Exotic superconducting states in the extended attractive Hubbard model

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Abstract
We show that the extended attractive Hubbard model on a square lattice allows for a variety of superconducting phases, including exotic mixed-symmetry phases with $d_{x^2-y^2} + i(s+s^*)$ and $d_{x^2-y^2} + p_x$ symmetries, and a novel $p_x + ip_y$ state. The calculations are performed within the Hartree–Fock Bardeen–Cooper–Schrieffer framework. The ground states of the mean-field Hamiltonian are obtained via a minimization scheme that relaxes the symmetry constraints on the superconducting solutions, hence allowing for a mixing of $s$-, $p$- and $d$-wave order parameters. The results are obtained within the assumption of uniform-density states. Our results show that extended attractive Hubbard model can serve as an effective model for investigating properties of exotic superconductors.

Keywords: unconventional superconductivity, attractive Hubbard model, chiral p-wave

(Some figures may appear in colour only in the online journal)
of unconventional, particularly the mixed OP symmetry, SC solutions [41, 42].

In this work, we unveil the exciting possibility of the existence of unconventional mixed symmetry SC states in an EAHM on a square lattice. A justifiable approximation on the nn attractive interaction followed by a general decoupling scheme together with an explicit minimization procedure allows us to construct comprehensive phase diagrams for the model. Superconducting phases with mixed OPs dominate the phase diagram. We present simple energetic arguments for the stability of mixed OP phases. Two of the unconventional mixed symmetry SC states in an EAHM for studying unconventional superconductivity. We also discuss the finite-temperature behavior and show that for certain densities the system undergoes multiple transitions before reaching a normal state at high temperature.

2. Model and method

2.1. Extended attractive Hubbard Hamiltonian

We begin with the EAHM defined on a 2D square lattice. The model is described by the Hamiltonian,

\[
H = -t \sum_{\langle ij \rangle, \sigma} \left[ c_{i \sigma}^\dagger c_{j \sigma} + H.c. \right] - \mu \sum_{\langle i \rangle} c_{i \sigma}^\dagger c_{i \sigma} \nonumber - U \sum_i n_{i \uparrow} n_{i \downarrow} - V \sum_i n_i n_j. \tag{1}
\]

Here \( c_{i \sigma} (c_{i \sigma}^\dagger) \) annihilates (creates) an electron at site \( i \) with spin \( \sigma \), \( \langle ij \rangle \) implies that sites \( i \) and \( j \) are nearest neighbours. \( \mu \) is the chemical potential, \( n_{i \sigma} = c_{i \sigma}^\dagger c_{i \sigma} \) is the electron number operator at site \( i \) and spin-projection \( \sigma \), and \( n_i = n_{i \uparrow} + n_{i \downarrow}. \) \( U \) and \( V \) denote the strengths of on-site and nearest neighbour attractive interactions, respectively. Using \( t = 1 \) as the basic energy scale, and restricting ourselves to zero temperatures (\( T = 0 \)), we are left with three independent parameters in the Hamiltonian, viz., \( U, V \) and \( \mu \).

Before we proceed with the study of the Hamiltonian equation (1), it is important to motivate the physical relevance of the EAHM as an effective lattice model. A possible realization of such a model via a competition of bare Coulomb repulsion and phonon-mediated effective attraction was already mentioned in the previous section. In general, the EAHM represents a physical situation where two independent mechanisms, one favouring on-site pairing and other favouring inter-site pairing, are simultaneously active [42]. These mechanisms then compete for superconducting order with different OP symmetries. A microscopic model for such a situation will depend of the specific details of the system. Nevertheless, the EAHM can serve as an elementary model to study such a competition among different SC states. Furthermore, it has been shown that a model with on-site repulsion and inter-site Ising type antiferromagnetic exchange can be mapped onto an on-site attractive model [43].

The existence of such mappings between attractive and repulsive models also makes it worthwhile to investigate the ordered states arising in purely attractive models. A promising avenue for realization of such models is ultracold Fermionic atoms in optical lattices [44–48]. The standard Hubbard model with both repulsive and attractive interactions has indeed been realized in these systems. Yet another possibility, which has so far been demonstrated for repulsive models, is the use of artificial crystals where semiconducting quantum dots can be patterned to form a two dimensional lattice [49].

We analyze the Hamiltonian in equation (1) by making a mean-field approximation for the interaction term [50]. In the inter-site attractive term we ignore the same-spin attraction parts \( n_{i \uparrow} n_{j \uparrow} \) and \( n_{i \downarrow} n_{j \downarrow}. \) This can be qualitatively justified for systems where superconductivity emerges in the vicinity of antiferromagnetism. The antiferromagnetic tendency ensures that electrons with opposite spin orientations are more likely to reside on neighbouring sites as compared to those with same spin orientation.

