Exact $SU(2)$ symmetry and $\eta$-pairing ground states in interacting fermion models with spin-orbit coupling

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We generalize the $\eta$-pairing theory in Hubbard models to the ones with spin-orbit coupling (SOC). Despite the broken $SU(2)$ spin symmetry, the $\eta$ pairing reveals an $SU(2)$ pseudospin symmetry in our spin-orbit coupled Hubbard model. In particular, we find that our exact results can be applied to a variety of spin-orbit coupled systems, whose noninteracting limit can be a Dirac semimetal, a Weyl semimetal, a nodal-line semimetal, and a Chern insulator. We then focus on a Dirac-semimetal Hubbard model with additional interactions and establish the stability regions in parameter space where the $\eta$-pairing states as well as charge-density-wave states can be constructed as exact ground states. The basic idea of the exact solution is to make the Hamiltonian frustration-free in some parameter regions. Our work uncovers an exact $SU(2)$ symmetry and establishes the exact superconducting ground states in spin-orbit coupled interacting systems, which may shed new light on the physics of strongly correlated systems with SOC.

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Introduction.—Exact results or solutions of interacting many-electron models beyond one spatial dimension are rare and highly appreciated. One important advance in studying the Hubbard model is the so-called $\eta$-pairing theory, which is an exact result due to Yang [1]. The $\eta$-pairing operator allows for the construction of exact eigenstates possessing off-diagonal long-range order (ODLRO) and reveals an $SU(2)$ pseudospin symmetry [2] of the Hubbard model. More importantly, the $\eta$-pairing states can serve as exact superconducting ground states in a class of strongly correlated electronic models [3–5], which is beyond the framework of BCS theory. Recent developments based on the $\eta$-pairing theory include the calculation of entanglement entropy of $\eta$-pairing states [6, 7] and the study of quantum thermalization physics in Hubbard models [8–11].

It is now recognized that spin-orbit coupling (SOC) can produce a wealth of topological phases and physical systems with SOC are currently under intense investigation. In particular, a number of theoretical understandings have been obtained for strongly correlated electronic systems with SOC [12–14]. Nevertheless, most of these theoretical investigations used various approximate methods such as mean field theory and more rigorous and clearer physical understanding of these systems deserves further studies. Therefore, exact results or solutions for spin-orbit coupled interacting electronic systems would be valuable.

In this work, we first show that Yang’s $\eta$-pairing theory can be generalized to a class of Hubbard models with SOC. The exact $SU(2)$ pseudospin symmetry can be then preserved in these systems, while the $SU(2)$ spin symmetry is broken due to SOC. We then apply these exact results to four concrete spin-orbit coupled systems including, in the noninteracting limit, a Dirac semimetal, a Weyl semimetal, a nodal-line semimetal, and a Chern insulator. Moreover, the $\eta$-pairing states can be stabilized as exact ground states by introducing additional bond interactions. In particular, we focus on an interacting Dirac-semimetal model on the square lattice. The basic idea of the exact solution is to make the Hamiltonian frustration-free in some parameter regions. It can then be shown that the $\eta$-pairing states with momentum $\pi$ and $0$, as well as charge-density-wave (CDW) states, can be constructed as exact ground states in different parameter regions, respectively.

Model and generalization of $\eta$ pairing.—The generic Hamiltonian for our spin-orbit coupled Hubbard models in arbitrary dimensions is given by

$$
H = H_0 + H_U
$$

$$
H_0 = \sum_k C_k^\dagger (a_k \sigma_x + b_k \sigma_y + c_k \sigma_z + \varepsilon_k \sigma_0) C_k
$$

$$
H_U = U \sum_i n_{i\uparrow} n_{i\downarrow}.
$$

(1)

The noninteracting part $H_0$ is written in momentum space, where $C_k^\dagger = (c_{k\uparrow}^\dagger, c_{k\downarrow}^\dagger)$. In $H_0$, the three momentum-dependent real coefficients $a_k, b_k, c_k$ with Pauli matrices $\sigma_x, \sigma_y, \sigma_z$ represent the SOC, and the term $\varepsilon_k$ with the identity matrix $\sigma_0$ is the usual energy band without SOC. The interacting part $H_U$ written in real space is the on-site Hubbard interaction, where $n_{i\sigma} = c_{i\sigma}^\dagger c_{i\sigma}$.

