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 T_c cuprates,[2] ruthenate,[3] organic conductors,[4] etc. The common feature of those compounds is the proximity of antiferromagnetic or ferromagnetic order. A vast number of studies have been 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; however, 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 that 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[5] in which all electrons form anisotropic pairs with spin 0 or spin 1, depending on a phase parameter [θ in (3)] 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 nontrivial in the present model, in which a model Hamiltonian is proved to exhibit condensation of unconventional electron pairs including spin-1 pairs.[6] A further advantage of our model is a relation to the proximity of magnetic orders. In a case in which there are no electron-hopping terms, the model exhibits antiferromagnetism at half-filling, when on-site repulsion terms of Hubbard-type are 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 $\Lambda=[1,L_1]\times[1,L_2]\cap\mathbb{Z}^2$ with periodic boundary conditions. It is assumed that L_1 is an odd positive integer and $L_2=L_1+2$. (We need these conditions to prove the uniqueness of the ground state, as we will show later.) We denote by $c_{x,\sigma}(c^\dagger_{x,\sigma})$ the annihilation (creation) operator for an electron with spin $\sigma=\uparrow,\downarrow$ at site x. They satisfy the anticommutation relations $\{c^\dagger_{x,\sigma},c^\dagger_{y,\tau}\}=\{c_{x,\sigma},c_{y,\tau}\}=0$ and $\{c^\dagger_{x,\sigma},c_{y,\tau}\}=\delta_{x,y}\delta_{\sigma,\tau}$. We denote by Φ_0 a state without electrons and by N_e the electron number.

The hopping part of our Hamiltonian is given by $H_{\mathrm{hop}}=\sum_{x,y\in\Lambda}\sum_{\sigma=\uparrow,\downarrow}t_{x,y}c^\dagger_{x,\sigma}c_{y,\sigma}$, 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.[7] Here, it is assumed that $t>0$ and $-1/4<\lambda<1/4$. In the wave space, it is represented as $H_{\mathrm{hop}}=\sum_{k\in\mathcal{K}}\sum_{\sigma=\uparrow,\downarrow}\varepsilon(k)\overline{c}^\dagger_{k,\sigma}\overline{c}_{k,\sigma}$, where $\varepsilon(k)=tg^2(k)$ with $g(k)=1-2\lambda\cos k_1-2\lambda\cos k_2$ for $k=(k_1,k_2)$, $\overline{c}_{k,\sigma}=1/\sqrt{|\Lambda|}\sum_{x\in\Lambda}e^{ik\cdot x}c_{x,\sigma}$, and

$$\mathcal{K}=\left\{\left(\frac{2\pi n_1}{L_1},\frac{2\pi n_2}{L_2}\right)\Big|n_l=0,\pm1,\ldots,\pm\frac{L_l-1}{2}\right\}. \quad (1)$$

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

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

$$a_{x,\sigma}=c_{x,\sigma}-\lambda\sum_{y\in\Lambda;|y-x|=1}c_{y,\sigma}, \quad (2)$$

$$b_{\theta,x,\sigma}=\sum_{y\in\Lambda;|y-x|=1}e^{-i\theta\cdot(y-x)}c_{y,\sigma} \quad (3)$$

with $\theta\in\{\alpha,\beta,\gamma\}$ where $\alpha=(0,0)$, $\beta=(0,\pi)$, and $\gamma=(\pi/2,\pi/2)$. The interaction discussed in this paper is at-

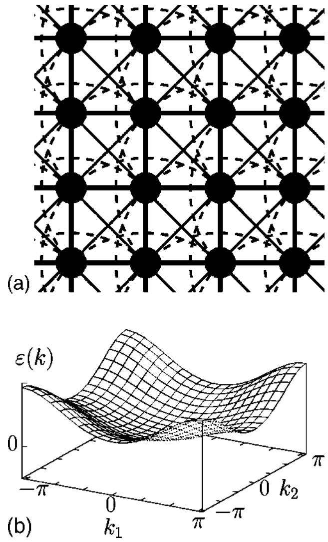

FIG. 1. (a) Lattice structure. (b) Dispersion relation.

