Effect of electron correlation on superconducting pairing symmetry

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Abstract. The role of electron correlation on different pairing symmetries are discussed in details where the electron correlation has been treated within the slave boson formalism. It is shown that for a pure s or pure d wave pairing symmetry, the electronic correlation suppresses the s wave gap magnitude (as well as the T_c) at a faster rate than that for the d wave gap. On the other hand, a complex order parameter of the form $(s + i\text{d})$ shows anomalous temperature dependence. For example, if the temperature (T_c^d) at which the d wave component of the complex order parameter vanishes happens to be larger than that for the s wave component (T_c^s), then the growth of the d wave component is arrested with the onset of the s wave component of the order parameter. In this mixed phase however, we find that the suppression in different components of the gap as well as the corresponding T_c due to coulomb correlation are very sensitive to the relative pairing strengths of s and d channels as well as the underlying lattice. Interestingly enough, in such a scenario (for a case of $T_c^s > T_c^d$) the gap magnitude of the d wave component increases with electron correlation but not T_c^d for certain values of electron correlation. However, this never happens in case of the s wave component. We also calculate the temperature dependence of the superconducting gap along both the high symmetry directions ($\Gamma - M$ and $\Gamma - X$) in a mixed $s + i\text{d}$ symmetry pairing state and the thermal variation of the gap anisotropy ($\frac{\Delta_{\Gamma-M}}{\Delta_{\Gamma-X}}$) with electron correlation. The results are discussed with reference to experimental observations.

PACS. 74.25.Dw Superconductivity phase diagrams – 74.62.-c Transition temperature variations – 74.20.Fg BCS theory and its development

1 Introduction

The correlated electron systems like the high temperature cuprate superconductors, show various anomalous physical properties in the normal as well as in the superconducting state. Along with the unsolved problems concerning the pairing mechanism in these exotic materials the question of order parameter symmetry is also not yet understood. In the weak coupling conventional BCS superconductors, superconductivity results from a pairing of electrons *via* phonon-mediated attractive electron-electron interaction which dominates the usual Coulomb repulsion at low temperature, and an energy gap $\Delta(k)$ appears in the quasiparticle spectrum. This energy gap is very nearly isotropic in k-space, so that the gap has the same magnitude and phase in all directions *i.e.*, an isotropic s-wave pairing state. In the high-T_c superconductors the pairing of charge carriers is established by experiments on flux quantization [1], *I-V* characteristics of Josephson tunnel junction [2] and Andreev scattering [3].

But the point contact tunneling [4] on various high-T_c materials and nuclear quadrupole/magnetic resonance and relaxation measurements [5] conclude that the energy gap function in these materials has considerable anisotropy. In high-T_c superconductors, measurements of the temperature dependence of the NMR Knight shift [5,6] of suitable nuclei in a superconductor ruled out the possibility of p-wave pairing but whether the pairing is of s-wave or d-wave type is not yet settled. The results of NMR experiments measuring Cu-relaxation rates by Martindale *et al.* [7], are in agreement with the prediction of d-wave pairing. Measurement of penetration depth λ at low temperatures [8] on $YBa_2Cu_3O_{6.95}$ supports d-wave pairing. Recent angle-resolved photoemission spectroscopy (ARPES) study [8] also suggests a d-wave state. However, there exist some experimental results like variation of penetration depth in $Nd_{2-x}Ce_xCuO_4$ [9], measurements of Josephson supercurrent for tunneling between Pb and $YBa_2Cu_3O_7$ [10] which does not correspond to the exact d-wave symmetry. Moreover, some photoemission studies on $Bi_2Sr_2CaCu_2O_{8+x}$ [11] are inconsistent with pure d-wave but are more consistent with a mixed state of s and d wave

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components. Kotliar [12] and Ruckenstein *et al.* [13] first introduced the concept of mixed s + id and s + d symmetries respectively. Their ideas of mixed configuration was to interpret the NMR and NQR data in the superconducting state of YBCO [14] and the Josephson critical current measurements in YBCO (superconductor-normal-superconductor) SNS junctions and YBCO/Pb junction [15].

Based on the discussions on the experimental situation about the determination of the order parameter symmetry in high temperature superconductors it is clear that there are various opinions about pairing symmetry in cuprates, which are known to be correlated system. Therefore, in the present paper the effect of Coulomb correlation on the superconducting state is considered based on a weak coupling theory. The role of electron correlation on different pairing symmetries are discussed in details where the electron correlation has been treated within the slave boson formalism. It is shown that for a pure s or pure d wave pairing symmetry, the electronic correlation suppresses the s wave gap magnitude (as well as the T_c) at a faster rate than that for the d wave gap. On the other hand, a complex order parameter of the form (s + id) shows anomalous temperature dependence. For example, if the temperature (T_c^d) at which the d wave component of the order parameter vanishes happens to be larger than that for the s wave component (T_c^s) then the growth of the d wave component is arrested with the onset of the s wave component of the order parameter. In this mixed phase however, it is shown that the suppression in different components of the gap as well as the corresponding T_c are very sensitive to the relative pairing strengths of s and d channels as well as the underlying lattice. Interestingly enough, in such a scenario (for a case of $T_c^s > T_c^d$) the zero temperature gap magnitude of the d wave component increases with electron correlation but not T_c^d for certain values of electron correlation. However, this never happens in case of the s wave component. We also calculate the temperature dependence of the superconducting gap along both the high symmetry directions ($\Gamma - M$ and $\Gamma - X$) in a mixed s + id symmetry pairing state and the thermal variation of the gap anisotropy ($\frac{\Delta_{\Gamma-M}}{\Delta_{\Gamma-X}}$) with electron correlation. The results are discussed with reference to experimental observations.

The lay out of the rest of the paper is as follows. In Section 2 we describe the effect of on-site coulomb correlation on weak coupling superconductivity. In this section we also present the slave boson approximation to the on-site coulomb correlation in the Hubbard model. Section 3 is devoted to describe the effect of electronic correlation on different order parameter symmetries. Effect of electron correlation on each order parameter symmetry is described sequentially in each subsection of this section with detailed discussions on the results. A comparison of the present study with ARPES results in high-T_c materials are described in Section 4. Finally, remarks have been made about the present calculation in the conclusion Section 5.

