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Pairing state symmetries of high-T_c superconductors: a comparative study using two Ginzburg–Landau models

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Abstract
An attempt has been made to resolve the issue regarding the pairing symmetry of high-T_c superconducting materials (cuprates). The properties of high-T_c superconductors, which are the signatures of the pairing symmetry of these materials, are being calculated by using the anisotropic s-wave Ginzburg–Landau (GL) theory, i.e. the anisotropic single-order parameter GL theory (ASGL), and is compared with those calculated in a recent work (Karmakar and Dey 2008 *J. Phys.: Condens. Matter* **20** 255218) by the isotropic d-wave GL theory involving mixed symmetry states of the order parameters, i.e. the isotropic two-order parameter GL theory (TIGL), over the entire range of applied magnetic field and temperature for arbitrary values of the GL parameter κ and vortex lattice symmetry. The results are further compared with suitable experimental data on the high-T_c superconducting cuprate $YBa_2Cu_3O_{7-\delta}$. It has been found that the TIGL model definitely gives a better match with the experimental data and is thus more suitable to describe the pairing state symmetries of the high-T_c superconducting cuprates.

1. Introduction

Determination of the pairing symmetry of high temperature superconductors (HTS) has proved to be a center of interest for both experimental and theoretical physicists. High-T_c superconducting cuprates are characterized by the presence of CuO_2 planes separated by CuO chains, and it is this layered structure of the material which has led to the presence of extreme anisotropy in the cuprates along with a short coherence length and high critical temperature. Experiments have suggested that this natural anisotropy of the planar crystal structure, combined with an s-wave pairing symmetry of the order parameter, can account for most of the properties of high temperature superconductors [2–5]. The problem, however, arises from the fact that the superconducting mechanism in high-T_c materials is most likely not phonon-mediated and the proposed unconventional mechanisms, such as antiferromagnetic spin fluctuation, support an unconventional pairing symmetry of the order parameter, namely d-wave pairing symmetry [6]. The possibility of a d-wave pairing symmetry, i.e. $d_{x^2-y^2}$ pairing state with lines of nodes in the energy gap, has been indicated by several experiments. Phase-sensitive experiments which directly probe the pairing state symmetry of the high-T_c superconductors [7, 8] have supported the presence of d-wave pairing symmetry. Phase coherence measurements by bimetallic dc SQUIDs [9], tricrystal junction measurements [10], etc, have indicated the presence of d-wave pairing symmetry in high-T_c superconductors. Apart from the phase-sensitive experiments, the d-wave pairing state symmetry of the high-T_c superconductors has been interpreted from the observed polarization dependence of the Raman scattering experiments [11]. However, none of these experiments could rule out the presence of a small s-wave order parameter component along with the predominant d-wave component. The presence of CuO chains in high-T_c cuprate gives rise to a small orthorhombic distortion in the CuO_2 planes which in turn leads to a mixed symmetry state between the order parameter components, where the bulk pairing mechanism is d-wave in nature along with a small admixture of an s-wave component [12]. In the case of orthorhombic materials, with the dominant order parameter component being d-wave in nature, a small s-wave component is always induced even in the absence of any perturbation. In the case of tetragonal systems, this s-wave component vanishes in bulk and can be induced only in the presence of external perturbations such as impurities, magnetic field, etc. Experimental manifestations of the presence of mixed symmetry state of order parameters in high-T_c superconductors have been many. For example, the field modulated critical current measurement experiment to obtain the pairing state symmetry of $YBa_2Cu_3O_{7-\delta}$ [13], momentum-resolved temperature dependence of the superconducting gap of $Bi_2Sr_2CaCu_2O_{8+x}$ [14], observation of Josephson supercurrents along the c direction in YBCO–Pb superconductor–insulator tunnel junctions [15], angle-resolved electron tunneling experiments [16], etc, have demonstrated the presence of a mixed symmetry state of the order parameter components. It is suggested that the mixed symmetry scenario can prove to be the origin of several unusual effects observed experimentally in HTS, namely the unusual upward curvature of the plot of temperature vs the upper critical magnetic field (H_{c2}) [17], the pseudogap effects in HTSs [18], the nonmagnetic impurity effects in HTSs leading to an energy gap [19] and the superconducting fluctuation effects in HTS [20] (for details see [1]). Along with the experimental observations, theoretical studies in this regard have also raised certain questions. It has been observed that the theoretical calculations of the reversible magnetization based on the single-order parameter (s-wave) mass anisotropic Ginzburg–Landau (ASGL) theory can be fitted very well with the experimental reversible magnetization data. Interestingly, the same experimental reversible magnetization data can also be fitted equally well with the data obtained theoretically from a two-order parameter (d-wave) isotropic Ginzburg–Landau (TIGL) theory involving the mixed symmetry state of the order parameter components [21]. Furthermore, from theoretical studies it has also been found that another characteristic feature of HTS, the experimentally observed oblique structure of its vortex lattice, can also be explained in terms of both the anisotropic single-order parameter (ASGL) theory [22, 23] and isotropic two-order parameter theory (TIGL) [1, 24].