2.2. General decoupling in the pairing channel

We now discuss how a general decoupling of the nearest-neighbour (nn) attractive interaction allows for possible mixed order parameter solutions. The interaction term is given by,

\[
H_{\text{int}} = -U \sum_i n_{i \uparrow} n_{i \downarrow} - V \sum_{\langle ij \rangle} n_i n_j. \tag{2}
\]

The Hartree–Fock decoupling in the pairing channel of the first term in equation (2) is straightforward, and leads to the replacement \( n_{i \uparrow} n_{i \downarrow} \rightarrow \langle c_{i \uparrow} c_{i \downarrow} \rangle \), \( \langle c_{i \uparrow} c_{i \downarrow} \rangle = (c_{i \uparrow}^\dagger c_{i \uparrow} c_{i \downarrow}^\dagger c_{i \downarrow} - \langle c_{i \uparrow} c_{i \downarrow} \rangle \langle c_{i \uparrow}^\dagger c_{i \uparrow} \rangle). \) The second term in equation (2) can be written as,

\[
H_{\text{int}}^{\text{nn}} = -V \sum_{i, \gamma = \uparrow, \downarrow} (n_{i \uparrow} + n_{i \downarrow}) (n_{i \uparrow} + n_{i \downarrow}). \tag{3}
\]

In the above, \( \gamma \) denotes the unit vectors \( +\hat{x} \) and \( +\hat{y} \) on the square lattice. Expanding further, we obtain four terms corresponding to each \( i, \gamma \) bond. These are \( n_{i \uparrow} n_{i \downarrow} + n_{i \downarrow} n_{i \uparrow}, n_{i \uparrow} n_{i \downarrow} + n_{i \downarrow} n_{i \uparrow}, n_{i \uparrow} n_{i \uparrow} + n_{i \downarrow} n_{i \downarrow}, n_{i \uparrow} n_{i \downarrow} + n_{i \downarrow} n_{i \uparrow}. \) As mentioned earlier, we assume that electrons with identical spin orientations are less likely to reside on nn sites, and taking an approximation we drop the \( \uparrow\uparrow \) and \( \downarrow\downarrow \) interaction terms. Rearranging the order of \( c \) operators, we can write the remaining terms as,

\[
H_{\text{int}}^{\text{nn}} \approx -V \sum_{i, \gamma = \pm \hat{x} \pm \hat{y}} \left[ c_{i \uparrow}^\dagger c_{i \downarrow}^\dagger c_{i \downarrow} c_{i \uparrow} + c_{i \uparrow} c_{i \downarrow}^\dagger c_{i \uparrow}^\dagger c_{i \downarrow} \right]. \tag{4}
\]

Implementing the mean-field decoupling in the pairing channel for the on-site and the nn interaction term, we obtain the mean-field Hamiltonian,

\[
H_{\text{MF}} = -t \sum_{\langle ij \rangle, \sigma} \left[ c_{i \sigma}^\dagger c_{j \sigma} + H.c. \right] - \sum_i \left[ \Delta c_{i \uparrow}^\dagger c_{i \downarrow}^\dagger + H.c. \right] - V \sum_{\langle ij \rangle} \left[ \Delta_{\gamma \uparrow} c_{i \uparrow}^\dagger c_{i \downarrow} + \Delta_{\gamma \downarrow} c_{i \downarrow}^\dagger c_{i \uparrow} + H.c. \right] + U \sum_i |\Delta_i|^2 + V \sum_{i, \gamma} [|\Delta_{\gamma \uparrow}|^2 + |\Delta_{\gamma \downarrow}|^2]. \tag{5}
\]
Note that in order to retain the generality of the decoupling we have introduced two different pair expectation values for a given pair of sites. These expectation values, $\Delta_{\gamma'}^{\uparrow} = \langle c_{\uparrow,1}^{\dagger} c_{\gamma'}^{\uparrow} \rangle$ and $\Delta_{\gamma'\gamma} = \langle c_{\downarrow,1}^{\dagger} c_{\gamma'}^{\uparrow} \rangle$, need not be equal, in principle. Indeed, if we assume that the pair satisfies antisymmetry under spin exchange, then $\Delta_{\gamma'}^{\uparrow} = \Delta_{\gamma'\gamma}^{\uparrow}$, and if the pair satisfies antisymmetry under site-index exchange then $\Delta_{\gamma'}^{\downarrow} = -\Delta_{\gamma'\gamma}^{\downarrow}$. In most studies a singlet condition on the pairing correlations is imposed and therefore the possibility of odd parity pairing in this model is left out. Here, we do not impose this symmetry constraint on our pairing correlations.

