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Dielectric instabilities and phase transitions in pseudospin-electron model of HTSC systems

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The possible dielectric instabilities and phase transitions in high-T_c superconductors are analyzed within the pseudospin-electron model involving Hubbard type electron correlations as well as their interaction with local anharmonic vibrational modes. The calculation of the dynamic dielectric susceptibility $\chi(\omega, \mathbf{q})$ is performed in the generalized random phase approximation. The instabilities with respect to the polarization and/or charge fluctuations are obtained from the temperature dependences of $\chi(\omega, \mathbf{q})$. The behavior of low-frequency modes in the vicinity of these instabilities is investigated. The case of the infinity narrow electron band is considered in details.

This report presents the results of the investigations of the dynamic dielectric susceptibility of the local anharmonic model in the theory of high-T_c superconductors. The model involves the characteristic features common for all high-T_c superconductors, i.e. the presence of two-dimensional tightly-bounded CuO_2 layers separated by the layers with soft dynamic configurations characterized by anharmonic effective potentials (e.g., anharmonic vibrations of apex oxygen ions of YBaCuO type compounds) [1,2].

In this context, the model Hamiltonian

$$H = \sum_i H_i + \sum_{ij\sigma} t_{ij}\, a^+_{i\sigma} a_{j\sigma}\,, \tag{1}$$

$$H_i = U n_{i\uparrow} n_{i\downarrow} + E_0 (n_{i\uparrow} + n_{i\downarrow}) + $$
$$+ g(n_{i\uparrow} + n_{i\downarrow}) S^z_i - \Omega S^x_i - h S^z_i \tag{2}$$

was proposed by Müller [3] (see also [4]). Hamiltonian (1) describes the strongly correlated electrons of CuO_2 sheets coupled with the local anharmonic vibrations represented by pseudospin variables.

In the Hubbard operators representation, the Hamiltonian (2) is diagonal for $\Omega = 0$, and for $\Omega \neq 0$ it can be reduced to the diagonal form with the help of rotational transformation $|R\rangle = \alpha_{Rr}\, |r\rangle$ (for details see [5,6]), which results in the Hamiltonian

$$H = \sum_{ir} \lambda_r X^{rr}_i + \sum_{ij\sigma} t_{ij}\, a^+_{i\sigma} a_{j\sigma} \tag{3}$$

with

$$\lambda_{r,\tilde r} = U\delta_{n_r,2} + E_0\, n_r \pm \frac{1}{2}\sqrt{(n_r g - h)^2 + \Omega^2} \tag{4}$$

and $a^+_{i\sigma} = \sum\limits_{mn} A^{\sigma}_{mn} X^{mn}_i$, $a_{i\sigma} = \sum\limits_{mn} A^{\sigma}_{mn} X^{nm}_i$. Here $n_1 = 0$, $n_2 = 2$, $n_3 = n_4 = 1$ $(n_r = n_{\tilde r})$ are the eigenvalues of electron number operator (the tilde indicates the states with $S^z_i = -1/2$). Operators $X^{mn}_i = |m\rangle\langle n|$ are defined on the basis of single-site vibronic states $|n_{i\uparrow}\,, n_{i\downarrow}\,, S^z_i\rangle$. The detailed consideration of single-electron spectrum of model (1) was performed in [5,6] in Hubbard-1 approximation. The interaction with the anharmonic mode splits energy levels of ordinary Hubbard model 0, E_0 and $2E_0 + U$ into sublevels (4) (vibronic states). As the result, each Hubbard single-electron band splits into four subbands.

The problem of the possible coexistence of ferroelectricity and superconductivity in high-T_c compounds is under discussion starting from the discovery of the high temperature superconductivity (see, e.g., [7,8]). There are no direct observations of ferroelectricity in high-T_c superconductors due to the presence of the small conductivity in the normal direction to the conducting planes CuO_2 but in some articles the observations of the pyro- and piezoelectric effects [9] and anomalies of dielectric susceptibility [10] were reported.

