Extended Hubbard Model with Unconventional Pairing in Two Dimensions

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We rigorously prove that an extended Hubbard model with attraction in two dimensions has an unconventional pairing ground state for any electron filling. The anisotropic spin-0 or anisotropic spin-1 pairing symmetry is realized, depending on a phase parameter characterizing the type of local attractive interactions. In both cases the ground state is unique. It is also shown that in a special case, where there are no electron hopping terms, the ground state has Ising-type Néel order at half-filling, when on-site repulsion is furthermore added. Physical applications are mentioned.

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Unconventional superconductivity with gap symmetries other than the conventional s-wave has been found ubiquitously in correlated electron systems. Examples include heavy fermions [1], high Tc cuprates [2], ruthenate [3], organic conductors [4], etc. The common feature of those compounds is proximity of antiferromagnetic or ferromagnetic order. A vast number of studies have been extensively devoted to revealing nature of these phenomena. So far, within the mean-field approach, it is recognized that effective electron-pair attraction depending on electron momentum can cause unconventional superconductivity, but, there still is no convincing evidence which model captures the mechanism truly. As a many-body problem, it is an extremely hard task to make a definite criterion to distinguish the validity of the models beyond the mean-field level. Indeed, electron systems exhibit various physical phenomena, relying on a subtle interplay between kinetic and interaction energies. It is thus desirable to rigorously establish the occurrence of unconventional pairing in concrete models of correlated electrons. The attempts in this direction will shed light on the mechanism for unconventional superconductivity and, in turn, give us useful information about possible sources of effective pair attraction in real materials.

In this paper, we rigorously construct a series of the electronic models having ground states with unconventional pairing symmetries. We consider a two-dimensional tight-binding model with attractive interactions which act on electrons occupying certain localized single-electron states (corresponding to ² and ³ below). For each even number of electrons, the model is proved to have the unique ground state ² in which all electrons form anisotropic pairs with spin 0 or spin 1, depending on a phase parameter (θ in ²) of the localized states. Here, we treat the model in two dimensions, since the case is most relevant to the experiments mentioned above. Extensions of the present method and idea to higher dimensional systems or other lattice structures are straightforward.

Remarkably, unlike usual mean-field Hamiltonians, our Hamiltonian conserves the electron number. The occurrence of the electron-pair condensation is thus non-trivial in the present model. To our best knowledge, this is the first time that a model Hamiltonian is proved to exhibit condensation of unconventional electron pairs including spin-1 pairs ³. Further advantage of our model is a relation to proximity of magnetic orders. In a case, where there are no electron hopping terms, the model exhibits antiferromagnetism at half-filling, when on-site repulsion terms of Hubbard-type are furthermore introduced. The model is expected to exhibit a quantum phase transition between the superconducting and the antiferromagnetic states, which is an essential feature of the cuprate superconductors, when parameters are varied away from an exactly solvable point in a parameter space.

Let us define the model. Let Λ be a rectangular lattice of the form Λ = [1, L₁] × [1, L₂] ∩ ℤ² with periodic boundary conditions. It is assumed that L₁ is an odd positive integer and L₂ = L₁ + 2. (We need these conditions to prove the uniqueness of the ground state as we will show later.) We denote by $c_{x,\sigma}(c_{x,\sigma}^\dagger)$ the annihilation (creation) operator for an electron with spin $\sigma = \uparrow, \downarrow$ at site $x$. They satisfy the anticommutation relations $\{c_{x,\sigma}, c_{y,\tau}\} = \{c_{x,\sigma}, c_{y,\tau}\}^\dagger = 0$ and $\{c_{x,\sigma}, c_{y,\tau}\} = \delta_{x,y}\delta_{\sigma,\tau}$. We denote by $\Phi_0$ a state without electrons and by $N_e$ the electron number.

