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Antiferromagnetism and superconductivity in a model with extended pairing interactions

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Abstract. The competition between antiferromagnetism and the $d+\mathrm{i}d$ superconducting state is studied in a model with near and next near neighbour interactions in the absence of any on-site repulsion. A mean field study shows that it is possible to have simultaneous occurrence of an antiferromagnetic and a singlet $d+\mathrm{i}d$ superconducting state in this model. In addition, such a coexistence generates a triplet $d+\mathrm{i}d$ superconducting order parameter with centre of mass momentum $Q=(\pi,\pi)$ *dynamically* having the same orbital symmetry as the singlet superconductor. Inclusion of next nearest neighbour hopping in the band stabilises the d_{xy} superconducting state away from half filling, the topology of the phase diagram, though, remains similar to the near neighbour model. In view of the very recent observation of a broad region of coexistence of antiferromagnetic and unconventional superconducting states in organic superconductors, the possibility of observation of the triplet state has been outlined.

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1 Introduction

Interests on the interplay between antiferromagnetism and superconductivity date back quite a while as in certain organic and heavy fermion superconductors, superconductivity is known to coexist with an antiferromagnetic (AF) phase at low temperatures [1,2]. In a recent study of the organic superconductor κ-$(ET)_2Cu[N(CN)_2]Cl$ the most complete phase diagram has been obtained as a function of pressure and a region of coexistence of unconventional SC and AF LRO is observed [3]. In the high T_c cuprates, the superconducting state abuts (albeit with a small gap) the AF state and recent inelastic neutron scattering [4,5] reveals considerable AF fluctuations deep inside the superconducting (SC) state in YBCO. There are, actually, quite a few similarities between the organic and high T_c superconductors [6]. Indeed, antiferromagnetism, in some theories, is considered to lie at the heart of the mechanism that drives unconventional superconductivity [7].

Several investigations were carried out [8] to study the phase diagram and nature of phase transitions between the AF state and the SC state in the context of the organic and heavy fermion superconductors. Meintrup *et al.* [9] proposed a model in the general context of antiferromagnetism and superconductivity in which nearest neighbour singlet pairing interaction was shown to accommodate both SC and AF states and their coexistence in certain range of parameters. These authors, and several others before them [10,11], showed that it is not necessary to have strong on-site repulsion to generate AF LRO. Correlated models with extended range of interactions can produce AF LRO and SC as well.

In a recently proposed SO(5) theory of superconductivity Zhang [12] considered a five-dimensional order parameter space $(\psi_1,\cdots,\psi_5)$ with $\psi_1+\mathrm{i}\psi_5$ being the SC order parameter and the remaining three constituting the AF moment. A rotation in this five-dimensional order parameter space, effected by the spin 1, charge 2, $\pi-$operators, ($\pi^\dagger_\alpha=\sum_k g(k)c^\dagger_{k+Q\uparrow}c^\dagger_{-k\downarrow}$, where $c^\dagger(c)$'s are the electron creation (destruction) operators and $Q=(\pi,\pi)$ in d = 2, leads to the transition from the AF to the SC state. In this theory, the triplet magnetic excitation of the quantum disordered phase is identified with this π-triplet mode in the SC phase. In an exact diagonalization study of the $t-J$ model [13], the dynamical correlation functions of the $\pi-$operators have been calculated and found to be non-zero. The existence of both AF and triplet pairing amplitude with net momentum Q was reported earlier in the mean-field study of a pairing Hamiltonian in the context of the heavy fermions and organic

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superconductors [8,14], although the conditions under which the triplet amplitude appears and the modifications of the phase boundaries due to this triplet amplitude were not dealt with. In a recent investigation, Kyung [15] considered explicit mean-field pairing interactions in the singlet and triplet channel with a repulsive on-site interaction to stabilize the d-wave SC state (over s-wave) and discussed the coexistence of a dynamically generated triplet SC pair amplitude and AF long range order (LRO). In this case, superconductivity is governed by the attractive interactions in the appropriate channels while the AF state owes its origin primarily to the on-site repulsion in the usual manner.

We start from a Hamiltonian with nearest and next nearest neighbour interaction and consider pairing in the d-wave and $d+\mathrm{i}d$-wave in the singlet (and later on in the triplet) channel along with the antiferromagnetic LRO. The on-site interaction is assumed to be small [16] (set to zero here) and both the LRO and off diagonal long range order (ODLRO) are governed by the same interactions in a manner similar to the case studied by Meintrup *et al.* [9] (where the on-site interaction was absent as well). Using a mean-field analysis, these authors studied the coexistence of different singlet SC and AF LRO states in their model. Related extended range models have been studied by numerical methods [10] and mean-field [11] theory earlier, although a detailed study with the possibility of several SC symmetries and AF order have not been undertaken.

There have been suggestions [17] for the existence of $d+\mathrm{i}d$ state in the high T_c systems followed by possible observation in a series of experiments [18,19]. Recently, it has been shown [20] from a renormalization group analysis of the fluctuations that the transition to $d+\mathrm{i}d$ state possesses a stable fixed point. Kino and Fukuyama [21] considered a model with only on-site repulsion for the organic superconductors in the intermediate coupling range (typically the on-site interaction is about half the band width). Such a model, although accounts for the AF phase and the metal-insulator transition, fails to explain the large SC phase observed in [3]. Extended range attractive interactions with the right symmetry are necessary to obtain these unconventional SC states. Additional processes discussed in reference [16], particularly in the large metallic region above the SC phase, possibly reduce the on-site interaction in the organic systems further.

