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Specific Heat Study of Distorted Iron based Superconductors

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Abstract. We have proposed here a mean field theoretical model in the coexistence of superconductivity and Jahn-Teller effect for the study of specific heat in iron based superconductors in presence of an external magnetic field. The superconducting gap and lattice strain energy expressions are calculated using the Zubarev's technique of double time electron Green's functions and solved numerically. The specific heat jump at the critical temperatures are observed.

Keywords: Iron pnictide superconductors, Jahn-Teller effect, Thermodynamic properties.

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1 Introduction

The discovery of electron doped iron pnictide ($LaOFeAs$) superconductors[1] has triggered intense research interest in condensed matter physics. The same is also the care for pnictide compounds $RFe\ (O_{1-x}F_x)$; where R = (Pr, Nd or Sm) having superconductivity above the transition temperature T_c=50 K. These compounds belong to the so called '1111' family. Besides the above pnictides, other types like $(A_{1-x}B_x)Fe_2As_2 (A = ba, Sr, Ca, B = K, Cs, Na)$ called "122" family of iron pnictides and $Fe(Se_xTe_{1-x})$ called "11" family have been discovered[2]. In all these compounds the Fe atoms form an equivalent superconducting layer. At present, the superconducting mechanism is under intensive investigations and their superconducting states remain elusive. There is still no established pairing state consistently explaining all the experimental data. The undoped "1111" and "122" parent compounds are semi-metals that undergo an Spin-Density Wave (SDW)-type antiferromagnetic transition in the temperature range of 100 -150K. In addition to this properties of magnetism a structural transformation takes place from a high-temperature tetragonal to low-temperature orthorhombic structure [3]. Upon doping, either with electrons or holes to the selective compounds [4, 5, 6] the antiferromagnetic transition is suppressed and superconductivity emerges.

The specific heat jump at the critical temperature T_c have been studied extensively[7,8, 10, 11, 12] for the above mentioned pnictide compounds. The specific heat is a fundamental property that probes directly the low energy electronic excitations near the Fermi energy and can give information on the density of states. The characteristics of phase transition, the phase diagram and fluctuation effects etc. can be studied from this thermodynamic property. The specific heat jump at the T_c for *s*-wave superconductors have been studied[9]. The temperature dependent specific heat can be expressed as $C(T) = \gamma T + \beta T^3 + \eta T^5$. At lower temperatures the electronic specific heat coefficient $\gamma \simeq C(T)/T$. Ding *et al*.[12] have observed γ = 81.0 and 83.7 mJ/molK^2 with applied magnetic fields 0T and 8T between the temperatures 14K and 20K for the $SmO_{1-x}F_xFeAs$ compound. This value of γ is much larger than the 1.0 mJ/mol K^2 observed by Sefat *et al*.[5] for $LaO_{0.89}FeAs(T_c = 28K)$. The temperature dependent specific heat have been studied by Johnston *et al*.[13] for $Ca_{0.32}Na_{0.32}Na_{0.68}Fe_2As_2$ in various magnetic fields. They have observed the specific heat coefficient γ for parent compound to be around 5.4 mJ/molK^2 which is in agreement with the previous results ranging between 4.7 and 8.2 mJ/molK^2 [14, 15].

Here we present the BCS model along with Jahn-Teller distortion and with external magnetic field applied to the system for the study of superconducting gap, lattice strain energy and electronic specific heat in the underdoped region before the onset of the superconductivity. Section 2 describes the mean-field theory of the model. Section 3 presents the calculations for the SC and JT order parameters and specific heat. The results and discussion are in section 4 and finally conclusion in section 5.