Motivated by the fact that large-scale charge inhomogeneities will not be allowed by long range Coulomb interactions in any real material, we search for uniform density solutions. Therefore, we focus on the SC phases that respect the translational symmetry of the Hamiltonian, and assume the above quantum expectation values to be independent of lattice sites, $\Delta_{\gamma} = \Delta_{\gamma'} = \Delta_{\gamma'\gamma} = \Delta_{\gamma'\gamma'}$, leading to five complex-valued mean-field parameters. Given that the model is purely attractive, possibility of magnetic ordering is ruled out [43, 51]. The charge ordering may be present at special filling fractions such as half-filling. Furthermore, while on-site attraction leads to charge ordering at half filling, the inter-site attraction destabilizes such charge modulated order. Therefore, we have not considered the competition between charge- and spin-ordering and superconductivity. The competition between superconductivity and charge ordering has been discussed in the extended model with on-site attraction and inter-site repulsion [43, 51]. Among the different possibilities for SC order, we have considered those OPs that are spatially uniform, therefore, possibilities such as pair density wave or finite momentum pairing have not been considered. Going over to the Fourier space by using, $c_{\sigma}(\mathbf{k}) = \sum_{\mathbf{r}} e^{-i\mathbf{k} \cdot \mathbf{r}} c_{\sigma}(\mathbf{r})$, and $c_{\sigma}^\dagger(\mathbf{k}) = e^{-i\mathbf{k} \cdot \mathbf{r}} c_{\sigma}(\mathbf{r})$, $N_s$ being the number of sites, the Hamiltonian can be reduced to a $2 \times 2$ matrix form. The resulting Hartree–Fock Bardeen–Cooper–Schrieffer (HF-BCS) Hamiltonian in the Nambu spinor notation is,

$$H_{BF} = \sum_{\mathbf{k}} \left[ c_{\mathbf{k},\uparrow}^\dagger \begin{array}{cc} h_{11}(\mathbf{k}) & h_{12}(\mathbf{k}) \\ h_{12}(\mathbf{k})^* & h_{22}(\mathbf{k}) \end{array} \right] c_{\mathbf{k},\downarrow} + N_s \{ U|\Delta_0|^2 + V(|\Delta_0^+|^2 + |\Delta_0^-|^2 + |\Delta_0^+|^2 + |\Delta_0^-|^2) \}. \tag{5}$$

The matrix elements in the above equation are explicitly given by,

$$h_{11}(\mathbf{k}) = -2t(\cos k_x + \cos k_y) - \mu = -h_{22}(\mathbf{k})$$
$$h_{12}(\mathbf{k}) = -U\Delta_0 - V(\Delta_0^+ e^{-i\mathbf{k} \cdot \mathbf{r}} + \Delta_0^- e^{i\mathbf{k} \cdot \mathbf{r}} + \Delta_0^+ e^{-i\mathbf{k} \cdot \mathbf{r}} + \Delta_0^- e^{i\mathbf{k} \cdot \mathbf{r}}) = h_{21}(\mathbf{k}). \tag{6}$$

For a given set $\{\Delta\} \equiv \{\Delta_0, \Delta_0^+, \Delta_0^-, \Delta_0^{\uparrow}, \Delta_0^{\downarrow}\}$, we can diagonalize the electronic part of the Hamiltonian equation (5) via the Bogoliubov transformations,

$$\begin{bmatrix} c_{\mathbf{k},\uparrow} \\ c_{\mathbf{k},\downarrow} \end{bmatrix} = \begin{bmatrix} \alpha_\mathbf{k} & -\gamma_\mathbf{k} \\ \gamma_\mathbf{k} & \alpha_\mathbf{k} \end{bmatrix} \begin{bmatrix} \gamma_{k0}^{\dagger} \\ \gamma_{k1}^{\dagger} \end{bmatrix}, \tag{7}$$

where $\alpha_\mathbf{k}$ and $\gamma_\mathbf{k}$ are complex numbers satisfying $|\alpha_\mathbf{k}|^2 + |\gamma_\mathbf{k}|^2 = 1$ for all $\mathbf{k}$, and $\gamma, \gamma^\dagger$ are the annihilation and creation operators for Bogoliubov quasiparticles. The resulting quasiparticle dispersion is given by,

$$E_\mathbf{k} = \sqrt{\left[ -2t(\cos k_x + \cos k_y) - \mu \right]^2 + \Delta_0^2},$$
$$\Delta_0^2 = | -U\Delta_0 - V(\Delta_0^+ e^{-i\mathbf{k} \cdot \mathbf{r}} + \Delta_0^- e^{i\mathbf{k} \cdot \mathbf{r}} + \Delta_0^+ e^{-i\mathbf{k} \cdot \mathbf{r}} + \Delta_0^- e^{i\mathbf{k} \cdot \mathbf{r}}) |^2. \tag{8}$$