In the absence of SOC ($a_k = b_k = c_k = 0$), Yang finds that the so-called $\eta$-pairing operator $\eta_{\pi}^\dagger = \sum_{j,j'} e^{i\pi \cdot j} c_{j\uparrow}^\dagger c_{j'\downarrow}$ obeys the commutation relations $[H_0, \eta_{\pi}^\dagger] = -2\mu \eta_{\pi}$ and $[H_U, \eta_{\pi}^\dagger] = U \eta_{\pi}^\dagger$, where $\mu$ is the chemical potential and $\pi = (\pi, \pi, \pi)$ or $(\pi, \pi)$ for the cubic or square lattice. The total Hamiltonian and $\eta_{\pi}$ thus obey $[H, \eta_{\pi}^\dagger] = (U - 2\mu)\eta_{\pi}$, and one can construct many exact eigenstates $H(\eta_{\pi}^\dagger)^m |0\rangle = m(U - 2\mu)(\eta_{\pi}^\dagger)^m |0\rangle$ ($m = 0, 1, \ldots$)
possessing ODLRO.

In Yang’s observation, the key point that makes the possible η pairing is the fact that the energy band ε_{k} (for the cubic or square lattice without SOC) has the property ε_{k} + ε_{π−k} = −2μ (independent of k), which leads to the commutation relation [H_{0}, n_{π}^{\dagger}] = −2μ n_{π}.

Therefore, to generalize the η-pairing theory to Hubbard models with SOC, e.g., Eq.(1), we need some new constraints on the coefficients a_{k}, b_{k}, and c_{k}. To achieve these new constraints, we first define the η-pairing operator with a generic momentum Q as

\[ n_{Q}^{\dagger} = \sum_{k} c_{k}^{\dagger} c_{k}^{\dagger} \]  

(2)  

It can then be shown that

\[ [H_{0}, n_{Q}^{\dagger}] = \lambda n_{Q}^{\dagger}, \]  

(3)  

if a_{k}, b_{k}, c_{k}, ε_{k}, and Q satisfy the following equations

\[ a_{k} = a_{Q} - k, \quad b_{k} = b_{Q} - k, \]  

\[ \varepsilon_{k} + \varepsilon_{Q} - k + c_{k} - c_{Q} - k = \lambda, \]  

(4)  

where λ is a constant independent of k. The commutator of the Hubbard interaction and the η-pairing operator reads

\[ [H_{U}, n_{Q}^{\dagger}] = U n_{Q}^{\dagger}, \]  

(5)  

which holds for arbitrary Q. It follows from Eqs.(3) and (5) that the η-pairing operator is now an eigenoperator of the total Hamiltonian, namely

\[ [H, n_{Q}^{\dagger}] = (λ + U) n_{Q}^{\dagger}. \]  

(6)  

Therefore, one can construct many exact eigenstates \( H(n_{Q}^{\dagger})^{m}|0\rangle = m(λ + U)|n_{Q}^{\dagger}|^{m}|0\rangle \) possessing ODLRO.

The SU(2) spin symmetry is typically broken due to the SOC terms in Eq.(1). However, from Eq.(6), we see that our spin-orbit coupled Hubbard model possesses an exact SU(2) pseudospin symmetry when \( λ + U = 0 \). The term pseudospin is attributed to the antiferromagnetic states of f fermions, i.e., \( \mathcal{F}^{2}(n_{Q}^{\dagger})^{m}|0\rangle = \frac{N(N^{2} + 1)(η_{Q}^{\dagger})^{m}|0\rangle + J_{x}(n_{Q}^{\dagger})^{m}|0\rangle = (m - \frac{N}{2})(η_{Q}^{\dagger})^{m}|0\rangle \) (where \( J^{2} = \sum_{\alpha} J_{\alpha}^{2} \)), which break the f fermion’s spin symmetry and hence break the pseudospin symmetry.

Application of the generalized η-pairing theory.—Based on the above exact results for model (1), we find that the η pairing can exist in a variety of spin-orbit coupled systems. In particular, we apply these exact results to four concrete examples, which include three gapless and one gapped noninteracting topological phases due to SOC.

