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The study of interplay of charge density wave and spin density wave in cuprate systems

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Abstract A microscopic model is proposed to study the co-existence of charge density wave (CDW) and spin density wave (SDW) effects in high-T_c super- conductors in normal state under underdoping condition before the onset of super-conductivity The one particle electron Green's functions are calculated by Zubarev's technique The CDW and SDW gap parameters are calculated from their correlation functions and solved self-consistently taking into account the position of the impurity levels and the hybridisation between the impurity electron and the copper *d*-electrons The temperature dependence of CDW and SDW gap parameters are studied for different model parameters of the system

Keywords superconductivity, charge density wave, spin density wave

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The interplay of lattice distortions accompanied by charge density wave (CDW) and superconductivity (SC) is inherent to cuprates.The existence of structural instability arising due to partial Fermi surface destruction prevents even high transition temperature T_c.The thermal expansion measurements on underdoped $La_{2-x}M_xCuO_4$ (M=Ba,Sr)system show two lattice instabilities having $T_{d_1} \approx 32K$ and $T_{d_2} \approx 36K$, while $YBa_2CuO_{7-\delta}$ with $T_c \approx$ 49K has a single instability at $T_d \approx 90$ K [1].Both T_{d_2} and T_d are close to maximal T_c's in the corresponding optimally doped compounds. Anomalous lattice properties above T_c in $La_{2-x}M_xCuO_4$ are observed in ultrasound experiments [2], thermal expansion and specific

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heat measurements [1]. The structural and electronic phase transitions occur above T_c for $La_{2-x}M_xCuO_4$, $YBa_2CuO_{7-\delta}$ and Bi-Sr-Ca-Cu-O [3,4]. It is remarkable that $Bi_2Sr_2CaCu_2O_{8+\delta}$ has T_c = 84K and structural transition at $T_d \simeq 95K$,while Bi-Sr-Ca-Cu -Pb-O has $T_c \simeq 107$ K and $T_d \simeq 130$ K [5]. The occurrence of a CDW in Cu-O plane of $YBa_2CuO_{7-\delta}$ is observed in scanning tunneling microscopy [6]-[10]. Similarly, the high-T_c cuprates also exhibit the antiferromagnetic phase for low dopant concentrations.So the cuprates having two dimensional character are likely candidates for the existence of spin density wave (SDW) [11]. Schrieffer *et al* [12] have proposed the SDW state as one of the reasons for the enhancement of T_c. The SDW and CDW states arise from the nesting property of the Fermi surface in low dimensional systems.The SDW state arises due to Coulomb interaction between electrons while CDW state is a consequence of the electron phonon interaction in presence of perfectly nested pieces of Fermi surface. Ghosh *et al* [13]have reported the interplay of the SDW and superconductivity for the cuprates.In the present communication we report the interplay of the CDW and SDW phases in presence of impurity in normal phase before the onset of the superconductivity.

The Hamiltonian used in this model is given by

$$H_0 = \sum_{k\sigma} \varepsilon_k c^\dagger_{k\sigma} c_{k\sigma} + \Delta^c \sum_{k\sigma} c^\dagger_{k\sigma} c_{k+Q,\sigma} + \Delta^s \sum_{k\sigma} \sigma\, c^\dagger_{k\sigma} c_{k+Q,\sigma}$$

$$+V \sum_{k,\sigma} \left(c^\dagger_{k,\sigma} f_{k,\sigma} f^\dagger_{k,\sigma} c_{k,\sigma} \right) + \varepsilon_f \sum_{k\sigma} f^\dagger_{k,\sigma} f_{k,\sigma}. \quad (1)$$

The first term in H_0 describes the hopping of copper d-electron between adjacent sites. Here $c^\dagger_{k\sigma}, (c_{k\sigma})$ are the creation (annihilation) operators of the conduction electrons of copper.The hopping takes place between the neighbouring sites of copper with the dispersion $\varepsilon_k = -2t_0 \left[\cos(k_x) + \cos(k_y) \right]$.

