SUPERCONDUCTING ORDER PARAMETERS IN THE EXTENDED HUBBARD MODEL: A SIMPLE MEAN-FIELD STUDY

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The extended Hubbard model with nearest neighbor hopping and intersite interaction for a 2D square lattice has been studied within the frame work of a simple mean-field formalism. The self-consistent solutions of superconducting order parameters have been obtained for various fillings. The results indicate that superconducting pairing occurs on doping for the repulsive on-site U and attractive nearest neighbor V .

Keywords: Hubbard model; extended Hubbard model; nearest neighbor interaction; mean-field superconducting order parameter; repulsive on-site U ; attractive nearest neighbor V .

1. Introduction

Ever since the discovery of high temperature superconductors in layered oxides,¹ two dimensional Hubbard model is being studied very extensively by various analytical and numerical techniques.² The Hubbard model, originally designed to describe itinerant magnetism in narrow band systems, has been found to be a successful model for many strongly correlated electronic systems.³ Mott (metal-insulator) transition, band insulator with antiferromagnetic ordering, non-Fermi liquid behavior etc. are some of the well-investigated topics with the Hubbard model. Although the model is only exactly solvable in one dimension, a number of results have been obtained in the mean field approximation, occasionally including fluctuations. In 2-dimension mean field phase diagrams⁴ have been studied implying the richness of various ordered phases⁵ (e.g. charge density wave states, anti-ferromagnetism, para and ferromagnetism and singlet pairing states).

In 1987 Anderson⁶ made an important suggestion that the Hubbard model is a suitable candidate for high T_c superconductivity. Based on the observation that a Mott insulator when doped, becomes a superconductor, Anderson postulated that

upon doping, the loss of antiferromagnetic long range order produces a so-called “resonating valence bond” (RVB) phase — a quantum liquid of singlet pairs and stabilizes the ground state with a short range magnetic order. In the strong coupling limit Anderson and coworkers⁷ believed that superconductivity can appear in a mean field theory, where the pair excitations are formed in the strange normal state and these pair can undergo charged boson condensation, when the temperature is lowered. Although this idea has passed through several modifications in the past decade,⁸ there have been other serious suggestions even at the weak coupling level (e.g. spin bag,⁹ antiferromagnetic Fermi liquid¹⁰ and paramagnon exchange¹¹ models) that superconductivity can be found in a Hubbard model.

On the other hand, during the past few years there have been great efforts on the elaborate computer simulations on the question as to whether a Hubbard ($U > 0$)-only model can produce superconductivity. Recently Imada¹² showed strong numerical evidence against superconductivity in 2D U -only Hubbard model near half-filling. Consequently an obvious step is to include the next neighbor interaction in the so-called extended Hubbard model. There are now some evidence^{13–21} that onsite (U) and the next neighbor (V) interactions can produce pairing and hence the superconductivity. The parameters, U and V can be positive or negative which depend on the coupling of the electrons to phonons or to other bosonic modes of the system. A familiar example is a negative U model. The direct Coulomb interaction can be suppressed by the strong coupling of phonons as has been pointed out by Anderson²² in the context of amorphous semiconductors.

Apart from pure Hubbard model there are variants of it in various limits, known as t - J model family. Extensive numerical work has been reported on several mysterious anomalies in the normal phases, besides the superconducting states. Bulut²³ reviews effective pairing interaction which is repulsive at (π, π) momentum transfer, and enhanced single-particle spectral weight near the $(\pi, 0)$ and $(0, \pi)$ points of the Brillouin zone, create optimum conditions for $d_{[x]2-[y]2}$ -wave pairing. Maier *et al.*²⁴ examine superconducting instabilities of the doped repulsive 2D Hubbard model, which are studied in the intermediate to strong coupling regime with the help of the dynamical cluster approximation. To solve the effective cluster problem they employ an extended noncrossing approximation, which allows for a transition to the broken symmetry state. Roth’s two-pole approximation has been used by Calegari *et al.*²⁵ to investigate the role of d - p hybridization in the superconducting properties of an extended d - p Hubbard model. Metzner²⁶ examines the existence of d -wave superconductivity in the two-dimensional Hubbard model close to half-filling, by using a renormalization group analysis at the one-loop level.