The first example is a Dirac-semimetal Hubbard model on a square lattice. Its Hamiltonian is given by Eq.(1) with \( a_{k} = 2t' \sin k_{x}, b_{k} = 2t' \sin k_{y}, c_{k} = 0, \) and \( ε_{k} = -2t(\cos k_{x} + \cos k_{y}) - μ \). The lattice spacing has been set to unity throughout our paper. There are four Dirac points \( K = (n_{1}π, n_{2}π, n_{3}π) \) at \( U = 0 \), where \( n_{1,2,3} = 0 \) or 1. Substituting the expressions of \( a_{k}, b_{k}, c_{k} \) and \( ε_{k} \) into Eq.(4), we find that the η-pairing momentum \( Q = π \) and the constant \( λ = -2μ \).

Similarly, the next example we consider is a Weyl-semimetal Hubbard model on a cubic lattice [15]. Its Hamiltonian is given by Eq.(1) with \( a_{k} = 2t' \sin k_{x}, b_{k} = 2t' \sin k_{y}, c_{k} = 2t' \sin k_{z}, \) and \( ε_{k} = -2t(\cos k_{x} + \cos k_{y} + \cos k_{z}) - μ \). There are totally eight Weyl points \( K = (n_{1}π, n_{2}π, n_{3}π) \) at \( U = 0 \), where \( n_{1,2,3} = 0 \) or 1. As can be seen from Eq.(4), the η-pairing momentum \( Q = π \) and the constant \( λ = -2μ \). Notice that for our Dirac- or Weyl-semimetal Hubbard model, the original η-pairing theory [1] is recovered in the absence of SOC, e.g., \( t' = 0 \).

Our third example is a nodal-line-semimetal Hubbard model on a cubic lattice [15]. Its Hamiltonian is given by Eq.(1) with \( a_{k} = t(\cos k_{x} + \cos k_{y} - b), b_{k} = t' \sin k_{x}, c_{k} = 0, \) and \( ε_{k} = -μ \). At \( U = 0 \), upon expanding \( a_{k} \) and \( b_{k} \) near the \( k = 0 \) point, we obtain a nodal ring with radius \( \sqrt{2(2b)} \) pinned at the \( k_{z} = 0 \) plane. We notice that, from Eq.(4), the η-pairing momentum \( Q = (0, 0, π) \) and the constant \( λ = -2μ \).

The last example we consider is a Chern-insulator Hubbard model on a triangular lattice [16]. Its Hamiltonian is given by Eq.(1) with \( a_{k} = -2t \cos(\frac{π}{3} - \frac{\sqrt{3}π}{6}), b_{k} = -2t \cos(\frac{π}{3} + \frac{\sqrt{3}π}{6}), c_{k} = -2t \cos k_{z}, \) and \( ε_{k} = -μ \). This model breaks time-reversal symmetry and \( H_{0} \) has a nonzero band Chern number ±2. In the large-U limit, this system is described effectively by the triangular lattice Kitaev-Heisenberg spin model [16, 17]. We see that, from Eq.(4), the η-pairing momentum \( Q = 0 \) and the constant \( λ = -2μ \). Note that the η-pairing operator with \( Q = 0 \) is simply the s-wave Cooper-pairing operator in the usual BCS theory. In fact, the first generalization of η pairing to a triangular lattice was obtained by adding a staggered \( π/2 \) flux through each triangle plaquette [18], in the absence of SOC.

For the above four examples of spin-orbit coupled Hubbard model (1), the exact SU(2) pseudospin symmetry is respected when \( λ + U = 0 \), i.e., \( μ = U/2 \). We notice
that the pseudospin symmetry would lead to a vanishing pseudospin moment \((J_z) = \frac{1}{2}(n_i - 1)\) on each site, so the electron density is fixed at half filling (independent of the temperature) when \(\mu = U/2\).

**Construction of the exact \(\eta\)-pairing ground states.**—In general, the exact \(\eta\)-pairing eigenstates of the Hubbard model (1) are not ground states [1]. In fact, beyond one spatial dimension, the Hubbard model has no exact solution to this day. However, some extended Hubbard models containing additional interactions are exactly solvable by constructing the ground state wave functions explicitly [3–5, 19]. Following the method used in Ref. [19], we would further show that the \(\eta\)-pairing states can be constructed as the exact ground states of extended Hubbard models with SOC.

