A Model of Correlated Fermions with $d_{x^2−y^2}$ Superconductivity

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Motivated by the phenomenology of the high-Tc cuprates, a two dimensional fermionic model with attractive interactions is here discussed. The exact solution to the two particle problem leads to a bound state in the $d_{x^2−y^2}$ subspace. Numerical techniques suggest that the model has $d_{x^2−y^2}$ superconductivity (SC) in the ground state at low fermionic density. Within a self-consistent RPA diagrammatic study, the density dependence of the critical temperature is calculated. We argue that in the context of d-wave SC this model fulfills the role that the attractive on-site Hubbard model has played for s-wave SC. We also show that another candidate, the attractive “t-U-V” model, which has d-wave SC at the mean-field level is actually not useful as a realization of this family of condensates for a variety of reasons.

74.20.-z, 74.20.Mn, 74.25.Dw

The Hubbard model with an attractive on-site interaction has played an important role in the qualitative understanding of s-wave superconductors. Several interesting problems, like the crossover from the BCS regime to the region where Cooper pairs form a Bose Condensate (BC), can be addressed within this model using analytical and numerical techniques. Although the phononic degrees of freedom are not explicit, it is expected that the qualitative properties of the attractive Hubbard model are the same as those of more realistic, and difficult to study, electron-phonon Hamiltonians.

However, since evidence is accumulating that the high critical temperature (high-Tc) superconductors have a condensate with pairs formed in the $d_{x^2−y^2}$ channel, the relevance for the cuprates of the on-site attractive Hubbard model is questionable. In addition, studies of $H_{e2}$ in cuprates suggest that the Cooper pairs are only a few lattice spacings in size, locating the high-Tc materials in an intermediate region between the BCS and the BC limits. In this regime, the BCS mean-field (MF) approximation is not quantitatively accurate. Thus, it would be desirable to have a fermionic model with a $d_{x^2−y^2}$ superconducting ground state that can be studied with reliable non-perturbative diagrammatic and computational techniques in the small coherence length region. Results obtained in this framework could be directly compared with the cuprate phenomenology.

What model can provide the generalization of the attractive Hubbard model for the case of $d_{x^2−y^2}$ superconductivity? Current literature shows that many studies of d-wave superconductors are performed using the BCS MF approximation after introducing a proper attractive kernel in the gap equation to induce d-wave correlations. This approach is accurate in weak coupling where pairs are large, but it does not address the regime of small pairs which is more realistic for the cuprates. To improve these results, it is natural to consider as a first candidate for a model with d-wave SC the so-called “t-U-V” model where U is repulsive on-site, V is the strength of a density-density attraction at distance of one lattice spacing a, and t is the amplitude of a nearest-neighbors (n.n.) hopping term. In the MF approximation the phase diagram at half-filling of the t-U-V model (Fig.1a) indeed has an “island” of d-wave SC. However, note the small size of this phase caused by the competition with phase separation (PS) where electrons doubly occupy a macroscopic region of the cluster to minimize the energy. A recent study has shown that the effect of PS cannot be simply avoided by introducing a long-range Coulomb repulsion since in this situation PS may be replaced by a charge-density-wave (CDW) state rather than by SC. Thus, the competition SC-PS is subtle and not created by the absence of long-range interactions.

Using techniques more powerful than MF, in this paper we argue that the t-U-V model is not much useful for the study of d-wave superconductors. As a first indication of this problem, let us analyze the results obtained using Quantum Monte Carlo (QMC) and Exact Diagonalization (ED) techniques. Working at small U/t where the MF approximation predicts a d-wave condensate, first we have studied the competition with PS. This phase can be observed numerically with QMC simulations since in some regions of parameter space we found that the mean particle density converges to two very different results depending on the randomly chosen initial Hubbard-Stratonovich fields. Such a behavior is typical of systems with two competing minima in the free energy, as it happens in the presence of PS. In QMC the effect can already be seen even using small clusters of 16 and 36 sites, and working at relatively high temperatures $T = t/6$ to alleviate sign problems. As example, the presence of the two minima was numerically observed at $U/t = 1$ for $|V/t| > 0.55$, reducing the MF d-wave stability region (Fig.1a). Increasing the lattice size and reducing the temperature would only enhance the effect, since the tunneling probability would become negligible.
FIG. 1. (a) Mean-field phase diagram of the “t-U-V” model at half-filling. DS, SS, PS, CDW, and SDW denote d-wave SC, s-wave SC, phase separation, charge-density-wave, and spin-density-wave order, respectively; (b) $d_{x^2-y^2}$ pairing correlation vs distance $r$ obtained with QMC, on a $4 \times 4$ cluster, $T = t/6$, $U/t = 0.0$ and $V/t = -0.3$ i.e. within the MF d-wave region. The correlations are small at distances larger than one. Similar negative results were obtained for other couplings inside the MF d-wave region. The error bars are smaller than the dots; (c) Schematic representation of model Eq.(1). Fermions move within the same sublattice, and interact at distance one; (d) Binding energy $\Delta_B$ for the two-particle problem solved exactly using $t_{20} = 0.4t_{11}$, as example. States with the lowest energy in the $d_{x^2-y^2}$, extended-s and p-subspaces are shown. Similar results are found for $t_{20} > 0.5t_{11}$. If $t_{20} > 0.5t_{11}$, at small $|V|/t_{11}$ the actual ground state has p-wave, but it becomes again $d_{x^2-y^2}$-wave after a finite coupling is reached.