2 Effect of electron correlation on a weak coupling theory of superconductivity

The simplest model that describes the electron-electron interaction in a correlated system, like the high-T_c cuprates, is the single band Hubbard model. One of the major problems in solving the Hubbard model is how to treat the correlation exactly. One of the ways to do so is to take recourse to the slave boson formulation of Kotliar and Ruckenstein (KR) [18]. In this representation a set of four bosons are assigned for four possible occupancies of a lattice site. The bosonic fields which keep track of the four different occupations of a site 'i' are $e_i^\dagger(e_i)$, $s_{i\sigma/(-\sigma)}^\dagger(s_{i\sigma/(-\sigma)})$ and $d_i^\dagger(d_i)$ corresponding to creation (annihilation) of empty, single occupation with spin $\sigma/(-\sigma)$ and double occupation respectively. Of course the total probability of occupation of any site is one and it has to be respected. Secondly, the fermion number should be conserved at ith site in this slave boson representation. These two constraints are imposed by two conditions, completeness relation and charge conservation, written as,

$$e_i^\dagger e_i + \sum_\sigma s_{i\sigma}^\dagger s_{i\sigma} + d_i^\dagger d_i = 1 \qquad (1)$$

$$c_{i\sigma}^\dagger c_{i\sigma} = s_{i\sigma}^\dagger s_{i\sigma} + d_i^\dagger d_i. \qquad (2)$$

The Hubbard Hamiltonian is described as

$$H = \sum_{ij\sigma} t_{ij} c_{i\sigma}^\dagger c_{j\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow} - \mu \sum_{i\sigma} n_{i\sigma} \qquad (3)$$

where the first term is the usual tight binding Hamiltonian with the hopping integral t_{ij}, the second term denotes the intra-atomic Coulomb repulsion (U) between two electrons with opposite spins occupying the same site and the third term denotes the chemical potential (μ) which can take into account the deviation from half-filling. The prescription for the transformation of equation (3) in terms of the slave boson operators is given below:

$$\left.\begin{array}{rcl} n_{i\uparrow} n_{i\downarrow} & \longrightarrow & d_i^\dagger d_i \\ n_{i\sigma} & \longrightarrow & \tilde{n}_{i\sigma} \\ c_{i\sigma}^\dagger c_{j\sigma} & \longrightarrow & z_{i\sigma}^\dagger \tilde{c}_{i\sigma}^\dagger \tilde{c}_{j\sigma} z_{j\sigma} \end{array}\right\} \qquad (4)$$

where

$$z_{i\sigma} = (1 - d_i^\dagger d_i - s_{i\sigma}^\dagger s_{i\sigma})^{-\frac{1}{2}} (e_i^\dagger s_{i\sigma} + s_{i-\sigma}^\dagger d_i)$$
$$\times (1 - e_i^\dagger e_i - s_{i-\sigma}^\dagger s_{i-\sigma})^{-\frac{1}{2}} \qquad (5)$$

and $\tilde{c}_{i\sigma}^\dagger$ is the modified fermion creation operator. The form of $z_{i\sigma}$ is so chosen as to reproduce the correct band structure in the absence of correlation. The operators $(e_i^\dagger s_{i\sigma} + s_{i-\sigma}^\dagger d_i)$ in the equation (5) describe the hopping process of electron *i.e.*, if an electron hops from site 'i' to 'j', the slave bosons must simultaneously change at j and i. Depending on whether the site 'i' is singly or doubly occupied the bosonic state of 'i' must change from $s_{i\sigma}^\dagger$ to

$e_i^\dagger$ or from $d_i^\dagger$ to $s_{i-\sigma}^\dagger$. Thus there are two transition channels which add up, and the total transition probability must be equal to one. It is therefore useful to introduce a normalization factor, which guarantees the conservation of probability even in the mean-field theory.

Following KR the Hubbard Hamiltonian can be rewritten in terms of the slave boson operators as

$$\mathrm{H} = \sum_{ij\sigma} t_{ij} z_{i\sigma}^\dagger \tilde{c}_{i\sigma}^\dagger \tilde{c}_{j\sigma} z_{j\sigma} + U \sum_i d_i^\dagger d_i - \mu \sum_{i\sigma} \tilde{c}_{i\sigma}^\dagger \tilde{c}_{i\sigma}$$
$$+ \sum_{i\sigma} \lambda_{i\sigma}(\tilde{c}_{i\sigma}^\dagger \tilde{c}_{i\sigma} - s_{i\sigma}^\dagger s_{i\sigma} - d_i^\dagger d_i)$$
$$+ \sum_i \lambda_i'(1 - e_i^\dagger e_i - d_i^\dagger d_i - \sum_\sigma s_{i\sigma}^\dagger s_{i\sigma}) \quad (6)$$

where $\lambda_{i\sigma}$ and λ_i' are Lagrange multipliers which enforce the charge conservation and completeness relation (1,2) respectively. So the Coulomb interaction term is simplified and diagonalized with double occupancy operators but the kinetic energy part becomes complicated. The values of the boson field operators and the Lagrange multipliers are determined by minimizing the free energy of the system in the saddle point approximation, where all the bose operators and Lagrange multipliers are replaced by c-numbers. In this approximation the Hamiltonian is

$$\mathrm{H} = \sum_{ij\sigma} \tilde{q} t_{ij} \tilde{c}_{i\sigma}^\dagger \tilde{c}_{j\sigma} + (\lambda - \mu) \sum_{i\sigma} \tilde{c}_{i\sigma}^\dagger \tilde{c}_{i\sigma}$$
$$+ N\left[Ud^2 - 2\lambda(d^2 + s^2) + \lambda'(1 - d^2 - e^2 - 2s^2)\right] \quad (7)$$

where $\tilde{q} = \langle z_{i\sigma}^\dagger z_{j\sigma}\rangle$, e, d, s, λ, λ' are the saddle point values of the respective field operators, N is the number of sites, and in the case of paramagnetic ground state $s_\sigma = s_{-\sigma} = s$. The Hamiltonian of the system takes the simple form of an effective tight binding model with a modified hopping integral of the form $t_{ij} \longrightarrow \tilde{q} t_{ij}$, where the correlation effects are built in through the multiplicative factor $\tilde{q} = \langle z^\dagger z\rangle$. $\tilde{q}$ in general is a complicated function of the coulomb correlation u ($= \frac{U}{U_c}$, U_c being the Brinkmann-Rice value for metal-insulator transition) and the dopant concentration δ. In this approach solutions are obtained for the paramagnetic states for all values of u and band fillings that reproduces the correct Brinkmann-Rice result for metal-insulator transition at a critical value of correlation (U_c) at half-filling. Approximately, in the weak correlation limit $\tilde{q} = 1 - u^2$ and in case of strong correlation and small values of δ, $\tilde{q} = \frac{2\delta}{\sqrt{1-u^{-1}}}$ (for details please see Ref. [19,20]).

Now in order to study the effect of electron correlation on SC pairing symmetry we use a model Hamiltonian which contains in addition to a repulsive on-site coulomb correlation (7) term, a pairing term that leads to superconductivity (for our purpose). The pairing interaction is assumed to be due to some boson exchange (unknown) mechanism, as there exists no conclusive pairing mechanism for the high-T_c superconductivity. The pairing Hamiltonian in general may be written as,

$$\mathrm{H_p} = -\sum_{kk'} V_{kk'} c_{k\uparrow}^\dagger c_{-k\downarrow}^\dagger c_{-k'\downarrow} c_{k'\uparrow}. \quad (8)$$