For the sake of concreteness, let us consider a square lattice Dirac-semimetal model similar to the one discussed above. Besides the on-site Hubbard \(U\), we now introduce additional bond interactions, and the resulting new Hamiltonian can be expressed as

\[
H' = \sum_{x\text{-bonds}} h_{ij}^x + \sum_{y\text{-bonds}} h_{ij}^y,
\]

where the summation \(\sum_{x\text{-bonds}} (\sum_{y\text{-bonds}})\) runs over all the bonds along the \(x\) (\(y\)) direction of the square lattice. The bond Hamiltonians are given by

\[
h_{ij}^x = t (c_i^\dagger \sigma_x c_j + c_j^\dagger \sigma_x c_i) - \frac{\mu}{4} (n_i + n_j) + \frac{U}{4} (n_i n_j + n_i n_j),
\]

\[
h_{ij}^y = t (c_i^\dagger \sigma_y c_j + c_j^\dagger \sigma_y c_i) - \frac{\mu}{4} (n_i + n_j) + \frac{U}{4} (n_i n_j + n_j n_i),
\]

where \(c_i^\dagger = (c_i^\dagger, c_i^\dagger)\), \(n_i = n_i^\uparrow + n_i\downarrow\), and \(\sigma = -\sigma\). The noninteracting part \(t\) represents SOC which is responsible for the Dirac points in momentum space. The \(B\) term in Eq. (8) is known as the bond-charge interaction [20]. Note that it differs from the usual bond-charge interaction \(\sum_\sigma (c_i^\dagger \sigma_{x,j} + c_j^\dagger \sigma_{x,j}) (n_{i\sigma} + n_{j\sigma})\) by spin flips on the bonds, which can be thought of as due to SOC [21]. In addition, the terms \(V\) and \(P\) denote the nearest-neighbor Coulomb interaction and the pairing-hopping term, respectively.

To construct the exact ground states of Eq. (7), the basic idea is to identify some parameter regions where the Hamiltonian (7) is frustration-free: The ground states of Eq. (7) are simultaneous ground states of each and every local bond Hamiltonian \(h_{ij}^{x,y}\) in Eq. (8).

To find the parameter region (i.e., restrictions on \(U\), \(B\), \(V\), and \(P\) in the form of equalities and inequalities) where the \(\eta\)-pairing states are frustration-free ground states, let us diagonalize the local bond Hamiltonians (8). Here, each bond Hamiltonian \(h_{ij}^{x,y}\) has 16 local eigenstates and their respective energies, which are summarized in Table I. Notice that we have set \(B = -t\) in the calculation [3–5, 19]. For \(B \neq -t\), the local eigenstates become complicated and it is very difficult to see whether there exists a global frustration-free ground state [19].

We note that the \(\eta\)-pairing states with momentum \(\pi = (\pi, \pi)\), i.e., \((\eta^\pi)^\mu|0\rangle\), can be built completely from the local states \(|0\rangle\), \(|22\rangle\), and \(|20\rangle - |02\rangle\). Thus, \((\eta^\pi)^\mu|0\rangle\) will be the common ground states of all the bond Hamiltonians \(h_{ij}^x\) and \(h_{ij}^y\), if \(|0\rangle\), \(|22\rangle\), and \(|20\rangle - |02\rangle\) are local ground states. This requires that, from Table I, \(0 = \frac{U}{2} - \mu + 4V = \frac{U}{2} - \frac{\mu}{2} - P\) are the minimum eigenvalues, which yields the following constraints

\[
V = -\frac{P}{2} < 0, \quad \mu = \frac{U}{2} + 4V
\]

\[
U < \min(-8|t| - 4V, -4V).
\]

Therefore, inside this parameter region together with

**Table I:** This table summarizes the 16 local eigenstates and their respective eigenvalues of the bond Hamiltonians (8), for \(B = -t\). The 16 local bases are defined as follows: \(|00\rangle\) denotes the vacuum, \(|22\rangle\) = \(c_i^\dagger c_j^\dagger c_j^\dagger c_i^\dagger|00\rangle\), \(|20\rangle\) = \(c_i^\dagger c_j^\dagger c_j^\dagger c_i|00\rangle\), \(|02\rangle\) = \(c_i^\dagger c_j^\dagger c_i^\dagger c_j|00\rangle\), \(|\sigma\sigma\rangle\) = \(c_i^\dagger c_j^\dagger|0\rangle\), \(|\sigma0\rangle\) = \(c_i^\dagger c_j^\dagger|0\rangle\), \(|0\sigma\rangle\) = \(c_i^\dagger c_j^\dagger|0\rangle\), \(|0\rangle\) = \(c_i^\dagger c_j^\dagger|00\rangle\), and \(\{2\sigma\} = c_i^\dagger c_j^\dagger c_j^\dagger c_i|00\rangle\).