Using the above quasiparticle spectrum along with the purely classical terms in the mean-field Hamiltonian equation (6), we can compute the total energy $E$ of a general SC state specified by set $\{\Delta\}$. This is achieved by constructing HF-BCS states as the vacuum of Bogoliubov quasiparticle for the given set $\{\Delta\}$. Therefore, the problem now reduces to minimizing the total energy of such HF-BCS states w.r.t. the set $\{\Delta\}$ of pairing correlations. We want to emphasize here that in most previous studies a particular form of the SC OP is assumed a priori [42]. In contrast, we allow for different combinations of spatially uniform OPs.

### 2.3. Minimization scheme

To put our results in proper context, we observe the following relations between the pair expectation values defined above and the commonly used SC OPs,

$$\Delta_\sigma = \Delta_0, \quad \Delta_\sigma' = \frac{(\Delta_0^+ + \Delta_0^- + \Delta_0^+ + \Delta_0^-)}{4}, \quad \Delta_{d_{\sigma\sigma'}}, \quad \Delta_{d_{\sigma\sigma'}} = \frac{(\Delta_0^+ - \Delta_0^-)}{2}, \quad \Delta_{d_{\sigma\sigma'}} = \frac{(\Delta_0^- - \Delta_0^+)}{2}. \tag{9}$$

The $s$, $p$- and $d$-wave OPs defined above have their usual meaning. $\Delta_0$, denotes the OP for the extended s-wave order which arises due to inter-site attraction [52]. It is easy to see that the form-factors that enter the $\mathbf{k}$-space matrix acquire their typical pure-singlet or pure-triplet form in the limiting cases. Note that a general set $\{\Delta\}$ may break symmetries of the Hamiltonian equation (1). Such broken-symmetry states are indeed allowed at the mean-field level, and therefore to retain the generality of the discussion within the mean-field approach we have included such broken symmetry states in our variational set $\{\Delta\}$. In addition to the magnitude of the OPs in the minimum energy state, we also need to determine the relative phase angles between different OPs in the mixed states. Therefore, we carry out variational calculations for energy as a function of relative phase angle between different OPs. We illustrate the details in figure 1(a) where we assume the magnitudes of the order parameters $\Delta_\sigma$ and $\Delta_\sigma'$ to be finite, keeping all other OPs equal to zero, and compute the total energy with varying relative phase angle $\Phi$. Variation of $E/N_s$ as a function of $\Phi$ for the state described by OP $\Delta_0^+ + e^{i\Phi}\Delta_0^-$ is shown in figure 1(a). This allows us to determine the value of the phase angle corresponding to the minimum energy. This is defined as $\Phi_{\text{min}}$ for the pair of OPs selected. The variation in $\Phi_{\text{min}}$ with chemical potential is
shown in the inset in figure 1(b). Similarly, we are able to find $\Phi_{\text{min}}$ for other choices of OP pairs.

The results are summarized in figure 1(b) where we plot the variation in $\Phi_{\text{min}}$ for a different pairs of OPs as a function of chemical potential $\mu$. For s-wave and $d_{\sigma \rightarrow \sigma'}$-wave order, we find that $\Phi = \pm \pi/2$ leads to the minimum energy for any value of chemical potential $\mu$ (see figure 1(b)). Similarly, the relative phase angle between $p_x$ and $p_y$ order parameters, when both of them are assumed finite in magnitude, is $\pm \pi/2$. The relative angle $\Phi_{\text{min}}$ vanishes for $s$ and $d_{\sigma \rightarrow \sigma'}$, and $s$ and $p_z$ OP pairs. These results do not depend on the choice of $\mu$ values.

The relative angle between s-wave and $s'$-wave order parameters shows an interesting behavior. $\Phi_{\text{min}}$ is found to evolve with change in $\mu$. For $\mu = 0$, corresponding to the half-filled band, $\Phi_{\text{min}} = \pi/2$. It decreases monotonically and becomes zero near $\mu = -1$, which corresponds to $n \approx 0.7$ (see inset in figure 1(b)). However, we will see that $s$ and $s'$ OPs are found to be finite only in the low density regime. Therefore, we can safely assume the relative phase between these two OPs to be zero. For most range of parameters, the relative phase angle between different OP pairs is either 0 or $\pi/2$. The above analysis helps us in reducing the number of variational parameters used in the minimization scheme by assigning fixed values to these relative phases. This allows us to perform explicit minimization by discretizing the parameter space of five real valued variables corresponding to the magnitudes of $s$, $s'$, $p_x$, $p_y$- and d-wave OPs.