As indicated earlier, research with Hubbard model and its variants have been carried out intensely with many diverging point of view, even whether the Hubbard model is the right model for the superconductivity. In the absence of a general consensus and a definite proof, we consider the Hubbard model as a very basic many-body model that takes appropriately electron correlations. In this paper we consider a pedagogic view in terms of basic interactions and attempt a study of the

superconducting order parameters in an extended Hubbard Model and treat onsite interaction U and nearest neighbor interaction V as phenomenological parameters. In Sec. 2 we discuss the mean field superconducting order parameters from the extended Hubbard Hamiltonian within a generalized (a simple) Hartree-Fock approximation (GHFA) in the ground state. Self-consistent solutions are obtained by varying the parameters for various fillings in Sec. 3. The effective potential is found to be attractive in certain conditions and the results are discussed with its implication to high T_c superconductivity. We conclude with this simple picture that one can have a qualitative understanding of how the superconductivity is manifested through electron correlation only.

2. Mean-Field Superconducting Order Parameter

We consider an extended Hubbard Hamiltonian given by

$$H = - \sum_{ij\sigma} (t + \mu\delta_{ij}) C_{i\sigma}^+ C_{j\sigma} + \frac{1}{2} \sum_{ij\sigma\sigma'} (S_u U \delta_{ij} \delta_{\sigma-\sigma'} + S_v V) n_{i\sigma} n_{j\sigma'} \quad (1)$$

where $C_{i\sigma}^+$, $C_{i\sigma}$ and $n_{i\sigma} = C_{i\sigma}^+ C_{i\sigma}$ are the creation, destruction and number operators respectively at the site i with spin $\sigma = \uparrow$ or $\downarrow$. j is restricted only to the nearest-neighbor sites of the site i . μ stands for chemical potential. S_u , and S_v take care of the sign of the interactions. The three cases of interactions which we study are; (1) when both U and V are attractive, which mean $S_u = S_v = -1$; (2) when U is attractive and V is repulsive, here $S_u = -1$ and $S_v = +1$ and (3) when U is repulsive and V is attractive, i.e., $S_u = +1$ and $S_v = -1$. The Eq. (1), in Bloch representation becomes

$$H = H_0 + H_1, \quad (2a)$$

where

$$H_0 = - \sum_{ij\sigma} (\varepsilon_k + \mu) C_{k\sigma}^+ C_{k\sigma} \quad (2b)$$

$$H_1 = \frac{1}{2N} \sum_{kk'q\sigma\sigma'} (S_u U \delta_{ij} \delta_{\sigma-\sigma'} + z S_v V f_q) C_{k\sigma}^+ C_{k-q\sigma} C_{k'\sigma'}^+ C_{k'+q\sigma'} . \quad (2c)$$

Here N is the total number of sites $\varepsilon_k = z t f_k$ is the Fourier transform of hopping integral and $f_k = \frac{1}{Z} \sum_j \exp(ik \cdot r_j)$, z is the co-ordination number and r_j is the nearest-neighbor vector. Within the generalized Hartree-Fock approximation (GHFA) the singlet-superconducting order parameter for the square lattice at $T = 0$ is given by

$$\delta_k = - \frac{1}{N} \sum_{k'} (S_u U + z S_v V f_k f_{k'}) \frac{\Delta_{k'}}{[E_{k'}^2 + \Delta_{k'}^2]^{1/2}} \quad (3)$$

where

$$E_k = (z t + z S_v V \eta) f_k - \mu + \frac{n}{2} (S_u U + 2 z S_v V) \quad (4)$$

The mean value of carrier concentration, n , is given by

$$n = 1 - \frac{1}{N} \sum_k \frac{E_k}{[E_{k'}^2 + \Delta_{k'}^2]^{1/2}} \quad (5)$$

and the quantity η

$$\eta = \frac{1}{N} \sum_k \frac{f_k E_k}{[E_{k'}^2 + \Delta_{k'}^2]^{1/2}} \quad (6)$$

renormalizes the hopping integral. The expression for Δ_k , Eq. (3), is written as $\Delta_k = \Delta_0 + f_k \Delta_1$ for the superconducting order (SC) order parameter. So one gets, from Eq. (3), the coupled equations for the on-site and off-site component of the order parameters as (8), respectively. Now we perform self-consistent numerical calculations of the relevant equations.