While treating the electron correlations using salve boson formalism, the nature of the quasiparticles are no longer the bare electrons but the electronic quasiparticles of the correlated system (*i.e.* $\tilde{c}$). Therefore the bare electronic operators should be transformed accordingly as equation (4). As a consequence, the strength of the pairing interaction becomes $V_{kk'} \longrightarrow \tilde{q}^2 V_{kk'}$ when the $c_{k\sigma}(c_{k\sigma}^\dagger)$ are replaced by new quasiparticle operators $\tilde{c}_{k\sigma}(\tilde{c}_{k\sigma}^\dagger)$. Hence, the total Hamiltonian for the superconducting state in a correlated system can be written as,

$$\mathrm{H} = \mathrm{H_0} + \mathrm{H_B} + \mathrm{H_p} \quad (9)$$

where

$$\mathrm{H_0} = \sum_{k\sigma}(\tilde{q}\epsilon_k - \mu)\tilde{c}_{k\sigma}^\dagger \tilde{c}_{k\sigma} \quad (10)$$

$$\mathrm{H_B} = U\sum_i d_i^\dagger d_i - \sum_{i\sigma} \lambda_{i\sigma}(s_{i\sigma}^\dagger s_{i\sigma} + d_i^\dagger d_i)$$
$$+ \sum_i \lambda_i'(1 - e_i^\dagger e_i - \sum_\sigma s_{i\sigma}^\dagger s_{i\sigma} - d_i^\dagger d_i) \quad (11)$$

$$\mathrm{H_p} = -\sum_{kk'} V_{kk'} \tilde{q}^2 \tilde{c}_{k\uparrow}^\dagger \tilde{c}_{-k\downarrow}^\dagger \tilde{c}_{-k'\downarrow} \tilde{c}_{k'\uparrow} \quad (12)$$

where

$$\epsilon_k = -2t\left[(\cos k_x a + \gamma_1 \cos k_y a) + \gamma_2 \cos k_x a \cos k_y a\right],$$

where $\gamma_2 = \frac{2t'}{t}$, t and t' represent nearest neighbour and next nearest neighbour hopping respectively, $\gamma_1 = 1$ for square lattice and in presence of orthorhombic distortion $\gamma_1 < 1$.

Since in the saddle point approximation the bosonic part $\mathrm{H_B}$ is constant, so the effective Hamiltonian is given by

$$\mathrm{H} = \mathrm{H_0} + \mathrm{H_p}. \quad (13)$$

It can be seen from equation (12) that the pairing vertex between the correlated electrons mediated by some bosonic exchange is renormalized to $\tilde{q}^2 V_{kk'}$. Since $\tilde{q}^2$ deviates from unity ($\tilde{q}^2 < 1$ for $u \neq 0$), the SC-pairing amplitude will always be suppressed in presence of electron correlation, however, its details will depend on the value of u, δ and the nature of $V_{k,k'}$, is the main point of investigation in this work.

The SC order parameter in a correlated system may be defined as

$$\Delta(k) = \sum_{k'} \tilde{q}^2 V_{kk'} \langle \tilde{c}_{k'\uparrow}^\dagger \tilde{c}_{-k'\downarrow}^\dagger\rangle. \quad (14)$$

The Hamiltonian (13) is treated within the mean field theory (14) in order to yield the SC gap equation within a weak coupling theory as,

$$\Delta(k) = \sum_{k'} \tilde{q}^2 V_{kk'} \frac{\Delta(k')}{2E_{k'}} \tanh\left(\frac{E_{k'}}{2T}\right) \quad (15)$$

where the quasiparticle energy is given by

$$E_k^2 = (\tilde{q}\epsilon_k - \mu)^2 + |\Delta(k)|^2. \quad (16)$$

In the next section we will discuss about the different pairing symmetry and its effect in a correlated system.
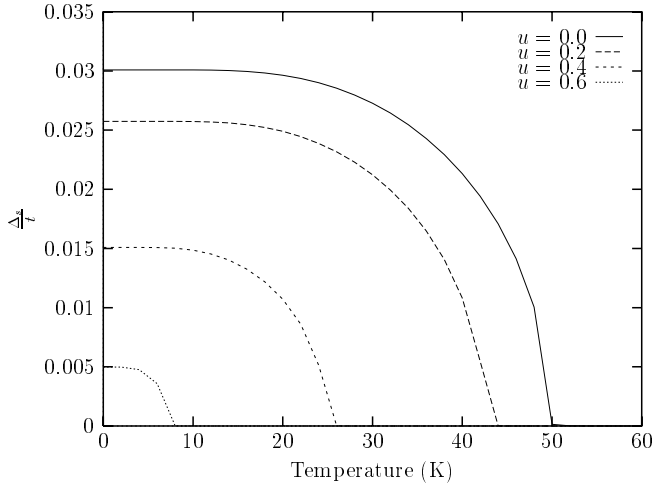
Fig. 1. Thermal variation of the isotropic s-wave gap ($v_s = 1$) for various values of the electron correlation ($u = U/U_c$) in a perfect square lattice (for other parameters, see text).

3 Effect of electron correlation on order parameter symmetry

Based on the nature of pairing potential, the symmetry of SC gap could be different. The pairing potential is usually assumed to have a separable form for simplicity *i.e.*,

$$V_{kk'} = V\eta_k\eta_{k'}. \tag{17}$$

Depending on the nature of the k-dependence of η_k one gets different symmetries such as (i) $\eta_k = $ constant, corresponds to an isotropic s-wave (conventional BCS) symmetry, (ii) $\eta_k = f(k)$, refers to an anisotropic s-wave symmetry, if $f(k)$ is a smooth function in the first Brillouin zone and is positive definite (*i.e.*, nodeless), (iii) $\eta_k = \cos k_x a + \cos k_y a$, corresponds to an extended s-wave pairing symmetry and (iv) $\eta_k = \cos k_x a - \cos k_y a$ corresponds to $d_{x^2-y^2}$ pairing symmetry. In the following we shall discuss only about the isotropic s-wave, the d-wave and a mixed symmetry state which will be defined later on.

3.1 Pure s-wave

The form of the pairing potential for isotropic s-wave symmetry is given by

$$V_{kk'} = v_s = \text{constant} \tag{18}$$

and the corresponding SC gap function $\Delta_k \equiv \Delta_s$. Hence the gap equation for a pure s-wave

$$\Delta_s = \tilde{q}^2 v_s \sum_{k'} \frac{\Delta_s}{2E_{k'}} \tanh(\frac{\beta E_{k'}}{2}) \cdot \tag{19}$$

The gap equation (19) can be solved analytically following the standard procedure of the BCS gap equation.
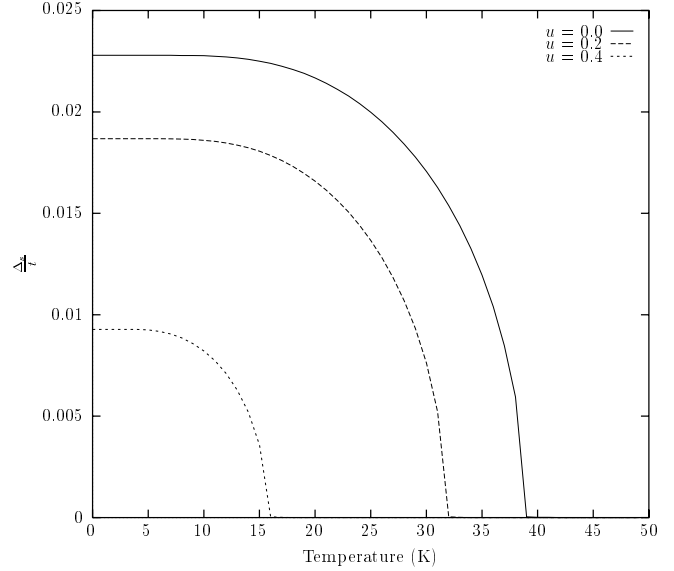

Fig. 2. Thermal variation of the isotropic s-wave gap ($v_s = 1$) in an orthorhombic lattice for various values of u (all other parameters being same as in Fig. 1).