traction between electrons in these localized states. The interaction part of our Hamiltonian is given by

$$H_{\mathrm{int},\theta} = -W\sum_{x\in\Lambda}\sum_{\sigma=\uparrow,\downarrow} b^{\dagger}_{\theta,x,-\sigma}b_{\theta,x,-\sigma}a^{\dagger}_{x,\sigma}a_{x,\sigma} \tag{4}$$

with $W>0$. One easily finds that the summand in (4) is bounded below by $-4(1+4\lambda^2)W$, which is attained by the states of the form $a^{\dagger}_{x,\sigma}b^{\dagger}_{\theta,x,-\sigma}\cdots\Phi_0$. This indicates that $H_{\mathrm{int},\theta}$ describes the attraction between two electrons with opposite spins.

The whole Hamiltonian of our model is given by

$$H_{\theta} = H_{\mathrm{hop}} + H_{\mathrm{int},\theta} + v_{\theta}\sum_{\sigma=\uparrow,\downarrow}\overline{c}^{\dagger}_{0,\sigma}\overline{c}_{0,\sigma}, \tag{5}$$

where $v_{\theta}=0$ if $\theta=\alpha$ and $v_{\theta}>0$ otherwise. The last term is added for a technical reason to show the uniqueness.

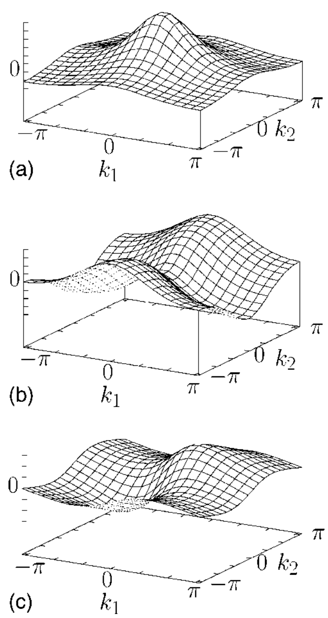

FIG. 2. Wave-vector dependence of $g_{\theta}(-k)/g(k)$. (a) $\theta=\alpha=(0,0)$. (b) $\theta=\beta=(0,\pi)$. (c) $\theta=\gamma=(\pi/2,\pi/2)$.

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

$$\{a^{\dagger}_{x,\sigma},\tilde{a}_{y,\tau}\} = \{\tilde{a}^{\dagger}_{x,\sigma},a_{y,\tau}\} = \delta_{x,y}\delta_{\sigma,\tau}. \tag{6}$$

Since $\{\tilde{a}^{\dagger}_{x,\sigma}\Phi_0\}_{x\in\Lambda}$ spans the single-electron Hilbert space, the b_{θ}-operators (3) are expanded as

$$b_{\theta,x,\sigma} = \sum_{y\in\Lambda}(U_{\theta})_{y,x}\tilde{a}_{y,\sigma}. \tag{7}$$

Here, the expansion coefficients $(U_{\theta})_{y,x}$ are given by $(U_{\theta})_{y,x}=\{a^{\dagger}_{y,\sigma},b_{\theta,x,\sigma}\}$. One finds that $(U_{\theta})_{x,y}=(U_{\theta})_{y,x}=(U_{\theta})^{*}_{y,x}$ for $\theta=\alpha,\beta$ while $(U_{\theta})_{x,y}=-(U_{\theta})_{y,x}=(U_{\theta})^{*}_{y,x}$ for $\theta=\gamma$.

