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Superconductivity in high-T_C cuprates using infinite U extended Hubbard model

Kuldeep Kholiya
Department of Applied Science, B.T. Kumaon Institute of Technology, Dwarahat, 263653, (INDIA)
E-mail: kuldeep_phy1@rediffmail.com
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Abstract : In the present investigation the expressions of the superconducting order parameter and carrier density using extended Hubbard model under $U\rightarrow\infty$ limit within the framework of Hubbard projection operator and ortho-fermions formalism have been derived. The present study shows that the next-nearest-neighbor hopping and inter-site interaction play an important role in the superconducting state of high-T_c cuprates in which, there exists strong electronic correlations and virtually $U\rightarrow\infty$ limit is justified

Keywords : Extended Hubbard model; Superconducting order parameter; Hubbard projection operator; Ortho-fermions formalism.

INTRODUCTION

On the basis of the planer electronic structure of cuprate superconductors Anderson[1] predicted that model fulfilling the electronic structure and strong correlation effects that exist in high-T_c cuprates is the two-dimensional Hubbard model[2]. It was further emphasized that to formulate a microscopic model of cuprates one has to take into account the orbital structure in the conducting CuO_2 planes, the main building blocks of cuprates and strong electron correlation effects as well. Mainly, one has to concentrate on the orbitals $Cu3d_{x^2-y^2}$, $O\,2P_x$ and $O2P_y$ in the CuO_2 plane of cuprates subject to hybridization and formation of as in plane band.

The recent photoemission experiments also suggested that there is a significant contribution coming out of next-nearest neighbour hopping energy as well as inter-site Coulomb interaction, due to existence of the long-range Coulomb correlations in these materials. The magnitude of Coulomb interaction at Cu $3d^9$ site is very large (of the order of 8-10 eV) in cuprates, in comparison with kinetic energy. In the light of the above facts the researcher working on the theoretical aspects of normal as well as superconducting state properties employed extended Hubbard model with nearest-neighbor and next-nearest-neighbor interactions and hopping energies.

Therefore during the last few years the Hubbard model containing nearest neighbor (N-N) and next-nearest-neighbor (N-N-N) interactions and hopping terms

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has been extensively studied[3-11] and within this model the emergence of superconductivity has been rigorously demonstrated under some conditions in these materials. Though, the exact solutions of Hubbard model have been reported for the only one-dimensional version of Hubbard model by Lieb and Wu[12] and as well as Muller-Hartman[13] and within the infinite dimensional limit by Kotliar and Ruckenstein[14]. In general for two and three-dimensional extended Hubbard model, which is relevant to high-T_c superconductivity in cuprates and strongly correlated electronic systems, there is so far, no satisfactory and mathematically tractable theoretical approach for realistic values of the electronic band-structure parameters in cuprates. Therefore, to study the Hubbard model, many approximate solutions and methods have been proposed[2,15,16]. There have also been several numerical simulations for finite system within the framework of Hubbard model[17] and its extensions.

For the system like cuprates in which intra-atomic interaction U is very large (≈10 eV), the calculation under $U \to \infty$ limit have also been attempted. Initially, Balserio and Foglio[18] have considered the model in which attractive inter-site interaction arises from the highly correlated electronic structure of the superconducting ceramic. They studied the Hubbard model in the limit of infinite Coulomb repulsion (i.e. $U \to \infty$) by employing standard decoupling techniques within the framework of Green's function formalism. They have derived the expressions of transition temperature T_c and the superconducting energy gap as a function of the various parameters of the model in superconducting state. Hirsch and Marsiglio[8] shown that superconductivity in these materials exists even in the presence of large Coulomb repulsion and transition temperature (T_c) increases with the hopping amplitude. They have discussed the various properties like tunneling density of states, specific heat, gap ratio and short coherence length as a function of hole density and various parameters of the Hamiltonian. Zhou *et al.*[19] have presented a mean-field calculation of the two-dimensional single-band Hubbard model based on Mori-projection operator formalism and calculated the various physical properties including the energy gap, effective hopping matrix element, local moment and fermi surface. They have also compared the results with those of the Hubbard-I approximation. Boer *et al.*[20] have also considered the extended Hubbard model and have shown that large class of these models has a superconducting ground state. They also studied the complete phase diagram of cuprates and concluded that the ground state of these systems is highly degenerate as is known for the $U \to \infty$ Hubbard model. Nazarenko *et al.*[21] have considered a two-dimensional fermionic model with attractive interaction for the underdoped high-T_c cuprates. They found that the exact solution leads to a two particle bound state in the $d_{x^2-y^2}$ subspace. They have also calculated the carrier density (holes) dependence of the transition temperature and suggested that the transition temperature increases with increase in carrier density but after a particular density, further increase in carrier density decreases the critical temperature. Harris *et al.*[22] on the basis of the angle-resolved photoemission spectroscopic measurements of the excitation gap in underdoped superconducting thin film of $Bi_2Sr_2Ca_{1-x}Dy_xCu_2O_{8+\delta}$ concluded that the transition temperature is reduced substantially on decreasing carrier concentration, while the decrease in the superconducting energy gap is very slow, which points towards a violation of the BCS mean-field results. Marsiglio[23] has considered the attractive Hubbard model in one-dimension and calculated the ground-state energy and energy gap in the first excited state using both, the Bethe-Ansatz equation and the variational BCS wave function approach. He found that the ground-state energies are always in very good agreement with experiment. Later, Maska[24] on the basis of the infinite-U Hubbard model calculated the electronic self-energy by projecting out the doubly occupied sites. Szabo and Gulacsi[25] have analysed the superconducting phase diagram of the extended Hubbard model supplemented with inter-site interaction and the next-nearest-neighbour hopping term in a mean-field approximation. They have emphasized the importance of different superconducting gap symmetries in the superconducting state and concluded that the thermodynamic properties are strongly influenced by next-nearest-neighbour contributions.