The hopping part of our Hamiltonian is given by $H_{\text{hop}} = \sum_{x,y\in \Lambda} \sum_{\sigma=\uparrow,\downarrow} t_{x,y} c_{x,\sigma}^\dagger c_{y,\sigma}$ where $t_{x,y} = (1 + 4\lambda^2)t$ if $x = y$, $t_{x,y} = -2\lambda t$ if $|x - y| = 1$, $t_{x,y} = 2\lambda^2 t$, if $|x - y| = \sqrt{2}$, $t_{x,y} = \lambda^2 t$ if $|x - y| = 2$, and zero otherwise ⁴. Here, it is assumed that $t > 0$ and $-1/4 < \lambda < 1/4$. In the wave space, it is represented as $H_{\text{hop}} = \sum_{k\in K} \sum_{\sigma=\uparrow,\downarrow} \varepsilon(k) c_{k,\sigma}^\dagger c_{k,\sigma}$ where $\varepsilon(k) = tg^2(k)$ with $g(k) = 1 - 2\lambda \cos k_1 - 2\lambda \cos k_2$ for $k = (k_1, k_2)$.

FIG. 1: (a) Lattice structure. (b) Dispersion relation.
€k,σ = \frac{1}{\sqrt{|Λ|}} \sum_{x \in Λ} e^{ik \cdot x} c_{x,σ}, \quad \text{and}

\mathcal{K} = \left\{ \left( \frac{2\pi n_1}{L_1}, \frac{2\pi n_2}{L_2} \right) \mid n_i = 0, \pm 1, \ldots, \pm \frac{L_i - 1}{2} \right\}. \quad (1)

The lattice structure and the single-electron dispersion relation are shown in Figs. 1(a) and (b).

Let us introduce new fermion operators corresponding to the single-electron states localized in the vicinity of site \(x \in Λ\) as follows:

\begin{align*}
    a_{x,σ} &= c_{x,σ} - λ \sum_{y \in Λ; |y-x|=1} c_{y,σ}, \quad (2) \\
    b_{θ,x,σ} &= \sum_{y \in Λ; |y-x|=1} e^{-iθ(y-x)} c_{y,σ} \quad (3)
\end{align*}

with \(θ \in \{α, β, γ\}\) where \(α = (0, 0), β = (0, π)\) and \(γ = (π/2, π/2)\). The interaction discussed in this paper is attraction between electrons in these localized states. The interaction part of our Hamiltonian is given by

\[ H_{int,θ} = -W \sum_{x \in Λ, σ=↑,↓} b_{θ,x,σ}^\dagger b_{θ,x,σ} a_{x,σ}^\dagger a_{x,σ} \quad (4) \]

with \(W > 0\). One easily finds that the summand in (4) is bounded below by \(-4(1+Λ^3)W\), which is attained by the states of the form \(a_{x,σ}^\dagger b_{θ,x,σ}^\dagger \cdots Φ_0\). This indicates that \(H_{int,θ}\) describes attraction between two electrons with opposite spins.

The whole Hamiltonian of our model is given by

\[ H_θ = H_{hop} + H_{int,θ} + v_0 \sum_{σ=↑,↓} c_{0,σ}^\dagger c_{0,σ} \quad (5) \]

where \(v_0 = 0\) if \(θ = α\) and \(v_0 > 0\) otherwise. The last term is added for a technical reason to show the uniqueness.

To state our main result, we need to introduce further notation. Let \(G\) be the Gram matrix for the a-operator \(a\) whose matrix elements are given by \((G)_{x,y} = \{a_{x,σ}^\dagger a_{y,σ}\}\). By a straightforward calculation, one finds that \(G\) is regular and that its inverse matrix is given by \((G^{-1})_{x,y} = 1/|Λ| \sum_{k \in Κ} g^{-2}(k) e^{ik \cdot (x-y)}\). Thus, it is possible to define dual operators of the a-operator as \(\tilde{a}_{x,σ} = \sum_{y \in Λ} (G^{-1})_{y,x} a_{y,σ}\), which satisfy

\[ \{a_{x,σ}^\dagger, \tilde{a}_{y,σ}\} = \{\tilde{a}_{x,σ}^\dagger, a_{y,σ}\} = δ_{x,y} δ_{σ,τ}. \quad (6) \]

Since \{\tilde{a}_{x,σ}^\dagger Φ_0\}_{x \in Λ} spans the single-electron Hilbert space, the \(b_{θ}\)-operators \(b\) are expanded as

\[ b_{θ,x,σ} = \sum_{y \in Λ} (U_θ)_{y,x} \tilde{a}_{y,σ}. \quad (7) \]

Here, the expansion coefficients \((U_θ)_{y,x}\) are given by \((U_θ)_{y,x} = \{a_{y,σ}^\dagger b_{θ,x,σ}\}\). One finds that \((U_θ)_{x,y} = (U_θ)^*_{x,y}\) for \(θ = α, β\) while \((U_θ)_{x,y} = -(U_θ)^*_{x,y}\) for \(θ = γ\).

