Since the PEM is similar to the Holstein model, and may be considered as a double-level approximation of the latter one, the ME approximation is expected to be satisfactory in the limits of non-half filling, low temperatures, and small Ω. It is worth noting that we have made the zero-approximation for the Green Fermi-functions G by analogy with what was done in [37], where the possibility of the SC appearance in the Hubbard model was examined in the $U \to \infty$ limit.

2. Phase Transitions to SC and CDW

In [30], taking the weak interaction limit, we considered the thermodynamics of the simplified ($U = 0$) PEM in the normal phase, and constructed the phase diagrams for both the zero and non-zero Ω. We showed that, depending on the chemical potential position, the system might undergo a transition to either a modulated or another homogeneous phase, with the latter having the different average values of S^z or electron concentration, and, in what follows, being referred to as the low-temperature homogeneous phase (LTHP). Now, our aim is to construct the phase diagrams for various values of Ω, taking into account that the SC transition may occur. In what follows, we will consider the $\mu = \text{const}$ regime.

A way to find the SC transition temperature is to determine a temperature, at which the susceptibility in the superconducting channel diverges. The condition, this temperature can be found from, implies that the scattering matrix

$$T_{\omega_1\omega_2}(k_1, k_2) = -T\chi^0_{\omega_1}(k_1)\Gamma^0_{\omega_1\omega_2}(k_1, k_2) \tag{28}$$

has a single eigenvalue [1, 38]. A specific feature of this procedure is that we are dealing with the imaginary discrete Matsubara's frequencies $i\omega_n = i(2n+1)\pi T$, that enables us to specialize to the $T_{\omega_1\omega_2}(k_1, k_2)$ matrix discrete in frequencies. To simplify the calculations, we will neglect the renormalization of the unperturbed vertex part performed according to Eq. (25), assuming that $\Gamma^0 \approx -g^2\Sigma$. Such an approximation is similar to the non-renormalized ME approximation in the Holstein model [1]. It should be noted that the requirement that the denominator in Eq. (25) equals zero at $\omega_1 = \omega_2$ coincides with condition (3), under which the static dielectric susceptibility diverges, implying the transition to CDW [29–31]. For this reason, we may neglect the Γ^0 vertex renormalization only in the high-temperature phase, when the system still not underwent a transition to CDW. Thereby, we confine ourselves to the consideration of a possibility of the transition to SC only from the high temperature phase. To go beyond this limit, i.e. to consider a transition from CDW to SC, we should use the complete expression for the $\Gamma^0_{\omega_1\omega_2}(k_1, k_2)$ vertex part.

As results from our simplification, the unperturbed vertex part doesn't depend on the wave vector, and thus, we can sum over the wave vectors k_1, k_2, k_3 in the Larkin equation (27). In this case, to determine the transition temperature, a unit eigenvalue of the matrix

$$\tilde{T}_{\omega_1\omega_2} = -T\sum_{k_1}\chi^0_{\omega_2}(k_1)\Gamma^0_{\omega_1\omega_2} \tag{29}$$

should be found at first. Then, of all the temperatures within the (T, h) plane which provide a unit eigenvalue for the $\tilde{T}_{\omega_1\omega_2}$ matrix, the highest one should be chosen as the critical SC transition temperature. It is this phenomenon that can be called as the absolute instability of the high-temperature phase with respect to the SC ordering. For the CDW case, the critical temperature can be determined from Eq. (3). Using the equations obtained in the MFA [29], we can calculate the mean values of both the electron concentration n and pseudospin $\eta = \cos\theta\langle\sigma^z\rangle_0$:

$$n = \frac{1}{N}\sum_{k\sigma}(e^{\beta(g\eta+t_k-\mu)}+1)^{-1} \equiv \frac{1}{N}\sum_{k\sigma}f(E_k-\mu) \tag{30}$$

$$\eta = \frac{h-gn}{2\lambda}\,\mathrm{tg}(\frac{\beta\lambda}{2}).$$

In our calculations, we take the direct sum over the two-dimensional square lattice. As the units of distance and energy, we choose a lattice constant a and a half-width of the electron band W, respectively. In the MFA, the band energy reads $E(k) = g\eta + t_k$, where $t_k = \frac{W}{2}(\cos k_x + \cos k_y)$ [29, 30].