However, we solve the gap equation numerically as the same will not be possible to solve analytically in case of d-wave as well as for the complex order parameter (discussed later on). All the parameters are expressed in units of t. However, at the end temperature has been expressed in Kelvin assuming $t = 0.3$ eV (realistic for copper oxide system), in order to examine, the real transition temperatures. For a set of parameter values $\omega_c = 0.6$ (cut-off value), $v_s = 1.0$ we present the numerical results in Figures 1 and 2. Figure 1 describes the temperature variation of the pure s-wave gap for a perfect square lattice whereas Figure 2 represents that for a distorted lattice ($t_x \neq t_y$, *i.e.*, $\gamma_1 = 0.95$) with next nearest neighbouring hopping $t' = 0.02t$. It is evident from both Figures 1 and 2 that the magnitude of Δ_s as well as the corresponding T_c decreases sharply with u. Furthermore, for the same set of parameter not only that the magnitude of Δ_s and T_c is less in the distorted case (*cf.* Fig. 2) than that for the perfect square lattice but also the fall in T_c with increasing u is more in comparison to the former case. So, the suppressive effect of electronic correlation on Δ_s and T_c is comparatively more in the orthorhombic phase (this may be clearer from Fig. 5) as will be discussed in the later subsections.

3.2 Pure d-wave

In case of the pure $d_{x^2-y^2}$ symmetry the pairing potential is given by

$$V_{kk'} = v_d(\cos k_x - \beta' \cos k_y)(\cos k'_x - \beta' \cos k'_y) \tag{20}$$

and the corresponding gap function is assumed as,

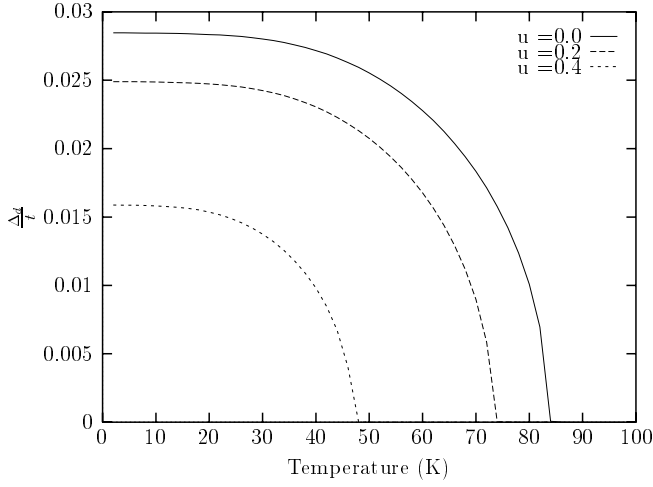$$\Delta_d(k) = \Delta_d^0(\cos k_x - \beta' \cos k_y) \tag{21}$$

Fig. 3. Thermal variation of the pure d-wave gap ($v_{\mathrm{d}} = 0.5$) for various values of the electron correlation in a perfect square lattice (for other parameters see text).
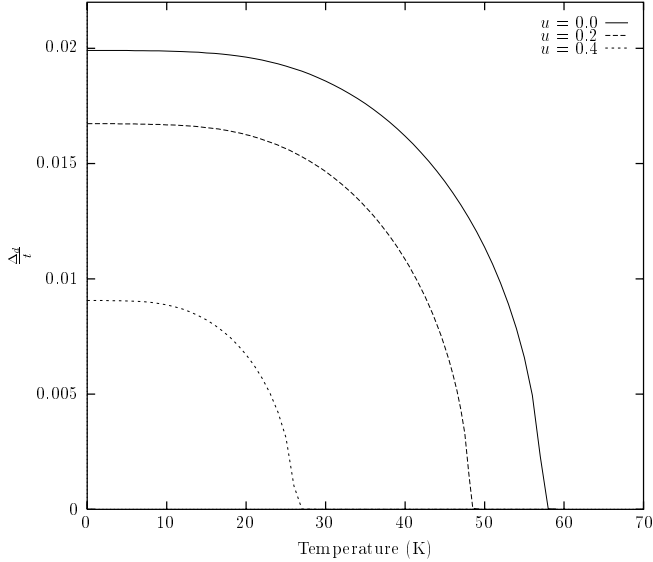

Fig. 4. Thermal variation of the pure d-wave gap ($v_{\mathrm{d}} = 0.5$) for various values of electron correlation in an orthorhombic lattice (with all the parameters being same as Fig. 3).

where v_{d} and Δ_{d}^0 represent the strength of the d-wave pairing potential and the amplitude of the gap function respectively. Where $\beta' = 1$ or $\beta' < 1$ corresponding to a square lattice or a orthorhombic lattice. So the resulting gap equation is written as

$$\Delta_{\mathrm{d}}^0 = \tilde{q}^2 v_{\mathrm{d}} \sum_{k'} \frac{\Delta_{\mathrm{d}}^0 (\cos k_x' - \beta' \cos k_y')^2}{2E_{k'}} \tanh\left(\frac{\beta E_{k'}}{2}\right). \tag{22}$$

In Figures 3 and 4 we show the thermal variation of the d-wave gap for the set of parameter values $\omega_{\mathrm{c}} = 0.6$, $v_{\mathrm{d}} = 0.5$ for square ($\gamma_1 = \beta' = 1$) and orthorhombic ($\gamma_1 = \beta' = 0.95$) lattices with next nearest neighbour hopping

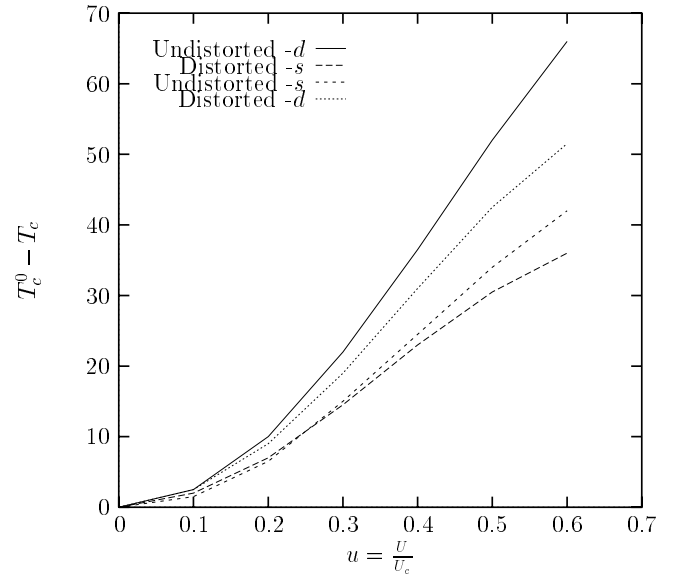**Fig. 5.** Change in T_{c} due to correlation for pure-s and pure-d wave gaps (in square and orthorhombic lattices) where $T_{\mathrm{c}}^0 \equiv T_{\mathrm{c}}(u = 0)$.