Using \((U_θ)_{x,y}\), let us define

\[ ζ_θ = Φ \sum_{x,y \in Λ} (U_θ)_{x,y} \tilde{a}_{x,σ}^\dagger \tilde{a}_{y,σ}, \quad (8) \]

which are the creation operators for electron-pairing states. The main result in this paper is as follows:

Theorem. Suppose \(λ ≠ 0\) and consider \(H_θ \) with \(W = t/4\) and fixed \(N_θ\) less than \(2|Λ|\). When \(N_θ\) is even, the ground state is unique, has zero energy, and is given by

\[ Φ_{θ,N_θ} = (ζ_θ^N_θ) Φ_0. \quad (9) \]

For odd \(N_θ\) the ground state has positive energy.

Before proceeding to the proof, we discuss the properties of \(H_{int,θ}\) and pairing states.

By using the Fourier transforms of the c-operator, the fermion operators \(a_{x,σ}^\dagger, b_{θ,x,σ}^\dagger\) are expanded as

\[ a_{x,σ}^\dagger = \frac{1}{\sqrt{|Λ|}} \sum_{k \in Κ} g(k) e^{ik \cdot x} c_{k,σ}^\dagger, \quad (10) \]

\[ b_{θ,x,σ}^\dagger = \frac{1}{\sqrt{|Λ|}} \sum_{k \in Κ} g(k) e^{ik \cdot x} c_{k,σ}^\dagger, \quad (11) \]

where \(g(k) = 2(cos(k_1 + θ_2) + cos(k_2 + θ_2))\) for \(k = (k_1, k_2)\) and \(θ = (θ_1, θ_2)\). One also finds from (10) that \(\tilde{a}_{x,σ}^\dagger = 1/\sqrt{|Λ|} \sum_{k \in Κ} g^{-1}(k) e^{ik \cdot x} c_{k,σ}^\dagger\). Substitution of this and (11) into \(ζ_θ\) yields \(ζ_θ = Φ \sum_{x,y \in Λ} a_{x,σ}^\dagger a_{y,σ}\), which follows from (6) and (7), yields

\[ ζ_θ = \sum_{k \in Κ} g(k) c_{k,σ}^\dagger c_{-k,τ}^\dagger. \quad (12) \]

The precise expressions of \(g_θ(k)\) are given by \(g_α(k) = 2(cos k_1 + cos k_2), g_β(k) = 2(cos k_1 - cos k_2),\) and \(g_γ(k) = -2(sin k_1 + sin k_2)\) (see Fig. 2). These mean that \(ζ_θ^\dagger \) and \(ζ_θ\) correspond to anisotropic spin-0 pairs while \(ζ_θ\) corresponds to an anisotropic spin-1 pair.

We find from (12) that \(H_{int,θ}\) is expressed in the wave space as

\[ H_{int,θ} = -\frac{1}{|Λ|} \sum_{k,k',q \in Κ} W_{k,k',q} g(k) c_{k,σ}^\dagger c_{-k,τ}^\dagger c_{k',σ}^\dagger c_{-k',τ}^\dagger \quad (13) \]

\[ W_{k,k',q} = W(g(k + q)g(k' - q)g(k')g(κ)g(k) + g(k + q)g(k' - q)g(k')g(κ)g(k)). \quad (14) \]
One notices that our interaction Hamiltonian expressed as above contains scattering processes of electron pairs with non-zero total momentum. It should be also noted that for scattering processes with zero total momentum, only which are discussed in mean-field-type arguments, the amplitudes $W_{k,-k,q}^\theta = 2Wg(k+q)g_\theta(k)g(k)g(k)$ become either positive or negative, depending on values of $q$ and $k$. Nevertheless, the ground states are the superpositions of products of the electron pairs with zero total momentum.

