Topological phase in a $d_{x^2-y^2} + (p + ip)$ superconductor in presence of spin-density-wave

Amit Gupta and Debanand Sa
Department of Physics,
Banaras Hindu University, Varanasi-221 005

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We consider a mean-field Hamiltonian for a $d_{x^2-y^2} + (p + ip)$ superconductor(SC) in presence of spin-density-wave(SDW) order. This is due to the fact that the non-commutativity of any two orders produces the third one. The energy spectrum of such a Hamiltonian is shown to be gapped and it yields a topological phase in addition to the conventional one. A phase diagram characterizing different topological phases is constructed. The Chern numbers and hence the nature of the topological phases are determined. The edge state spectrum and the possibility of whether the vortex state harbouring the zero modes are discussed.

The subject of topological systems in condensed matter is one of the most active field of research at present and is developing in rapid pace. Topological phases are characterized by the existence of both the gapless edge states as well as the gapped bulk states. In order to have topological phase, one ought to have an gap in the energy spectrum separating the ground state from the excited states. In such a case, one can define a smooth deformation in the Hamiltonian which does not close the bulk gap. This is due to the fact that one gapped state can not be deformed into another gapped state in a different topological class unless a quantum phase transition occurs when the system become gapless. This field has attracted a lot of interest due to its wide range of applicability in various areas of condensed matter systems such as, quantum Hall effect, superconductors, $Z_2$ topological insulators(spin Hall insulators) etc. The topological phases are crucially dependent on some particular symmetries of the system such as time reversal(TR), space inversion(SI), particle-hole(PH) and chiral etc. The gapless edge states are topologically stable against those perturbations that do not break the symmetries of the system. The topologically protected gapless edge states play important role in determining the transport properties of the system. The total number of topologically protected edge modes in a given system is associated with the topological numbers such as the Thouless-Kohmoto-Nightingale-den Nijs(TKNN) number (the first Chern number) for the systems without time reversal symmetry and the $Z_2$ invariant in case of time reversal invariant systems.

The two-dimensional(2D) topological insulators were theoretically predicted by Bernevig et. al. and experimentally observed in HgTe/CdTe quantum wells. Such an insulator was already proposed by Kane and Mele in 2005. These quantum states of matter belong to a class which is invariant under TR symmetry and the spin-orbit (SO) coupling is essential to achieve this. Soon after, it was generalized to superconductors and superfluids. In 2D, the classification of topological SC is similar to that of topological insulators. For example, the TR breaking SC are classified by an integer $N$ similar to that of quantum Hall insulators whereas TR invariant SC are represented by a $Z_2$ invariant in 2D and 1D. The TR breaking topological SC have attracted a lot of attention recently due to their relation to non-Abelian statistics and their potential application to topological quantum computation. The nature of the low-energy gapless edge states in such systems are non-trivial. They imply fractionalization of quasi-particles as well. For example, in a vortex core of a spinless $p + ip$ SC, the zero mode is described by a Majorana fermion which is half of a conventional fermion. Such a vortex with a Majorana fermion obeys non-Abelian statistics which is crucial for the construction of fault-tolerant quantum computers. The existence of zero energy Majorana mode in a vortex core characterizes the topological order in the system.

The search for the possible realization of topological phases in condensed matter systems is an intriguing and challenging issue. This involves novel concepts as well as potential applications. In this communication, we consider a coexistence phase of singlet SC and SDW which induces a triplet SC component. This is precisely due to the non-commutativity of the former two orders. The singlet SC is taken to be of $d_{x^2-y^2}$ symmetry whereas the SDW order parameter is of $s$-wave and the triplet SC is of $p + ip$ type symmetry. Such a Hamiltonian is shown to yield a non-trivial coexistence phase which is topological in addition to the conventional one. A phase diagram characterizing different topological phases is constructed. The Chern numbers and hence the nature of the topological phases are determined. The edge state spectrum and the vortex state in such system are also discussed.