$t' = 0.02t$ respectively. The qualitative trend of behaviors for the thermal variation of the gap parameter remains almost unaltered *i.e.*, the magnitude of the gap as well as the T_{c} reduces with u. In case of orthorhombic lattice the SC gap and T_{c} is smaller than that of the undistorted one.

Figure 5 shows the variation of $T_{\mathrm{c}}^0 - T_{\mathrm{c}}$ *versus* u for s and d wave symmetry in distorted and undistorted lattice. T_{c}^0 is the SC T_{c} for $u = 0$. It is evident from Figure 5 that for distorted lattice the effect of u on T_{c} is more than the undistorted one for both s and d wave symmetry. It may be compared from Figures 1 and 3 that for an increase in u from 0 to 0.4 there is a reduction in T_{c} about 50% and 44% for the s and the d wave gaps respectively. The same when compared between Figures 2 and 4 the reduction in T_{c} is about 58% and 54% for the s and d-wave respectively. Therefore, in general the coulomb correlation affects the s-wave symmetry largely in comparison to the d-wave gap.

3.3 Mixed s + id order parameter symmetry

In the mixed symmetry state there is a mixture of both s and d wave order parameter and a phase difference of $\mathrm{e}^{i\frac{\pi}{2}}$ is considered [21]. The generalized form of the pairing interaction causing the superconductivity is given by

$$V_{kk'} = v_{\mathrm{s}} + v_{\mathrm{d}}(\cos k_x - \beta' \cos k_y)(\cos k_x' - \beta' \cos k_y') \tag{23}$$

where v_{s} and v_{d} correspond to the strengths of s and d wave channel interactions. And the corresponding s + id wave order parameter is taken as,

$$\Delta(k) = \Delta_{\mathrm{s}} + i\Delta_{\mathrm{d}}^0(\cos k_x - \beta' \cos k_y). \tag{24}$$

Substituting equations (23) and (24) into equation (15) and separating the real and imaginary parts of the equation, we obtain gap equations for coupled s and d wave
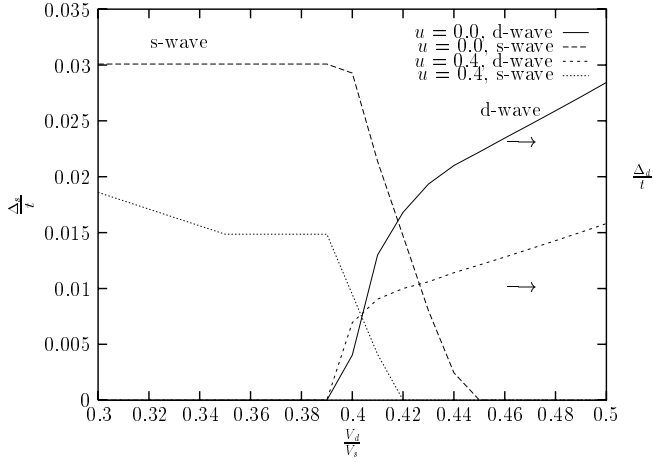
Fig. 6. Phase diagram of a s + id superconductor, where the amplitudes of the s-wave and d-wave component of the order parameter in a square lattice is plotted as a function of their relative strength v_d/v_s for different values of electron correlation at $T = 10$ K.

Fig. 7. Thermal variation of the amplitudes Δ_s and Δ_d (in units of t) of the complex order parameter $(s + id)$ for different values of electron correlation at $v_d/v_s = 0.4$ in a perfect square lattice (all other parameters are kept fixed as earlier figures).

components given by

$$\Delta_s = \tilde{q}^2 v_s \sum_{k'} \frac{\Delta_s}{2E_{k'}^{\mathrm{mix}}} \tanh\left(\frac{\beta E_{k'}^{\mathrm{mix}}}{2}\right) \qquad (25)$$

and

$$\Delta_d^0 = \tilde{q}^2 v_d \sum_{k'} \frac{\Delta_d^0 (\cos k_x' - \beta' \cos k_y')^2}{2E_{k'}^{\mathrm{mix}}} \tanh\left(\frac{\beta E_{k'}^{\mathrm{mix}}}{2}\right) \qquad (26)$$

with

$$E_k^{\mathrm{mix}\,2} = (\tilde{q}\epsilon_k - \mu)^2 + \Delta_s^2 + \Delta_d^{0\,2}(\cos k_x - \beta' \cos k_y)^2. \qquad (27)$$

Self-consistent solution of equations (25, 26) gives Δ_s and Δ_d^0 in a mixed $(s + id)$ wave state and for either $v_d = 0$ or $v_s = 0$ the coupled gap equations reduce to pure s-wave or pure d-wave (as discussed in the earlier subsections) respectively. To note, the difference between (19) and (25) as well as that between (22) and (26) lies mainly with the difference between E_k and E_k^{mix}. Here we performed the self-consistent solution of (25) and (26) with a cut off $\omega_c = 0.6$ (as in the earlier cases of a pure s or a d wave scenario).

In case of mixed $s + id$ symmetry with v_d and v_s both being finite, Figure 6 shows the phase diagram where the magnitudes of the order parameters with different symmetry at a temperature of 10 K are plotted against the ratio of the strength of interactions (v_d/v_s) for different u for the square lattice. This phase diagram has three regions, the region where only s-wave solution exists *i.e.*, for $v_d/v_s < 0.45$, only d-wave solution exists *i.e.*, for $v_d/v_s > 0.39$ and both the s and d wave solution co-exist for $0.39 < v_d/v_s < 0.45$. For finite electron correlation $u = 0.4$ the region with mixed symmetry shrinks to within
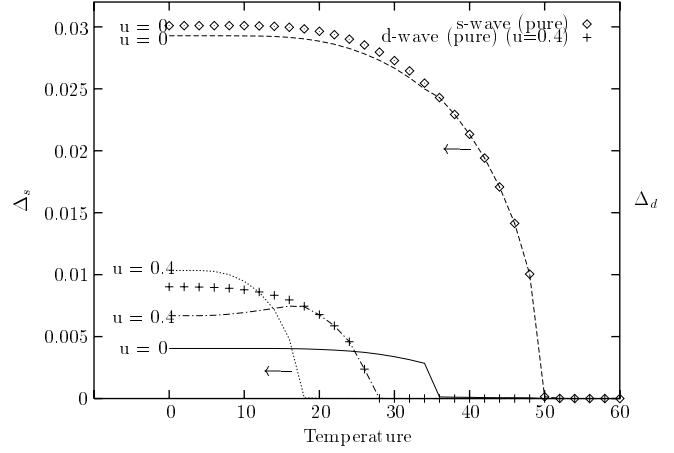
$0.39 < v_d/v_s < 0.42$ with larger decrease in the magnitude of the s-wave gap compared to that for the d-wave component. To note, with the electron correlation increased (to $u = 0.4$) the region (in terms of v_d/v_s) where the s-wave solution exists reduces (to $v_d/v_s < 0.42$), but that for the d-wave remains unchanged although the magnitude is suppressed. It is also important to note that the magnitudes of the s or d-wave component gaps with correlation depends crucially on the relative strength of interaction v_d/v_s.