The issue thus still remains controversial regarding the actual pairing symmetry of the high-T_c cuprates, and there is insufficient consensus about the fact of whether a mixed symmetry state scenario (d-wave with an admixture of s-wave order parameter component) is required or an anisotropic s-wave pairing symmetry scenario would suffice to explain the various observed properties of high-T_c superconducting cuprates. The issue could not be addressed earlier in depth, as earlier theoretical studies are restricted to an applied magnetic field near the upper (H_{c2}) and lower (H_{c1}) critical fields. Moreover, in many of the studies an approximate expression of s-wave order parameter in terms of d-wave is obtained from the leading order behavior of the two-order parameter GL theory [24–26] which in turn reduces the problem to an effective single-order parameter theory.

In this work we address the issue about the nature of pairing symmetry of the order parameter in HTS. For this we study two different Ginzburg–Landau (GL) theories: (i) a single-order parameter (s-wave) GL theory with the effect of anisotropy being taken into account as the in-plane mass anisotropy (ASGL) and (ii) an isotropic two-order parameter (d-wave) GL theory in states of mixed symmetry (TIGL). In the present work, several new and experimentally observable properties of the high-T_c material, such as the vortex core radius, penetration depth, etc, are being calculated by using the ASGL model for the first time. These properties were not calculated or presented in [22] where some of the results of the ASGL model were being presented. As for the TIGL model, the various experimentally relevant properties are been depicted in [1]. The results, though representing the mixed symmetry scenario to be a strong candidate to explain the pairing symmetry of high-T_c materials, however, fails to shed light on the fact whether this candidature of the mixed symmetry scenario is stronger than that of an anisotropic (s-wave) single-order parameter model. This can be achieved by carrying out a comparative study of the results obtained by these two models (ASGL and TIGL) along with the relevant experimental data corresponding to the properties of the high-T_c cuprates, which are signatures of its pairing symmetry, and this is exactly the work that has been depicted in the present paper. The theoretical studies are being carried out over the entire range of applied magnetic field ($H_{c1} \ll H \ll H_{c2}$) and temperature, where the fully coupled nonlinear GL equations are being solved for arbitrary values of the GL parameter κ and vortex lattice symmetry. Also for the TIGL model, no leading order behavior has been used for the s-wave order parameter component.

2. Theoretical formalism

The two-dimensional average GL free energy density for the anisotropic single-order parameter GL theory (ASGL) can be written in dimensionless units as [22, 27]

$$f_{\mathrm{ASGL}} = \langle -\omega + \omega^2/2 + \vec{\nabla}\omega\mathbf{\Lambda}\vec{\nabla}\omega/4{\kappa_y}^2\omega + \omega\vec{Q}\mathbf{\Lambda}\vec{Q} + (\vec{\nabla}\times\vec{Q})^2\rangle \tag{1}$$

where $\langle\cdots\rangle = \frac{1}{V}\int \mathrm{d}\mathbf{r}\cdots$ denote spatial average, $\psi(x,y) = \omega(x,y)^{1/2}\exp[\mathrm{i}\phi(x,y)]$ is the superconducting order parameter with $\omega = |\psi|^2 \leqslant 1$, $\mathbf{Q}(x,y) = \mathbf{A}(x,y) - \nabla\phi(x,y)/\kappa_y$ is the supervelocity, $\kappa_y = \lambda_y/\xi_y$ is the GL parameter and $\mathbf{\Lambda}$ is the mass anisotropy tensor given by $\mathbf{\Lambda} = \begin{pmatrix} m_y/m_x & 0 \\ 0 & 1\end{pmatrix}$.