Therefore, most of the theoretical investigations attempted so far on the superconductivity in cuprates are within the extended Hubbard model[18-25] as mentioned above (with on-site and inter-site interactions). Some of the authors have considered both these interactions

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repulsive while some other have taken inter-site interaction attractive and on-site interaction repulsive in one-band and two-band Hubbard like models within mean-field as well as beyond mean-field approximations. The 2D-strongly interacting systems like cuprates in the limit $U \to \infty$ have also been studied using Hubbard projection operator formalism to avoid double occupancy because under this limit there may be only one particle either of spin up or of spin down in any orbital state. As in cuprates, there exist very strong on-site Coulomb correlations in the superconducting state as well, therefore, to study the superconductivity in high-T_c cuprates one has to take care of these strong electron correlation effects. To take care of strong correlation effects Mishra and Rajasekaran[26] have constructed the algebra of the creation and destruction operators for spin ½ particles obeying a new exclusion principle which is modified Pauli's exclusion principle. If the on-site Coulomb interaction becomes very large, virtually $U \to \infty$ limit may be applied as in cuprates, then an orbital state shall not contain more than one particle (whether spin up or spin down). These authors have also discussed the applicability of this ortho-Fermions algebra for infinite U-Hubbard model and emphasized its applicability for strongly correlated electronic systems like high-T_c cuprates. Recently, Mishra[27] have also demonstrated the two-main methods the Gutzwiller projection technique and the Nested-Bethe ansatz, to handle the electronic systems with very large electronic correlations. He concluded that in $U \to \infty$ limit the Bethe-ansatz solution leads to decoupling between the spin and charge degrees of freedom. Whereas in the Gutzwiller approach, the usual antisymmetry of space and spin coordinates is maintained.

More recently, Kishore and Mishra[28] studied the thermodynamics of infinite U Hubbard model within ortho-Fermions statistics (i.e. Fermions with infinitely large Coulomb interaction). They have shown that at least in one-dimension the fermions with exclusion of double occupancy of particles behave as free ortho-Fermions. They have further emphasized to extend these one dimensional result of infinite U Hubbard model to ascertain the accuracy of existing approximate solution of the Hubbard model for higher dimensions applicable for the strongly correlated electron system like high-T_c cuprate superconductors.

Thus, in the light of above facts the aim of the present paper is to study the superconducting state in high-T_c cuprate superconductors by considering an extended Hubbard model Hamiltonian with $U \to \infty$ limit within Hubbard projection operator formalism as well as the ortho-Fermions quantum approach and obtain the expressions of superconducting order parameter and carrier density as a function of various parameters of the model Hamiltonian.

THEORETICAL FORMULATION

Superconductivity in the extended Hubbard model in $U \to \infty$ limit (Hubbard projection operator formalism)

The electronic structure of CuO_2 planes, the basic building blocks of high temperature cuprate superconductors, can be described well within the framework of tight-binding Hubbard Hamiltonian[6,7]. Further, it has been pointed out that in cuprates there are strong electron correlations at Cu $3d^9$ site even in the superconducting state. Besides this the electronic band structure and core level photoemission experiments also predict a significant contribution of next-nearest-neighbour hopping energy and inter-site Coulomb interaction[25] in these materials even in the superconducting state. Thus, to study the superconductivity in cuprates we will consider the extended Hubbard model with attractive inter-site interaction. The model Hamiltonian may be given as:

$$\mathbf{H} = \sum_{ij\sigma} \mathbf{t}_{ij} \mathbf{C}^{+}_{i\sigma} \mathbf{C}_{j\sigma} + \sum_{ij'\sigma} \mathbf{t'}_{ij'} \mathbf{C}^{+}_{i\sigma} \mathbf{C}_{j'\sigma} + \mathbf{U} \sum_{i\sigma} \mathbf{n}_{i\sigma} \mathbf{n}_{i-\sigma} - \frac{1}{2} \sum_{ij\sigma\sigma'} \mathbf{V}_{ij} \mathbf{n}_{i\sigma} \mathbf{n}_{j\sigma'} - \mu \sum_{i\sigma} \mathbf{C}^{+}_{i\sigma} \mathbf{C}_{i\sigma} \quad (1)$$

where, V_{ij} is an attractive nearest neighbour inter-site interaction, and we have not gone to discuss about the origin of this attraction, t_{ij} is the nearest-neighbour hopping energy, $t'_{ij'}$ is the next-nearest-neighbour hopping energy, U is the on-site Coulomb interaction, μ is the chemical potential of the system.