| Eigenvalue | \(h_{ij}^x\) | \(h_{ij}^y\) |
|-------------|-------------|-------------|
| \(0\) | \(|00\rangle\) | \(|00\rangle\) |
| \(\frac{U}{2} - \mu + 4V\) | \(|22\rangle\) | \(|22\rangle\) |
| \(\frac{U}{2} - \frac{\mu}{2} + P\) | \(|20\rangle \pm |02\rangle\) | \(|20\rangle \pm |02\rangle\) |
| \(\pm t - \frac{\mu}{2}\) | \(|\sigma\sigma\rangle\) | \(|\sigma\sigma\rangle\) |
| \(\pm t + \frac{\mu}{2} + 2V\) | \(|\sigma0\rangle \pm |0\sigma\rangle\) | \(|\sigma0\rangle \pm |\sigma|0\sigma\rangle\) |
| \(|\sigma2\rangle \mp |2\sigma\rangle\) | \(|\sigma2\rangle \mp |2\sigma\rangle\) |
$B = -t$, the exact ground states of our interacting Dirac-semimetal model (7) are $(\eta \pi)^m |0\rangle$ ($m = 0, 1, ..., N$).

In the same way, one can establish the parameter region in which the $\eta$-pairing states with momentum $0$ become the exact ground states. $(\eta \pi)^m |0\rangle$ is now built completely from the local states $|00\rangle$, $|22\rangle$, and $|20\rangle + |02\rangle$, which have to be made local ground states. Again from Table I, we get the following constraints

$$
V = \frac{P}{2} < 0, \quad \mu = \frac{U}{2} + 4V \\
U < \min(-8|t| - 8V_1 - 4V) \quad (10)
$$

It is interesting to see that the CDW state $|\text{CDW}\rangle = \prod_{i \in A \cup B} c_i^\dagger c_i |0\rangle$ can also be an exact ground state, where $A$ and $B$ are the two sublattices of square lattice. Notice that $|\text{CDW}\rangle$ can be constructed completely from the local states $|20\rangle$ and $|02\rangle$, we get the following constraints

$$
P = 0 \\ \\
U < \min(-4|t| + \mu, 4V, 2\mu) \\ \\
V > \max\left(\frac{|t|}{2} + \frac{\mu}{8}, \frac{U}{16} + \frac{\mu}{8}\right) \quad (11)
$$

Eqs.(9)-(11) are exact results that establish the stability regions of superconducting (i.e., the $\eta$-pairing states) and CDW ground states. We thus see that, for sufficiently small $U$, superconducting ground states are stabilized by attractive $V$ and finite $P$, whereas a repulsive $V$ (without $P$) favors a CDW ground state. In fact, the interactions $V$ and $P$ lift the degeneracy between the $\eta$-pairing and the CDW states: When $V = P = 0$, the local ground states in Table I are $|00\rangle$, $|20\rangle$, $|02\rangle$, and $|22\rangle$ for $B = -t, U = 2\mu < -4|t|$. In this case, the ground-state space of Eq.(7) is spanned by the bases $\prod_{i \in A \cup B} (c_i^\dagger c_i) l_i |0\rangle$ ($l_i = 0, 1$) and is highly degenerate, which contains both the $\eta$-pairing states (with arbitrary momenta) and the CDW states.

Summary.—In summary, we have generalized Yang’s $\eta$-pairing theory to a class of Hubbard models with SOC. The $\eta$ pairing reveals an $SU(2)$ pseudospin symmetry in these spin-orbit coupled Hubbard models, even though the $SU(2)$ spin symmetry is broken due to SOC. Based on our exact results, we apply the $\eta$-pairing theory to four concrete spin-orbit coupled Hubbard models, which include three gapless and one gapped topological phases in the noninteracting limit. We then focus on an interacting Dirac-semimetal model on the square lattice. We have established the stability regions in parameter space where the $\eta$-pairing states with momentum $\pi$ and $0$, as well as CDW states, can be constructed as exact ground states. The basic idea of the exact solution is to make the Hamiltonian frustration-free in some parameter regions.

Based on our exact results and solutions, we identify an exact $SU(2)$ symmetry and establish the exact superconducting ground states in spin-orbit coupled interacting systems. This work may motivate future works to study the possible exotic quantum phases in strongly correlated systems and real materials with nonnegligible SOC.

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