In addition to this problem, in the regime where PS is not observed in our analysis, a QMC simulation still does not show enhanced d-wave correlations at $T = t/6$. Defining the operator that destroys a d-wave local pair as $\Delta_i^d \equiv \hat{c}_{i\uparrow} \hat{c}_{i\downarrow} + \hat{c}_{i\downarrow} \hat{c}_{i\uparrow}$, with $\hat{x}, \hat{y}$ unit vectors along the axis, then the ground state pairing correlation is $C_d(r) = \langle \Delta^d_i \Delta^d_{i+r} \rangle$. Fig.1b shows that $C_d$ decays to zero with distance. Actually, results at $U, V = 0$ are very similar to Fig.1b. We also performed ED studies on $4 \times 4$ clusters that are in excellent agreement with the QMC data. While the QMC result does not rule out the stability of d-wave SC at $T < t/6$, it shows that (i) the small region of possible d-wave SC cannot be easily studied with current state-of-the-art computational studies beyond the MF approximation, and (ii) obviously in such a weakly correlated regime, Cooper pairs can only be large in size contrary to the high-Tc phenomenology. In addition, note also that the tentative d-U-V model occurs at half-filling with all electrons pairing to form the condensate. However, it would be desirable to have a model where a small density of carriers forms pairs, mimicking the expected hole-pairing of the cuprates. The t-U-V model at low electronic density has s-wave SC rather than d-wave, complicating matters further. An inescapable conclusion of this analysis is that it is necessary to go beyond the t-U-V model for a proper study of effective fermionic models for d-wave SC. It is remarkable that in spite of the recent huge effort devoted to the study of d-wave SC in the cuprates, the analog of the attractive Hubbard model for $d_{x^2-y^2}$ pairs still seems unknown.

The main purpose of this paper is to discuss a fermionic model for $d_{x^2-y^2}$ SC which solves the problems found in the t-U-V Hamiltonian. Analyzing the model studied here with computational techniques, it presents strong pairing correlations in the d-wave channel, and PS does not cause serious problems. The Hamiltonian contains an attractive n.n. density-density interaction at distance $a$, as in the t-U-V model, but it differs from it in the fermionic dispersion which in the new model is dominated by hopping within the same sublattice, i.e. linking next-nearest-neighbor (n.n.n.) sites. This model was discussed before in the context of the “Antiferromagnetic van Hove”(AFVH) scenario for the cuprates where the high $T_c$ is induced by a large peak in the hole density of states (DOS) caused by antiferromagnetism. The intra-sublattice dispersion is natural if holes move in a nearly antiferromagnetic background that is energetically costly to disturb. The attractive interaction has its origin in AF correlations. In Ref. the model was studied only within a MF approximation, but here we substantially improve the analysis using computational and self-consistent diagrammatic techniques. The Hamiltonian of the proposed model candidate for d-wave SC is

$$H = \sum_{\alpha\beta} \epsilon_{AF}(k) |c_{\alpha\beta}^\dagger c_{\alpha\beta} + h.c.| - |V| \sum_{\langle ij \rangle} n_i n_j,$$