Fig. 1 shows the dependences of the wave vector of the CDW-modulation $\vec{q} = (q, q)$, the CDW transition

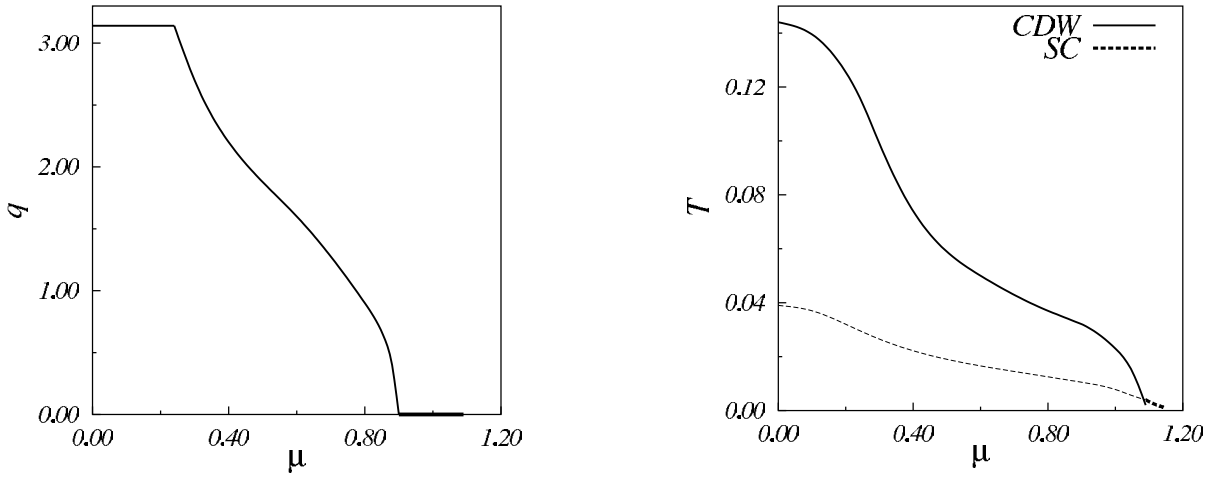


Fig. 1. The wave vector of the CDW-modulation $\vec{q} = (q, q)$, the temperature of the absolute instability of the high-temperature phase with respect to the transitions to CDW (solid line) and SC (bold dashed line) as functions of the chemical potential, for $\Omega = 0.06$ and $g = 0.5$

temperature (solid line), and the SC transition temperature (bold dashed line) on the chemical potential, for $\Omega = 0.06$. Since the picture is symmetric with respect to $\mu = 0$, only positive values of the chemical potential are presented. As is seen, the $q = \pi$ case is realized for small absolute values of the chemical potential $|\mu|$, i.e. for μ located near the band center. As $|\mu|$ grows, the system undergoes the transition to the CDW with the incommensurate lattice period modulation. Further increase in μ gives rise to the transition to the LTHP, and finally, when the chemical potential is located near the band edges ($|\mu| \leq W + g/2$ in an ordered state of pseudospins), the transition to SC occurs (bold dashed line). The transition to SC marked by the thin dashed line is not realized in reality. This line denotes a multitude of the points of the high-temperature phase instability with respect to the SC appearance, when there is no CDW transition, i.e. when a renormalization of the unperturbed Γ^0 vertex part is neglected. It should be noted, that for $\Omega = 0$, the transition to SC doesn't onset, since the effective interaction between electrons becomes static and hence, according to the Anderson theorem, SC ordering can't appear [32]. In this case, the transition to the LTHP persists up to the values of the chemical potential which are located near the band edges, $|\mu| = W + g/2$. When $\Omega \neq 0$, the range of μ, for which CDW appears, gets narrowed and the transition to SC becomes feasible. It is difficult to find the limit value of $|\mu|$, at which the SC transition still persists, because the transition temperature is low. The transition to SC is thought to may occur up to $|\mu| = W + g/2$, independent of the Ω value, provided that $\Omega \neq 0$.

Fig. 2 presents the dependences of the wave vector of the CDW modulation, the CDW transition temperature (solid line), and the SC transition temperature (bold dashed line) on the chemical potential, for $\Omega = 0.2$. It is seen that, upon an increase in Ω, there is no transition to the LHTP, and the CDW transition temperature is reduced in comparison with Fig. 1. Dotted line shows the temperature of the transition to the phase with $q = \pi$, i.e. to that with the double lattice period modulation (the so-called chess-board phase). In [1–4], the appearance of the incommensurate phase wasn't observed for the Holstein model, and the phase transition was concluded only to be either to the chess-board phase or to the SC one. As is seen from Fig. 2, there is a region of the phase space where the transition to the CDW with the incommensurate lattice period modulation is possible, and this region is rather large for the small values of Ω.