In cuprates the on-site Coulomb interaction U is very large in comparison with the hopping energy and inter-site interaction, therefore, virtually $U \to \infty$ limit may be an approximate starting point. Under this limit we will eliminate doubly occupied sites and left with the

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singly occupied lower band. Because of the exclusion of doubly occupied states, the on-site Coulomb interaction serve to reduce the phase space available to the electronic system. In order to formulate this effect ($U \to \infty$), we use the algebra of the projection operators which will avoid double occupancy of the states.

Let $a_{k\sigma}$ and $a^{+}_{k\sigma}$ be the projection operators corresponding to the operators $C_{k\sigma}$ and $C^{+}_{k\sigma}$. It can be shown[29] that the operators $a_{k\sigma}$ and $a^{+}_{k\sigma}$ satisfy the such algebraic relations so that only single occupied site are taken care of as:

$$\mathbf{a_{i\sigma} = \left(1 - n_{i-\sigma}\right) C_{i\sigma}} \quad \textbf{(2a)}$$

$$\mathbf{[a_{k\sigma}, a^{+}_{k'\sigma'}] = [\delta_{kk'} - n_{-\sigma}(k'-k)]\delta_{\sigma\sigma'} + \delta_{\sigma-\sigma'} n_{\sigma-\sigma}(k'-k)} \quad \textbf{(2b)}$$

In the absence of long range magnetic order these Hubbard projection operators satisfy the following simplified anti-commutation relation as:

$$\mathbf{[a_{k\sigma}, a^{+}_{k'\sigma'}] = (1 - \langle n_{-\sigma}\rangle)\ \delta_{\sigma\sigma'}\delta_{kk'}} \quad \textbf{(2c)}$$

$$\mathbf{[a_{k\sigma}, a_{k'\sigma'}] = [a^{+}_{k\sigma}, a^{+}_{k'\sigma'}] = 0} \quad \textbf{(2d)}$$

Thus, in $U \to \infty$ limit (the doubly occupied sites are excluded) the Hamiltonian given by equation (1) transformed to:

$$\tilde{H} = \sum_{ij\sigma}(t_{ij} - \mu) a^{+}_{i\sigma} a^{+}_{j\sigma} + \sum_{ij'\sigma} t'_{ij'}\, a^{+}_{i\sigma} a^{+}_{j'\sigma} - \frac{1}{2}\sum_{ij\sigma\sigma'} V_{ij} a^{+}_{i\sigma} a^{+}_{i\sigma} a^{+}_{j\sigma'} a_{j\sigma'} \quad \textbf{(3)}$$

The above Hamiltonian (3) can be written in the momentum space by performing usual Fourier transformation as:

$$\tilde{H} = \sum_{k\sigma}(\epsilon_k - \mu)\ a^{+}_{k\sigma} a_{k\sigma} - \frac{V}{2N}\sum_{\substack{kk'q \\ \sigma\sigma'}} a^{+}_{k\sigma} a_{k+q,\sigma}\ a^{+}_{k'\sigma'}\, a_{k'-q\sigma'} \quad \textbf{(4)}$$

Now the Hamiltonian given by equation (4) may be linearize within BCS mean field approach as:

$$\tilde{H} = \sum_{k\sigma} \tilde{\epsilon}_k\ a^{+}_{k\sigma} a_{k\sigma} - \frac{1}{2}\ \sum_{k\sigma}\left\{\Delta^{*}_{k\sigma} a_{-k-\sigma} a_{k\sigma} + \Delta_{k\sigma} a^{+}_{k\sigma} a^{+}_{-k-\sigma}\right\} \quad \textbf{(5)}$$

where,

$$\tilde{\epsilon}_k = \epsilon_k - \frac{V}{2}\left(1 - \langle n_{-\sigma}\rangle\right) - \mu\ ,$$

$$\epsilon_k = -2t\left(\mathrm{Cos}\, k_x + \mathrm{Cos}\, k_y\right) - 4t'\ \mathrm{Cos}\ k_x \mathrm{Cos}\, k_y\ ,$$

$$\Delta^{*} = \frac{V}{N}\sum_{k\sigma} \langle a^{+}_{k\sigma}\ a^{+}_{-k-\sigma}\rangle\ ,\ \Delta = \frac{V}{N}\sum_{k\sigma} \langle a_{k\sigma}\ a_{-k-\sigma}\rangle \quad \textbf{(6)}$$

Where Δ^{*} is the superconducting order parameter.

Now, in our present analysis within Hubbard projection operator formalism, to obtain the self-consistent expressions for superconducting order parameter and carrier density as a function of various parameters of the model Hamiltonian, we apply the Green's function equation of motion technique[30] and drive the equation of motion for Greenn's function $G^{\sigma}(k,\omega) = \left\langle\left\langle a_{k\sigma} \middle| a^{+}_{k\sigma}\right\rangle\right\rangle_{\omega}$ as:

$$\omega G^{\sigma}(k,\omega) = \frac{1}{2\pi}\left\langle\left[a_{k\sigma}, a^{+}_{k\sigma}\right]\right\rangle + \left\langle\left\langle\left[a_{k\sigma}, \tilde{H}\right] a^{+}_{k\sigma}\right\rangle\right\rangle_{\omega} \quad \textbf{(7)}$$