$$\Delta_0 = -\frac{US_u}{N} \sum_k \frac{(\Delta_0 + f_k \Delta_1)}{[E_{k'}^2 + \Delta_{k'}^2]^{1/2}}, \quad (7)$$

and

$$\Delta_1 = -\frac{zS_v V}{N} \sum_k \frac{f_k (\Delta_0 + f_k \Delta_1)}{[E_{k'}^2 + \Delta_{k'}^2]^{1/2}}, \quad (8)$$

respectively. Now we perform self-consistent numerical calculations of the relevant equations.

3. Numerical Results

Rewriting $E_k = t_0 f_k - \mu_0$ where, from Eq. (4) $t_0 = zt + zS_v V \eta$, $\mu_0 = \mu - n(S_u U + 2zS_v V)/2$ and defining band width $W = 2zt\gamma$, here, $\gamma = \max|f_k|$, it is convenient to study Eqs. (5) to (8) in terms of the dimensionless variables of the system. The dimensionless parameters are $\alpha = U/W$ and $\beta = zV/W$. In what follows, we define the dimensionless variables $\Delta_0 = \Delta_0/W$, $\Delta_1 = \Delta_1/W$ and $\mu_0 = \mu_0/W$. The k -space integration of the Eqs. (2.5) to (2.8) is easily done, assuming that f_k is a variable such that $0 \leq f_k \leq \gamma$. This approximation is equivalent to a square density of states model. With the square density of states model, the pairing is taking place in the whole Brillouin zone, contrary to the BCS model. However, if one includes the van-Hove singularity in the density of states, then the strength of the Cooper pairing increases. After some algebra, the coupled Eqs. (5) to (8) are simplified and we get

$$\mu_0 = \frac{1}{2X_0} [-X_1 - (X_1^2 - 4X_0 X_2)^{1/2}] \quad (9)$$

$$X_0 = t_0^2 - (\delta t_0 - \Delta_0 \Delta_1 S_u / \alpha)^2; \quad X_1 = -2t \Delta_0 \Delta_1 \quad (10)$$

$$X_2 = (\Delta_0 \Delta_1)^2 + \gamma^2 (\delta t_0 - \Delta_0 \Delta_1 S_u / \alpha)^4 - [\Delta_0^2 + \gamma^2 C] (\delta t_0 - \Delta_0 \Delta_1 S_u / \alpha)^2 \quad (11)$$

Other coupled equations are

$$2\gamma\sqrt{C}(t_0\mu_0 - \Delta_0\Delta_1)[(\delta t_0 - \Delta_0\Delta_1 S_u/\alpha)^2 - C] \\ = -(\delta t_0 - \Delta_0\Delta_1 S_u/\alpha)(t_0\Delta_0 + \mu_0\Delta_1)^2 \sinh\left[\frac{2\gamma\sqrt{C}(\delta\Delta_1 + t_0\Delta_0 S_u/\alpha)}{t_0\Delta_0 + \mu_0\Delta}\right] \quad (12)$$

$$-\frac{2\Delta_1}{\beta} C S_v = 2t_0\Delta_0(\delta - \mu_0 S_u/\alpha) + \Delta_1(\delta\mu_0 + \Delta_0^2 S_u/\alpha) \\ - \Delta_1 \frac{(t_0\mu_0 - \Delta_0\Delta_1)}{(\delta t_0 - \Delta_0\Delta_1 S_u/\alpha)} \quad (13)$$

and

$$\eta_v = -\frac{1}{2C} [2\Delta_0\Delta_1(\delta - \mu_0 S_u/\alpha) - t_0(\delta\mu_0 + \Delta_0^2 S_u/\alpha)] \\ - \frac{t_0}{2C} \frac{(t_0\mu_0 - \Delta_0\Delta_1)}{(\delta t_0 - \Delta_0\Delta_1 S_u/\alpha)} \quad (14)$$

where $C = t_0^2 + \Delta_0^2$. The above four equations Eq. (9) and Eqs. (12)–(14) are solved for the unknown Δ_0 , Δ_1 and μ_0 self-consistently as a function of system's parameters α , β and δ . Here $\delta = 1 - n$, is taken positive definite to account for the hole density.