A preliminary report of the coexistence of and competition between the singlet superconducting $d_{x^2-y^2}$, d_{xy}, $d_{x^2-y^2}+\mathrm{i}d_{xy}$ (the so called $d+\mathrm{i}d$ state) states and AF LRO in a model similar to that of Meintrup *et al.* with extended range of interaction has been presented recently by two of us [22]. We extend this calculation and show in the present work that in the presence of such coexisting singlet SC order parameter and AF LRO, a triplet pairing amplitude with centre of mass momentum Q is dynamically generated even if there is no explicit interaction in the Hamiltonian in that channel. It is not *a-priori* obvious that the dynamical generation of the triplet amplitude should occur in a model where the AF and SC states are governed by combinations of the same interactions. In the model considered by Kyung [15] the relative strength of these two competing states are governed primarily by separate and independent interaction parameters. We also figure out how the phase diagram gets modified in the presence of the triplet pairing amplitude in the present model. In Section 2 we discuss the model under consideration. Section 3 concerns with the results, discussion and concluding remarks.

2 Model and calculations

The model studied here incorporates antiferromagnetic LRO and superconductivity and is given by the Hamiltonian [22]

$$\mathbf{H} = \sum_{k,\sigma} \xi_{\mathbf{k}} c^{\dagger}_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma} + \sum_{\langle ij\rangle\sigma} V_{ij} n_{i\sigma} n_{j-\sigma} + \sum_{\langle\langle ij\rangle\rangle\sigma\sigma'} \tilde{V}_{ij} n_{i\sigma} n_{j\sigma'} \quad (1)$$

where the sum over $\langle ij\rangle$ extends over near neighbour and $\langle\langle ij\rangle\rangle$ over next near neighbour sites. We take V_1 and V_2 as the corresponding interaction strengths (both V_1 and V_2 are negative) and write $\xi_{\mathbf{k}} = \epsilon_{\mathbf{k}} - \mu$. In the absence of an on-site repulsion, this model is perhaps the simplest that produces AFM as well as superconductivity in the $d+\mathrm{i}d$ channel.

Elementary physical reasoning shows how an AF state appears in this Hamiltonian. In the classical limit ($t_{ij}=0$) the Hamiltonian has near-neighbour attractive density-density interaction (amongst opposite spins) that leads to AF spin correlation (of Ising symmetry) among nearest neighbour spins. An on-site repulsive term would have stabilised this further and the region of AF LRO would extend in the phase space. The second neighbour attractive density-density correlation term is spin independent and stabilises a d_{xy} order in the quantum limit. The regions of stability of $d_{x^2-y^2}$, d_{xy} and the $d+\mathrm{i}d$ state for the range of values of V_1 and V_2 have been discussed in [25]. Extensive literature exists for models in the opposite limit of repulsive extended range interactions where the classical limit gives rise to charge density waves [23]. In the absence of V_2, Monte-Carlo calculations [10] of model (1) shows AF phase at all densities. At half-filling the ground state is Néel ordered while away from half-filling there is evidence for phase separation between AF ordered and empty domains. Mean-field analysis [9] captures much of these features qualitatively, although a realistic description of the phase separation eludes such calculations as expected.

In order to use mean-field description for the symmetry-broken states we define the operators corresponding to the singlet and triplet SC order parameters in real space [16]

$$\Lambda_{i,s} = \frac{1}{4}\sum_{\delta,\sigma} \sigma c_{i+\delta,\sigma} c_{i,-\sigma} \phi(\delta) \qquad \text{and}$$

$$\Lambda_{i,t} = \frac{1}{4}\sum_{\delta,\sigma} c_{i+\delta,\sigma} c_{i,-\sigma} \phi(\delta), \quad (2)$$

where δ is the usual near-neighbour translation vector and a choice of the form factor $\phi(\delta)$ with $\phi_1(\delta) = 1$ for $\delta = (\pm 1, 0)$ and $\phi_1(\delta) = -1$ for $\delta = (0, \pm 1)$ (with $\phi_1(\delta) = 0$ for all other choice of δ) ensures that the SC OP has $d_{x^2-y^2}$ symmetry. For d_{xy} symmetry, one takes the form factor (the only non-zero terms) ϕ as $\phi_2(\delta) = 1$ for $\delta = (\pm 1, \pm 1)$ and $\phi_2(\delta) = -1$ for $\delta = (\pm 1, \mp 1)$. The operator corresponding to the AF order parameter is the well known form $\sum_\sigma \sigma c^\dagger_{i,\sigma} c_{i,\sigma}$. Writing the AF, singlet and triplet SC order parameters as ($\sigma = \pm 1$)

$$\sum_\sigma \langle \sigma c^\dagger_{i,\sigma} c_{i,\sigma} \rangle = b_0 \mathrm{e}^{\mathrm{i}\mathbf{Q}\cdot\mathbf{r}_i} \tag{3a}$$

$$\frac{1}{4}\sum_{\delta,\sigma} \langle \sigma c_{i+\delta,\sigma} c_{i,-\sigma} \rangle (\phi_1(\delta) + \mathrm{i}\phi_2(\delta)) = \Delta_s \tag{3b}$$

and

$$\frac{1}{4}\sum_{\delta,\sigma} \langle c_{i+\delta,\sigma} c_{i,-\sigma} \rangle (\phi_1(\delta) + \mathrm{i}\phi_2(\delta)) = \Delta_t \mathrm{e}^{\mathrm{i}\mathbf{Q}\cdot\mathbf{r}_i}. \tag{3c}$$