In order to investigate the possible instabilities of the system with respect to the polarization or charge density fluctuations the semi-invariant Matsubara's Green functions

$$K^{AA'}_{lm}(\tau - \tau') = \langle \tilde T \tilde A_l(\tau) \tilde A'_m(\tau')\rangle^c \tag{5}$$

(where A, $A' = n, S^z$), which determine the corresponding contributions to the transverse dielectric susceptibility ($\chi^{AA'} = K^{AA'}$ and $\chi^{AA'} = K^{AA'} - K^{An}K^{nA'}/K^{nn}$ for regimes $\mu = \text{const}$ and $n = \text{const}$, respectively), were calculated. In the case of YBaCuO structure the pseudospin component of the transverse polarization vector ($A = S^z$) is connected with the apex oxygen motion in the double well potential and the electron component ($A = n$) with the electron charge redistribution between the CuO$_2$ layers and other structure elements (reservoir of the electrons which fix the value of the chemical potential).

In the case of zero hopping $t_{ij} = 0$ the exact expressions for correlation functions $\chi^{AA'}(\omega_n) = \chi^{AA'}_{s,\alpha}(\omega_n) + \chi^{AA'}_d(\omega_n)$ ($\alpha = \mu$ or n) are obtained:

$$\chi^{SS}_{s,\mu}(\omega_n) = \frac{\beta}{4}\delta(\omega_n)\left[\sum_{r=1}^{4}\cos^2 2\varphi_r(b_r + b_{\tilde{r}}) - \left(\sum_{r=1}^{4}\cos 2\varphi_r(b_r - b_{\tilde{r}})\right)^2\right], \tag{6}$$

$$\chi^{nS}_{s,\mu}(\omega_n) = \chi^{Sn}_{s,\mu}(\omega_n) = \beta\delta(\omega_n)\left[(1 - \tfrac{n}{2})\cos 2\varphi_2(b_2 - b_{\tilde{2}}) - \tfrac{n}{2}\cos 2\varphi_1(b_1 - b_{\tilde{1}}) + (1 - n)\cos 2\varphi_3(b_3 - b_{\tilde{3}})\right],$$

$$\chi^{nn}_{s,\mu}(\omega_n) = \beta\delta(\omega_n)[n(1 - n) - 2(b_3 + b_{\tilde{3}})]$$

in $\mu = \text{const}$ regime and

$$\chi^{SS}_{s,n}(\omega_n) = \frac{\beta}{4}\delta(\omega_n)\left[\sum_{r=1}^{4}\left(\frac{\cos 2\varphi_r}{\operatorname{ch}\beta/2\,[(n_r g - h)^2 + \Omega^2]^{1/2}}\right)^2 (b_r + b_{\tilde{r}}) + \right.$$
$$\left. + \left(\cos 2\varphi_1 \operatorname{th}\frac{\beta}{2}\sqrt{h^2 + \Omega^2} + \cos 2\varphi_2 \operatorname{th}\frac{\beta}{2}\sqrt{(2g - h)^2 + \Omega^2} - 2\cos 2\varphi_3 \operatorname{th}\frac{\beta}{2}\sqrt{(g - h)^2 + \Omega^2}\right)^2 \frac{\gamma(b_3 + b_{\tilde{3}})^2}{1 - 2(1 - \gamma)(b_3 + b_{\tilde{3}})}\right] \tag{7}$$

$\chi^{nS}_{s,n}(\omega_n) = \chi^{Sn}_{s,n}(\omega_n) = 0$, $\chi^{nn}_{s,n}(\omega_n) = 0$ in $n = \text{const}$ regime ($\cos 2\varphi_r = (n_r g - h)/[(n_r g - h)^2 + \Omega^2]^{1/2}$). Here

$$b_p = \left[\sum_r e^{-\beta\lambda_r}\right]^{-1} e^{-\beta\lambda_p}$$

is the semi-invariant of the first order. The terms with factors $\delta(\omega_n)$ contribute to the so-called isothermal susceptibility. Dynamical part of susceptibility is determined by the pseudospin contribution

$$\chi^{SS}_d(\omega_n) = \frac{1}{2}\sum_{r=1}^{4}\frac{\Omega^2(b_r + b_{\tilde{r}})\operatorname{th}\beta/2\sqrt{(n_r g - h)^2 + \Omega^2}}{\sqrt{(n_r g - h)^2 + \Omega^2}\,[(n_r g - h)^2 + \Omega^2 - (i\omega_n)^2]} \tag{8}$$

and appears only at non-zero tunneling frequency Ω. Its poles gives the energies of the pseudospin excitations. One can see from (6) and (7) that the character of the temperature dependence of the susceptibility (in the same manner as for the Ising model) strongly depends on the values of the longitudinal and transversal fields h and Ω. The change of the electron concentration which may be caused by the charge redistribution between the reservoir and conducting layers reflects in the change of the intensities of the low-frequency excitations (Fig. 1).