2. Theoretical Model

Here we consider the model Hamiltonian[16] for the *s*-wave pairing interaction within the same orbitals and the same strength of interactions for the two orbitals and the mean-field Hamiltonian for a JT distorted and SC state in presence of the external magnetic filed. The Hamiltonian is defined as

$$H = H_0 + H_{JT} + H_I \,. \tag{1}$$

Here H_0 describes the hopping of conduction electrons between the neighbouring sites of the two degenerate orbitals and is given by

$$H_0 = \sum_{\alpha,k,\sigma} (\varepsilon_k - \sigma B)(c^{\dagger}_{\alpha,k,\sigma} c_{\alpha,k,\sigma}) \tag{2}$$

Through the Jahn-Teller interaction the electron density in the degenerate band is coupled to the static elastic strain. The interaction is described by

$$H_{JT} = \sum_{k,\sigma} Ge\left(c^{\dagger}_{1,k,\sigma} c_{1,k,\sigma} - c^{\dagger}_{2,k,\sigma} c_{2,k,\sigma}\right) + \frac{1}{2} C_0 e^2 \tag{3}$$

Here *G* is the strength of the JT coupling and e is the strength of uniform lattice strain defined as

$$e = -\frac{G}{C_0} \sum_{k,\sigma} \left(\left\langle c^{\dagger}_{1,k,\sigma} c_{1,k,\sigma} \right\rangle - \left\langle c^{\dagger}_{2,k,\sigma} c_{2,k,\sigma} \right\rangle \right), \tag{4}$$

where C_0 is the elastic constant. The expression for lattice strain is found by the minimization of the free energy of the electron including the elastic energy. The free energy is defined as

$$F = -k_B T \sum_{k,i} ln\left(1 + exp[\pm \beta \omega_i(k)]\right) + \frac{1}{2} C_0 e^2 \tag{5}$$

with $\beta = \frac{1}{k_B T}$, k_B is the Boltzmann constant and i = 1, 2. On minimizing the free energy with respect to the parameter e such that $\frac{\partial F}{\partial e} = 0$, one can find the self-consistent equation for the corresponding gap equation of strain e. The spontaneous splitting of the bands and building up of strain indicates a structural transition. This building up of strain leads to lattice elastic energy $\frac{1}{2} C_0 e^2$. The lattice strain splits the single degenerate band into two bands with energies $E_{1,2k} = \varepsilon_k \pm G_e$.

Now the superconductivity is considered including the intra-band pairing coupling for both the bands by the Hamiltonian as

$$H_I = -\Delta_{sc} \sum_{k} \left(c^{\dagger}_{1,k,\uparrow} c^{\dagger}_{1,-k,\downarrow} + c^{\dagger}_{2,k,\uparrow} c^{\dagger}_{2,-k,\downarrow} + h.c \right), \tag{6}$$

where Δ_{sc} is the amplitude of the SC gap and is defined as

$$\Delta_{sc} = -\sum_{k,\sigma} \tilde{V}_k \left(\left\langle c^{\dagger}_{1,k,\uparrow} c^{\dagger}_{1,-k,\downarrow} \right\rangle + \left\langle c^{\dagger}_{2,k,\uparrow} c^{\dagger}_{2,-k,\downarrow} \right\rangle \right), \tag{7}$$

where $\tilde{V}_k$ is the effective attractive interaction in BCS limit and $\tilde{V}_k = -V_0$ for $\varepsilon_k < \hbar w_D$ or 0.

3. Calculation of order parameters and specific heat

The double time single particle electron Green's functions are calculated by Zubarev's technique[17]. The Green's functions for the orbitals 1 and 2 are defined as

$$A_1(k,w) = \left\langle\left\langle c_{1,k,\uparrow}; c^{\dagger}_{1,k,\uparrow} \right\rangle\right\rangle_w \;;\; A_2(k,w) = \left\langle\left\langle c^{\dagger}_{1,-k,\downarrow}; c^{\dagger}_{1,k,\uparrow} \right\rangle\right\rangle_w$$

$$B_1(k,w) = \left\langle\left\langle c_{2,k,\uparrow}; c^{\dagger}_{1,k,\uparrow} \right\rangle\right\rangle_w \;;\; B_2(k,w) = \left\langle\left\langle c^{\dagger}_{2,-k,\downarrow}; c^{\dagger}_{1,k,\uparrow} \right\rangle\right\rangle_w . \qquad (8)$$

In these Green's functions four-fold band energies $\pm w_\alpha (\alpha = 1$ to 4) are observed in the presence of the external magnetic field B as

$$\pm w_1 = -B \pm \sqrt{E^2_{1,k} + \Delta^2} \;;\; \pm w_2 = -B \pm \sqrt{E^2_{2,k} + \Delta^2} \,,$$

$$\pm w_3 = B \pm \sqrt{E^2_{1,k} + \Delta^2} \;;\; \pm w_4 = B \pm \sqrt{E^2_{2,k} + \Delta^2} \,,$$

where the quasi-particle bands $E_{1,2k}$ are given $E_{1,2k} = \varepsilon_k \pm Ge$.