I. THEORETICAL FORMULATION

Motivated from the recent spectroscopic experimental results on the appearence of a nodal gap on the deeply underdoped cuprate SC, there has been few studies to uncover such new and unexpected re-
In an earlier work, we have already discussed about the topological study of d-wave SC in presence of SDW order and compared with the above cuprates data[33]. However, from the study of the group algebra[34, 35], it is known that the coexistence of any two non-commuting order parameters produces a third order parameter. In case of SDW and d-wave superconductivity, there is a third, dynamically generated, order parameter[36]. This happens to be a triplet SC here. In the present work, we consider the coexistence of SDW and d-wave superconductivity which can generate a triplet and non-zero center of mass superconducting order parameter. We thus start with a Hamiltonian on a 2D square lattice as,

$$H = \sum_{k,\sigma} \xi_k c_{k,\sigma}^\dagger c_{k,\sigma} + \frac{U}{N} \sum_{k,k'} c_{k,\psi}^\dagger c_{k+Q,\psi}^\dagger c_{k',Q,\psi} c_{k',\psi}^\dagger + \sum_{k,k'} V^1(k,k') c_{k,\psi}^\dagger c_{k-Q,\psi}^\dagger c_{k',\psi} c_{k',Q,\psi}^\dagger + \sum_{k,k'} V^2(k,k') c_{k,\psi}^\dagger c_{k-Q,\psi}^\dagger c_{k',-Q,\psi}^\dagger c_{k',\psi}^\dagger. \quad (1)$$

Here, $\xi_k$ is the bare dispersion, $U$ is the onsite Coulomb interaction, $V^{1,2}$ are the pairing strengths for d-wave and p-wave superconductivity and $N$ is the number of sites. We model the bare dispersion in the tight-binding approximation on a 2D square lattice as $\xi_k = -2t(\cos k_x + \cos k_y) - 4t' \cos k_x \cos k_y - \mu$. $c_{k,\sigma}$ (c_{k}\sigma) denotes creation (annihilation) operator of the electron with spin $\sigma = (\uparrow, \downarrow)$ at $k = (k_x, k_y)$. Here, $\sum_{\sigma}$ is the sum of $k$ over the reduced Brillouin zone (RBZ). We express the wave-vector $k$ in units of $\pi/\alpha$, with ‘$\alpha’ the lattice parameter of the underlying lattice. $Q = (\pi, \pi)$ is the SDW nesting vector in 2D. We assume here a commensurate SDW so that $k + Q = k - Q$. The staggered spin magnetization is defined as $M_0 = -\frac{1}{N} \sum_{k,\sigma} \sigma < c_{k+Q,\sigma}^\dagger c_{k,\sigma} >$. Since we will be discussing about three order parameters below, the crystal symmetry of them should be such that the commutator of any two of them should give the third one. For this reason, if $V^1$ is assumed to be of singlet d-wave symmetry, the SDW state guarantees that $V^2$ should be of triplet type. So we get the singlet interaction $V^1_{k,k'} = V^1_{k,k'} s_k s_{k'}$ and $V^2_{k,k'} = V^2_{k,k'} p_k p_{k'}$, where $s_k = \frac{1}{2}(\cos k_x - \cos k_y)$ and $p_k = \sin k_x + i \sin k_y$. We assume that $V^{1,2}$ are attractive. The SC order parameters are defined as, for singlet state, $\Delta_{k'} = \Delta_{0} s_{k'} = V^1_{0} s_{k'} \sum s_k < c_{k,\uparrow} c_{k,\downarrow} > = V^1_{0} s_{k'} \sum s_k < c_{k+Q,\uparrow} c_{k+Q,\downarrow} >$. On the other hand, the triplet order is decoupled in the main band and in the magnetic band as $\Delta_{k'} = \Delta_{0} p_{k'} = V^2_{0} p_{k'} \sum p_k < c_{k,\uparrow} c_{k,\downarrow} > = \Delta_{0} (\sin k_x + i \sin k_y) = \Delta_{1,k} + i \Delta_{2,k}$. While $\Delta_{0} = V^2_{0} p_{k'} \sum p_k < c_{k,\uparrow} c_{k+Q,\downarrow} >$. This is the reason why the time-reversal symmetry remains invariant in the triplet SC state. After substituting these mean-field orders, the total Hamiltonian reads as,