We obtain $\left[a_{k\sigma}, \tilde{H}\right]$ within Hubbard projection operators for Hamiltonian (5) and finally obtain:

$$\omega G^{\sigma}(k,\omega) = \frac{1}{2\pi}\left(1 - \langle n_{-\sigma}\rangle\right) + \tilde{\epsilon}_k\ \left(1 - \langle n_{-\sigma}\rangle\right) G^{\sigma}(k,\omega)$$

$$+ \Delta_k\left(1 - \langle n_{-\sigma}\rangle\right)\left\langle\left\langle a^{+}_{-k-\sigma} \middle| a^{+}_{k\sigma}\right\rangle\right\rangle \quad \textbf{(8)}$$

In Equation (8) there is one additional Green's function $\left\langle\left\langle a^{+}_{-k-\sigma} \middle| a^{+}_{k\sigma}\right\rangle\right\rangle$, now we define this Green's function as:

$$\omega\left\langle\left\langle a^{+}_{-k-\sigma} \middle| a^{+}_{k\sigma}\right\rangle\right\rangle = \frac{1}{2\pi}\left\langle\left[a^{+}_{-k-\sigma}, a^{+}_{k\sigma}\right]\right\rangle + \left\langle\left\langle\left[a^{+}_{-k-\sigma}, \tilde{H}\right] a^{+}_{k\sigma}\right\rangle\right\rangle \quad \textbf{(9)}$$

and finally obtain the following equation:

$$\left\langle\left\langle a^{+}_{-k-\sigma} \middle| a^{+}_{k\sigma}\right\rangle\right\rangle_{\omega} = \frac{\Delta^{*}_{k}\left(1 - \langle n_{-\sigma}\rangle\right) G^{\sigma}(k,\omega)}{\omega + \left(1 - \langle n_{-\sigma}\rangle\right)\tilde{\epsilon}_k} \quad \textbf{(10)}$$

Substituting Equation (10) into (9) we get:

$$G^{\sigma}(k,\omega) = \frac{1}{2\pi}\frac{\left(1 - \langle n_{-\sigma}\rangle\right)}{\omega - \left(1 - \langle n_{-\sigma}\rangle\right)\tilde{\epsilon}_k - \dfrac{\left(1 - \langle n_{-\sigma}\rangle\right)^2 \left|\Delta_k\right|^2}{\omega + \left(1 - \langle n_{-\sigma}\rangle\right)\tilde{\epsilon}_k}} \quad \textbf{(11)}$$

Substituting: $\left(1 - \langle n_{-\sigma}\rangle\right)\tilde{\epsilon}_k = \tilde{\epsilon}_{kn}$ **and** $\left(1 - \langle n_{-\sigma}\rangle\right)\Delta_k = \tilde{\Delta}_k$ into Equation (11) we have:

$$G^{\sigma}(k,\omega) = \frac{1}{2\pi}\frac{\left(1 - \langle n_{-\sigma}\rangle\right)\left(\omega + \tilde{\epsilon}_{kn}\right)}{\omega^2 - \left(\tilde{\epsilon}_{kn}\right)^2 - \left|\tilde{\Delta}_k\right|^2} \quad \textbf{(12)}$$

Which we can rearranged in the following form:

$$G^{\sigma}(k,\omega) = \frac{1}{2\pi}\frac{\left(1 - \langle n_{-\sigma}\rangle\right)\left(\omega + \tilde{\epsilon}_{kn}\right)}{\left(\omega - E_{kn}\right)\left(\omega + E_{kn}\right)} \quad \textbf{(13)}$$

where, $E_{kn} = \sqrt{\left(\tilde{\epsilon}_{kn}\right)^2 + \left|\tilde{\Delta}_k\right|^2}$

From Equation (13) using the standard procedure for correlation function[30] the distribution of the charge carriers may be obtained as:

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$$\langle \mathbf{n}_{\sigma} \rangle = \frac{1}{2}\sum_{\mathbf{k}} \left(1 - \langle \mathbf{n}_{-\sigma} \rangle\right) \left(1 - \frac{\tilde{\in}_{\mathbf{kn}}}{\mathbf{E}_{\mathbf{kn}}} \tanh \frac{\mathbf{E}_{\mathbf{kn}}}{2\mathbf{k}_{\mathbf{B}}\mathbf{T}}\right) \quad (14)$$

Substituting (13) into (10) we can also have:

$$\left\langle\left\langle \mathbf{a}^{+}_{-\mathbf{k}-\sigma} \middle| \mathbf{a}^{+}_{\mathbf{k}\sigma} \right\rangle\right\rangle_{\omega} = \frac{1}{2\pi} \frac{\tilde{\Delta}^{*}_{\mathbf{k}} \left(1 - \langle \mathbf{n}_{-\sigma} \rangle\right)}{\left(\omega - \mathbf{E}_{\mathbf{kn}}\right)\left(\omega + \mathbf{E}_{\mathbf{kn}}\right)} \quad (15)$$

From Equation (15) the superconducting order parameter may be obtained in a straight forward way as:

$$\Delta^{*} = -\sum_{\mathbf{k}} \mathbf{V}\left(1 - \langle \mathbf{n}_{-\sigma} \rangle\right) \frac{\tilde{\Delta}^{*}_{\mathbf{k}}}{2\mathbf{E}_{\mathbf{kn}}} \tanh\left(\frac{\mathbf{E}_{\mathbf{kn}}}{2\mathbf{k}_{\mathbf{B}}\mathbf{T}}\right) \quad (16)$$

From Equations (14) and (16), we study the superconducting order parameter as a function of inter-site interaction, carrier concentration, hopping parameter as well as temperatures in high-T_c cuprates. Eq. (16) is just the modified BCS-superconducting order parameter form. A close examination of equation (14) and (16) reveal that these are coupled integral equations and required a self-consistent numerical computation.