3. Results and discussions

3.1. Order parameters and phase diagram

We focus our discussion on the variations in $U/t$ and $\mu$ for a fixed value of $V/t = 4$. Direct minimization is carried out by varying different real-valued OPs and relative phase factors among them. The density dependence of SC OPs corresponding to minimum total energy are plotted in figures 2(a) and (d). For small $U$, the high-density regime is dominated by $d_{\sigma \rightarrow \sigma'}$ and $p_z$ OPs. Both $p_z$ and $p_y$ are finite in the intermediate density range. At further lower densities OPs with $p_y$, $s$ and $s'$ (also called extended-$s$) symmetries are finite. Eventually, the low-density regime supports $s$ and $s'$ OPs (see figures 2(a) and (b)).

For larger values of on-site attraction, $\Delta_{p_y}$ and $\Delta_{p_z}$ remain zero, and instead $\Delta_{s ureal}$ and $\Delta_{d_{\sigma \rightarrow \sigma'}}$ together with s-wave OP become finite (see figure 2(c)). Finally, in the limit of large $U$, $s$ and extended-$s$ OPs dominates. We simultaneously track the values of relative phase angles between these OPs in the minimum energy state, allowing us to describe the specific combination of the mixed SC OPs. The step-like behavior in the density dependence of OPs is a consequence of the discretization of the parameter space and should not be misunderstood as a finite-size effect. For $V = 4$ and $U = 2$, the OPs are allowed to vary with an increment of 0.01 (0.02) for $p_y$ and $p_z$ ($s$, $s'$ and $d_{\sigma \rightarrow \sigma'}$).

We have ensured that the step-size used for a given choice of Hamiltonian parameters does not effect the observed trends. We will further discuss finite-size effects in section 3.3.

We summarize the results in the form of a $n - U$ phase diagram in figure 3. Most notably, a chiral $p_x + i p_y$ order is present in the density range $0.35 < n < 0.55$ in the limit of weaker on-site attraction. Within this interaction regime, $p_x$ order also mixes with $d_{\sigma \rightarrow \sigma'}$ and extended s-wave order for different electronic densities. The possibility of chiral $p$-wave order in the extended repulsive Hubbard model has been pointed out within fluctuation exchange approximation [53, 54]. The $d_{\sigma \rightarrow \sigma'} + p_x$ order is particularly stable over a large density regime. This is intriguing as a number of experiments on cuprates report on the possibility of a secondary unconventional OP in addition to the dominant $d_{\sigma \rightarrow \sigma'}$ order. The secondary OP is proposed to be either s-wave or p-wave. Interestingly, phases with $d_{\sigma \rightarrow \sigma'} + i [s + s']$ and $d_{\sigma \rightarrow \sigma'} + p_z$ OPs reside next to each other in the density regime $0.6 < n < 1$. Moreover, for smaller values of $V$ we also find a pure $d_{\sigma \rightarrow \sigma'}$ order in the low-doping regime. This will be discussed later in section 3.4. From the angular dependence of the gap function it is easy to see that some of the OPs break the rotational symmetry of the lattice (see figures 3(b)–(e)). Such spontaneously-broken-symmetry states are allowed in our explicit minimization approach. Note further that the inversion symmetry is also spontaneously
density of states (TDOS) in different phases. Normalized TDOS is defined as,
\begin{equation}
N(\omega) = \frac{1}{N_0} \sum_k \left[ |i\delta(\omega - E_k) + |\omega| \delta(\omega + E_k)|^2 \right],
\end{equation}
where \( E_k \) is the energy dispersion for Bogoliubov quasiparticles and \( N_0 \) measures electron-like amplitude in the quasiparticle state labeled by wave vector \( k \). TDOS can be directly probed by tunneling experiments and therefore characterization of different mixed OP states in terms of TDOS is desirable [61, 62].

Mixing of a \( p_x \) component in the \( d_{x^2-y^2} \) superconductivity completely modifies the TDOS structure and opens a clean gap much like that present in the simple s-wave superconductors (see figure 4(a)). Indeed, the nodes present in the \( d_{x^2-y^2} \) gap function are removed by the presence of \( i\Delta_{p_x} \sin k_x \) term. Multiple coherence peaks in the TDOS are also clearly observed. In fact, it is easy to see why a mixing of \( p \)-wave component is energetically favoured. The system gains energy by pushing the eigenenergies further away from the chemical potential by opening a clean gap. The chiral \( p \)-wave order and the mixed \( s + s^* + p_x \) orders also support a clean gap in the TDOS (see figure 4(b)). The \( s + s^* \) ordering shows the expected TDOS with the coherence peaks residing right at the gap edge. In the \( d_{x^2-y^2} + i[s + s^*] \) state the features corresponding to s-wave and \( d \)-wave ordering are present at larger value of electronic density (see figure 4(d)). For the smaller density, the \( d \)-wave component reduces and the TDOS appears s-wave-like. The occurrence of a \( d + i s \) phase in extended Hubbard model has also been reported previously [36]. Recent ARPES data on cuprates is consistent with the presence of a secondary OP that opens a gap at the nodal points of the pure \( d \)-wave OP [63].