The SC order parameters are chosen to be of $d_{x^2-y^2}$ and d_{xy} symmetries as the interactions V_1 and V_2 are known to favour [20,25,26] superconductivity in such orbital symmetries. The presence of AF order in the model (1) has already been indicated. The superconducting order parameter Δ_s, which is a spin singlet with d-wave orbital symmetry, can have a non-zero value when the underlying pairing state is spatially homogeneous. On the other hand, the order parameter Δ_t that we write down here should be thought of as a non-zero expectation value of the $\pi-$operator of the SO(5) theory and is generated only dynamically [24]. It can be non-zero provided that the expectation value of the annihilation operators in (3c) changes sign on alternating bonds. The resulting Δ_t is thus a staggered order parameter: it changes sign from site to site in the same way as the antiferromagnetic order parameter (3a) does.

Using the Hartree-Fock approximation with these order parameters and going over to Fourier space we get a Hamiltonian in quadratic form as

$$\begin{aligned}\mathbf{H}_{\mathrm{MF}} = &\sum_{k,\sigma} (\epsilon_{\mathbf{k}} - \tilde{\mu}) c^\dagger_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma} \\ &+ b_{\mathrm{m}} \sum_k [(c^\dagger_{\mathbf{k}\uparrow} c_{\mathbf{k+Q}\uparrow} - c^\dagger_{\mathbf{k}\downarrow} c_{\mathbf{k+Q}\downarrow}) + \mathrm{h.c.}] \\ &+ \sum_k (\Delta^*_s(\mathbf{k}) c_{-\mathbf{k}\downarrow} c_{\mathbf{k}\uparrow} + \mathrm{h.c.}) \\ &+ \sum_k [\Delta^*_t(\mathbf{k})(c_{-\mathbf{k}\downarrow} c_{\mathbf{k+Q}\uparrow} + c_{-\mathbf{k-Q}\downarrow} c_{\mathbf{k}\uparrow}) + \mathrm{h.c.}].\end{aligned} \tag{4}$$

Here $\Delta_s(\mathbf{k}) = \frac{1}{2}\Delta_1(\cos k_x - \cos k_y) + \mathrm{i}\Delta_2 \sin k_x \sin k_y$ and $\Delta_t(\mathbf{k}) = \frac{1}{2}\Delta_{t1}(\cos k_x - \cos k_y) + \mathrm{i}\Delta_{t2} \sin k_x \sin k_y$ are the pairing amplitudes in the singlet and triplet channel respectively; $b_{\mathrm{m}} = Ab_0$ with $A = zV_1 + zV_2$ (z is the coordination number). The tight binding energy dispersion on a square lattice that we use involves upto next-near neighbour hopping in conformity with the range of interactions considered. The dispersion is $\epsilon_{\mathbf{k}} = -2t(\cos k_x + \cos k_y) + 4t' \cos k_x \cos k_y$ where t is the near neighbour and t' is the next near neighbour hopping integral. Here $\tilde{\mu} = \mu - nz(V_1 + V_2)$ and we use μ to denote $\tilde{\mu}$ in the foregoing analysis.

The potential and the SC order parameters are expanded [26,27] in the usual basis functions (B_1 representation of C_{4v}) $\eta_1(\mathbf{k}) = \frac{1}{2}(\cos k_x - \cos k_y)$ and $\eta_2(\mathbf{k}) = \sin k_x \sin k_y$. Expanding in these bases $V(\mathbf{k},\mathbf{k}') = \sum_i V_i \eta_i(\mathbf{k})\eta_i(\mathbf{k}')$ and $\Delta_{\mathbf{k}} = \sum_{\mathbf{k}'} V(\mathbf{k},\mathbf{k}') \Gamma_{\mathbf{k}'} \equiv \sum_i V_i \Delta_i \eta_i(\mathbf{k})$ where $\Delta_i = \sum_{\mathbf{k}} \eta_i(\mathbf{k}) \Gamma_{\mathbf{k}}$ (and $\Gamma_{\mathbf{k}} = \langle \sum_\sigma c_{\mathbf{k}\sigma} c_{-\mathbf{k}\sigma} \rangle$). $V(\mathbf{k},\mathbf{k}')$ comes from the Fourier transform of the second and third terms of the Hamiltonian (1) (described in detail in Ref. [26]).