Using $(U_{\theta})_{x,y}$, let us define

$$\zeta^{\dagger}_{\theta} = \sum_{x,y\in\Lambda}(U_{\theta})_{x,y}\tilde{a}^{\dagger}_{x,\uparrow}\tilde{a}^{\dagger}_{y,\downarrow}, \tag{8}$$

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

Theorem. *Suppose* $\lambda\neq 0$ *and consider* H_{θ} *with* $W=t/4$ *and fixed* N_{e} *less than* $2|\Lambda|$. *When* N_{e} *is even, the ground state is unique, has zero energy, and is given by*

$$\Phi_{\theta,N_{\mathrm{e}}} = (\zeta^{\dagger}_{\theta})^{N_{\mathrm{e}}/2}\Phi_0. \tag{9}$$

For odd N_{e} *the ground state has positive energy.*

Before proceeding to the proof, we discuss the properties of $H_{\mathrm{int},\theta}$ and pairing states.

By using the Fourier transforms of the c-operator, the fermion operators $a^{\dagger}_{x,\sigma}$, $b^{\dagger}_{\theta,x,\sigma}$ are expanded as

$$a^{\dagger}_{x,\sigma} = \frac{1}{\sqrt{|\Lambda|}}\sum_{k\in\mathcal{K}}g(k)e^{ik\cdot x}\overline{c}^{\dagger}_{k,\sigma}, \tag{10}$$

$$b^{\dagger}_{\theta,x,\sigma} = \frac{1}{\sqrt{|\Lambda|}}\sum_{k\in\mathcal{K}}g_{\theta}(k)e^{ik\cdot x}\overline{c}^{\dagger}_{k,\sigma}, \tag{11}$$

where $g_{\theta}(k)=2[\cos(k_1+\theta_2)+\cos(k_2+\theta_2)]$ for $k=(k_1,k_2)$ and $\theta=(\theta_1,\theta_2)$. One also finds from (10) that $\tilde{a}^{\dagger}_{x,\sigma}=1/\sqrt{|\Lambda|}\Sigma_{k\in\mathcal{K}}g^{-1}(k)e^{ik\cdot x}\overline{c}^{\dagger}_{k,\sigma}$. Substitution of this and (11) into $\zeta^{\dagger}_{\theta}=\Sigma_{x\in\Lambda}\tilde{a}^{\dagger}_{x,\uparrow}b^{\dagger}_{\theta,x,\downarrow}$, which follows from (7) and (8), yields

$$\zeta^{\dagger}_{\theta} = \sum_{k\in\mathcal{K}}\frac{g_{\theta}(-k)}{g(k)}\overline{c}^{\dagger}_{k,\uparrow}\overline{c}^{\dagger}_{-k,\downarrow}. \tag{12}$$

The precise expressions of $g_{\theta}(k)$ are given by $g_{\alpha}(k)=2(\cos k_1+\cos k_2)$, $g_{\beta}(k)=2(\cos k_1-\cos k_2)$, and $g_{\gamma}(k)=-2(\sin k_1+\sin k_2)$ (see Fig. 2). These mean that $\zeta^{\dagger}_{\alpha}$ and $\zeta^{\dagger}_{\beta}$ correspond to anisotropic spin-0 pairs, while $\zeta^{\dagger}_{\gamma}$ corresponds to an anisotropic spin-1 pair.

We find from (10) and (11) that $H_{\mathrm{int},\theta}$ is expressed in the wave space as

$$H_{\mathrm{int},\theta}=-\frac{1}{|\Lambda|}\sum_{k,k',q\in\mathcal{K}}W^{\theta}_{k,k',q}\overline{c}^{\dagger}_{k+q,\uparrow}\overline{c}^{\dagger}_{k'-q,\downarrow}\overline{c}_{k',\downarrow}\overline{c}_{k,\uparrow},\qquad(13)$$

$$W^{\theta}_{k,k',q}=W[g(k+q)g_{\theta}(k'-q)g_{\theta}(k')g(k)+g_{\theta}(k+q)g(k'-q)g(k')g_{\theta}(k)].\qquad(14)$$