Furthermore for $v_d/v_s \sim 0.39$ the s-wave gap decreases with u while d-wave gap increases slightly from its value compared to that at the uncorrelated case. This is because the rate of decrease of s-wave gap is more rapid than the d wave gap with correlation. For a clearer observation, the variation in the temperature dependence of the s-wave and d-wave component of the gap parameters in the mixed state (for $v_d/v_s = 0.4$) with electronic correlation is shown in Figure 7. The graph with diamond shows pure s-wave gap for the uncorrelated case ($v_s = 1$, $v_d = 0$). In the mixed state $v_d/v_s = 0.4$ (and in the absence of correlation), the s-wave gap has value slightly less than that of the pure case (the dashed line). With increasing correlation, $u = 0.4$, while the magnitude of s-wave gap is suppressed strongly (dotted line), that of the d-wave gap acquires higher value than the $u = 0$ case (the solid line). Nevertheless, the d-wave T_c (T_d^c) is higher for the uncorrelated case than that with correlation. Hence, in the lower temperature regions there is a competing effect between the s and d-wave gap parameters in the mixed symmetry region; with the appearance of the s-wave order parameter the d-wave gap is suppressed for the $u = 0.4$ case (the dash dotted line). The d-wave gap attains its highest value where the s-wave component gap amplitude vanishes. In this figure, the curve with ++ sign represents the pure d-wave gap with all the parameters being same ($v_d = 0.4$); demonstrating the arresting of the growth of the d-wave
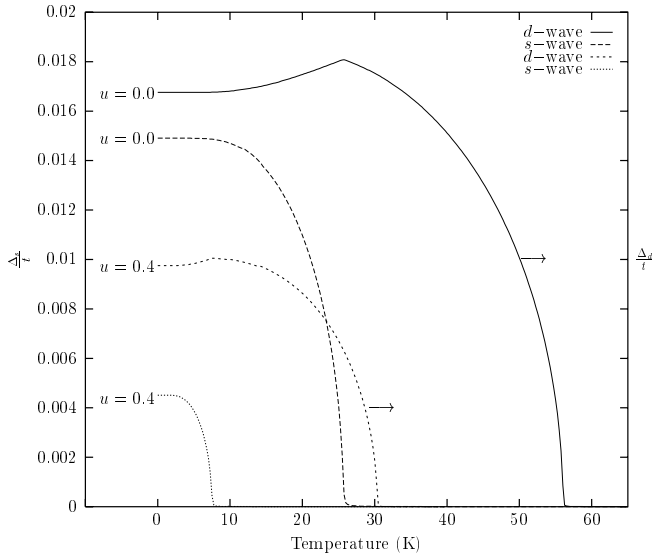
Fig. 8. Thermal variation of Δ_{s} and Δ_{d} of the complex order parameter $(\mathrm{s}+i\mathrm{d})$ for different values of electron correlation at $v_{\mathrm{d}}/v_{\mathrm{s}} = 0.42$ in a perfect square lattice (all other parameters are same as earlier figures).

Fig. 9. Thermal variation of Δ_{s} and Δ_{d} of the complex order parameter $(\mathrm{s} + i\mathrm{d})$ for different values of electron correlation at $v_{\mathrm{d}}/v_{\mathrm{s}} = 0.45$ in a perfect square lattice.

component with the opening up of the s-component gap in the mixed phase.

Figures 8 and 9 show the variation of s-wave and d-wave gap parameters for different u as the ratio of the strengths of interactions increases close to and beyond the values corresponding to the co-existence regions (for $u = 0.4$) *i.e.*, at $v_{\mathrm{d}}/v_{\mathrm{s}} = 0.42$ and $v_{\mathrm{d}}/v_{\mathrm{s}} = 0.45$ respectively. The gap magnitude for both the order parameter symmetry decreases with electron correlation, however, the rate of decrease is different for s and d in the mixed state which depends on $v_{\mathrm{d}}/v_{\mathrm{s}}$ ratio as well as the electron correlation. Here for the uncorrelated case it is clearly visible that the growth of d-wave component of the gaps is arrested with the onset of the s-wave component gap. In fact a detailed investigations of Figures 7 to 9 will demonstrate that in the mixed phase within the coexistence regime *i.e.*, $0.39 < v_{\mathrm{d}}/v_{\mathrm{s}} < 0.42$, the suppression in different components of the gap as well as the corresponding $T_{\mathrm{c}}^{\mathrm{s}}$ are very sensitive to the relative pairing strengths of s and d channels.

So far all the calculations for the mixed phase, were carried out for the square lattice. However, it was seen in case of the pure s and d phases that the introduction of orthorhombicity causes reduction in both, the magnitude of the order parameters as well as the corresponding $T_{\mathrm{c}}^{\mathrm{s}}$. So the effect of orthorhombicity on the mixed phase is now investigated. The phase diagram for different order parameter symmetry as a function of the $v_{\mathrm{d}}/v_{\mathrm{s}}$ ratio is depicted in Figure 10 for the orthorhombic distortion and finite next nearest neighbouring interaction. The s-wave and d-wave gap has lesser magnitude in the distorted lattice than that for the perfect square lattice in mixed s+id state and the region of s and d co-existence is shifted to smaller $v_{\mathrm{d}}/v_{\mathrm{s}}$ value and is shrunk to smaller region of area
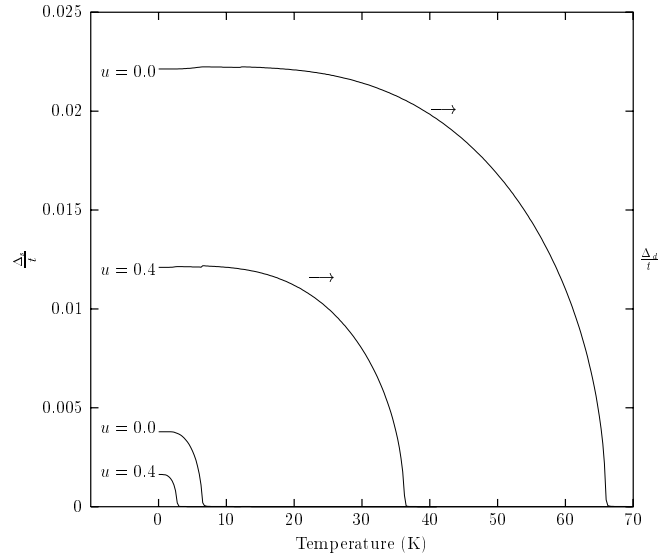
compared to the undistorted lattice. Similar to the phase diagram in Figure 6, the value of $v_{\mathrm{d}}/v_{\mathrm{s}}$ for the occurence of d-wave component does not change with u whereas that for the s component changes from $v_{\mathrm{d}}/v_{\mathrm{s}} < 0.48$ (for $u = 0$) to $v_{\mathrm{d}}/v_{\mathrm{s}} < 0.46$ (for $u = 0.4$). With a higher value of Coulomb correlation ($u = 0.4$) the s−d mixing region reduces further along with a large suppression in the magnitude of s-wave and d-wave gap parameters. It is noticable that the s-wave component suffers larger suppression in magnitude of the gap than that for the d-wave. The on-site Coulomb correlation strength u as well as the isotropic pairing strength v_{s} both being isotropic in nature, the s-wave gap magnitude is largely affected by Coulomb correlation, whereas due to extended nature of the d-wave component it is less affected by correlation. However, we note that in the mixed phase, depending on the value of $v_{\mathrm{d}}/v_{\mathrm{s}}$ the effect of electron correlation on transition temperatures $T_{\mathrm{c}}^{\mathrm{d}}$ or $T_{\mathrm{c}}^{\mathrm{s}}$ is very different. This is due to the fact that in the mixed phase none of the components (s or d) follow BCS like temperature variation. This has sometime led to increase in the gap magnitude with u but reduction in the $T_{\mathrm{c}} (\equiv T_{\mathrm{c}}^{\mathrm{d}})$ (*cf.* Fig. 7).