The order parameters can be treated as variational parameters with the trial Hamiltonian H_{MF}. The corresponding free energy functional is given by

$$\tilde{F} = F_0 + \langle H - H_{\mathrm{MF}} \rangle_0 \tag{5}$$

where $\langle ... \rangle_0$ denotes average with respect to $\rho_0 = \exp[-H_{\mathrm{MF}}/kT]/Z_0$ and $F_0 = -kT \ln(Z_0)$. The self-consistency equations for the order parameters are obtained by minimising the free-energy functional $\tilde{F}$.

$$1 = \frac{1}{2N}\sum_{\mathbf{k}} \sum_{\gamma=+,-} A \left(1 + \frac{\mu^2 \gamma}{\alpha(\mathbf{k})}\right) \frac{1}{E_\gamma(\mathbf{k})} \tanh \frac{E_\gamma(\mathbf{k})}{2T} \tag{6}$$

$$1 = \frac{1}{2N}\sum_{\mathbf{k}} \sum_{\gamma=+,-} \frac{V_1 \eta_1^2(\mathbf{k})}{E_\gamma(\mathbf{k})} \tanh \frac{E_\gamma(\mathbf{k})}{2T} \tag{7}$$

$$1 = \frac{1}{2N}\sum_{\mathbf{k}} \sum_{\gamma=+,-} \frac{V_2 \eta_2^2(\mathbf{k})}{E_\gamma(\mathbf{k})} \tanh \frac{E_\gamma(\mathbf{k})}{2T} \tag{8}$$

$$\begin{aligned}\Delta_{t1} = &-\frac{1}{2N}\sum_{\mathbf{k}} \sum_{\gamma=+,-} \frac{\gamma}{\alpha(\mathbf{k})} V_1 \Delta_1 \eta_1^2(\mathbf{k}) \\ &\times \mu A b_0 \frac{1}{E_\gamma(\mathbf{k})} \tanh \frac{E_\gamma(\mathbf{k})}{2T}\end{aligned} \tag{9}$$

$$\begin{aligned}\Delta_{t2} = &-\frac{1}{2N}\sum_{\mathbf{k}} \sum_{\gamma=+,-} \frac{\gamma}{\alpha(\mathbf{k})} V_2 \Delta_2 \eta_2^2(\mathbf{k}) \\ &\times \mu A b_0 \frac{1}{E_\gamma(\mathbf{k})} \tanh \frac{E_\gamma(\mathbf{k})}{2T} \cdot\end{aligned} \tag{10}$$

The self-consistency equations (6–10) provide a set of five coupled equations to be solved numerically. What is interesting is that although we have not included any pairing interaction in the triplet channel, the triplet amplitudes Δ_{t1} and Δ_{t2} are non-zero. The simultaneous co-existence of $\Delta_{1,2}$ and b_0 ensures the existence of this non zero amplitude.

One could, of course, include additional pairing interactions W_1 and W_2 explicitly in the Hamiltonian (1) in the triplet channels with preferred symmetries and obtain the self-consistency equations. (An alternative and quite commonly used approach is to include such terms in the mean-field Hamiltonian (4) as in Kato and Machida [8] and Kyung [15], rather than derive them from microscopic interactions.) This would modify all the equations (6–10) but the nature of the phase diagrams remains qualitatively similar (discussed later). For the sake of completeness, we write down the equations for the triplet amplitudes including W_1 and W_2 and note that they reduce to (9) and (10) without $W_{1,2}$.

$$\Delta_{t1} = \frac{1}{2N}\sum_{\mathbf{k}}\sum_{\gamma=+,-}\Bigg[W_1\Delta_{t1}\eta_1^2(\mathbf{k}) + \frac{\gamma}{\alpha(\mathbf{k})}V_1\Delta_1\eta_1^2(\mathbf{k}) \times\left(V_1W_1\Delta_1\Delta_{t1}\eta_1^2(\mathbf{k}) + V_2W_2\Delta_2\Delta_{t2}\eta_2^2(\mathbf{k}) - \mu A b_0\right) + \frac{\gamma}{\alpha(\mathbf{k})}\epsilon_{\mathbf{k}}^2 W_1\Delta_{t1}\eta_1^2(\mathbf{k})\Bigg]\frac{1}{E_\gamma(\mathbf{k})}\tanh\frac{E_\gamma(\mathbf{k})}{2T} \quad (11)$$

and

$$\Delta_{t2} = \frac{1}{2N}\sum_{\mathbf{k}}\sum_{\gamma=+,-}\Bigg[W_2\Delta_{t2}\eta_2^2(\mathbf{k}) + \frac{\gamma}{\alpha(\mathbf{k})}V_2\Delta_2\eta_2^2(\mathbf{k}) \times\left(V_1W_1\Delta_1\Delta_{t1}\eta_1^2(\mathbf{k}) + V_2W_2\Delta_2\Delta_{t2}\eta_2^2(\mathbf{k}) - \mu A b_0\right) + \frac{\gamma}{\alpha(\mathbf{k})}\epsilon_{\mathbf{k}}^2 W_2\Delta_{t2}\eta_2^2(\mathbf{k})\Bigg]\frac{1}{E_\gamma(\mathbf{k})}\tanh\frac{E_\gamma(\mathbf{k})}{2T}\cdot \quad (12)$$