The superconductivity in extended Hubbard model in the limit U→∞ : (Ortho-Fermions approach)

As pointed out in the introduction the Hubbard model and its various extensions are suitable for the study of superconductivity in high-T_c cuprates In the high-T_c cuprates the on-site Coulomb interaction is found to be very large as compared to other parameters. Thus, under such situation U→∞ limit may be applicable in cuprates which impose the condition that no two holes can reside on the same site. Therefore, in the limit of U→∞ the Pauli's exclusion principle, will be modified, according to which, "two electrons having opposite spin can occupy the same orbital state" and mathematically expressed as:

$$\mathbf{a}^{+}_{\mathbf{i}\alpha}\mathbf{a}^{+}_{\mathbf{i}\alpha} = \mathbf{0}$$

where, $\alpha = \sigma$ or $\bar{\sigma}$.

Recently, for the systems like the high temperature cuprates where the limit U→∞ is justified, a new exclusion principle applicable for U→∞ limit case was developed by Mishra and Rajasekaran[26]. According to which "an orbital state should not contain more than even one particle, whether spin up or down" and mathematically given as:

$\mathbf{a}^{+}_{\mathbf{i}\alpha}\mathbf{a}^{+}_{\mathbf{i}\beta} = \mathbf{0}$ where, $\alpha, \beta = \sigma$ or $\bar{\sigma}$

Mishra and Rajasekaran[26] also developed the algebra for such Fermionic system and named as ortho-Fermion which satisfies the following anti-commutation relations:

$$\mathbf{a}_{\mathbf{i}\alpha}\mathbf{a}_{\mathbf{j}\beta} + \mathbf{a}_{\mathbf{j}\alpha}\mathbf{a}_{\mathbf{i}\beta} = \mathbf{0} \quad (17a)$$

$$\mathbf{a}_{\mathbf{i}\alpha}\mathbf{a}^{+}_{\mathbf{j}\beta} = \delta_{\alpha\beta}\left(\delta_{\mathbf{ij}} - \sum_{\gamma} \mathbf{a}^{+}_{\mathbf{j}\gamma}\mathbf{a}_{\mathbf{i}\gamma}\right) \quad (17b)$$

where, α, β and γ will be σ (up spin) $\bar{\sigma}$ (down spin) and represent a modified Pauli's exclusion principle. These anti-commutation relations show that in the ortho-Fermions statistics there can be only exchange of particle sites and the spin degree's of freedom get frozen. So while applying this ortho-Fermion approach for strongly correlated electronic systems one has to be careful about this fact during the decoupling approximations used.

Now in our present analysis, within the framework of ortho-Fermions approach in U→∞ limit we obtain the self-consistent expressions for superconducting order parameter and carrier density as a function of various parameters of the model Hamiltonian given by equation (1). We apply the Green's function equation of motion technique for the Green's function $<< C_{k\sigma} | C^{+}_{k\sigma} >>$ as:

$$\omega\left\langle\left\langle \mathbf{c}_{\mathbf{k}\sigma} \middle| \mathbf{c}^{+}_{\mathbf{k}\sigma} \right\rangle\right\rangle_{\omega} = \frac{1}{2\pi}\left\langle\left[\mathbf{c}_{\mathbf{k}\sigma}, \mathbf{c}^{+}_{\mathbf{k}\sigma}\right]\right\rangle + \left\langle\left\langle\left[\mathbf{c}_{\mathbf{k}\sigma}, \tilde{\mathbf{H}}\right] \middle| \mathbf{c}^{+}_{\mathbf{k}\sigma} \right\rangle\right\rangle \quad (18)$$

Where $\tilde{\mathrm{H}}$ is the fourier transformed Hamiltonian of equation (1).

To solve the Equation (18) we find $\left[c_{K\sigma}, \tilde{H}\right]$. During the calculation to decouple the higher order Green's function terms we have used the following rules Mishra and Rajasekaran[26]:

(i) From the given string of the operators product expression, we form all compact anti-normal pairs. The compact anti-normal pair (CAP) is defined to be an anti-normal pair between a_m and a^{+}_n such that no unpaired a or a^{+} appears between a_m and a^{+}_n. We denote CAP by the symbol $\smile$ e.g. $a_m a_n a^{+}_k$, $a_m a_n a^{+}_k a^{+}_l$

(ii) If the spin on the a and a^{+} appearing in any of the CAP are not matched the given string of the operators product vanishes and so does its normal product e.g. $a_{\bar{K}} a_{\bar{l}} a_m a^{+}_n a^{+}_{\bar{p}} a^{+}_q = 0$