In the case of $\theta = \gamma$, if we consider a Hamiltonian $H'_\theta$ obtained by replacing $H^\text{int}_\gamma$ with $H^\text{int}_\theta$ as

$$H^\text{int}_\theta = -W \sum_{x} \sum_{\sigma = \uparrow, \downarrow} b^\dagger_{\theta,x,\sigma} b_{\theta,x,\sigma} a_{x,\sigma},$$

which is interpreted as attraction between electrons with the same spin, the following states become ground states for $H'_\theta$. It is noted that the fully-polarized pairing states $\Phi_{\gamma,N,\uparrow,0}$ and $\Phi_{\gamma,0,N,\downarrow}$ are stable for the on-site repulsion or the ferromagnetic interaction. These results may have some relevance to recently discovered materials exhibiting the superconductivity as well as the ferromagnetism 3,10.

In the following, we shall prove the theorem for $\theta = \beta, \gamma$. The case of $\theta = \alpha$ can be proved in a similar but slightly simpler way.

Proof of Theorem for $\theta = \beta, \gamma$. We first note that, by using the $a$-operator, $H^\text{hop}$ is rewritten as $H^\text{hop} = t \sum_x \sum_{\sigma = \uparrow, \downarrow} a^\dagger_{x,\sigma} a_{x,\sigma}$. Then, using this representation of $H^\text{hop}$ as well as $W = t/4$, we obtain

$$H_\theta = W \sum_{x} \sum_{\sigma = \uparrow, \downarrow} a^\dagger_{x,\sigma} b_{\theta,x,\sigma} a_{x,\sigma} + v_\theta \sum_{\sigma = \uparrow, \downarrow} c^\dagger_{0,\sigma} c_{0,\sigma}. \quad (15)$$

Since all the operators in the right hand side are positive semidefinite, a state which is annihilated by these operators is a ground state, having zero energy. We show that this is the case for $\Phi_{\theta,N_e}$ in 8.

It follows from 6, 11 and $(b^\dagger_{\theta,x,\sigma})^2 = 0$ that

$$b^\dagger_{\theta,x,\sigma} a_{x,\sigma} \Phi_{\theta,N_e} = b^\dagger_{\theta,x,\sigma} \left( \sum_{y} (U^t_{\theta})_{x,y} a^\dagger_{y,\sigma} + \zeta_0 a_{x,\sigma} \right) = \zeta_0 b^\dagger_{\theta,x,\sigma} a_{x,\sigma}. \quad (16)$$

Noting that $(U^t_{\beta})_{x,y}$ and $(U^t_{\gamma})_{x,y}$ are symmetric and anti-symmetric, respectively, with respect to the exchange of $x$ and $y$, we similarly obtain $b^\dagger_{\theta,x,\sigma} a_{x,\sigma} \Phi_{\theta,N_e} = \zeta_0 b^\dagger_{\theta,x,\sigma} a_{x,\sigma}$. These relations imply that $\Phi_{\theta,N_e}$ is a zero-energy state of the first term in the right hand side of 13. Furthermore, using $c_{0,\sigma} = 1/\sqrt{|A|} \sum_{x \in A} (1 - 4\lambda)^{-1} a_{x,\sigma}$ and

$$\sum_{x \in A} b^\dagger_{\theta,x,\sigma} = 0, \quad (17)$$

which follow from straightforward calculations, we find that $c_{0,\sigma} \Phi_{\theta,N_e} = \zeta_0 c_{0,\sigma}$. This together with the above result leads to $H_\theta \Phi_{\theta,N_e} = 0$. Therefore, $\Phi_{\theta,N_e}$ is a ground state of $H_{\theta}$. To see that $\Phi_{\theta,N_e}$ is actually a non-zero state, one rewrites $\zeta_0$ as

$$\zeta_0 = \sum_{x \in A \setminus \{0\}} (a^\dagger_{x,\uparrow} - a^\dagger_{0,\uparrow}) b^\dagger_{\theta,x,\downarrow} \quad (18)$$

by use of 17. Since each set of $\{ (a^\dagger_{x,\sigma} - a^\dagger_{0,\sigma}) \Phi_{0} \}_{x \in A \setminus \{0\}}$ and $\{ b^\dagger_{\theta,x,\sigma} \Phi_{0} \}_{x \in A \setminus \{0\}}$ is linearly independent 11, $\Phi_{\theta,N_e}$ is non-vanishing.