One notices that our interaction Hamiltonian expressed as above contains scattering processes of electron pairs with nonzero total momentum. It should be also noted that for scattering processes with zero total momentum, which only are considered in mean-field-type arguments, the amplitudes $W^{\theta}_{k,-k,q}=2Wg(k+q)g_{\theta}(k+q)g_{\theta}(k)g(k)$ 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'_{γ} obtained by replacing $H_{\mathrm{int},\gamma}$ with $H'_{\mathrm{int},\gamma}=-W\Sigma_{x\in\Lambda}\Sigma_{\sigma=\uparrow,\downarrow}b^{\dagger}_{\gamma,x,\sigma}b_{\gamma,x,\sigma}a^{\dagger}_{x,\sigma}a_{x,\sigma}$, which is interpreted as attraction between electrons with the same spin, the following states become ground states for $\lambda\neq 0$ and $W=t/4$: $\Phi_{\gamma,N_{\mathrm{e},\uparrow},N_{\mathrm{e},\downarrow}}=(\zeta^{\dagger}_{\gamma,\uparrow})^{N_{\mathrm{e},\uparrow}/2}(\zeta^{\dagger}_{\gamma,\downarrow})^{N_{\mathrm{e},\downarrow}/2}\Phi_0$ with even positive integers $N_{\mathrm{e},\uparrow}$ and $N_{\mathrm{e},\downarrow}$ less than $|\Lambda|$, where the pairing operators are given by $\zeta^{\dagger}_{\gamma,\sigma}=\Sigma_{x,y\in\Lambda}(U_{\gamma})_{x,y}\tilde{a}^{\dagger}_{x,\sigma}\tilde{a}^{\dagger}_{y,\sigma}$.[8] For $N_{\mathrm{e},\uparrow}\neq N_{\mathrm{e},\downarrow}$, $\Phi_{\gamma,N_{\mathrm{e},\uparrow},N_{\mathrm{e},\downarrow}}$ has a finite value of $(N_{\mathrm{e},\uparrow}-N_{\mathrm{e},\downarrow})/2$, an eigenvalue of the third component of the total spin. This means that the coexistence of ferromagnetism and spin-1 pair condensation is realized in the ground states of H'_{γ}. It is noted that the fully polarized pairing states $\Phi_{\gamma,N_{\mathrm{e},\uparrow},0}$ and $\Phi_{\gamma,0,N_{\mathrm{e},\downarrow}}$ are stable for the on-site repulsion or the ferromagnetic interaction. These results may have some relevance to recently discovered materials exhibiting superconductivity as well as ferromagnetism.[9,10]

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_{hop} is rewritten as $H_{\mathrm{hop}}=t\Sigma_x\Sigma_{\sigma}a^{\dagger}_{x,\sigma}a_{x,\sigma}$. Using this representation of H_{hop} as well as $W=t/4$, we then obtain

$$H_{\theta}=W\sum_{x\in\Lambda}\sum_{\sigma=\uparrow,\downarrow}a^{\dagger}_{x,\sigma}b_{\theta,x,-\sigma}b^{\dagger}_{\theta,x,-\sigma}a_{x,\sigma}+v_{\theta}\sum_{\sigma=\uparrow,\downarrow}\overline{c}^{\dagger}_{0,\sigma}\overline{c}_{0,\sigma}.\qquad(15)$$

Since all the operators in the right-hand side are positive semidefinite, a state that is annihilated by these operators is a ground state, having zero energy. We show that this is the case for $\Phi_{\theta,N_{\mathrm{e}}}$ in (9).