The SC and JT order parameters defined in eqns.(7) and (4) respectively are calculated from the Green's functions A_i and B_i = (i =1,2) to be

$$1 = -g \int_{-w_D}^{w_D} d\varepsilon_k \left[\frac{1}{w_1 - w_2} F_1(w) - \frac{1}{w_3 - w_4} F_2(w) \right] \qquad (9)$$

and

$$e = -G \frac{N(0)}{C_0} \int_{-\frac{w}{2}}^{\frac{w}{2}} d\varepsilon_k \left[\frac{1}{w_1 - w_2} \{F_3(w) + F_5(w)\} - \frac{1}{w_3 - w_4} \{F_4(w) + F_6(w)\} \right] \qquad (10)$$

respectively with the SC coupling $g = N(0)V_0$g and $N(0)$ being the density of states (DOS) of conduction electrons and the integration is carried out within the cut-off energy w_D. The different functions $F_i(w)$ (i = 1 to 6) are given by

$$F_1(w) = \frac{1}{e^{\beta w_1} + 1} - \frac{1}{e^{\beta w_2} + 1} \;;\; F_2(w) = \frac{1}{e^{\beta w_3} + 1} - \frac{1}{e^{\beta w_4} + 1} \,,$$

$$F_3(w) = \frac{w_1 + \varepsilon_{2k}}{e^{\beta w_1} + 1} - \frac{w_2 + \varepsilon_{2k}}{e^{\beta w_2} + 1} \;;\; F_4(w) = \frac{w_3 + \varepsilon_{4k}}{e^{\beta w_3} + 1} - \frac{w_4 + \varepsilon_{4k}}{e^{\beta w_4} + 1} \,,$$

$$F_5(w)=\frac{-w_1+\varepsilon_{1k}}{e^{-\beta w2}+1}-\frac{w_1+\varepsilon_{1k}}{e^{-\beta w2}+1}\ ;\ F_6(w)=\frac{-w_3+\varepsilon_{3k}}{e^{-\beta w3}+1}-\frac{-w_3+\varepsilon_{3k}}{e^{-\beta w3}+1}\ ,$$

where $\varepsilon_{1,2k}=\varepsilon_k+Ge\mp B$ and $\varepsilon_{3,4k}=\varepsilon_k-Ge\mp B$ respectively.

The entropy and specific heat at constant volume can be calculated from the free energy for the system expressed in eqn.(5) in terms of the quasi-particle energies. The four quasi-particle energies are w_{ik} (i =1 to 2) and are written as $w_{ik}=(-1)^i B\pm\sqrt{E_{ik}^2+\Delta^2}$ with $E_{ik}=\varepsilon_k\pm Ge$. The entropy S per particle from the relation is $S=-(\partial F/\partial T)_v$ which leads to the well-known expression[18].

$$S=-\sum_{w_i>0}\left[f(w_i)\,ln\,f(w_i)+f(-w_i)\,ln\,f(-w_i)\right], \tag{11}$$

where $f(w)$ is the Fermi distribution function. From the expression of entropy $S(T)$ the specific heat at constant volume can be calculated as

$$C_v=T\left(\frac{\partial S}{\partial T}\right). \tag{12}$$

The superconducting gap parameter Δ and the JT gap parameter Ge are solved self-consistently. To perform the numerical calculations, we have considered the bandwidth of conduction band $W = 8t_0$, where t_0 is the hopping integral and all the quantities entering in eqns.(9) and (10) are made dimensionless by dividing with $2t_0$. The non-dimensional parameters are the SC gap parameter $z=\frac{\Delta_{sc}}{2t_0}$, the lattice strain e, reduced temperature $t=\frac{k_BT}{2t_0}$, the magnetic field $b=\frac{B}{2t_0}$, the SC coupling constant $g=N(0)V_0$ and the JT coupling constant $g_1=\frac{G}{2t_0}$. The interplay of SC gap parameter z and JT gap parameter $e'(=g_1\times e)$ are studied in absence of external magnetic field.