3.1. The influence of U on Δ_0 , Δ_1 and μ_0

In the absence of an extended Hubbard interaction, $V = 0$, the s -wave SC order parameter (since, Δ_1 comes out to be zero) is given by a simple expression,

$$\Delta_1 = \gamma t_0(1 - \delta^2)^{1/2} \sinh(\gamma t_0/\alpha)^{-1}, \quad (15)$$

while the chemical potential obtained from Eq. (9) is

$$\mu_0 = -\delta\gamma t_0 \coth(\gamma t_0/\alpha). \quad (16)$$

With the inclusion of V , the above simple expression of Δ_0 gets coupled to Δ_1 . In all our calculations we have taken, $\gamma = 1$. We discuss here the solutions of Eq. (9) and Eqs. (12)–(14) for $\beta = 0.5$, $\delta = 0.5$ while α is varied from 0 to 1. We choose $\delta = 0.5$ because the order parameters at this value of δ show maximum deviation (see Sec. 3e) in the results from the U Hubbard model's results. Fig. 1(a) shows the results for Δ_0 . As expected, Δ_0 gets enhanced with attractive V as compared with the values of the U Hubbard model, while it gets suppressed in the region where $\alpha < \beta$ for repulsive V . For all values of α at fixed β , Δ_0 obeys an inequality $-\Delta_0(-U, +V) \leq -\Delta_0(-U, V = 0) \leq -\Delta_0(-U, -V)$. From the qualitative behavior of Δ_0 , it is clear that, when U is attractive, a repulsive or an attractive V only renormalizes the effect of U in a simple manner, i.e., the V seems to get either added or subtracted to U . However, for a repulsive U , the mean field equations still provide an effective attractive interaction required for SC pairing, though its magnitude is very small as is evident from the values of Δ_0 . With repulsive U , the

Fig. 1. (a) Δ_0 versus α at $\beta = 0.5$ and $\delta = 0.5$. The --- curve is the U Hubbard model's values for Δ_0 . In all the figures, the curves with --- mark corresponds to the case when U and V are attractive. The -+ curves are the results for attractive U and repulsive V , while +- curves represent the repulsive U and attractive V , respectively. (b) Δ_1 versus α at $\beta = 0.5$ and $\delta = 0.5$. (c) Δ_1 versus α at $\beta = 0.5$ and $\delta = 0.5$. (d) μ_0 versus α at $\beta = 0.5$ and $\delta = 0.5$. The --- curve is the U Hubbard model's values for μ_0 .

(d)

Fig. 1. (Continued).

behavior of Δ_0 changes drastically — it shows a non-BCS kind of take-off for small values of α and goes to a constant for $\alpha > 0.45$.

The extended-wave pairing as a function of α is shown in Figs. 1(b) and 1(c). Notice, that for attractive V , Δ_1 becomes negative, however, $\Delta = \Delta_0 + \gamma\Delta_1$ remains positive definite for all values of α . For the case of repulsive V , no SC pairing exist ($\Delta_0 = 0$, $\Delta_1 = 0$) for small values of α (e.g., for $\alpha < 0.16$). Pairing starts building as α is increased away from 0.16 and acquires a maximum value around $\alpha = 0.46$. Note that, the strong attractive U does not promote the extended-wave pairing, for attractive or repulsive V . In fact, U suppresses it (6.1) monotonically. For repulsive U , Δ_1 decreases exponentially and gets saturated for larger values of α [see Fig. 1(c)]. A glance at the magnitudes of Δ_0 and Δ_1 shows that the SC pairing is dominated by the extended-wave pairing in the case of repulsive U .