The energy eigenvalues $E_\gamma(\mathbf{k})$ used above are

$$E_\gamma(\mathbf{k}) = \left[b_{\rm m}^2 + |\Delta_s(\mathbf{k})|^2 + |\Delta_t(\mathbf{k})|^2 + \epsilon_{\mathbf{k}}^2 + \mu^2 + 2\gamma\alpha(\mathbf{k})\right]^{1/2} \quad (13)$$

where $\alpha(\mathbf{k}) = \left[(V_1W_1\Delta_1\Delta_{t1}\eta_1^2(\mathbf{k}) + V_2W_2\Delta_2\Delta_{t2}\eta_2^2(\mathbf{k}) - \mu b_{\rm m})^2 + \epsilon_{\mathbf{k}}^2(\mu^2 + |\Delta_t(\mathbf{k})|^2)\right]^{1/2}$ with $W_{1,2}$ set to zero in equations (6–10). In order to obtain the phase diagram in the temperature-density plane, the particle density n is calculated from $n = -\frac{\partial F}{\partial \mu}$ as

$$n = 1 + \frac{1}{2N}\sum_{\mathbf{k}}\sum_{\gamma=+,-}\Bigg[\mu + \frac{\gamma}{\alpha(\mathbf{k})}\Bigg[(-Ab_0) \times\left(V_1W_1\Delta_1\Delta_{t1}\eta_1^2(\mathbf{k}) + V_2W_2\Delta_2\Delta_{t2}\eta_2^2(\mathbf{k}) - \mu A b_0\right) + \epsilon_{\mathbf{k}}^2\mu\Bigg]\Bigg]\frac{1}{E_\gamma(\mathbf{k})}\tanh\frac{E_\gamma(\mathbf{k})}{2T}\cdot \quad (14)$$

Note that $\xi_{\mathbf{k}} + \xi_{\mathbf{k+Q}} = 0$ when $t' = 0$. The $\mathbf{k}$-sums run over half the Brillouin zone to accommodate the zone folding due to AF state.

3 Results and discussion

It is straightforward to check that these self-consistency equations reduce to simpler and well known forms in the limit of pure phases (either AF or SC). Setting Δ_t and Δ_s zero in equation (7), we recover $E_\gamma(\mathbf{k}) = -\mu - \gamma\sqrt{(b_{\rm m}^2 + \epsilon_{\mathbf{k}}^2)}$ (where γ, as before, is ± 1) and $\alpha(\mathbf{k}) = \sqrt{(b_{\rm m}^2 + \epsilon_{\mathbf{k}}^2)}$. This leads to the well known self consistency equation for AF order parameter $1/A = -\frac{1}{2}\sum_{\mathbf{k},\gamma=\pm 1}\frac{\gamma\tanh\beta E_\gamma(\mathbf{k})/2}{\alpha(\mathbf{k})}$. Similar reduction occurs in the equations for singlet or triplet SC order parameters in the absence of other two. The complete solutions of the non-linear coupled set of equations (6–11) have been obtained numerically. Before discussing these solutions and the resulting phase diagrams, we examine some of the equations critically.

The structure of these self-consistency equations for the order parameters lend themselves to some interesting conclusions as noted earlier. The amplitude Δ_{t1} has a finite value even when the pairing interaction in the triplet channel with corresponding symmetry is zero, provided the AF (b_0) and the $d_{x^2-y^2}$ SC order parameters (Δ_1) are non-zero simultaneously. In exactly similar manner Δ_{t2} gets *dynamically generated* when both AF and d_{xy} SC order parameters (*i.e.*, b_0 and Δ_2) appear simultaneously while the pairing interaction (W_2) is zero in equation (10). Simultaneous presence of AF and singlet $d + {\rm i}d$ SC state dynamically generates the triplet $d + {\rm i}d$ SC state. This is a reflection of the fact that the presence of spin density wave order parameter $\langle c_{\mathbf{k},\uparrow}^\dagger c_{\mathbf{k+Q},\uparrow}\rangle$ and singlet SC order parameter $\langle c_{\mathbf{k},\uparrow}^\dagger c_{-\mathbf{k},\downarrow}^\dagger\rangle$ can lead to a coupling in the triplet channel $\langle c_{\mathbf{k+Q},\uparrow}^\dagger c_{-\mathbf{k},\downarrow}^\dagger\rangle$. Note that the symmetries of the order parameters for singlet and triplet SC states have to be the same. A glance at the terms causing the dynamical generation of triplet SC order parameters in equations (9) and (10) reveals that they contain a factor $\eta_i^2(\mathbf{k})$ of which one $\eta_i(\mathbf{k})$ term comes from spin singlet amplitude and the other comes from the spin triplet term. For the dynamical generation of triplet SC order parameters, it is necessary that both of them have the same symmetry or at least non-orthogonal. At half filling ($\mu = 0$) these terms responsible for the dynamical generation of triplet amplitudes vanish and there will be no triplet SC state in the absence of W_1 or W_2.