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We solve $\left[c_{k\sigma}, \tilde{H}\right]$ within ortho-Fermions algebra using normal product rules as above for Hamiltonian given by Equation (1) and finally obtained the equation of motion as:

$$\omega\left\langle\left\langle c_{k\sigma}\middle|c_{k\sigma}^{+}\right\rangle\right\rangle_{\omega} = \frac{1}{2\pi}\left(1-\langle n_{k-\sigma}\rangle\right)+\epsilon_k\left\langle\left\langle c_{k\sigma}\middle|c_{k\sigma}^{+}\right\rangle\right\rangle-\frac{V}{2}\left\langle\left\langle c_{k\sigma}\middle|c_{k\sigma}^{+}\right\rangle\right\rangle$$

$$+\frac{V}{2N}\sum_{\substack{k'q\\ \sigma_1}}\left\langle\left\langle c_{k'\sigma_1}^{+}c_{k+q\sigma}c_{k'-q\sigma_1}\middle|c_{k\sigma}^{+}\right\rangle\right\rangle+\frac{V}{2N}\sum_{\substack{k_1q\\ \sigma_1}}\left\langle\left\langle c_{k_1\sigma_1}^{+}c_{k-q\sigma}c_{k_1+q\sigma_1}\middle|c_{k\sigma}^{+}\right\rangle\right\rangle \quad (19)$$

We linearize the higher order Green's functions in Equation (19) in to lower one by retaining desired correlations important in the superconducting phase, and finally obtained:

$$\omega\left\langle\left\langle c_{k\sigma}\middle|c_{k\sigma}^{+}\right\rangle\right\rangle = \frac{1}{2\pi}\left(1-\langle n_{k-\sigma}\rangle\right)+\tilde{\epsilon}_k\left\langle\left\langle c_{k\sigma}\middle|c_{k\sigma}^{+}\right\rangle\right\rangle + \Delta_k\left\langle\left\langle c_{-k-\sigma}^{+}\middle|c_{k\sigma}^{+}\right\rangle\right\rangle \quad (20)$$

where, $\tilde{\epsilon}_k=\epsilon_k-\frac{V}{2}\left(1-\langle n_{k\sigma}\rangle\right)-\mu$ and $\Delta = \frac{V}{N}\sum_{k\sigma}\langle a_{k\sigma}a_{-k-\sigma}\rangle$ (21)

In Equation (20) there is one additional Green's function $\left\langle\left\langle c_{-k-\sigma}^{+}\middle|c_{k\sigma}^{+}\right\rangle\right\rangle$. Now we define this Green's function as:

$$\omega\left\langle\left\langle c_{-k-\sigma}^{+}\middle|c_{k\sigma}^{+}\right\rangle\right\rangle_{\omega} = \frac{1}{2\pi}\left\langle\left[c_{-k-\sigma}^{+}, c_{k\sigma}^{+}\right]\right\rangle+\left\langle\left\langle\left[c_{-k-\sigma}^{+}, H\right]\middle|c_{k\sigma}^{+}\right\rangle\right\rangle \quad (22)$$

and following the earlier procedure finally obtain the equation of motion as:

$$\omega\left\langle\left\langle c_{-k-\sigma}^{+}\middle|c_{k\sigma}^{+}\right\rangle\right\rangle = -\tilde{\epsilon}_k\left\langle\left\langle c_{-k-\sigma}^{+}\middle|c_{k\sigma}^{+}\right\rangle\right\rangle+\Delta_k^{*}\,G^{\sigma}(k,\omega) \quad (23)$$

where,

$$\Delta^{*} = \frac{V}{N}\sum_{k\sigma}\left\langle c_{k\sigma}^{+}c_{-k-\sigma}^{+}\right\rangle \quad (24)$$

Substituting the value of $\left\langle\left\langle c_{-k-\sigma}^{+}\middle|c_{k\sigma}^{+}\right\rangle\right\rangle$ from Equation (23) to (20) the final expression for $G^{\sigma}(k,\omega)=\left\langle\left\langle c_{k\sigma}\middle|c_{k\sigma}^{+}\right\rangle\right\rangle$, Green's function comes out as:

$$G^{\sigma}(k,\omega) = \frac{1}{2\pi}\frac{\left(1-\langle n_{k-\sigma}\rangle\right)\left(\omega+\tilde{\epsilon}_k\right)}{\left(\omega+E_k\right)\left(\omega-E_k\right)} \quad (25)$$

where,

$$E_k = \sqrt{\tilde{\epsilon}_k^{2}+\left|\Delta_k\right|^{2}} \quad (26)$$

From Equation (25) on applying the standard procedure the distribution of the charge carriers may be given as:

$$\langle n_{\sigma}\rangle = \frac{1}{2}\sum_{k}\left(1-\langle n_{-\sigma}\rangle\right)\left(1-\frac{\tilde{\epsilon}_k}{E_k}\tanh\frac{E_k}{2k_BT}\right) \quad (27)$$

Again to find the expression for superconducting order parameter we solve Equations (23) and (25) to obtain $\left\langle\left\langle c_{-k-\sigma}^{+}\middle|c_{k\sigma}^{+}\right\rangle\right\rangle$ as:

$$\left\langle\left\langle c_{-k-\sigma}^{+}\middle|c_{k\sigma}^{+}\right\rangle\right\rangle = \frac{\Delta_K^{*}}{2\pi}\frac{\left(1-\langle n_{k-\sigma}\rangle\right)}{\left(\omega+E_k\right)\left(\omega-E_k\right)} \quad (28)$$

From the Green's function given by above Equation (28) using the standard procedure we calculated the superconducting order parameter as:

$$\Delta^{*} = -\sum_{k} V\left(1-\langle n_{-\sigma}\rangle\right)\frac{\Delta_k^{*}}{2E_k}\tanh\left(\frac{E_k}{2k_BT}\right) \quad (29)$$

From Equation (27) and (29) one can study the superconducting order parameter as a function of inter-site interaction, carrier concentration, as well as temperatures in high-T_c cuprates. A close examination of Equation (27) and (29) reveal that these are coupled integral equation and require a self-consistent numerical computation.