The representation 18 of $\zeta_0$ motivates us to introduce the following lemma, from which the other statements in the theorem follow.

Lemma. Suppose $\lambda \neq 0$. Any zero-energy state of $H_\theta$ with $\theta = \beta, \gamma$, $W = t/4$ and $N_e$ less than $2|A|$ (where $N_e$ is not fixed) is expanded as

$$\sum_{A \subseteq \Lambda \setminus \{0\}} \phi_A \left( \prod_{x \in A} (a^\dagger_{x,\uparrow} - a^\dagger_{0,\uparrow}) \right) \left( \prod_{x \in A} b^\dagger_{\theta,x,\downarrow} \right) \Phi_0 \quad (19)$$

where the coefficients $\phi_A$ satisfy $\phi_A = \phi_{A'}$ for any subsets $A, A'$ such that $|A| = |A'|$.

This lemma implies that the ground state energy for odd $N_e$ is positive. Suppose that there are two linearly independent zero-energy states for fixed even $N_e$. Since both of these states must satisfy the statement in the lemma, we find that the one is always represented by the other, which contradicts the assumption. Therefore, the ground state for fixed even $N_e$ is unique. $\blacksquare$

Proof of Lemma. The parameter $\theta$ is assumed to be $\beta$ or $\gamma$ in this proof. Let us define $\tilde{a}^\dagger_{0,\sigma} = c_{0,\sigma}$ and $\tilde{a}^\dagger_{x,\sigma} = a_{x,\sigma} - a_{0,\sigma}$ for $x \in \Lambda \setminus \{0\}$ and also define $b^\dagger_{0,\sigma} = c_{0,\sigma}$ and $b^\dagger_{\theta,x,\sigma} = b_{\theta,x,\sigma}$ for $x \in \Lambda \setminus \{0\}$. These new operators satisfy the anticommutation relations

$$\{ \tilde{a}^\dagger_{0,\sigma}, \tilde{a}^\dagger_{x,\sigma} \} = \{ b^\dagger_{0,\sigma}, b^\dagger_{\theta,x,\sigma} \} = 0 \quad (20)$$

for $x \in \Lambda$. Furthermore, each set of $\{ \tilde{a}^\dagger_{x,\sigma} \Phi_{0} \}_{x \in \Lambda}$ and $\{ b^\dagger_{\theta,x,\sigma} \Phi_{0} \}_{x \in \Lambda}$ is linearly independent and spans the single-electron Hilbert space. Thus, the collection of states $\Phi_{(A,B)} = (\prod_{x \in A} \tilde{a}^\dagger_{x,\sigma}) (\prod_{x \in B} b^\dagger_{\theta,x,\sigma}) \Phi_0$ with subsets $A$ and $B$ such that $|A| + |B| = N_e$ forms a complete basis for the $N_e$-electron Hilbert space. Here, the spin index $\upsilon$ is fixed to either $\uparrow$ or $\downarrow$.

Let $\Phi$ be an arbitrary zero-energy state of $H_\theta$ with $W = t/4$. We first expand $\Phi$ in terms of the basis states $\Phi_{(A,B)}$ as $\Phi = \sum_{A,B \subseteq \Lambda} \phi_{(A,B)} \Phi_{(A,B)}$ with coefficients $\phi_{(A,B)}$. To be a zero-energy state, $\Phi$ must satisfy $c_{0,\sigma} \Phi = 0$.
Taking account of the above results, we rewrite \( \Phi \) as \( \Phi = \Phi(\{A\} \setminus \{0\}) \) with \( \Phi(\{A\} \setminus \{0\}) \) does not contain a nearest-neighbor site \( y \) of \( x_0 \) but does contain next-nearest-neighbor site \( y' \) in the same direction. (The sites \( x_0, y, y' \) are in the same axis.) For this set of sites, \( F_{y,y'}^{x_0} \) is non-zero. Then, by checking the coefficient of \( \Phi(\{A\} \setminus \{0\}) \), we have \( \text{sgn}[y,y';A] \phi_A + \text{sgn}[y,y';B] \phi_B = 0 \) where \( \phi_A \) is defined for \( x \in A \) and \( \phi_B \) is defined for \( x \in B \).