The second and third terms in H_0 describe the mean field CDW and SDW states. In high-T_c systems oxygen atoms surrounding the central Cu-atom form an octahedron. The structural evidences show that the neighbouring Cu-O octahedra are enlarged and contracted alternately. As a result ,Cu-atoms acquire disproportionate charges, because of the two different Cu-O bond lengths.This indicates to the existence of strong electron-phonon interaction. The presence of the nested pieces of Fermi surface and the disproportionate charges of Cu-site stabilizes the system with Fermi surface instability by the formation of the charge density wave (CDW).Long range antiferromagnetic order present in cuprates owes its origin to itinerant electrons in the system.The presence of the Fermi surface instability due to the existence of the nested pieces of Fermi surface results in the formation of a spin density wave (SDW). The Δ^c and Δ^s are respectively the CDW and SDW order parameters given by

$$\Delta^c = -V_0 \sum_{k\sigma} \left\langle c^\dagger_{k,\sigma} c_{k+Q,\sigma} \right\rangle, \quad (2)$$

$$\Delta^s = -U_0 \sum_{k\sigma} \sigma \left\langle c^{\dagger}_{k,\sigma} c_{k+Q,\sigma} \right\rangle, \tag{3}$$

where V_0 and U_0 being respectively the attractive and repulsive strengths and Q being the nesting wave vector.The nesting of pieces of the Fermi surface separated by the wave vector Q responsible for the formation of CDW and SDW results in the electron-hole symmetry.

$$\varepsilon_{k\pm Q} = -\varepsilon_k \, . \tag{4}$$

The fourth term of eq.(1) describes a weak hybridisation between the f-level of the rare earth ion and the Cu-3d electron band. This is mostly in influenced by the degree of a dispersionless hybridization strength (V). The fifth term in H_0 describes the intra f-electron kinetic energy term with the dispersionless renormalized f-level energy ε_f of the rare-earth ion and $f^{\dagger}_{i,k,\sigma}$, $(f_{i,k,\sigma})$ are the creation (annihilation)operators of the localised electrons.

We calculate one electron Green 's function using the Hamiltonian H_o given in eq.(1) for the CDW and SDW of the cuprate system in presence of impurity by using Zubarev 's technique [14].The Green's functions $A_i(k,w)$(i = 1 – 4) involved in these calculations are defined as

$$A_1(k,\omega) = \left\langle\left\langle c_{k,\sigma}; c^{\dagger}_{k,\sigma} \right\rangle\right\rangle_{\omega},$$

$$A_2(k,\omega) = \left\langle\left\langle c_{k+Q,\sigma}; c^{\dagger}_{k,\sigma} \right\rangle\right\rangle_{\omega},$$

$$A_3(k,\omega) = \left\langle\left\langle f_{k,\sigma}; c^{\dagger}_{k,\sigma} \right\rangle\right\rangle_{\omega},$$

$$A_4(k,\omega) = \left\langle\left\langle f_{k+Q,\sigma}; c^{\dagger}_{k,\uparrow} \right\rangle\right\rangle_{\omega} . \tag{5}$$

The four coupled equations involving four Green 's functions are solved and are given below.

$$A_1(k,\omega) = \left(\frac{1}{2\pi}\right)\left[\frac{\left((\omega+\varepsilon_k)(\omega+\varepsilon_f)-v^2\right)(\omega-\varepsilon_f)}{|D_\sigma(\omega)|}\right], \tag{6}$$

$$A_2(k,\omega) = \left(\frac{1}{2\pi}\right)\left[\frac{\left(\Delta^c+\Delta^s\sigma\right)\left(\omega^2-\varepsilon_f^2\right)}{|D_\sigma(\omega)|}\right], \tag{7}$$

$$A_3(k,\omega)=\left(\frac{1}{2\pi}\right)\left[\frac{v\left((\omega+\varepsilon_k)(\omega+\varepsilon_f)-v^2\right)}{|D_\sigma(\omega)|}\right], \tag{8}$$

$$A_4(k,\omega)=\left(\frac{1}{2\pi}\right)\left[\frac{\left(\Delta^c+\Delta^s\sigma\right)\left(\omega^2-\varepsilon_f^2\right)}{|D_\sigma(\omega)|}\right], \tag{9}$$

where

$$|D_\sigma(\omega)|=\left[\omega^4-\omega^2P_\sigma+Q_\sigma\right]. \tag{10}$$

The four quasi particle bands for the up-spin are $\pm\omega_{1,2}$ and the four quasi particle bands for the down-spin are $\pm\omega_{3,4}$

$$\pm\omega_{1,2}=\left[\frac{P_1\pm\sqrt{P_1-4Q_1}}{2}\right]^{1/2},$$

$$\pm\omega_{3,4}=\left[\frac{P_3\pm\sqrt{P_2-4Q_1}}{2}\right]^{1/2}, \tag{11}$$

where P_1 Q_1 are for the up-spins and P_2, Q_2 are for down spins :

$$P_1=E_{1,k}^2+\varepsilon_f^2+2V^2;\ Q_1=E_{1,k}^2\varepsilon_f^2-2\varepsilon_k\varepsilon_fV^2+V^4,$$

$$P_2=E_{2,k}^2+\varepsilon_f^2+2V^2;\ Q_2=E_{2,k}^2\varepsilon_f^2-2\varepsilon_k\varepsilon_fV^2+V^4, \tag{12}$$

$$E_1^2=\varepsilon_k^2+\left(\Delta^c+\Delta^s\right)^2;\ \ E_2^2=\varepsilon_k^2+\left(\Delta^c-\Delta^s\right)^2. \tag{13}$$