Fig. 3 shows the dependences of the temperature of the transition to CDW with the modulation wave vector $\vec{q} = (\pi, \pi)$ (solid line) and SC transition temperature (bold dashed line) on the chemical potential for $\Omega = 0.4$. For such large values of Ω, there is no transition to the LTHP or the phase with the incommensurate lattice period modulation. In other words, the system may undergo only the transition either to the chess-board phase or to the SC one.

Let us estimate the SC transition temperature. Given $W \approx 0.5$ eV and $g \approx 0.25$ eV, the maximum value of

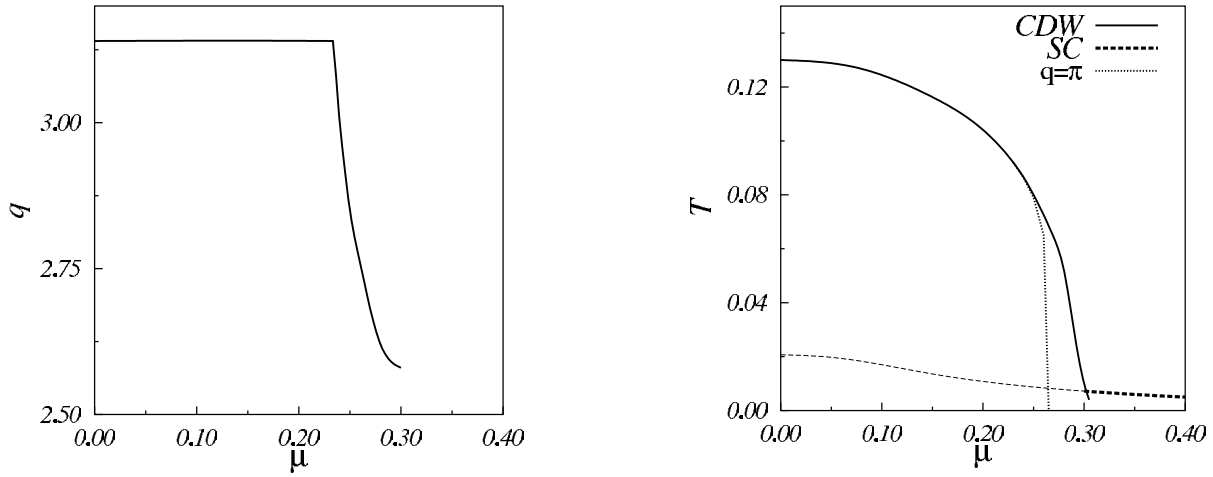


Fig. 2. The wave vector of the CDW-modulation $\vec{q} = (q, q)$, the temperature of the absolute instability of the high-temperature phase with respect to the transitions to CDW (solid line) and SC (bold dashed line) as functions of the chemical potential, for $\Omega = 0.2$ and $g = 0.5$. Dotted line shows the temperature of the transition to the phase with the modulation wave vector $\vec{q} = (\pi, \pi)$

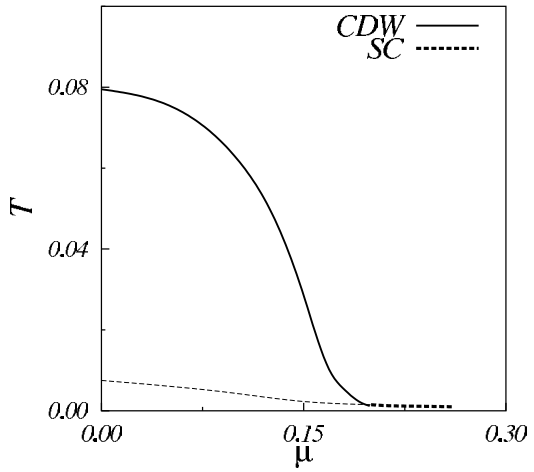


Fig. 3. Dependence of the temperature of the absolute instability of the high-temperature phase with respect to the transitions to CDW (solid line) and SC (bold dashed line) on the chemical potential, for $\Omega = 0.4$ and $g = 0.5$. The wave vector of the modulation is $\vec{q} = (\pi, \pi)$

the SC transition temperature is found to be $T^{\rm SC}_{\rm max} \approx 10 \div 40$ K. Making this estimation, we have taken into account that the SC transition occurs at non-half filling, because the system turns into CDW at $\mu = 0$. It is seen from Figs. 1—3 that, if there wasn't the CDW transition, the SC transition temperature would be several times greater than the obtained values of $T^{\rm SC}_{\rm max}$, at which the SC transition may actually occur. This agrees with the conclusions obtained for PEM in [33], where calculations were performed by analogy with the scheme used for the Eliashberg equations in the limit of the weak electron-phonon interaction, provided that the renormalization of the pseudospin excitement energy is neglected. According to the estimations carried out in [10], if there was no CDW, the SC transition temperature would be $T^{\rm SC} \approx 40$ K at the band filling close to a half.