We further investigate the nature of various phases in terms of their edge-state spectra. To this end, we perform calculations on a \( 20 \times 200 \) stripe by imposing periodic boundary conditions only along the \( y \) direction and plotting the spectra as a function of \( k_y \). Two of the new phases obtained from our calculations turn out to be trivial as no edge states are found to appear inside the SC gap (see figures 5(c) and (d)). The chiral

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**Figure 3.** (a) Phase diagram in the \( U-n \) parameter space for intersite attraction strength \( V = 4t \). The results are obtained via brute-force minimization of total energy using a \( 16 \times 16 \) \( k \)-point grid for different combinations of OPs described in text. The phase diagram is constructed from the data similar to that presented in figure 2. The dashed horizontal lines are the cuts corresponding to the data shown in figure 2. The angular dependence of the magnitude of the OP for, \( b \) \( d_{x^2-y^2} + p_x \), \( c \) \( p_x + ip_y \), \( d \) \( s + s^* + p_x \), and \( e \) \( d_{x^2-y^2} + i[s + s^*] \) symmetries. Dashed lines in \( b \) correspond to pure-\( d_{x^2-y^2} \) and pure \( p_x \) OP symmetries.

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**Figure 4.** (a) Density of states for electrons in different phases at different values of average electronic density. These calculations are performed on \( 600 \times 600 \) \( k \)-point grid. A Lorentzian broadening of 0.01 is used.
$p$-wave superconductor shows the expected non-trivial behaviour wherein counter-propagating edge states appear in the gap (see figure 5(b)) [64]. An intriguing situation occurs for $d_{x^2-y^2} + p_x$ superconductor where pairs of states are present on each edge (see figure 5(a)). While the topology of the bulk band will remain trivial in this case as the states traverse back to their respective original band, the presence of such mid-gap states will have observable consequences. Indeed, if such a situation can be realized in a real material, then the surface spectroscopy with voltage bias smaller than the gap value will have contributions from the edge states. This is in contrast to the situation where such states are absent, and only Andreev reflection contributions are observed in tunnelling.

3.3. Finite-size effects and $V-n$ phase diagram

Although the detailed discussion for the phase diagram has been presented for $V=4t_1$, it is important to discuss the dependence of results on the specific choice of the inter-site interaction strength. Before we present results for smaller values of $V$, it is instructive to discuss the role of lattice sizes used for calculations. In figure 6 we show the dependence of OPs on number of lattice sites, $N_s$, for different values of $V$. Since explicit minimization on larger lattices is time consuming, we have made use of the self-consistent approach for obtaining data on larger lattices. Starting with some initial values of OP set $\{\Delta\}$, we can calculate different pair correlations using the set of equations,

$$
\begin{align*}
\Delta_0 &= 1/N_s \sum_k u_kv_k^* (2f(E_k) - 1) \\
\Delta_i^+ &= 1/N_s \sum_k e^{ikx} u_kv_k^* (2f(E_k) - 1) \\
\Delta_i^- &= 1/N_s \sum_k e^{-ikx} u_kv_k^* (2f(E_k) - 1) \\
\Delta_i^+ &= 1/N_s \sum_k e^{iky} u_kv_k^* (2f(E_k) - 1) \\
\Delta_i^- &= 1/N_s \sum_k e^{-iky} u_kv_k^* (2f(E_k) - 1).
\end{align*}
$$

(12)

In the above, $E_k$ are the eigenvalues, $f(E_k)$ denotes the Fermi function and $u_k$, $v_k$ are the coefficients that appear in the Bogoliubov transformation equation (8). We then repeat this procedure of diagonalizing the Hamiltonian for a given set $\{\Delta\}$ and recalculating the set $\{\Delta\}$ using equation (12) until the parameters converge within an accuracy limit of $10^{-6}$. We have preferred explicit minimization over the above self-consistent approach for the reason that in a multivariable parameter space self-consistent solutions may lead to metastable states. However, the availability of results from explicit minimization guides our choice of initial set $\{\Delta\}$ and hence the self-consistency approach can then be used to obtain results on much larger lattices.

For $V=4$ the results obtained on $N_s=16^2$ are representative of thermodynamic-limit behaviour (see figure 6(a)). For smaller values of $V$, one needs to perform calculations on progressively larger lattices in order to obtain reliable results.