Similarly, the two-dimensional average free energy density for the isotropic two-order parameter GL theory (TIGL) can be written as [1, 21]

$$\begin{aligned} f_{\mathrm{TIGL}} = \langle[&\alpha_s\omega_s - \omega_d + \beta_1\omega_s^2 + \beta_2\omega_d^2 + (\beta_3 + 2\beta_4\cos(2\phi)) \\ &\times \omega_s\omega_d + (\omega_s+\omega_d)Q^2 + (\vec{\nabla}\omega_s)^2/4\omega_s\kappa^2 \\ &+ (\vec{\nabla}\omega_d)^2/4\omega_d\kappa^2 + 2\epsilon_v\{\cos(\phi)[((\nabla_y\omega_s)(\nabla_y\omega_d) \\ &- (\nabla_x\omega_s)(\nabla_x\omega_d))/(4\kappa^2(\omega_s\omega_d)^{1/2}) \\ &+ (Q_y^2 - Q_x^2)(\omega_s\omega_d)^{1/2}] + \sin(\phi)[(Q_y(\nabla_y\omega_s) \\ &- Q_x(\nabla_x\omega_s))(\omega_d/4\kappa^2\omega_s)^{1/2} - (Q_y(\nabla_y\omega_d) \\ &- Q_x(\nabla_x\omega_d))(\omega_s/4\kappa^2\omega_d)^{1/2}]\} + (\vec{\nabla}\times\vec{Q})^2\,]\rangle \end{aligned} \tag{2}$$

where $s(x,y) = \omega_s(x,y)^{1/2}\exp[\mathrm{i}\phi_s(x,y)]$, $d(x,y) = \omega_d(x,y)^{1/2}\exp[\mathrm{i}\phi_d(x,y)]$ are the superconducting order parameter components with $\omega_s = |s^2| \leqslant 1$, $\omega_d = |d^2| \leqslant 1$.

High precision numerical iteration techniques have been developed to solve the corresponding nonlinear GL equations for arbitrary values of the applied magnetic field ($H_{c1} \ll H \ll H_{c2}$), temperature, GL parameter and symmetry of the vortex lattice [1, 21, 22]. Before proceeding further one

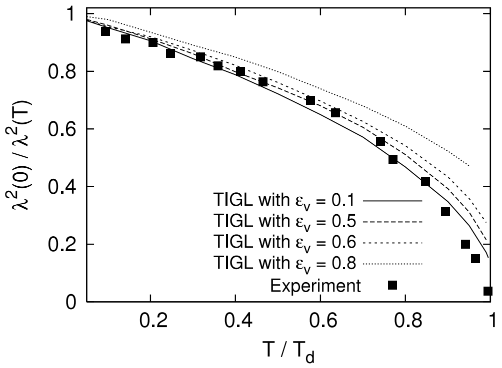

Figure 1. Comparison of temperature dependence of the penetration depth calculated by using different values of the coupling parameter ϵ_v for the TIGL model with experiment [30]. Other parameter values are $\alpha_s/|\alpha_d| = 1.4$, $\beta_1 = \beta_2 = \beta_3 = \beta_4$, $\kappa = 72$ with $b = 0.004$ ($H = 0.5$ T) and phase difference $\phi = (\phi_d - \phi_s) = \pi/2$.

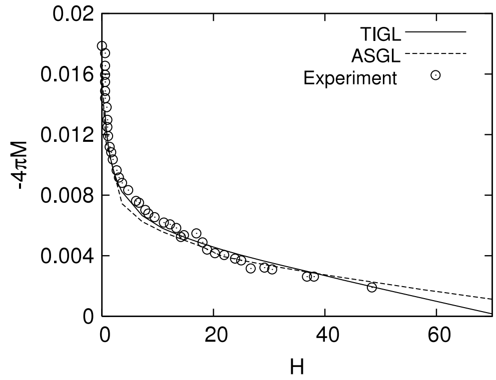

Figure 2. Comparison of the reversible magnetization data calculated by two different Ginzburg–Landau models (ASGL and TIGL) with the experimental data of $YBa_2Cu_3O_{7-\delta}$ [28]. Parameter values used are $\gamma = 2$, $\epsilon_v = 0.1$. Other parameters are the same as in figure 1.