The chemical potential μ_0 is plotted in Fig. 1(d). The two points are to be noted about μ_0 . First μ shows a jump as V is switched-on from repulsive to attractive interaction. Second, μ_0 remains constant up to certain values of α , when α is small. This region where μ_0 is constant is in proximity with non-SC phase. For large α , μ_0 decreases linearly with α . In the SC phase, μ_0 decreases with α . In the case of repulsive U , μ_0 starts from 0 and decreases with α , and for $\alpha > 0.2$ it acquires a constant values.

3.2. The influence of V on Δ_0 , Δ_1 and μ_0

Note that it due to the k -dependence of Δ_k which couples Δ_0 to the V . The effect of an extended Hubbard interaction on SC pairing is shown in Figs. 2(a) and 2(b) for various values of β (β varies from 0 to 1) at $\alpha = 0.5$ and $\delta = 0.5$. At the origin of β axis are the results of U Hubbard model, where, the only pairing exhibited is the s -wave pairing. Now if we switch-on an attractive V , then physically one

(a)

(b)

(c)

Fig. 2. (a) Δ_0 versus β at $\alpha = 0.5$ and $\delta = 0.5$. (b) Δ_1 versus β at $\alpha = 0.5$ and $\delta = 0.5$ and (c) μ_0 versus β at $\alpha = 0.5$ and $\delta = 0.5$.

expects, the SC-pairing to get enhanced, while the reverse effect should be observed for the repulsive case. As shown in Fig. 2(a), Δ_0 increases linearly with attractive V almost till $\beta = 1$. While for repulsive V , Δ_0 decreases comparatively faster with β and deviates from linearity also, as we know that, for $+U$ Hubbard model, in the mean field approximation, there is no s -wave pairing. However, one expects SC-pairing with attractive V if its magnitude is greater than some critical value. This critical value depends upon the magnitude of repulsive U . In this case when $\alpha = 0.5$, we find that s -wave pairing starts building when $\beta > 0.5$ and increases rapidly in a non-exponential manner with β and gets saturated for $\beta > 0.8$. In the mean field calculations, we find that there is a qualitative difference in the behavior of s -wave pairing due to an on-site Hubbard interaction and an extended Hubbard interaction.

Figure 2(b) shows the variations of Δ_1 with β . For an attractive V , Δ_1 becomes negative, while it is positive for repulsive V . In both the cases it varies linearly with β . Notice, that the magnitude of Δ_1 is larger than Δ_0 for repulsive U , manifesting the dominance of the extended-wave pairing.

The values of μ_0 [see Fig. 2(c)] increases with attractive V as compared with the U Hubbard model's values. For repulsive V , it decreases. In the case when U is repulsive, μ_0 shows little variation with β for $\beta > 0.48$.

3.3. The influence of δ on Δ_0 , Δ_1 and μ_0

The dependence of Δ_0 on δ is shown in Figs. 3(a) for $\alpha = 0.2$, and $\beta = 0.5$. We have chosen $\alpha < \beta$ because, as we shall see latter on that for these values of interaction parameters, SC order parameter exhibits an interesting phase diagram. In U Hubbard model, Δ_0 is proportional to $\sqrt{1 - \delta^2}$, [see Eq. (15)]. The inclusion of an attractive V produces qualitative changes in Δ_0 it decreases faster than $\sqrt{1 - \delta^2}$ for intermediate values of δ . In the above mean field calculations, one finds that, the s -wave pairing is maximum at half-filling and vanishes as expected at no carrier concentration, i.e., at $\delta = 1$. Since we took $\alpha > \beta$, so one expects a destabilizing effect of pairing with repulsive V at some critical carrier concentration. Which happens for $n \geq 0.42$. However, the s -wave pairing which has been maximum at half-filling for attractive U , got completely suppressed to zero for repulsive U , see Fig. 3(b). This can be seen from Eq. (12), that for repulsive U , the only solution of Δ_0 at half-filling is $\Delta_0 = 0.0$. Departure from half-filling starts building s -wave pairing and it acquires a maximum value at $\delta = 0.75$ then it vanishes in the usual way like $\sqrt{1 - \delta^2}$ at $\delta \rightarrow 1$.