The expression for CDW gap of eq.(2) is written as

$$\Delta^c=-g\int_{-\omega/2}^{\omega/2}d\varepsilon_k\left[\phi_{k,\uparrow}+\phi_{k,\downarrow}\right], \tag{14}$$

where the CDW coupling parameter $g = N(0)V_0$ with $N(0)$ being the density of states of the conduction electron at the Fermi level.The correlation function given in bracket of eq.(14) are calculated for the Green's function given in eq.(7) and given by

$$\phi_{k,\uparrow}=\frac{\Delta^c+\Delta^s}{2\left(\omega_1^2-\omega_2^2\right)}[F_{11}],$$

$$\phi_{k,\downarrow} = \frac{\Delta^c - \Delta^s}{2\left(\omega_3^2 - \omega^2\right)}[F_{22}],$$

$$F_{11} = \left[\frac{\left(\omega_2^2 - \varepsilon_f^2\right)}{\omega_2}\tanh\frac{\beta\omega_2}{2} - \frac{\left(\omega_2^2 - \varepsilon_f^2\right)}{\omega_1}\tanh\frac{\beta\omega_1}{2}\right], \tag{15}$$

$$F_{22} = \left[\frac{\left(\omega_4^2 - \varepsilon_f^2\right)}{\omega_4}\tanh\frac{\beta\omega_4}{2} - \frac{\left(\omega_3^2 - \varepsilon_f^2\right)}{\omega_3}\tanh\frac{\beta\omega_3}{2}\right]. \tag{16}$$

Similarly, the expression for SDW gap of eq. (3) is written as

$$\Delta^s = -g_1\int_{-\omega/2}^{\omega/2} d\varepsilon_k\left[\phi_{k,\uparrow} + \phi_{k,\downarrow}\right], \tag{17}$$

where the SDW coupling is $g_1 = N(0)U_0$ .The physical quantities involved are made dimensionless by dividing them by $2t_0$. They are

$$Z_1 = \frac{\Delta^c}{2t_0};\; Z_2 = \frac{\Delta^s}{2t_0};\; d = \frac{\varepsilon_f}{2t_0};\; v = \frac{V}{2t_0},$$

$$g = N(0)V_0;\quad g_1 = N(0)\,U_0\,.$$

The charge density wave (CDW)parameter (Z_1) and the spin density wave (SDW) parameter (Z_2) are solved self-consistently in normal phase.The temperature variation of Z_1 is shown in Figure 1 and that of Z_2 is shown in the inset of Figure 1. Both the parameters show similar temperature variations.The Z_1 and Z_2 slowly decreases and become minimum at the same temperature *i.e.* the CDW transition temperature (T_c) equals the SDW transition temperature (T_s) with $T_c = T_s \simeq$ 0.125.The gap parameters at T = 0 K are Z_1 (0) = 0.0174 and Z_2 (0) = 0.017. The CDW coupling g = 4.0 is much larger than the SDW coupling g_1 = 1.0.

The temperature variation of the SDW parameters for different values of the CDW coupling is shown in Figure 2. The SDW gap parameter (Z_2) decreases slightly with increase of the CDW coupling (g) similar to the charge density gap CDW. The temperature (T_c))remaining unchanged.The CDW gap also decreases with the increase of the CDW coupling [see inset of Figure 2].

The effect of SDW coupling (g_1) on the CDW gap parameter (Z_1) is shown in Figure 1. The increase of SDW coupling suppresses the CDW gap (Z_1) throughout the temperature

We have solved self-consistently, the gap equations of the CDW and the SDW phases in normal phase in presence of the impurity level (*d*) and the hybridization (*V*). Both the gaps Z_1 and Z_2 show slow temperature decrease with temperature and form a minima for $T_c \simeq T_s$ and increase beyond the temperature T_c. A large CDW coupling (g ~4) changes the CDW gap and the SDW gap. Now, the SDW coupling (g_1 ~ 1.25) suppresses both the gap parameters in normal phase. The hybridization between the impurity *f*-level and the conduction band enhances both the gaps due to introduction of lattice distortion in the system.

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