Figure 11 shows the variation of s and d wave component with electron correlations for $v_{\mathrm{d}}/v_{\mathrm{s}} = 0.45$. Similar to the square lattice the s and d wave gap parameters in the pure state take higher values than that in the mixed state for same parameter values v_{d}, v_{s} and u. This figure has to be contrasted with Figure 9. With the introduction of orthorhombicity the nature of the temperature variations of the different gap components changes abruptly. It is worth noting that in the pure s or pure d wave cases (discussed earlier) the orthorhombicity suppresses both the magnitude of the order parameters and the corresponding $T_{\mathrm{c}}^{\mathrm{s}}$ (*cf.* Fig. 1 to Fig. 4). However in the mixed state, because of the interplay between the two components of the order

Fig. 10. Phase diagram of a s + id superconductor where the amplitudes s-wave and d-wave component of the order parameter is drawn against their relative pairing strength in an orthorhombic lattice for different electron correlations ($T = 10$ K).
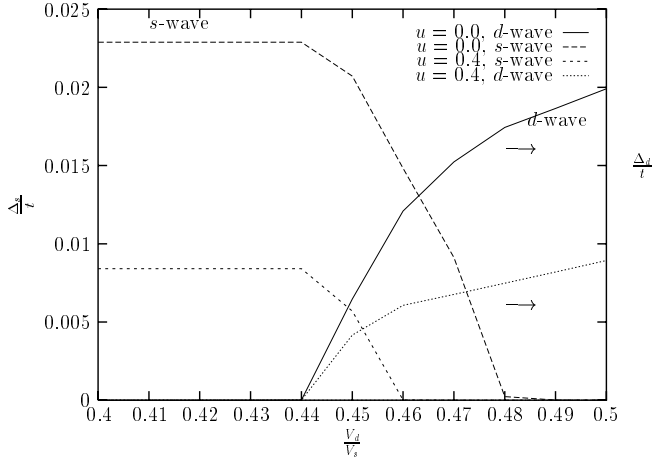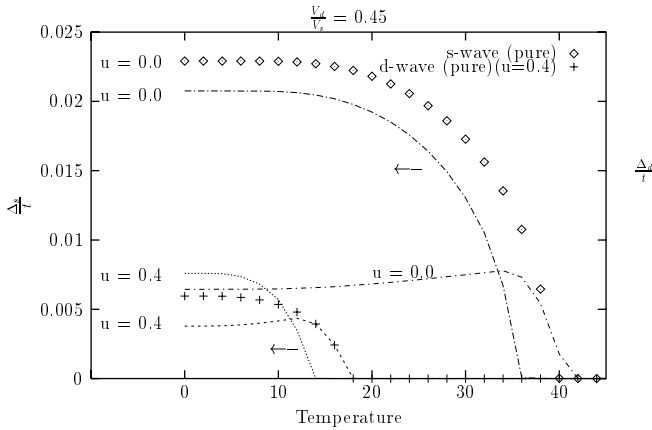

Fig. 11. Thermal variation of Δ_s and Δ_d of the complex order parameter (s + id) for different values of electron correlation in an orthorhombic lattice at $v_d/v_s = 0.45$.

4 Temperature dependent gap anisotropy in a correlated system

There are three broad catagories of experiments, which had been used to probe the symmetry of the superconducting gap function [8–10, 16, 22, 23] namely (i) magnetization and transport, (ii) spectroscopies and excitations and (iii) Josephson measurements. The most direct and fundamental probe of the gap magnitude in superconductors is angle resolved photoemission spectroscopy (ARPES), which indicates a highly anisotropic gap in high T_c compounds.

The main features observed from ARPES by different groups of experimentalists are summarized below: Shen *et al.* [23] observed that the SC-gap has (a) maximum magnitude along $\Gamma - M$ direction (Cu–O bond direction in real space); (b) minimum magnitude (negligible spectral weight) along $\Gamma - X(Y)$ direction (diagonal to the Cu–O bond) and there is a monotonic increase in the magnitude of the gap from its smallest value along the $\Gamma - X$ direction, thereby confirming true anisotropy. The authors of [23] argue that these results are consistent with $d_{x^2-y^2}$ symmetry of the gap. However, the data on the momentum-resolved temperature dependence of the SC gap of Bi-2212 by Ma *et al.* [11] is not only in contradiction with Shen *et al.* [23] but also it shows some exciting features. For measurements of the temperature dependence of the gap, the angle resolved photoemission data have been taken for temperatures ranging from 36 to 95 K along the $\Gamma - M$ as well as in the $\Gamma - X$ (40 to 95 K) high symmetry directions. The photoemission SC condensate spectral area along $\Gamma - M$ direction exists till the bulk transition temperature, $T_c = 83$ K. The measured SC gap is almost independent of the temperature at lower temperatures and retains its maximum value even up to temperature 85% of its T_c. But most interesting features to note is that, the photoemission condensate spectral area is remarkably weaker at 40 K in the $\Gamma - X$ direction compared to that in the $\Gamma - M$ direction, indicating a smaller size of the gap. The size of the gap at 36 K in the $\Gamma - M$ direction is 16 meV whereas that in the $\Gamma - X$ direction is 10 meV (at $T = 40$ K). The finite gap magnitude along $\Gamma - X$ direction below T_c ruled out the possibility of simple d-wave pairing [16]. However, at 70 K when the gap along the $\Gamma - M$ direction retains 90 to 100% of its full value, but becomes indistinguishable from zero along the $\Gamma - X$ line. This may be taken as a signature of a two component order parameter, $d_{x^2-y^2}$ type close to T_c and a mixture of the both s and d otherwise. Moreover, the significant point is that, due to the unconventional temperature dependence of the SC gap in different parts of the Brillouin zone, the temperature dependent gap anisotropy *i.e.*, the ratio $\frac{\Delta_{sc}(\Gamma - M)}{\Delta_{sc}(\Gamma - X)}$ is enhanced closed to T_c. In the present section we show that the above peculiarity in the temperature dependence of the SC gap is a natural consequence of the mixed s + id symmetry and in a correlated system the gap anisotropy increases with electron correlation.