It follows from (6) and (7), and $(b^{\dagger}_{\theta,x,\sigma})^2=0$ that

$$b^{\dagger}_{\theta,x,\downarrow}a_{x,\uparrow}\zeta^{\dagger}_{\theta}=b^{\dagger}_{\theta,x,\downarrow}\left(\sum_{y\in\Lambda}(U_{\theta})_{x,y}\tilde{a}^{\dagger}_{y,\downarrow}+\zeta^{\dagger}_{\theta}a_{x,\uparrow}\right)=\zeta^{\dagger}_{\theta}b^{\dagger}_{\theta,x,\downarrow}a_{x,\uparrow}.\qquad(16)$$

Noting that $(U_{\beta})_{x,y}$ and $(U_{\gamma})_{x,y}$ are symmetric and antisymmetric, respectively, with respect to the exchange of x and y, we similarly obtain $b^{\dagger}_{\theta,x,\uparrow}a_{x,\downarrow}\zeta^{\dagger}_{\theta}=\zeta^{\dagger}_{\theta}b^{\dagger}_{\theta,x,\uparrow}a_{x,\downarrow}$. These relations imply that $\Phi_{\theta,N_{\mathrm{e}}}$ is a zero-energy state of the first term in the right-hand side of (15). Furthermore, using $\overline{c}_{0,\sigma}=1/\sqrt{|\Lambda|}\Sigma_{x\in\Lambda}(1-4\lambda)^{-1}a_{x,\sigma}$ and

$$\sum_{x\in\Lambda}b^{\dagger}_{\theta,x,\sigma}=0,\qquad(17)$$

which follow from straightforward calculations, we find that $\overline{c}_{0,\sigma}\zeta^{\dagger}_{\theta}=\zeta^{\dagger}_{\theta}\overline{c}_{0,\sigma}$. This, together with the above result, leads to $H_{\theta}\Phi_{\theta,N_{\mathrm{e}}}=0$. Therefore, $\Phi_{\theta,N_{\mathrm{e}}}$ is a ground state of H_{θ}. To see that $\Phi_{\theta,N_{\mathrm{e}}}$ is actually a nonzero state, one rewrites $\zeta^{\dagger}_{\theta}$ as

$$\zeta^{\dagger}_{\theta}=\sum_{x\in\Lambda\setminus\{0\}}(\tilde{a}^{\dagger}_{x,\uparrow}-\tilde{a}^{\dagger}_{0,\uparrow})b^{\dagger}_{\theta,x,\downarrow}\qquad(18)$$

by use of (17). Since each set of $\{(\tilde{a}^{\dagger}_{x,\sigma}-\tilde{a}^{\dagger}_{0,\sigma})\Phi_0\}_{x\in\Lambda\setminus\{0\}}$ and $\{b^{\dagger}_{\theta,x,\sigma}\Phi_0\}_{x\in\Lambda\setminus\{0\}}$ is linearly independent,[11] $\Phi_{\theta,N_{\mathrm{e}}}$ is nonvanishing.

The representation (18) of $\zeta^{\dagger}_{\theta}$ 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_{θ} with $\theta=\beta,\gamma$, $W=t/4$ and N_{e} less than $2|\Lambda|$ (where N_{e} is not fixed) is expanded as

$$\sum_{A\subset\Lambda\setminus\{0\}}\phi_A\left(\prod_{x\in A}(\tilde{a}^{\dagger}_{x,\uparrow}-\tilde{a}^{\dagger}_{0,\uparrow})\right)\left(\prod_{x\in A}b^{\dagger}_{\theta,x,\downarrow}\right)\Phi_0,\qquad(19)$$

where the coefficients ϕ_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. □

Proof of Lemma. The parameter θ is assumed to be β or γ in this proof. Let us define $\tilde{a}'_{0,\sigma}=\overline{c}_{0,\sigma}$ and $\tilde{a}'_{x,\sigma}=\tilde{a}_{x,\sigma}-\tilde{a}_{0,\sigma}$ for $x\in\Lambda\setminus\{0\}$ and also define $b'_{\theta,0,\sigma}=\overline{c}_{0,\sigma}$ and $b'_{\theta,x,\sigma}=b_{\theta,x,\sigma}$ for $x\in\Lambda\setminus\{0\}$. These new operators satisfy the anticommutation relations

$$\{\tilde{a}'^{\dagger}_{0,\sigma},\tilde{a}'_{x,\sigma}\}=\{b'^{\dagger}_{\theta,0,\sigma},b'_{\theta,x,\sigma}\}=\delta_{0,x}\qquad(20)$$