On the contrary, for attractive U (and for attractive or repulsive V) Δ_1 is zero at half-filling, see Fig. 3(c). The zero solution of Δ_1 at half-filling, $\mu_0 = 0$, can be trivially seen from the GHFA equations for zero or non-zero values of Δ'_0 . As $\delta \rightarrow 1$, Δ_1 seems to vanish like $\sqrt{1 - \delta^2}$. With attractive U and repulsive V , the variation in Δ_1 is small and it (Δ_1) vanishes at $\delta = 0.58$. For repulsive U , Δ_1 is zero for $\delta \leq 0.05$ and as δ increases further, like Δ_0 , Δ_1 passes through a maximum

(a)

(b)

(c)

Fig. 3. (a) Δ_0 versus δ at $\alpha = 0.2$ and $\beta = 0.5$. The --- curve is the U Hubbard model's values for Δ_0 . (b) Δ_0 versus δ at $\alpha = 0.2$ and $\beta = 0.5$. (c) Δ_1 versus δ at $\alpha = 0.2$ and $\beta = 0.5$. (d) Δ_1 versus δ at $\alpha = 0.2$ and $\beta = 0.5$. (e) μ_0 versus δ at $\alpha = 0.2$ and $\beta = 0.5$.

(d)

(e)

Fig. 3. (Continued).

around $\delta = 0.75$, than drops to zero with the usual mean field manner. The results are plotted in Fig. 3(d). The qualitative features of the SC diagram, defined by $\Delta = \Delta_0 + \gamma\Delta_1$ as a function of δ for the case of weak repulsive U and comparatively stronger V .

The chemical potential μ_0 for U Hubbard model (under the mean field approximation) is a linear function of δ , see Eq. (16). With the inclusion of V , μ_0 remains linear for $\delta < 0.2$ and $\delta > 0.8$ for all the cases of interactions. The slope of μ_0 is determined by the case of interaction — for small δ the slope is largest for attractive U and repulsive V , and it is smallest for repulsive U and attractive V . At intermediate values of δ , μ_0 shows maximum departure from the $-\gamma t_0 \coth(\gamma t_0/\alpha)$ which is the slope of μ_0 for U Hubbard model. For non-SC phase which is observed in repulsive V when $\delta > 0.58$, μ_0 varies linearly like $-\gamma t_0$ (see Eq. (3.1)). At the level of chemical potential, one can identify (within the mean-field approximation) the transition

from a SC-phase to non-SC phase from the slope of μ_0 against μ . One notice that μ_0 varies non-linearly in SC phase or linearly with slope $-\gamma t_0 \coth(\gamma t_0/\alpha)$ as in U Hubbard model, while in the non-SC phase ($\Delta_0 = 0.$, $\Delta_1 = 0$), it varies linearly with slope $-\gamma t_0$.

4. Conclusions

The reliability of the present mean-field calculations is restricted to the regions where electron correlations are not too strong ($\alpha < 1$ and $\beta < 1$) and the carrier concentration is not too low. This situation is physically appropriate for superconducting phase of the oxides. One knows that on doping the carriers are delocalized reducing the strong short-range correlations. A doped material is a poor insulator in comparison with an undoped one. For stronger correlations, deviation²⁷ from the above results are expected. In summary, we found, that the contribution to the pairing from on-site interaction is always stronger than the off-site interaction, except for the case when U is repulsive, where pairing is dominated by extended wave pairing. The effect of V on μ_0 and order parameters, shows linear dependence in the whole range of its variation, again except for the case when U is repulsive. The deviation of Δ_0 and μ from the U Hubbard results due to the inclusion of V is also discussed. The SC-phase diagram versus doping in the repulsive U and attractive V case has to be carefully analysed that would make a connection with the quasi-particle energy²⁸ for experimental comparison.

In summary, we have investigated possibilities of superconducting order in an extended Hubbard model with onsite U and nearest neighbor interaction V as phenomenological parameters. While we are aware that a huge number of papers have been written on this aspect, our aim has been to provide in this work a simple and a pedagogic generalized mean-field picture. We demonstrate the manifestation of superconductivity arising out of purely electronic interactions over a broad range of parameters in particle density and interaction strengths.

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