The self-consistency equations for the order parameters are solved numerically for different values of the interaction strengths V_1, V_2, W_1 and W_2 in the presence of nearest ($t' = 0$) and next nearest neighbour hopping ($t' \neq 0$). The corresponding phase diagrams are shown in Figures 1–5 in the doping ($x = n - 1$), temperature (T) plane. In this calculation, all energies and temperatures are scaled in units of t. In Figure 1, where $V_1 = -0.17$, $V_2 = -0.08$, $W_1 = W_2 = 0$, the ground state is antiferromagnetic at half filling for $t' = 0$. As we move slightly away from half filling, a phase appears where the order parameters corresponding to AF, $d_{x^2-y^2}$-SC and the π-triplet SC with $d_{x^2-y^2}$ symmetry are simultaneously present. Note that the triplet SC phase appears even though the pairing

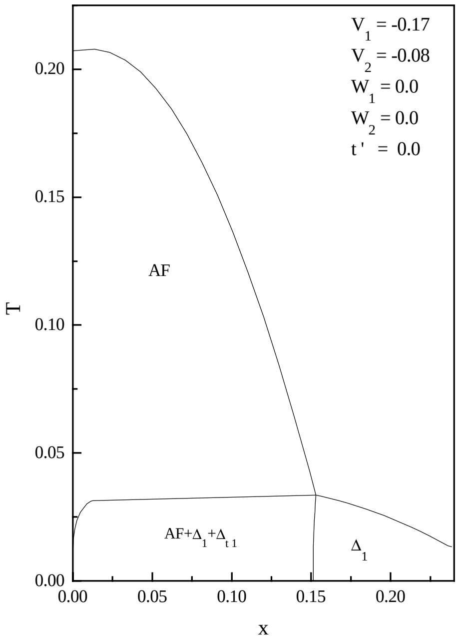


Fig. 1. Phase diagram in doping $x = n - 1$ and temperature (T) plane for $V_1 = -0.17$, $V_2 = -0.08$, $W_1 = W_2 = 0$ and $t' = 0$. All energies are measured in units of t.

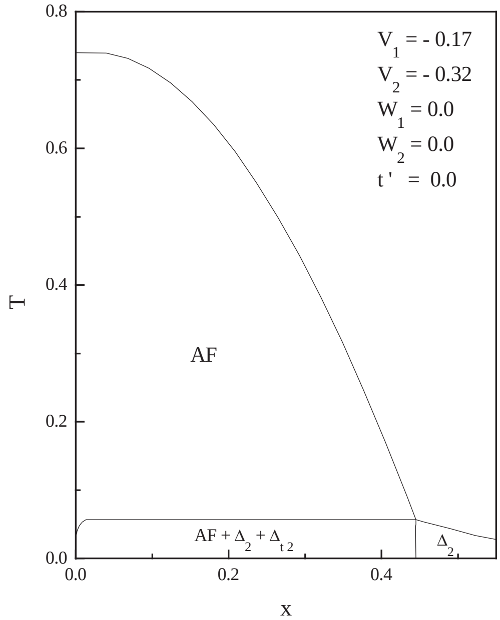


Fig. 2. Phase diagram in doping and temperature plane for $V_1 = -0.17$, $V_2 = -0.32$, $W_1 = W_2 = 0$, $t' = 0$.

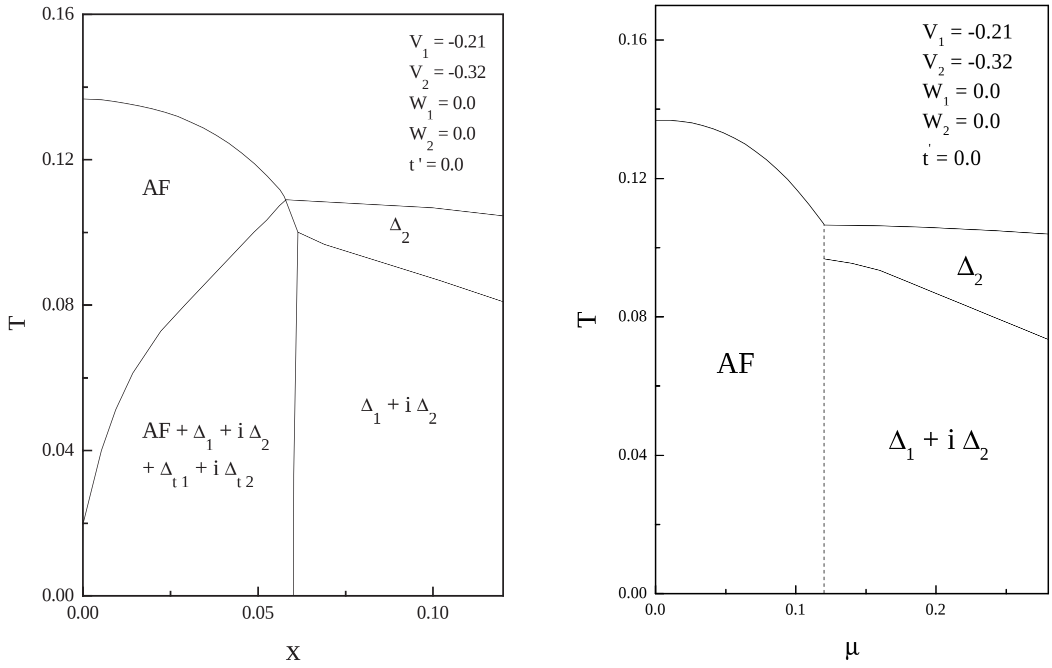
potential in the triplet channel (W_1) is zero. This phase is generated *dynamically* in the presence of the other two phases. In the region where different ordered phases coexist, the system actually phase separates [9]: there is a first order transition between the SC and the AF states. In the mean-field theory there is a single phase boundary that separates the two phases, whereas in an actual system, with long range interactions, there could be multiple domains of one phase in another. Finally, far away from half filling we get an SC-only phase having $d_{x^2-y^2}$ symmetry.