Whereas at $n = \text{const}$ regime the chemical potential is always in one of the subbands (or between them), in the regime $\mu = \text{const}$ it becomes possible that the chemical potential goes out from (or enters into) the energy band. If the chemical potential moves inside the band with the change of the electric field, then the electron concentration (average occupancy of states) in layer changes. This can correspond to the so-called electric-field effect observed in HTSC compounds [11].

The influence of the electron hopping on the charge and pseudospin correlation functions is analyzed in

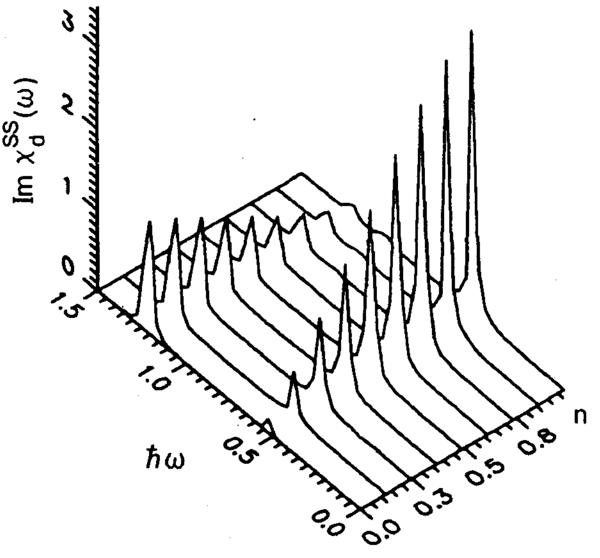

Fig. 1. Imaginary part of $\chi_d^{SS}(\omega)$ vs. electron concentration n ($h/g = 1.1, \Omega/g = 0.5, T/g = 0.5$).

the case $\Omega = 0$ which is simpler for consideration. For $\Omega = 0$, the Green's functions (5) can be expressed in terms of functions $K_{lm}^{(pq)}(\tau - \tau') = \langle \widetilde{T}\widetilde{X}_l^{pp}(\tau)\widetilde{X}_m^{qq}(\tau')\rangle_c$ the Fourier transforms of which can be presented in the form [12]

$$K(\omega_n, \mathrm{q}) = \beta \{b(\mathrm{q}) + {}'\Pi(0, \mathrm{q})b(\mathrm{q})\Pi'(0, \mathrm{q}) +$$

$$+ {}'\Pi(0, \mathrm{q})b(\mathrm{q}) + b(\mathrm{q})\Pi'(0, \mathrm{q})\}\delta(\omega_n) + \Pi''(\omega_n, \mathrm{q}) \,, \tag{9}$$

where the «full» semi-invariant of the second order satisfies the Dyson type equation $b(\mathrm{q}) = b + b\Pi(0, \mathrm{q})b(\mathrm{q})$.
The last term in (9) determines the dynamic part of susceptibility.

Summing up the diagrams determining renormalized loops Π, $'\Pi$, Π', Π'', we have restricted ourselves to the contributions from the ladder diagrams with antiparallel lines (so-called generalized random phase approximation [13]) constructed by zero-order loops Π_0, $'\Pi_0$, Π_0', Π_0'' (see, [12,14]).

The numerical calculations of the static dielectric susceptibility $\chi_\perp(\mathrm{q}, 0)$ were performed for different points of the Brillouin zone. We may separate three regions corresponding to different values of asymmetry parameter h ($h < 0$, $0 < h < g$, $h > g$) with different behavior of susceptibility. This is caused by the rearrangement of the single-electron spectrum at the points $h = 0$ and $h = g$ [6].

In the case opposite to $t_{\mathrm{q}} = 0$ the presence of the electron transfer leads to the appearance of divergences on the temperature dependences of the functions χ_n^{SS} and χ_μ^{SS} (existing in the certain range of parameter values)*. Out of the vicinity of this divergence the temperature behavior of the pseudospin component of susceptibility is similar to the one obtained in the case of zero hopping.