should mention about the selection of the parameters used in the numerical calculations. For the ASGL model, there are only two parameters, the GL parameter $\kappa_y = \kappa = \kappa_{avg}$ and the mass anisotropy parameter $\gamma = m_x/m_y$. For both of these, the values as determined from the experiment on the high-T_c superconducting material YBCO are being used, i.e. $\kappa = \kappa_{avg} = 72$ [28] and $\gamma = 2$ [22]. For the TIGL model, the major contribution of the s-wave order parameter component arises from the mixed gradient coupling term. The parameters $\alpha's$ and $\beta's$ are related to each other through various inequalities [24, 25] and the linear stability analysis have suggested that, for the contribution of the s-wave order parameter component, the concentration has to be mainly focused on the mixed gradient coupling term and the other coupling terms of s-and d-wave order parameter components, i.e. the β_3, β_4, etc, terms are not important for the generation of the s-wave order parameter component. This fact has been verified by calculating the properties associated with the high-T_c superconductors with different combinations of $\alpha's$ and $\beta's$. It has been found that the various combinations do not lead to a significant effect on the different properties associated with the material, thus re-establishing the fact that the most important term in the free energy functional for the generation of the s-wave order parameter component is the mixed gradient coupling term with the corresponding parameter being ϵ_v. For the parameters $\alpha's$ and $\beta's$ the parameter values used are the same as in [24], while for the parameter ϵ_v, the value has been determined from the best fit of the theoretical results calculated by the TIGL model with the experimental data of the temperature dependence of the penetration depth in HTS. The value of ϵ_v determined from this fit amounts to 0.1, a value consistent with the theoretical work carried out by Feder *et al* [29], where they have studied the d-wave superconductor involving an admixture of the s-wave order parameter component by using two different models, namely the extended Hubbard model and the anti-ferromagnetic van Hove model. They have found that both the models suggest a gradient coupling parameter of $\epsilon_v \approx 0.1$–0.4.

Knowing the solutions, some of the experimentally relevant properties of HTS, such as penetration depth of the magnetic field, vortex core radius, reversible magnetization, shear modulus of the vortex lattice and their variations with temperature and applied magnetic field, are being calculated.

3. Numerical calculations, results and discussion

As mentioned above, to determine the value of the mixed gradient coupling parameter ϵ_v, first the temperature dependence of the penetration depth for different values of the mixed gradient coupling parameter ϵ_v is computed and the results are being compared with the experimental data of the high-T_c material $YBa_2Cu_3O_{7-\delta}$ [30]. The results are shown in figure 1, where it can be seen that the best fit with the experimental data is obtained for $\epsilon_v = 0.1$. Thus, for the rest of the TIGL calculations the value of $\epsilon_v = 0.1$ is used. Strictly speaking, GL theory is valid near T_c. However, it is generally assumed that the GL models yields fairly good results at any temperature. A further improvement of the theoretical models can be achieved by invoking an extension of the GL theories for high-T_c superconductors over the entire range of temperature, an approach that will parallel the work carried out by Lipavsky *et al* [31] for the low-T_c superconductors.

The computed reversible magnetization results as obtained from the two models are being compared with experiment. This is shown in figure 2. It can be seen from the figure that the experimental reversible magnetization data (available up to the maximum applied field $H \sim 45$ [28]) can be fitted very well with both the models as mentioned above. However, for the present study, when the reversible magnetization calculation is extended to higher applied field ($H > 45$) the results from these two models start to deviate and the deviation increases with increase in the applied field. Therefore to check which of the models gives a better fit with experiment, reversible magnetization experiments data should be made available for higher applied fields.

The result mentioned so far, i.e. the reversible magnetization though favoring the mixed symmetry scenario of the order parameters, however, fails to develop a clear consensus regarding the same. Thus, to have a clearer picture of the pairing symmetry in these materials the next obvious step

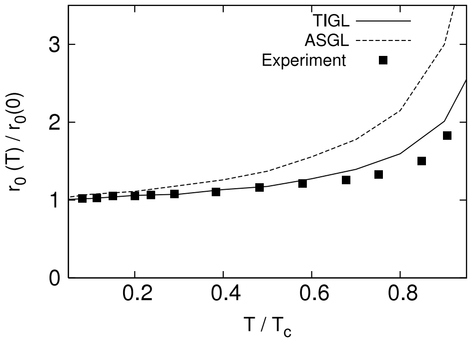

Figure 3. Comparison of temperature dependence of the vortex core radius calculated by using two different GL models (ASGL and TIGL) with the experimental data [32]. Parameter values are the same as in figure 2 and $b = 0.004$, i.e. $H = 0.5$ T.