For example, for $V=0.5$ one needs to use $N_s \approx 100^2$ (see figure 6(d)). This restricts the use of our explicit minimization procedure to $V \geq 1.5$. To illustrate further the point about finite size effects, we obtain results for $V=1.5$ using $N_s = 32^2$. As one can anticipate by looking at figure 6(c), $N_s = 32^2$ should lead to results representative of the thermodynamic limit. Nevertheless, fluctuations are expected to be present. We indeed find that while the overall trends for the OPs are well behaved, considerable fluctuations in the $n$-dependence are present (see figure 7). Comparing the results with those presented in figure 2(a), we find that the trends in terms of OP symmetries are similar. For small density, $s$- and extended $s$-wave OPs are finite while all other OPs remain zero. Near $n=0.3$, $p_x + ip_y$ order emerges while $s + s^*$ disappears. This is followed by the appearance of $d_{x^2-y^2} + p_x$ order near $n=0.5$ and finally pure $d$-wave order is present for $n \geq 0.7$. The trends for $U=1.0$ (figure 7(b)) are similar to those just described. The key difference w.r.t. the results for $V=4$ are the following: (i) The $s + s^* + p_x$ state is absent, and (ii) a pure $d_{x^2-y^2}$ state is present for $V=1.5$. 

![Figure 5. (a)-(d) Bogoliubov quasiparticle dispersions for different SC states obtained by using open (periodic) boundary condition along $x$ ($y$) direction. Edge states disperse across the SC gap for, (a) $p_x + ip_y$ and for (b) $d_{x^2-y^2} + p_x$ OP symmetries.](image)

![Figure 6. Variation of $\Delta_{d_{x^2-y^2}}$ and $\Delta_{p_x}$ with number of lattice sites $N_s$ for (a) $V=4.0$, (b) $V=2.0$, (c) $V=1.5$ and (d) $V=0.5$. All the results are for $U=0$. Note the logarithmic scale on $x$-axis. The electronic density values are specified in the plots.](image)
compute energy for the following phases: (i) calculations using other. Limiting the variational set of OPs allows us to perform regime. Additionally, all the OPs defined in equation (10) set covers most of the non-trivial OPs found in the large

Figure 7. Order parameters as a function of density for $V = 1.5t$. Note that a pure $d_{x^2-y^2}$ symmetry of the order parameter is present close to half-filling for both $U = 0.2t$ and $U = t$. The results are obtained via explicit minimization on $32 \times 32$ k-point grid.

Figure 8. Phase diagram in the $V$-$n$ parameter space for on-site attraction strength $V = t$. The results are obtained via minimization using a $32 \times 32 (512 \times 512)$ k-point grid for $V \geq 1.5 (V < 1.5)$.

For a comprehensive picture of the type of SC OPs present in the $U - V - n$ parameter space, we show $V - n$ phase diagram for $U = 1$. Most of the interesting superconducting states appearing in the EAHM are covered within the $U - n$ (figure 3) and $V - n$ (figure 8) phase diagrams. Given that we need to perform calculations on larger lattices for smaller $V$, we had to further restrict our OP choices for completing the $V - n$ phase diagram. For $V \geq 1.5$ we have used $N_x = 32^2$, and the minimization over the entire parameter space is performed. For smaller values of $V$ ($V \leq 1.5$), we specifically compute energy for the following phases: (i) $s + s^*$, (ii) $s + s^* + p_x$, (iii) $p_x + i p_y$ and (iv) $d_{x^2-y^2} + p_x$. This variational set covers most of the non-trivial OPs found in the large $V$ regime. Additionally, all the OPs defined in equation (10) are allowed to exist in pure form without mixing with each other. Limiting the variational set of OPs allows us to perform calculations using $N_x = 512^2$, and therefore the results can be trusted for smaller values of $V$. A particularly interesting question is how a weak inter-site attraction effects the phase diagram of the on-site attractive model. In the purely on-site attractive model ($U \neq 0, V = 0$), $s$-wave SC order is present at all fillings except at $n = 1$ where a charge ordered state is degenerate with the $s$-wave SC state. Switching on inter-site attractive term $V$, we find that the extended $s$-wave order is induced leading to the $s + s'$ SC phase. Unconventional SC states begin to appear in the regime where the inter-site scale $V$ dominates over the on-site term $U$. In this regime, we recover SC states with $s + s^* + p_x$, $p_x + i p_y$, $d_{x^2-y^2}$ and $d_{x^2-y^2} + p_x$ symmetries. Note that unlike the repulsive model where $U$ is the dominant energy scale over $V$, the hierarchy of these scales may be reversed in the attractive model. This is easy to see by recalling that the effective attractive couplings in the EAHM emerge as the sum of two contributions, the bare Coulombic repulsion and, say, the phonon-mediated attraction. If the spatial dependence of the phonon-mediated attraction happens to be weaker than $1/r$, then $|V| > |U|$ with both $U$ and $V$ being negative is a likely scenario. In fact, repulsive $U$-attractive $V$ model can be seen as an extreme case of reversed hierarchy of the EAHM where the phonon-mediated attraction can overcome the inter-site repulsion while it cannot overcome the on-site repulsion.