4 Results and Discussion

A standard set of parameters is chosen as g = 0.032, g_1 = = 0.180, band-width W = $1eV$, cutoff energy $w_D \simeq 250K$ to perform numerical calculations for temperature dependence of $z(t)$ and $e'(t)$. The inset of fig.1 shows the temperature dependence of the SC gap $z(t)$ and the JT gap $e'(t)$. The JT gap is suppressed in the coexistence phase with the SC gap. The SC transition temperature $t_c \simeq 0.011$ is approximately equal to 28K and the distortion temperature $t_d \simeq 0.019$ is approximately equal to 48K[16]. The temperature dependent electronic specific heat (C_v) is computed numerically and plotted in fig.1 in corresponds to the temperature dependent JT and SC gaps as shown in inset of this figure. The linearity of the specific heat in the paramagnetic phase for temperature $t > t_d$ $\simeq$0.019 is clearly shown. The specific heat shows a jump at the JT transition temperature t_d $\simeq$0.019 and then decreases towards the lower temperatures upto the SC transition temperature t_c. It shows another jump at the SC transition temperature t_c $\simeq$0.011and then further decreases towards lower temperatures. The electronic coefficient of the specific heat γ is determined to be 5.75$mJ/molK^2$ which is in agreement with the values ranging between 4.7 and 8.2$mJ/molK^2$ [13, 14, 15] for iron based superconductors.

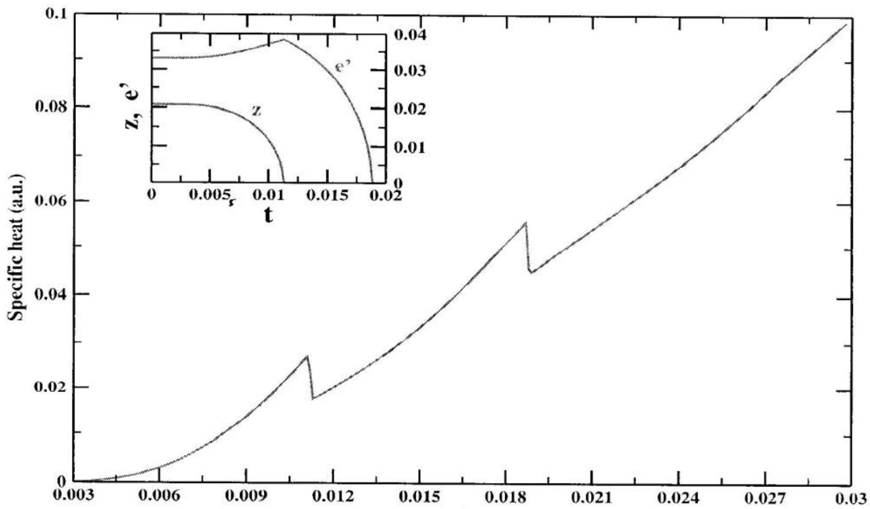

Fig.1. The plot of electronic Specific heat vs. reduced temperature *t* for fixed values of SC coupling constant g = 0.032, JT coupling constant g_1 = 0.180 and external magnetic field b = 0T. The inset is the self-consistent plots of SC gap (z) JT gap (e′) vs. reduced temperature (t) for the same values of g, g_1 and b.

The effect of the SC coupling constant g on the specific heat C_v is shown in fig.2. The SC transition temperature t_c decreases with the increase of the SC coupling g with the decrease of the SC gap throughout the temperature range as shown in the inset of fig.2 but the JT transition temperature t_d does not change with g however the JT gap is suppressed in the coexistence state.