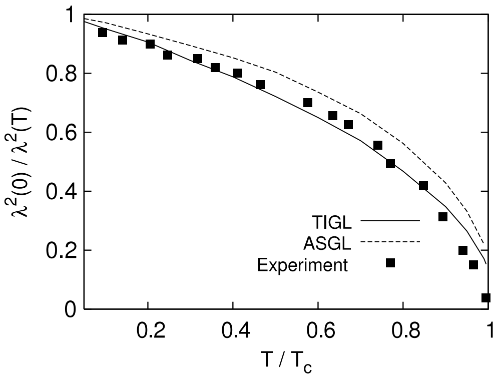

Figure 4. Comparison of temperature dependence of the penetration depth calculated by using two different GL models (ASGL and TIGL) with the experimental data [30]. Parameter values are the same as in figure 3.

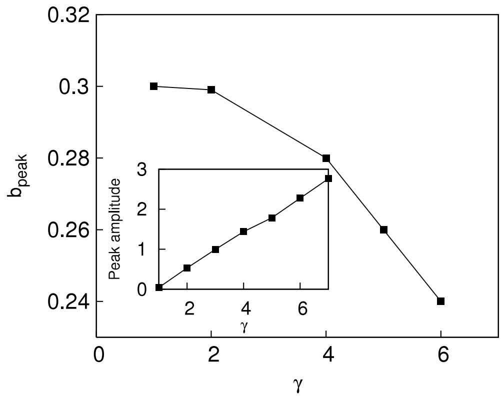

Figure 5. Variation of peak position (b_{peak}) and peak amplitude (inset) of the shear modulus (c_{66}) profile with mass anisotropy parameter γ for the ASGL model with $\kappa = 72$.

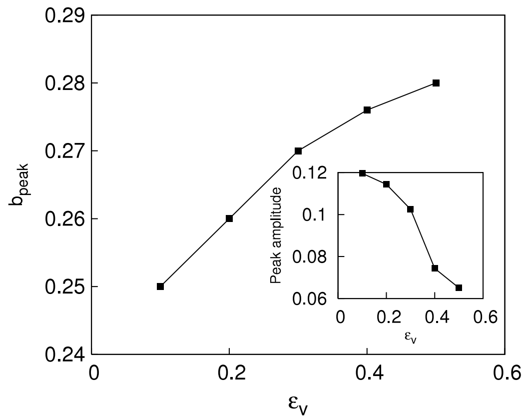

Figure 6. Variation of peak position (b_{peak}) and peak amplitude (inset) of the shear modulus (c_{66}) profile with ϵ_v for the TIGL model. Parameter values are the same as in figure 1.

is to probe the properties which are dependent on the local spatial behavior of the system such as the vortex core radius, penetration depth, shear modulus (c_{66}) of the vortex lattice, etc. Figures 3 and 4 show the variation of the vortex core radius and penetration depth, respectively, with temperature as obtained from the two models and their comparison with experimental data [30, 32]. It can be seen from the figures that the TIGL model results gives a much better fit with experimental data at all temperatures as compared to the ASGL model results. The shear modulus of the vortex lattice (c_{66}) is an important quantity as it gives information regarding the stability of the vortex lattice and thus its melting. It is a numerically computable quantity which gives the stiffness of the vortex lattice against thermal instabilities. The two important quantities which can be determined from the shear modulus of the vortex lattice are the peak amplitude and peak position (b_{peak}) of c_{66}. While the peak amplitude gives the maximum magnitude of c_{66}, the peak position suggests the magnetic field induction at which the value of c_{66} becomes maximum. In the present work it has been found that the peak amplitude and the peak position of c_{66} calculated by the two GL models show a striking dissimilarity among themselves. For the ASGL model it has been seen that the b_{peak} (value of the magnetic induction for which c_{66} attains a maximum) decreases with increase of the mass anisotropy parameter while for the TIGL model it increases with increase of the coupling parameter ϵ_v. This is shown in figures 5 and 6, respectively. The increase in the b_{peak} value with ϵ_v implies that the vortex lattice of HTS should melt at a higher applied magnetic field for higher values of ϵ_v. Similarly, calculation of the variation of the peak amplitude of c_{66} with parameters γ and ϵ_v also shows contrasting behavior for the two models (insets of figures 5 and 6, respectively). For the ASGL model the peak amplitude of c_{66} increases with γ, which indicates that the mass anisotropy does not favor melting of the vortex lattice. On the other hand, for the TIGL model the peak amplitude of c_{66} decreases with increase of ϵ_v which suggests that a larger coupling of the s-wave order parameter component leads to a softer vortex lattice and thus favors its melting.