Figure 2 describes the phase diagram with a larger value of $V_2 = -0.32$ keeping the other parameters same as in Figure 1. The phase diagram has the same topology as in Figure 1, but an increased V_2 favours the d_{xy} state over the $d_{x^2-y^2}$ and hence the three phase region now comprises of AF, d_{xy}-SC and the π-triplet SC having d_{xy} symmetry. As before, the triplet SC phase exists (with a different symmetry compared to Figure 1, being forced by the d_{xy} symmetry of the corresponding singlet phase now) even without the pairing interaction W_2.

The generic phase diagram of the model remains similar to either Figure 1 or Figure 2 as the ratio $\frac{V_1}{V_2}$ is changed. As noted earlier [22], simultaneous appearance of an AFM phase with $d+\mathrm{i}d$ SC can be observed in a narrow regime of parameter space with strongly suppressed AFM region. In a similar vein, we observe in Figures 3–5, a non-zero value of both AFM and $d+\mathrm{i}d$ order parameter (along with the dynamically generated triplet amplitude), when the interaction strength corresponding to AFM amplitude is suppressed ($A = zV_1$). The x-T phase diagram for $V_1 = -0.21$, $V_2 = -0.32$ with $W_1 = W_2 = 0$ and $t' = 0$ is shown in Figure 3a. At half filling the ground state is antiferromagnetic as usual. On increasing the filling slightly a phase appears where AF, $d_{x^2-y^2} + \mathrm{i}d_{xy}$ SC and the triplet $d_{x^2-y^2} + \mathrm{i}d_{xy}$ SC amplitudes are simultaneously non-zero. The triplet superconducting amplitude is generated *dynamically* and has the same symmetry as of the singlet SC state as expected. On increasing the doping we get a singlet $d_{x^2-y^2} + \mathrm{i}d_{xy}$ SC phase. Note that at a higher temperature in the phase diagram, there is a region where only the pure d_{xy} phase survives. The same phase diagram can be drawn in the temperature-chemical potential plane (Fig. 3b), a situation that obtains in some experiments where it is difficult to dope the system while as a function of pressure there are interesting phase transitions observed. It is quite interesting to note the similarity between the phase diagram shown in Figure 3b here with Figure 1 in Lefebvre *et al.* [3]. The symmetry of the SC phase abutting the AF phase in our model depends on the values of the parameters V_1 and V_2. A dynamical generation of triplet pairing amplitude, therefore, remains a distinct possibility in the region of coexistence of AF and SC phases in the organic superconductors and further experiments are needed to ascertain this. We did not extend our study of the model to the high temperature normal state properties and it remains to be observed if strong pairing fluctuations render the single particle properties of that state unusual.

In the phase diagram shown in Figure 4 pairing potentials for π triplet SC state are taken to be finite. The topology of the phase diagram remains the same as in Figure 3. The phase boundaries shift to provide a larger triplet region only and no separate triplet SC region arises even if the values of W_1 and W_2 are made comparable to those of V_1 and V_2.

In the phase diagram of Figure 5 we introduced a small $t' = 0.03$ without changing V_1 and V_2 and keeping $W_1 = W_2 = 0$. Changing the band structure with a



(a) (b)

Fig. 3. (a) Appearance of the dynamically generated triplet state for $V_1 = -0.21$, $V_2 = -0.32$, $W_1 = W_2 = 0$, $t' = 0$. All five amplitudes are non-zero in the region of coexistence. In (b) is shown the same phase diagram in the T-μ plane. The dashed line represents a first order transition, while the solid lines stand for second order transitions.

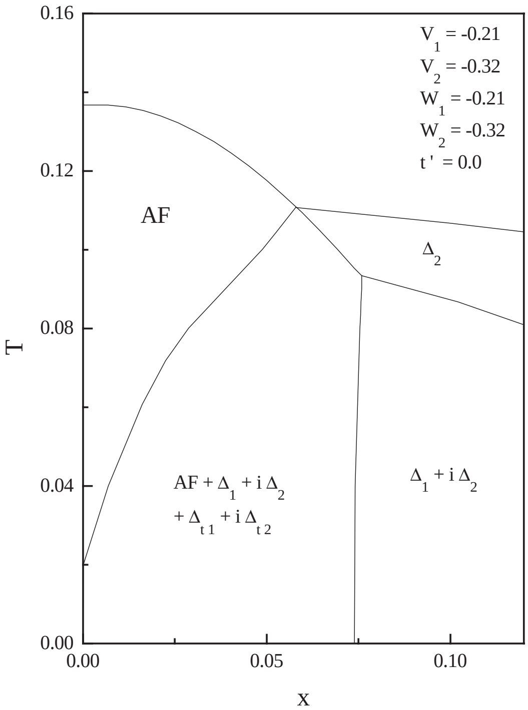


Fig. 4. No major change appears in the phase diagram with $W_1 = -0.21$ and $W_2 = -0.32$ in comparison to Figure 3. The triplet phase occupies slightly larger region in the phase diagram.