(1)

where $\alpha = A, B$ indicates the sublattice; $\epsilon_{AF}(k) = 4t_{11} \cos k_x \cos k_y + 2t_{20}(\cos 2k_x + \cos 2k_y)$ is the dispersion; $t_{11}, t_{20}, V$ are parameters; and $n_i$ is the number operator, with the rest of the notation standard (see Fig.1c). The operators $c$ satisfy anticommutation relations. They do not have a spin index, but carry a sublattice index which plays a similar role. Particles are distributed such that half of them are in each sublattice. Intuitively the particles described by Eq.(1) represent “holes” in the cuprates. It is straightforward, and very instructive, to solve exactly the two particle problem using Eq.(1). Defining the binding energy as $\Delta_B = E_2 - 2E_1$, where $E_n$ is the ground state energy of the $n$-particles subspace, the results are shown in Fig.1d for extended-s, $d_{x^2-y^2}$ and p-wave symmetries. The lowest energy state has $\Delta_B < 0$, signaling the presence of a bound state, and it corresponds to $d_{x^2-y^2}$-symmetry. At small $|V|$, i.e. for weakly bounded particles, $\Delta_B$ is very small in absolute value, but still negative. Studying the average distance between the
two particles we observed that at \( |V|/t_{11} \approx 2 \) in Fig.1d, the pair size is already close to its maximum value of one lattice spacing defining the strong coupling regime. 

FIG. 2. (a) Two fermions in the large \( |V| \) limit of Eq.(1) showing the \( d_{x^2−y^2} \)-wave character of the bound state; (b) Two fermions in the large \( |V| \) limit of the \( t-U-V \) model. The bound state is \( s \)-wave; (c) \( d_{x^2−y^2} \) pairing correlations vs distance \( r \) for model Eq.(1) at \( T=0 \) studied with ED techniques on a 32 site cluster. The couplings are \( |V|/t_{11} = 1.0 \), \( t_{20}/t_{11} = 0.4 \), and \( x \) is indicated. Correlations in the \( s \)- and \( p \)-channels are negligible.

What is the origin of the \( d \)-wave symmetry in the ground state of the two-body problem? Consider the large \( |V| \) limit, and let us analyze the movement of one particle around the other as schematically shown in Fig.2a. In this regime, the energy is minimized when the interparticle distance is one lattice spacing at all times. Keeping particle B fixed at a given site, the problem now amounts to solving an effective four-site hopping Hamiltonian of particle A moving along the four n.n. sites to B using the hoping amplitude \( t_{11} \) along the diagonal. Here it is important to observe that the sign of \( t_{11} \) is chosen as a positive number by the requirement that the minimum in the dispersion is at \( p = (\pi/2, \pi/2) \) or \( (0, 0) \), as it is natural in problems of holes in antiferromagnets. The signs of \( t_{11} \) and \( t_{20} \) are physically relevant, unlike the sign of a n.n. hopping that can be changed by suitable transformations on a square lattice. Then, the ground state of the effective four-site problem corresponds to selecting a phase alternating in sign for particle A (Fig.2a). This leads to a \( d_{x^2−y^2} \) bound state, providing a real-space intuitive explanation for the appearance of \( d \)-wave pairs which complements those based on the perturbative interchange of magnons. We remark that this simple result found in Eq.(1) is not present in the \( t-U-V \) model. If the n.n.n. hopping (Fig.2a) is replaced by the n.n. hopping of the t-U-V model, then the ground state phases of particle A orbiting around B at large \( |V| \) are as shown in Fig.2b. They correspond to an s-wave bound state.

The presence of \( d_{x^2−y^2} \) bound states in the two body problem of Eq.(1) suggests SC in the same channel at finite particle density. However, CDW and PS states are also favored by a particle-particle attraction and thus an explicit calculation is needed to verify the existence of a SC condensate. For this purpose, we exactly calculated the ground-state pairing correlations \( C_d(r) \) on a \( \sqrt{32} \times \sqrt{32} \) site cluster using ED techniques. The operator is the same used before for the t-U-V model, simply switching the spin indices for sublattice indices. In order to avoid possible complications with the potentially dangerous PS regime, in the study shown in Fig.2c an intrasublattice density-density repulsive interaction of strength \( |V|/\sqrt{2} \) and \( |V|/2 \) at distances \( \sqrt{2}a \) and \( 2a \), respectively, was also included in the Hamiltonian. The results at \( |V|/t_{11} = 1.0 \), \( t_{20} = 0.4t_{11} \), and at realistic densities \( x = 6/32 \approx 0.19 \) and \( 8/32 = 0.25 \), are shown in Fig.2c. The robust tail suggests strong pairing correlations in the ground state. Thus, with Hamiltonian Eq.(1) supplemented by mild assumptions to avoid PS it is possible to obtain numerical signals of \( d \)-wave SC, unlike the results obtained before for the t-U-V model. 