$$H = \sum_{k,\sigma} \xi_k c_{k,\sigma}^\dagger c_{k,\sigma} + M_0 \sum_{k,k'} \sigma c_{k+Q,\sigma} c_{k,\sigma} + \sum_k \Delta_{1} c_{k,\uparrow}^\dagger c_{k,\downarrow}^\dagger + c_{k,\downarrow}^\dagger c_{k,\uparrow} + \sum_k \Delta_{2} c_{k,\uparrow}^\dagger c_{k-Q,\uparrow}^\dagger + \sum_k \Delta_{2} c_{k,\uparrow} c_{k+Q,\uparrow}^\dagger + \sum_k \Delta_{2} c_{k,\downarrow} c_{k-Q,\downarrow}^\dagger + \sum_k \Delta_{2} c_{k,\downarrow}^\dagger c_{k+Q,\downarrow}^\dagger$$

where $\xi_k^+ = -4t' \cos k_x \cos k_y - \mu$ and $\xi_k^- = -2t(\cos k_x + \cos k_y)$. In the above Hamiltonian, the nesting property in the band dispersion i.e. $\xi_{k+Q} = \xi_k$, $\xi_{k+Q} = -\xi_k^-$ and the order parameters $\Delta_{1,k+Q} = -\Delta_1(c_{k+Q,a-\cos k_y}) = -\Delta_1$ and $\Delta_{2,k+Q} = -\Delta_2$ have been employed. In the momentum space, the Hamiltonian can be expressed as, $H = \sum_k \psi_k^\dagger H(k) \psi_k$ where the four-component spinor $\psi_k$ is, $\psi_k = (c_{k,\uparrow}, c_{k-Q,\downarrow}, c_{k-Q,\downarrow}, c_{k+Q,\downarrow})$. Thus, the Hamiltonian matrix $H(k)$ in this basis is written as,
The second equation in Eqn.(5) is met only when 
and the non-trivial regions as shown in Fig.2. We will
explore the Chern number associated with such phases in the next section.

II. PHASE DIAGRAM AND THE CHERN NUMBER

To examine the topological phase transition(TPT), it is convenient to use the dual Hamiltonian instead of the original one. This can be done through a constant unitary transformation matrix $D$ as,

$$
\mathcal{H}(k) = D \mathcal{H}(k) D^\dagger,
$$

resulting

$$
\mathcal{H}^D(k) = 
\begin{pmatrix}
\xi_k^+ + \xi_k^- & \Delta_{k}^2 - \Delta_{k}^1 & \Delta_{k}^1 M_0 & 0 \\
\Delta_{k}^2 + \xi_k^+ & -\xi_k^- - M_0 & -\xi_k^+ - M_0 & -\Delta_{k}^1 \\
\Delta_{k}^1 & -\xi_k^- - M_0 & -\xi_k^- & -\Delta_{k}^1 \\
0 & -\xi_k^- & -\xi_k^- & -\xi_k^- M_0
\end{pmatrix}.
$$

In the limit $t \to 0$, the dual Hamiltonian $\mathcal{H}^D(k)$ in the leading order around $k = (0,0)$ and $(\pi, \pi)$ gives rise to the following two $2 \times 2$ block-Hamiltonian as,
\[
H^D(k) = \begin{pmatrix}
-4t' - \mu + M_0 & \Delta_3^2(k_x + ik_y) \\
\Delta_2^2(k_x - ik_y) & 4t' + \mu - M_0 \\
0 & 0 \\
0 & 0 \\
4t' + \mu + M_0 & -\Delta_2^2(k_x - ik_y) \\
-\Delta_2^2(k_x + ik_y) & -4t' - \mu - M_0
\end{pmatrix}.
\] (9)

We notice here that the above dual Hamiltonian have a close similarity to the Hamiltonian of the spinless chiral \( p + ip \) superconductor discussed in [8].

In order to study the phase diagram of this Hamiltonian one needs to determine the phase boundaries corresponding to gapless regions since the topological invariants can not change without closing the bulk gap. For the present model, the critical lines are determined by solving equation (8), i.e., \( M_0 = \pm (4t' + \mu) \) for the upper(lower) blocks in the case with \( k = (0,0) \) and \( (\pi,\pi) \). The phase becomes topological in the region when \( M_0 < \pm (4t' + \mu) \) whereas it is trivial for \( M_0 > \pm (4t' + \mu) \).

Similarly, one can draw a phase diagram for any \( k \) point in the RBZ. e.g., for \( k = (0,\pi) \) and \( (\pi,0) \), we get the same condition for the topological phase transition to occur from second condition of Eqn. (5), i.e. \( (4t' - \mu) \neq 0, \Delta_3^2 = 0 \). This leads to the following Eqn. of the critical lines \( M_0^2 = (4t' - \mu)^2 \). The topological phase exist in the region \( M_0 < \pm (4t' - \mu) \) whereas it is trivial for \( M_0 > \pm (4t' - \mu) \).