Repeating the same argument for all \( x \in \{A\} \setminus \{0\} \), we reach the conclusion that \( \phi_A = \phi_A' \) whenever \( |A| = |A'| \), which completes the proof of the lemma.

Now let us consider the case of \( \lambda = 0 \) at half-filling with the inclusion of the on-site repulsion. Here, we further assume that \( v_0 = 0 \) for all \( \theta \) and that \( L_1 \) and \( L_2 \) are even integers. In this case the Hamiltonian becomes \( H_{x,y} = W \sum_{x,y} c_{x,y}^{\dagger} c_{x,y} + U \sum_{x,y} c_{x,y}^{\dagger} c_{x,y} c_{x+1,y} c_{x+1,y} + \sum_{x,y} c_{x,y}^{\dagger} c_{x,y} c_{x+1,y} c_{x+1,y} - \sum_{x,y} c_{x,y}^{\dagger} c_{x,y} c_{x,y} + \sum_{x,y} c_{x,y}^{\dagger} c_{x,y} c_{x,y} c_{x,y} \).

One can readily find that the Hamiltonian \( H_0 \) does not possess spin rotational symmetry. In the case of \( \theta = \alpha, \beta \), however, we can construct an isotropic model with the ground state \( \Phi(\{A\}) \) as follows. Let us define \( H_{\text{int},0} = W \sum_{x,y} (a_{x,y}^{\dagger} b_{x,y} - a_{x,y} b_{x,y}^{\dagger} c_{x,y}^{\dagger} c_{x,y}) + \sum_{x,y} c_{x,y}^{\dagger} c_{x,y} c_{x,y} c_{x,y} \).

A straightforward calculation yields that \( H_{\text{int},\theta} = \sum_{x,y} c_{x,y}^{\dagger} c_{x,y} c_{x,y} c_{x,y} \).

A construction of an isotropic model for the spin-1 pairing case and detailed investigation of perturbed models of ours in both spin-0 and 1 cases are left as an interesting future study.
with \( k \in \mathcal{K} \). Since \( L_1 \) and \( L_2 \) are odd integers and differ by \( 2 \), \( g_\theta(k) \) with \( \theta = \beta, \gamma \) become zero if and only if \( k = (0,0) \). Thus, the dimension of the kernel of \( G_\theta \) with \( \theta = \beta, \gamma \) is one. This together with \( \text{(17)} \) proves the linear independence. In the case of \( \theta = \alpha \), all \( g_\alpha(k) \) are non-zero, so that \( \{b_{\alpha,x,\sigma}^\dagger \Phi_0\}_{x \in \Lambda} \) is linearly independent.

[12] Recall the relation \( \zeta_\theta^j = \sum_{x} a_{x,\downarrow}^\dagger b_{x,\downarrow}^\dagger = \sum_{x} b_{x,\uparrow}^\dagger a_{x,\uparrow}^\dagger \) for \( \theta = \alpha, \beta \), and use \( \text{(18)} \).

[13] We note that \( H_{\text{int},\theta} + H'_{\text{int},\theta} \) is rewritten as \( \frac{W}{4} H_{\text{hop}} + W \sum_x \{S_\alpha^a \cdot S_\beta^b - \frac{3}{4} n_\sigma^a n_\tau^b \} \) where \( n_\sigma^a = \sum_{\sigma} a_{x,\sigma}^\dagger a_{x,\sigma}^\dagger \), \( (S_\alpha^a)^{(l)} = \sum_{\sigma,\gamma} a_{x,\sigma}^\dagger p_{\sigma,\gamma}^{(l)} a_{x,\gamma} \) with the Pauli matrices \( p^{(l)} \), and \( n_\sigma^b \) etc. are defined similarly for the \( b \)-operator.