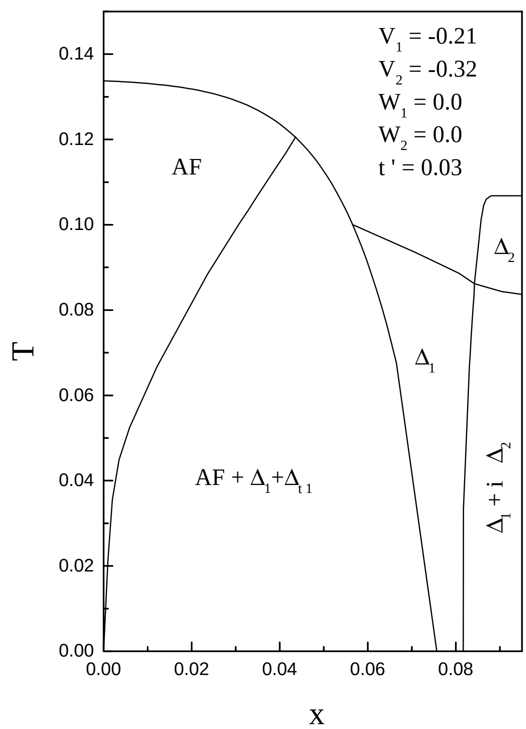


Fig. 5. A non-zero small $t' = 0.03$ changes the phase diagram with the sliver of $d_{x^2-y^2}$ SC state appearing in between with no d_{xy} state in the coexistence region. Both W_1 and W_2 have been kept zero.

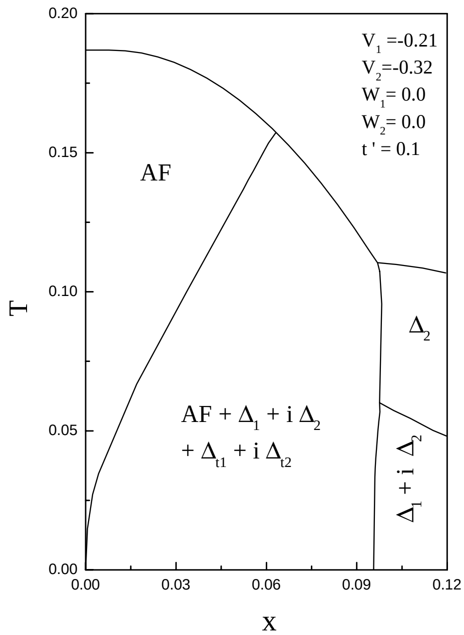


Fig. 6. A larger $t' = 0.1$ gives rise to the region of coexistence of all five amplitudes again. The d_{xy} component stabilises on increasing t'.

non zero t' is known [25] to favour the d_{xy} state over the $d_{x^2-y^2}$ state. But simultaneously, the chemical potential shifts for a particular doping on introduction of t'. These two effects act counter to each other in the term $\xi_{\mathbf{k}}+\xi_{\mathbf{k+Q}}$ (which is -2μ if $t' = 0$). As a result, we get a small sliver of pure $d_{x^2-y^2}$ component before the $d+\mathrm{i}d$ phase and the coexistence region therefore has AF, Δ_1 and the dynamically generated Δ_{t1}. At high temperature we get a pure d_{xy} SC phase, below which a $d_{x^2-y^2}+\mathrm{i}d_{xy}$ state appears. On increasing the next near neighbour hopping, the d_{xy} phase stabilises and the sliver of $d_{x^2-y^2}$ state disappears (Fig. 6). There is a combined region of AF and $d+\mathrm{i}d$ state in both singlet and triplet channel. The triplet part is, of course, dynamically generated here as $W_1 = W_2 = 0$. For the purpose of demonstration, we have shrunk the region of pure AF phase around half filling in Figure 6. We also observe that in our model the on-site Coulomb interaction term has been set to zero. Presence of this term, at least at the mean-field level, will not change the phase diagram qualitatively [15]; although the region of stability of the AF phase increases with such a term.

In conclusion, we have demonstrated the possibility of simultaneous presence of a spin density wave and superconductivity in the $d + \mathrm{i}d$ channel in a model with only extended pairing interactions. As it turns out that such simultaneous appearance of AF and singlet SC order parameter leads to a spontaneous generation of a triplet SC amplitude with the same symmetry even when the corresponding pairing interaction in the triplet channel is absent. Though we do not intend to propose the present model for the organic superconductors, the nature of phase diagrams we obtained from a generic correlated electronic model that produces coexistence of AF and singlet SC state bears similarity to the ones obtained for them. Since the dynamical generation of the triplet amplitude rests only on the coexistence of AF and singlet SC order, we believe it would be interesting to see if further measurements in the organic superconductors like κ-$(ET)_2Cu[N(CN)_2]Cl$ reveal the presence of unconventional superconductivity in the triplet channel as well.

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