3.4. Finite temperature behaviour

It is interesting to also study the finite-temperature evolution of the ground-state phase diagram. The simplest scenario for the finite temperature behaviour in a mean-field scheme is that each of the superconducting phases have an associated $T_c$ and a normal state is obtained for $T > T_c$. However, within our approach we can perform the explicit minimization at finite $T$ and investigate into more general possibilities. Indeed, we uncover an interesting possibility of multiple phase transitions. We find that one superconducting order can disappear and another one can appear upon raising temperature before a normal non-superconducting state is finally obtained at high temperature. To demonstrate this, we plot the $T$-dependence of the SC OPs for a few representative average electronic densities for $V = 4t$ and $U = 2t$ (see figure 9).

We find that the $d_{x^2-y^2} + p_x$ state at $n \approx 0.7$ gives way to a pure $d_{x^2-y^2}$ state, and finally to a non-superconducting state upon increasing temperature (figure 9(a)). Similarly, $p_x + i p_y$ state at $n \approx 0.45$ melts into a $d_{x^2-y^2} + s^* + p_x$ state at intermediate temperatures, before leading to a non-superconducting state (figure 9(b)). Generally the $p$-wave order seems to disappear at lower temperatures leading to a different intermediate temperature state. The conventional scenario is found for $n \approx 0.2$ where $s + d_{x^2-y^2}$-wave ordering disappears.
at $T/t = 1.2$ and a non-superconducting state is directly obtained. Of course, the $T_C$ scales obtained within mean-field theory are not reliable. However, the feature that one superconducting order disappears and gives way to another is likely to be robust and can be tested in future studies involving more sophisticated methods such as the auxiliary field quantum Monte Carlo. Note that in our calculations the chemical potential is adjusted to obtain a specific target density and the full minimization is performed at every trial value of chemical potential. There are still variations in density of the order of $\sim 0.01$ (see inset in panel (d)) which cause some fluctuations in the $T$-dependence of order parameters. The overall trends, however, are robust.

4. Conclusion

In conclusion, we have shown that the EAHM treated without imposing symmetry constraints presents an exciting possibility for hosting a variety of SC states with mixed OP symmetries. Our approach allowed for competition between SC orders of $s$- and $d$-wave type. The resulting phase diagram hosts some very interesting SC phases. Most notable of these are, (i) the chiral $p$-wave state, (ii) states with mixed $d$-wave and $p$-wave, and with $s$-wave, extended $s$-wave and $p_\pm$ symmetries, and (iii) a $d_{x^2−y^2} + i[s + s^*]$ SC phase. To the best of our knowledge, the possibility of such mixed order-parameter phases has not been explored in the EAHM [65]. We should add that the SC phases obtained in this work are the broken-symmetry solutions of the mean-field Hamiltonian. Further work is required to test the stability of such exotic states in treatments of the model that go beyond mean-field. The comprehensive mean-field phase diagrams presented here should serve as a reference for future studies. Some experiments on cuprates report the possibility of a mixed $s$ and $d$ wave order [5], while a possible mixing of a $p$-wave component with the $d$-wave order has been inferred via thermal transport measurements [66]. Experiments on Sr$_2$RuO$_4$ indicate a chiral $p_x + i p_y$-wave order. Similarly, $p$-wave SC OP is consistent with experiments on Bechgaard salts TMTSF$_2$PF$_6$ and TMTSF$_2$ClO$_4$ [14–18, 67]. Although a microscopic theory of superconductivity in some of these systems is still awaited, our results suggest that EAHM can serve as the effective model for a number of such unconventional superconductors. It is particularly interesting to see the possibility of topologically non-trivial SC states being realized in the EAHM. One of the promising avenues for experimental realization of such states is in the ultracold Fermionic atoms trapped in optical lattices [47, 48]. Given the presence of various non-trivial SC phases, a number of interesting questions can be further asked for the EAHM. Indeed, the effect of non-magnetic and magnetic impurities, influence of Zeeman and Peierls’s terms arising from an external magnetic field, effects of next-nearest hopping, etc are some of the problems that can be readily addressed using the present model. The model can be made material specific by estimating the values of effective on-site and nn electron-electron attractions. Such model studies can help in a microscopic characterization of various mixed-symmetry states and can be useful in improving our understanding of the rich experimental data available on unconventional superconductors.

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