RESULT AND DISCUSSION

We have derived the expressions of the superconducting order parameter and carrier density using extended Hubbard model under $U\rightarrow\infty$ limit within the framework of Hubbard projection operator and ortho-fermions formalism. The expression of superconducting order parameter given by Equation (16), just have the BCS form but it depend on carrier concentration, inter-site interaction energy and temperature as well. It can be seen from this equation that at exact half-filling i.e. ($<n_{\sigma}>=1$), the superconductivity vanishes (i.e. $\Delta\rightarrow 0$). This is in accordance with the observed experimental facts where in the absence of doping (there is one particular site), the cuprates behave as insulator due to very strong electron co-relation at Cu $3d^9$ site. Now to study the superconducting order parameter as a function of temperature we solve Equation (16) self-consistently, numerically, by extending the summation over k-values into an integration. During the numerical calculation we have considered $_k = \Delta_0$ (Cos k_x – Cos k_y), i.e. d-wave symmetry in the superconducting order parameter as suggested by several workers[31,32].

In Figure 1, we have plotted superconducting order parameter (Δ) vs. temperature for different values of hole concentration, keeping t = 350 meV, t' = 30 meV and V = 4325 meV, fixed. It is clear from the Figure 1, that initially the Δ and hence the transition temperature (T_c) increases on increasing hole concentration (n=0.15–0.18). But, for the further increase in hole concentration (n = 0.19), away from optimal doping, the transition temperature again starts decreasing. This is in accord with the experimental and the theoretical results of the Balserio and Foglio[18] and de Mello *et al.*[10] for the extended Hubbard model with an attractive inter-site interaction.

In Figure 2, we have plotted superconducting order parameter (Δ) vs. temperature, for different values of the attractive inter-site interaction (V), keeping t = 355 meV, t' = 30 meV and n = 0.2 fixed. It is clear from Figure 2, that on increasing the inter-site interaction the transition temperature increases. This is in accordance with the results of Balserio and Foglio[18] as well as experimental observations in these systems.

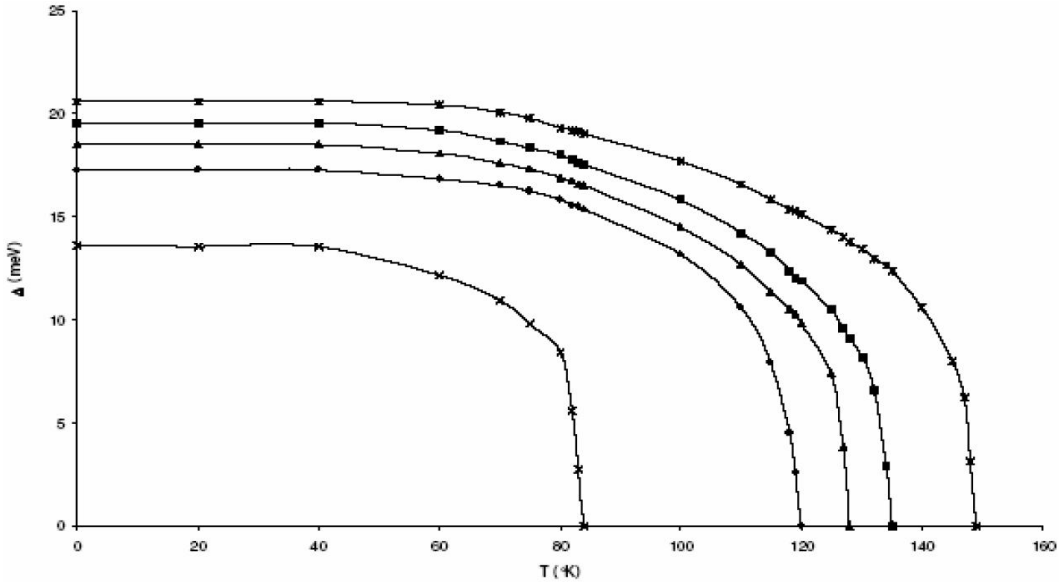

Figure 1 : The variation of Δvs. T with (a) n=0.15 (cross), (b) n=0.16 (circle), (c) n=0.19 (triangle), (d) n=0.18 (square), (e) n=0.17 (star). The other parameters are t=350 meV, t′=30 meV and V=4325 meV.