In the gap equations (25, 26) Δ_s and Δ_d^0 represents the amplitudes of the s and d wave gaps respectively. Since Δ_s represents the isotropic s-wave gap so it retains its

parameters, the orthorhombicity together with next nearest neighbour hopping enhances the relative magnitude of the s-wave component whereas reduces that of the d-wave when compared with respect to the perfect square lattice for same value of v_d/v_s (*cf.* Figs. 9 and 11). Considering the case of $u = 0.4$ from Figures 9 and 11 it would be self-evident that the T_c^d in the orthorhombic phase reduces very largely from its value for the square lattice, whereas T_c^s in the orthorhombic phase increases strongly. On the other hand unlike the undistorted lattice, with the mixed symmetry (*cf.* Fig. 6), where the d-wave component can have higher magnitude for higher u close to $v_d/v_s = 0.4$; in presence of orthorhombic distortion the d-wave order parameter never acquire higher magnitude for higher u, for any value of v_d/v_s, as is clear from Figure 10 as well as Figure 11.
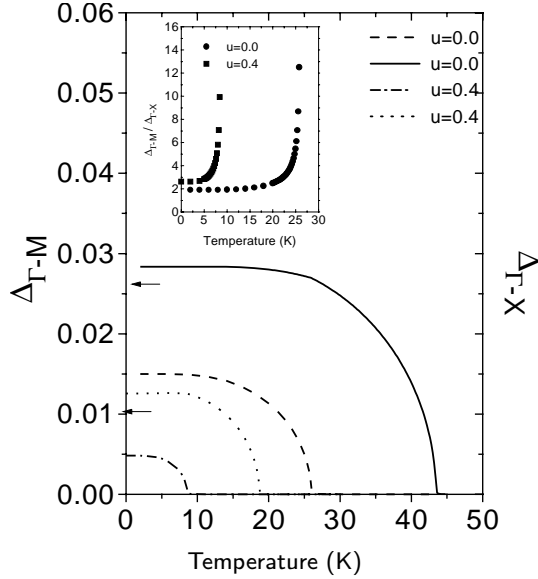
Fig. 12. Temperature variation of the superconducting gap along the two high symmetry directions for $u = 0.0$, 0.4 in the mixed $s + id$ phase. The inset figure depicts the ratio of the superconducting gap along the two high symmetry directions ($\frac{\Delta_{\mathrm{sc}}(\Gamma - M)}{\Delta_{\mathrm{sc}}(\Gamma - X)}$) with temperature for $u = 0.0$, 0.4.

constant maximum value for any k_x and k_y direction whereas magnitude of Δ_{d} varies with k_x and k_y direction due to the multiplicative factor ($\cos k_x - \cos k_y$). In the $\Gamma - \bar{M}(M)$ direction *i.e.*, $(\pm \pi, 0)$, $(0, \pm \pi)$, ($\cos k_x - \cos k_y$) acquires maximum magnitude ∓ 2, while in the $\Gamma - X(Y)$ direction $(\pm \frac{\pi}{2}, \pm \frac{\pi}{2})$ ($\cos k_x - \cos k_y$) is zero identically. So it is expected that the d-wave gap parameter will attain its maximum at $\Gamma - M(\bar{M})$ points and minimum at $\Gamma - X(Y)$ points, however s-wave gap is constant all over the Fermi surface. Considering the energy spectrum of the mixed phase E_k^{mix} we write $\Delta(\Gamma - M)$ and $\Delta(\Gamma - X)$ as

$$\Delta(\Gamma - M) = \sqrt{\Delta_{\mathrm{s}}^2 + 4\Delta_{\mathrm{d}}^2} \tag{28}$$

and

$$\Delta(\Gamma - X) = \Delta_{\mathrm{s}}. \tag{29}$$

Hence the ratio which is a measure of gap anisotropy can be written as

$$\frac{\Delta(\Gamma - M)}{\Delta(\Gamma - X)} = \frac{\sqrt{\Delta_{\mathrm{s}}^2 + 4\Delta_{\mathrm{d}}^2}}{\Delta_{\mathrm{s}}} . \tag{30}$$

Figure 12 shows the variation of $\Delta(\Gamma - M)$ and $\Delta(\Gamma - X)$ for $u = 0$ and $u = 0.4$ in an orthorhombic lattice with $v_{\mathrm{d}}/v_{\mathrm{s}} = 0.46$. The $\Delta(\Gamma - M)$ is larger and almost constant with temperature till $\Delta(\Gamma - X)$ is zero, then $\Delta(\Gamma - M)$ falls to zero at the T_{c}. The decrease of $\Delta(\Gamma - M)$ with u is much less than that for the $\Delta(\Gamma - X)$. The inset of Figure 12 depicts the temperature dependent gap anisotropy in a correlated case. The ratio $\frac{\Delta(\Gamma - M)}{\Delta(\Gamma - X)}$ is almost constant at

lower temperatures and increases faster near the temperature where $\Delta(\Gamma - X) = \Delta_{\mathrm{s}}$ is going to be zero. $\frac{\Delta(\Gamma - M)}{\Delta(\Gamma - X)}$ ratio is higher for higher correlation. This feature is however not an unique consequence of $s + id$ pairing symmetry *e.g.*, similar results are also obtained in a modified version of spin bag [24] mechanism of superconductivity.

5 Conclusion

We have presented a detailed study of the effect of electron correlation on pairing symmetry within a weak coupling theory. The method used to treat electron correlation is the slave boson formalism of KR [23] which reproduces the Brinkmann-Rice value of metal-insulator transition (U_{c}) correctly in the paramagnetic state. The value of u used in this work is always less than 1 (*i.e.* $U < U_{\mathrm{c}}$) so that weak coupling mean field theory of superconductivity can be applied. All through out the present calculation we restricted to half-filled situation. Within this study we found that electron correlation has important effect on pairing symmetry. The detailed nature of order parameter, its temperature variation as well as magnitude depends very sensitively with electron correlation and the nature of underlying lattice considered. Few interesting features of interplay between the different components of the order parameter with electron correlation has been demonstrated (in the $s + id$ picture). Such study may have some bearings to the high temperature superconductors. However, we have made no effort to understand the mechanism of superconductivity for cuprates in this work. The electron correlation always affect the pure s-wave gap more than the pure d-wave symmetry gap irrespective of the underlying lattice. In the mixed $s + id$ phase, the suppression in different components of the gap as well as the corresponding T_{c} are very sensitive to $v_{\mathrm{d}}/v_{\mathrm{s}}$ and the underlying lattice. Assuming the $s + id$ nature of the order parameter, the measured temperature dependent gap anisotropy from the ARPES of Ma *et al.* [11] can be understood on which the role of electron correlation has been emphasized. However, such a picture is not unique [24].

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