The question as to what occurs in the system as the tunnel splitting frequency grows further is also of great interest. It was shown in [29] that, at $\mu = 0$, the critical temperature of the transition to the phase with the double lattice period modulation, $T_c^{\rm CDW}$, decreases with the increase in Ω according to the exponential law: $T_c^{\rm CDW} \sim \exp\left(-\frac{\pi\sqrt{\Omega W}}{g\sqrt{2}}\right)$. It follows from the analysis of the behavior of the $\tilde{T}_{\omega_1,\omega_2}$ matrix elements (Eq. (29)) that the SC transition temperature, $T_c^{\rm SC}$, changes with Ω in a similar way. In this case, for $\mu = 0$, $T_c^{\rm SC}(\Omega \to \infty) \approx T_c^{\rm CDW}(\Omega \to \infty)$. As is seen from Figs. 1 — 3, with the increase in $|\mu|$, the CDW transition temperature falls more rapidly than the SC one. Thus, for the non-zero values of the chemical potential, provided that Ω is sufficiently large, the SC transition temperature is expected to be higher than the CDW one, and there will only be the transition to SC. However, as was noted above, to make the correct analysis of the competition between these transitions, the renormalized Γ^0 vertex should be used when solving Eq. (28) and determining $T_{\rm SC}$. In addition, when Ω values are sufficiently large, the applicability of the approximation used to derive this equation becomes unjustified.

Conclusions

In this work, the possibility of the appearance of the SC ordering has been studied in the PEM with the tunnel splitting of levels in the limit of the weak pseudospin-electron interaction. The phase diagrams in the (T, μ) and (q, μ) planes have been constructed. When the chemical potential is located near the band center (the case of half-filling, $\mu \approx 0$), the transition to the phase with the modulation of the lattice period is found to occur. For the non-half filling case, the SC transition may appear, provided that the tunnel frequency Ω is nonzero.

The results obtained for the two-dimensional PEM are similar to those obtained for the infinite-dimensional Holstein model, although the phonon coordinates are continuous in the latter, whereas, in the former, the pseudospin variable takes on only two values. Contrary to the studies [1–4], we have revealed that the transitions to either the incommensurate phase or LTHP is possible too. Though the authors of [1] admitted that the incommensurate phase might exist within a very narrow region of the phase diagram, we have shown that, in our case, this area is rather extensive, when Ω is not large. In addition, the papers mentioned did not study the influence of the change in the phonon frequency on the phase diagram shape. It was only noted that, at small frequencies, the SC transition temperature went to zero. As has been shown by us, in the case of the PEM, the range of the chemical potential values, within which the SC transition may occur, becomes gradually narrowed as Ω decreases, and finally, disappears at $\Omega = 0$.

It should be noted that the conditions for the SC to appear, which are found by us for PEM, supplement the results of the analysis made both within the scheme of the Eliashberg equations [33], where the consideration was confined to the case with the electron band filling close to a half, and on the basis of the quantum Monte Carlo simulations [15]. In [15], it was only established that SC might appear at low temperatures, but the transition to CDW was not studied. As follows from our study, the presence of the CDW phase gives rise to the fact that, for the PEM, the transition to SC occurs at the non-half filling beyond the region of the existence of CDW.

The mechanism that leads to SC, which we have considered in this paper, as also the traditional phonon one, does not result in the high values of T_c, and apparently thus, it does not explain the HTSC phenomenon.

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НАДПРОВІДНІСТЬ У ПСЕВДОСПІН-ЕЛЕКТРОННІЙ МОДЕЛІ

Т.С. Мисаковіч, І.В. Стасюк

Р е з ю м е

Досліджується статична сприйнятливість у надпровідному каналі для локально ангармонічної кристалічної системи з сильними електронними кореляціями в рамках псевдоспін-електроної моделі (ПЕМ) з тунельним розщепленням рівнів при слабкій псевдоспін-електронній взаємодії. В режимі $\mu =$ const є можливість фазового переходу до фази з модуляцією періоду гратки у випадку, коли хімпотенціал знаходиться поблизу центра зони. При відмінному від половинного заповненні зони та ненульовій частоті тунелювання Ω виявлено перехід до надпровідної фази. Досліджено вплив тунельного розщепленя на фазові переходи.