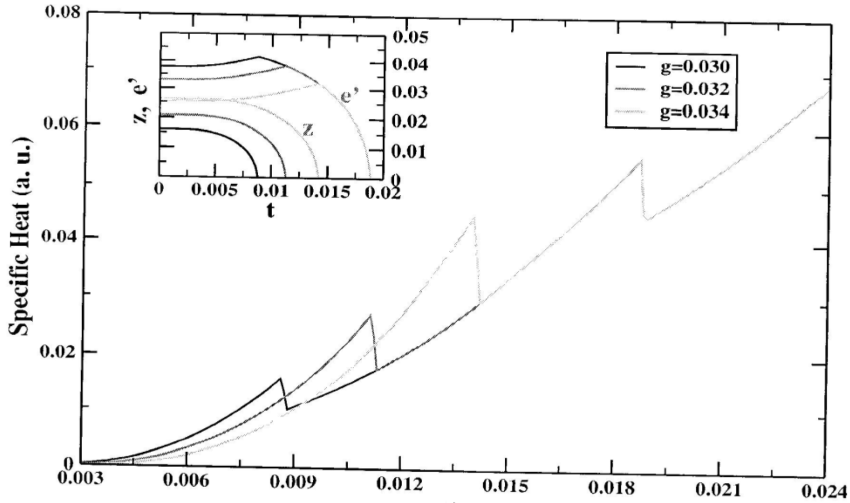

Fig.2. The plots of electronic Specific heat vs. reduced temperature t for fixed values of JT coupling constant g_1= 0.180 and external magnetic field b = 0T and different values of SC coupling constant g = 0.030, 0.032 and 0.034. The inset is the self-consistent plots of SC gap (z) JT gap (e') vs. reduced temperature (t) for the same values of g, g_1 and b.

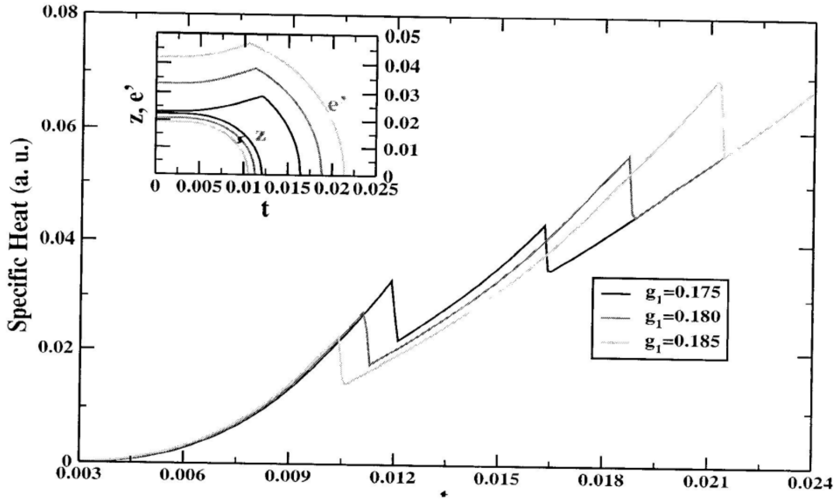

Fig.3. The plots of electronic Specific heat vs. reduced temperature t for fixed values of SC coupling constant g = 0.032 and external magnetic field b = 0T and different values of JT coupling constant g_1 = 0.175, 0.180 and 0.185. The inset is the self-consistent plots of SC gap (z) JT gap (e') vs reduced temperature (t) for the same values of g, g_1 and b.

The effect of the JT coupling constant g_1 on the specific heat C_v is shown in fig.3. The inset of this figure shows the temperature dependence of the JT and the SC gaps with the variation of the JT coupling g_1. As g_1 increase from 0.0175 to 0.185 the SC transition temperature increases with the increase of the SC gap throughout the temperature range but the JT transition temperature decreases with the decrease of the JT gap throughout the range of temperature.

5. Conclusion

The mean field Hamiltonian for the coexistence of the superconductivity and the Jahn-Teller effect is solved by using Zubarev's technique of the double time electron Green's function. The SC gap and the lattice strain energy expressions are derived and solved numerically self-consistently and observed their effect on one another in the coexistence phase. The specific heat expression is derived from the free energy expression and solved numerically, which shows the paramagnetic linear phase and the jumps at the SC and JT transition temperatures.

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