The variation of the shear modulus with temperature for the ASGL and TIGL models as plotted in figures 7 and 8, respectively, also shows contrasting behavior. Both the models show that vortex lattice melting is favored at higher temperatures, which is in agreement with the vortex phase boundary as observed experimentally in a single crystal of $YBa_2Cu_3O_{7-\delta}$ [33]. However, for a given temperature, the increase of c_{66} with γ for the ASGL model suggests that the

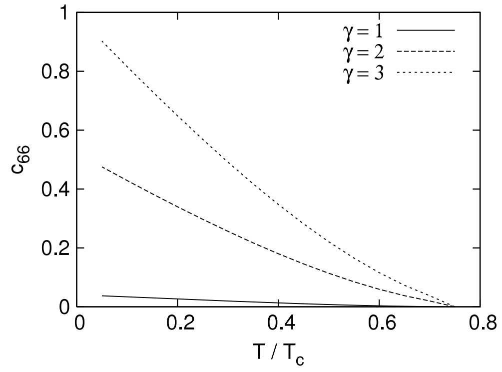

Figure 7. Variation of the shear modulus (c_{66}) of the vortex lattice with temperature for the ASGL model for different values of the mass anisotropy parameter γ. The other parameter used is $\kappa = 72$.

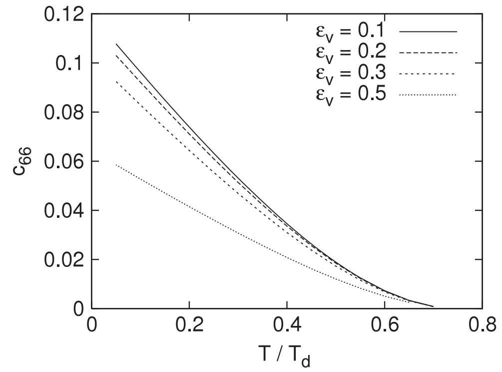

Figure 8. Variation of the shear modulus (c_{66}) of the vortex lattice with temperature for the TIGL model for different values of the coupling parameter ϵ_v. Other parameter values are the same as in figure 1.

vortex lattice will melt for lower ab-plane mass anisotropy, contrary to the popular belief that the presence of anisotropy favors melting of the vortex lattice in HTS. On the other hand, the decrease of c_{66} with increasing ϵ_v for the TIGL model suggest that melting is favored at stronger coupling between the order parameters. In order to verify these contrasting observations, experiments should be carried out to determine the variation of vortex phase boundary of HTS with the mass anisotropy parameter γ.

4. Conclusion

In conclusion, a systematic study has been carried out to resolve the issue regarding the pairing symmetry of high-T_c cuprate superconductors. For this, various experimentally relevant properties of the high-T_c materials are calculated in the framework of an anisotropic s-wave GL theory (ASGL) and the results are compared with those obtained by an isotropic d-wave GL theory (TIGL) involving the mixed symmetry state of the order parameter components, along with the suitable experimental data for HTS. The study shows that the best fit of the theoretical results with the experiment are obtained with the isotropic two-order parameter (TIGL) model of HTS in states of mixed symmetry. Even the properties of HTS which are dependent on the local spatial behavior of the system and are the signatures of the pairing symmetry of these materials, as calculated by the TIGL model, show a very good match with the experimental data as compared to those calculated by the ASGL model. The anisotropic single-order parameter (ASGL) model not only fails to provide better agreement with experimental results as compared to the TIGL model, but also gives results which are in contradiction to the experimentally observed behavior, such as the vortex lattice melting in HTS.

Thus, the isotropic d-wave GL theory (TIGL) involving mixed symmetry states of the order parameter components can be considered to be a far better candidate for describing the actual pairing state symmetry of high-T_c superconducting materials. However, as mentioned in the previous section, in order to explain the contrary scenarios presented by the two models regarding the melting of the vortex lattice, further experiments, which can probe the variation of the vortex phase boundary of HTS with mass anisotropy, are the call of the day.

It must, however, be noted that in the present work the effect of impurity and thermal fluctuations have not been considered. Thermal fluctuation is an important property especially in the case of the high temperature superconductors and thus its presence is likely to affect the various properties associated with these materials.

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