For $h > 0$ and $h < g$ such divergences exist only at $\mathrm{q} = 0$ (Γ-point) and can be treated as the manifestation of the dielectric type instabilities which appear in the pseudospin subsystem (i.e. system of anharmonic oscillators) under the influence of the effective interactions. The denominator in the expression for susceptibility χ^{SS} becomes zero at the temperature of the divergency T^*. This denominator is connected with the factor $(1 - \hat{b}\hat{\Pi})^{-1}$, which appears as the result of the summation of polarization loop series. The total loop Π_{ij}^{rs} describes the effective interaction between the states $|r\rangle$ and $|s\rangle$ of the cells i and j via conducting electrons. The corresponding phase diagram T^* vs. n and q (where q is changed along the Γ-M line in the

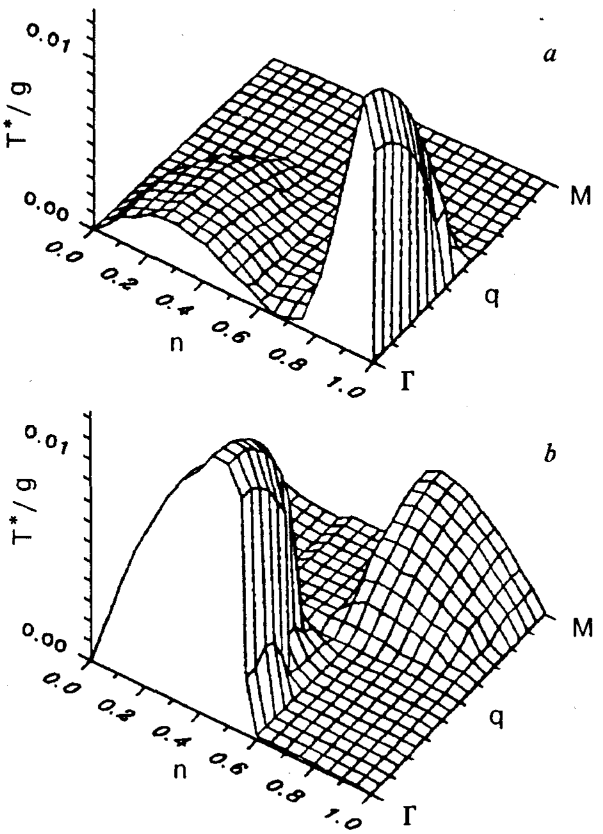

Fig. 2. T^* vs. n and q at $h/g = 1.05$ (*a*) and $h/g = 0.9$ (*b*) ($U \to \infty$, $W/g = 0.2$).

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* These divergences are very similar to the one reported in Ref. 10 for $YBa_2Cu_3O_{7-\delta}$.

$2D$ Brillouin zone) is shown in Fig. 2,*a*, where the surface limiting the stability region is plotted.

For $0 < h < g$ besides the dielectric instability at Γ point the instability at $\mathbf{q} = (\pi/a, \pi/a)$ (M point) with respect to the charge ordering is manifested (Fig. 2,*b*). This instability at M point corresponds to the one obtained within the mean field approximation (MFA) [14].

The above mentioned singularities are observed on the temperature dependences of the isothermal susceptibilities. We have also considered the features of the dynamic susceptibility which for our model is determined only by the charge–charge correlation function χ^{nn}.

For the cases $h > g$ and $h < 0$ there is a divergence in the temperature dependence of dynamic susceptibility at the temperature T^{**} lower then the corresponding one for the isothermal susceptibility.

In order to get the dynamic susceptibility ($i\omega_n \to \hbar\omega$) one should calculate the zero-order loops Π_0, $'\Pi_0$, Π'_0, Π''_0. Their real and imaginary parts in the $2D$ case that is considered possess van Hove singularities and contain contributions from the intra- and interband transitions.

The corresponding changes in the low-energy spectrum (the frequency dependence of the susceptibility) are investigated. The complicated spectrum caused by the van Hove singularities at high temperatures is seriously changed in the vicinity of T^{**}. Here the spectral density of states indicates the presence of relaxation type mode. Its relaxation rate is the linear function of wave vector and the corresponding relaxation time follows the Curie–Weiss temperature dependence.

For the parameter values when the instability with respect to charge ordering exists there are no any divergences on the temperature dependences of the dynamic susceptibility and the anomalies of the temperature behavior of the low-frequency spectrum are absent. That means that the charge ordering instability obtained within the pseudospin-electron model is caused by the mean-field effects which is in agreement with the calculations performed in the mean-field approximation in [14].

The obtained considerable increase in the contribution into transverse dielectric susceptibility from pseudospin and electron subsystems can lead to the increasing of the effective interelectron coupling constant λ. The high values of $\chi_S(0)$ and especially the anomalies of this function can influence the transition into the superconducting phase.

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