Hamiltonian Eq.(1) can also be studied diagrammatically using Eliashberg-type equations. With this approach, we have calculated \( T_c \) vs \( x \) in the intermediate to strong coupling region. Working in Matsubara space and in natural units, we approximate the normal state proper self-energy by iteratively solving the equation

\[
\Sigma(k, \omega_n) = -\frac{T}{N} \sum_{q, \omega_n'} V_{eff}(k - q, \omega_n - \omega_n') G(q, \omega_n'),
\]

where \( N \) is the number of sites (we used a \( 32 \times 32 \) cluster for this calculation), \( T \) the temperature, \( \omega_n = (2n + 1)\pi T \) \((-\infty < n < +\infty)\), the full normal state one particle Green’s function satisfies \( G(k, \omega_n) = 1/(\omega_n - (\epsilon_{AF}(k) - \mu) - \Sigma(k, \omega_n)) \), and \( V_{eff}(k, \omega_n) \) is the RPA effective potential with particle-hole bubbles containing \( G \) rather than the noninteracting Green’s function, to make the calculation self-consistent. Once the normal state \( G \) is found, for the SC state we use

\[
\Phi(k, \omega_n) = \sum_{q, \omega_n'} M(k, q, \omega_n, \omega_n') \Phi(q, \omega_n'),
\]

where \( \Phi(k, \omega_n) \) is the anomalous self-energy which can be considered as an order parameter for SC, and

\[
M(k, q, \omega_n, \omega_n') = -\frac{1}{2} V_{eff}(k - q, \omega_n - \omega_n') G(q, \omega_n') G(-q, -\omega_n').
\]

We have solved Eqs.(2,3) self-consistently at different temperatures and densities, using as an energy cutoff ten times the bandwidth. The symmetry of the SC condensate is determined from the symmetry of the eigenvector of Eq.(3) corresponding to the largest eigenvalue. After all ring diagrams are summed up, this symmetry is \( d_{x^2−y^2} \).
The results for $T_c$ are shown in Figs. 3a,b compared to the MF approximation. Which in this model is equivalent to the Hartree-Fock (HF) approximation. The qualitative agreement is good, and quantitatively the self-consistent approach reduces $T_c$ at optimal doping by a factor $\sim 1.5$ still maintaining $T_c$ at a high value. No drastic further reductions of $T_c$ are expected by adding diagrams beyond RPA to the calculation. The reason is that in this model the vertex correction identically vanishes due to intrinsic features of the Hamiltonian Eq.(1), namely that particles move within the same sublattice, while the interaction is intersublattice. To understand this effect, consider the real space representation of the vertex correction contribution to the self-energy which is given by

$$\Sigma_{\text{vertex}}(r, \tau) = \sum_{\mathbf{e}_1, \mathbf{e}_2 = \mathbf{x}, \mathbf{y}} G(\mathbf{r} + \mathbf{e}_1, \mathbf{e}_2, -\tau) G(\mathbf{r} + \mathbf{e}_2, -\tau) G(\mathbf{r} + \mathbf{e}_1, \mathbf{e}_2, -\tau) G(\mathbf{r} + \mathbf{e}_2, -\tau).$$

It is clear that there is always a Green’s function that vanishes, irrespective of whether $\mathbf{r}$ connects the same or different sublattices. Finally, note that the values of $T_c$ shown in Fig.3a are realistic, and the presence of an “optimal” density is a consequence of a peak in the DOS of $\epsilon_{AF}(\mathbf{k})$.\[3\]

Summarizing, in this paper we studied a model for fermions moving on a 2D square lattice with intrasublattice hopping and attractive n.n. density-density interactions. Using numerical and analytical techniques we conclude that in this model (i) the two-body problem leads to a $d_{x^2-y^2}$-wave bound state in a natural way, and (ii) in the dilute limit the ground state has strong $d_{x^2-y^2}$ pairing correlations. We have also provided evidence that the t-U-V model actually does not show a clear signal of d-wave SC in computational studies, and the competition with PS prevents the analysis of its intermediate coupling regime. Thus, we conclude that the new model discussed here is the natural generalization to $d_{x^2-y^2}$ superconductivity of the attractive Hubbard model. The new model is based on the phenomenology of the high-Tc cuprates which near half-filling is dominated by antiferromagnetic fluctuations. Phenomenological studies of the influence of impurities, external fields, and other probes on $d_{x^2-y^2}$ superconductivity would become more accurate if model Eq.(1) replaces the t-U-V model.

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