Based on the finiteness of the Chern number given below, we propose a phase diagram in the in the former case (Fig. 2) in the \((\mu, M_0^2)\) plane which distinguishes the topological and non-topological phases. This is the new result of the present manuscript. Thus, it is obvious that both these phases are separated by a quantum phase transition line. The Chern numbers in the topological phases of Fig. 2 are calculated below.

It is well known that the topological phases can be characterized by Chern numbers. For a specific model Hamiltonian \( h(k) = \sum_\alpha d_\alpha(k)\sigma_\alpha \), with \( \sigma_\alpha \), the Pauli matrices and \( d_\alpha(k) = [d_1(k), d_2(k), d_3(k)] \), the Chern number can be calculated from the expression

\[
\mathcal{N} = \frac{1}{4\pi} \int d^2k \hat{d}(k) \cdot \left( \frac{\partial \hat{d}(k)}{\partial k_x} \times \frac{\partial \hat{d}(k)}{\partial k_y} \right),
\] (10)

where the unit vector \( \hat{d}(k) = d(k)/\sqrt{\sum d^2(k)} \) characterizes a map from the Brillouin zone vector \( k \) to unit sphere. The present model Chern number simply counts the number of times \( \hat{d}(k) \) wraps around the unit sphere as a function of \( k \). In the present model the Chern number for the case \( M_0 < \pm (4t' + \mu) \) is calculated as \( N = 1 \) whereas it vanishes when \( M_0 > \pm (4t' + \mu) \). In presence of SDW order, the \( p + ip \) SC state has odd parity and \( s_z = 0 \) symmetry which is a fully gapped system. Due to SDW order, it has \( U(1) \) spin rotation along say, \( z \)-axis and \( \pi_0(C_2) = Z \) which corresponds to class \( A \) in accordance with the symmetry classification of Altland and Zirnbauer [38]. This means that there are infinite number of distinct topological SC with \( s_z \) conservation and are labeled by an integer

FIG. 3. Edge-state spectrum of the coexistence phase of \( p_x + ip_y \) SC in presence of SDW order on a cylindrical geometry. Parameters are chosen as, \( t' = -0.30t \) eV, \( \Delta_0 = t, \mu = .25t \), \( M_0 = .3t \) for a lattice of \( N_x = 100 \) sites.

which is the Chern number [31]. This is associated with the number of chiral fermion edge modes.

III. EDGE STATES AND THE VORTEX STRUCTURE

In order to see the evolution of edge states in this model(coexistence of \( p + ip \) SC and SDW order), we studied it numerically on a cylindrical geometry with periodic boundary condition in \( y \)-direction and open boundary condition in \( x \)-direction. We solved the eigen-value problem where the Hamiltonian has been diagonalized on \( N_x = 100 \) sites. The energy dispersion \( E_k \) versus \( k_y \) has been obtained and hence the edge states has been shown in Fig. 3. As it is already been discussed in the previous section, two chiral edge states characterize the topological phase in this model.

It is well known that the vortex of a topological SC with odd topological quantum number \( \mathcal{N} \) carries an odd number of Majorana zero modes. The existence of such zero modes in the vortex core of a \( p + ip \) SC is shown to be due to index theorem [39, 40]. In the present case, since the SC is coexisting with SDW order, the topological classification is always trivial for class \( A \) in 1D. Since the existence of the zero modes in the vortex core is determined by the symmetry classification in one space dimension less, the topological \( p + ip \) SC with the chiral edge modes won’t support such zero energy vortex bound state [31].
IV. CONCLUSION

In conclusion, we summarize the main findings of the present manuscript. We consider a possible coexistence of singlet SC and SDW which induces a triplet SC component as well. The singlet SC is taken to be of $d_{x^2-y^2}$ symmetry whereas the SDW order parameter is of $s$-wave and the triplet SC is $p + ip$ type symmetry. Such a Hamiltonian is shown to yield a non-trivial coexistence phase which is topological in addition to the conventional one. A phase diagram characterizing different topological phases is constructed. The Chern numbers and hence the nature of the topological phases are determined. The edge state spectrum and the possibility of whether the vortex state harbouring the zero modes are discussed.

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