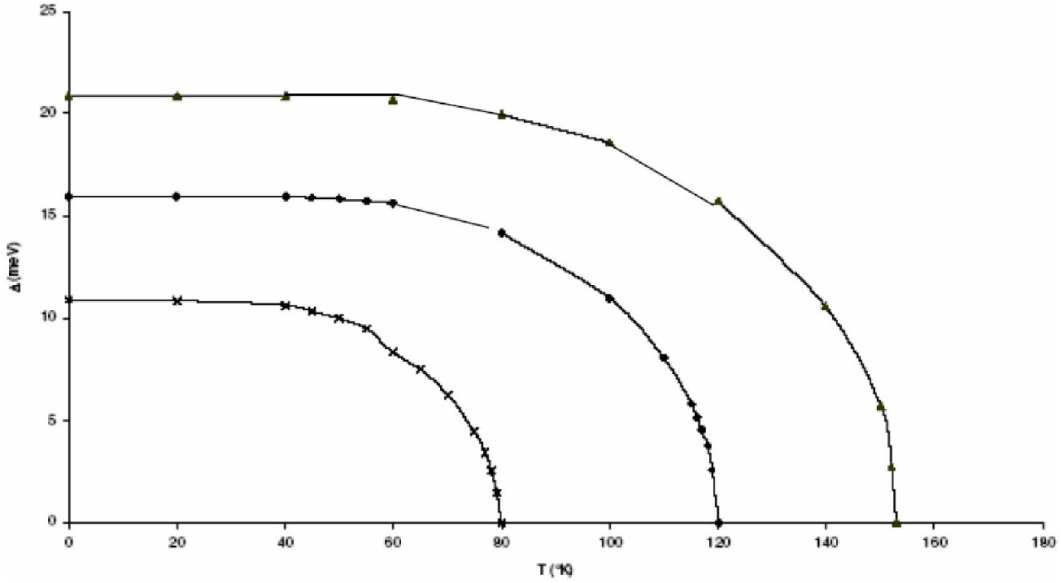

Figure 2 : The variation of Δ vs. T with (a) V=4475 meV (cross), (b) V=4500 meV (circle), (c) V=4525 meV (triangle). The other parameters are t=355 meV, t′=30 meV and n=0.2.

ORIGINAL ARTICLE

In Figure 3, we have plotted the BCS ratio ($2\Delta_0/k_BT_c$) vs. hole concentration around optimal doped regime in cuprates, keeping t = 350 meV, t' = 30 meV and V = 4325 meV, fixed. It is clear from Figure 3, that in the optimal doped region, the ratio ($2\Delta_0/k_BT_c$) comes out to be very close to the BCS ratio (3.52) but in the under-doped and over-doped regime the ratio ($2\Delta_0/k_BT_c$) deviates from the BCS ratio, in strongly correlated high-T_c cuprates. These results are in accordance with the results obtained by Szabo and Gulasci[25] for extended Hubbard model.

In the section 2.2 we have derived the expressions of the superconducting order parameter and carrier density using extended Hubbard model with in the framework of ortho-Fermions approach. The expression of superconducting order parameter in ortho-Fermions approach Equation (29) resembles with the expression of superconducting order parameter obtained in Hubbard projection operator formalism Equation (16). At T = 0°K, these two results just become identical. While in these two approaches, the temperature dependence of the superconducting order parameter is quite different. This is because in Hubbard projection operator formalism we consider the Fermions distribution and then project out the doubly occupied sites while in ortho-Fermions approach the doubly occupied sites are eliminated using new anti-commutation relations by modified exclusion principle which are much more microscopic.

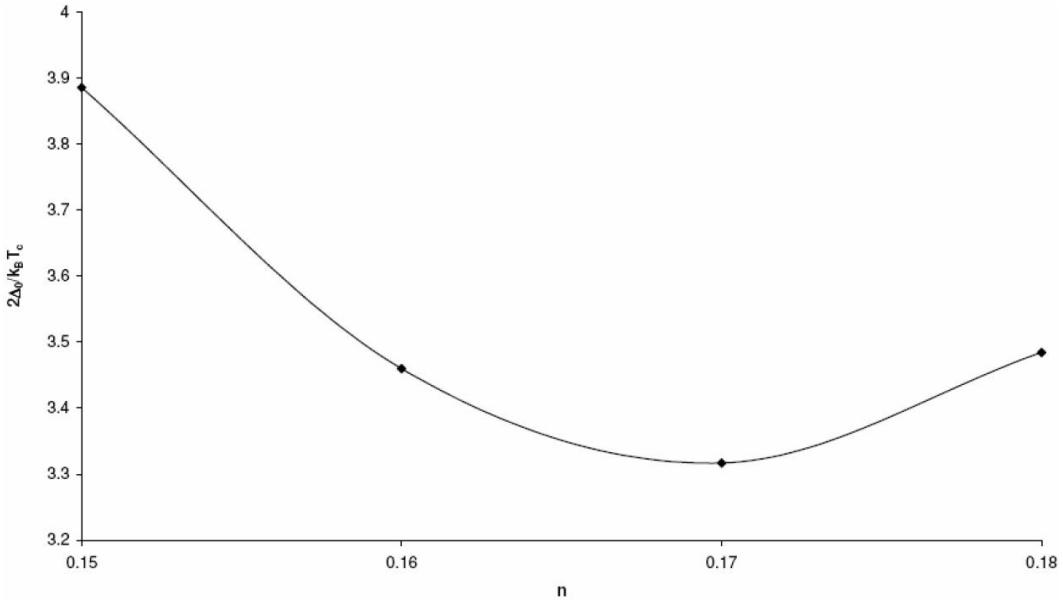

Figure 3 : The variation of $2\Delta_0/k_BT_c$. The other parameters are t=350 meV, t′=30 meV and V = 4325 meV.

Finally, it can be concluded that next-nearest-neighbour hopping and inter-site interaction play an important role in the superconducting state of high-T_c cuprates in which, there exists strong electronic correlations and virtually $U\rightarrow\infty$ limit is justified.

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