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 $\Phi^{\upsilon}_{(A,B)}=(\Pi_{x\in A}\tilde{a}'^{\dagger}_{x,\upsilon})(\Pi_{x\in B}b'^{\dagger}_{\theta,x,-\upsilon})\Phi_0$ with subsets A and B such that $|A|+|B|=N_{\mathrm{e}}$ forms a complete basis for the N_{e}-electron Hilbert space. Here, the spin index υ is fixed to either ↑ or ↓.

Let Φ be an arbitrary zero-energy state of H_{θ} with $W=t/4$. We first expand Φ in terms of the basis states $\Phi^{\downarrow}_{(A,B)}$ as $\Phi=\Sigma_{A,B\subset\Lambda}\phi_{(A,B)}\Phi^{\downarrow}_{(A,B)}$ with coefficients $\phi_{(A,B)}$. To be a zero-energy state, Φ must satisfy $\overline{c}_{0,\sigma}\Phi=0$ and $b^{\dagger}_{\theta,x,-\sigma}a_{x,\sigma}\Phi=0$ for $\sigma=\uparrow,\downarrow$ and $x\in\Lambda$. From the former condition and (20), we find that $\phi_{(A,B)}=0$ if 0 is contained in either A or B, or both. From the latter condition for $x_0\in\Lambda\setminus\{0\}$ with $\sigma=\downarrow$ and $\{\tilde{a}'^{\dagger}_{x,\sigma},a_{y,\sigma}\}=\delta_{x,y}$ for x, $y\in\Lambda\setminus\{0\}$, we obtain

$$\sum_{A,B\subset\Lambda\setminus\{0\}}\chi[x_0\in A, x_0\notin B]\mathbf{sgn}[x_0;A,B] \times \phi_{(A,B)}\Phi^{\downarrow}_{(A\setminus\{x_0\},B\cup\{x_0\})}=0, \qquad (21)$$

where $\mathbf{sgn}[\cdots]$ is a sign factor coming from exchanges of the fermion operators, and χ ["event"] takes 1 if "event" is true and 0 otherwise. Since all the terms in the left-hand side are linearly independent, we find $\phi_{(A,B)}=0$ if $x_0\in A$ in addition to $x_0\notin B$. This holds for any $x\in\Lambda\setminus\{0\}$, so that only the terms with A, B such that $A\subset B\subset\Lambda\setminus\{0\}$ can contribute to the expansion. Taking account of the above results, we rewrite Φ as $\Phi=\Sigma_{A,B\subset\Lambda;|A|\geqslant|B|}\phi'_{(A,B)}\Phi^{\uparrow}_{(A,B)}$ with new coefficients $\phi'_{(A,B)}$. Operating $\overline{c_{0,\sigma}}$ and $b^{\dagger}_{\theta,x_0,\downarrow}a_{x_0,\uparrow}$ on Φ in this form and repeating an argument similar to the above, we find that Φ is expanded in terms of $\Phi^{\uparrow}_{(A,B)}$ with A, B such that $A=B\subset\Lambda\setminus\{0\}$.

Any zero-energy state is thus written as $\Sigma_{A\subset\Lambda\setminus\{0\}}\phi_A\Phi^{\uparrow}_{(A,A)}$ where $\phi_A=\phi'_{(A,A)}$. We again consider the zero-energy state condition $b^{\dagger}_{\theta,x_0,\uparrow}a_{x_0,\downarrow}\Phi=0$ for $x_0\in\Lambda\setminus\{0\}$ and derive conditions on ϕ_A. Here, it is noted that $b_{\theta,x_0,\sigma}$ is expanded as $b_{\theta,x_0,\sigma}=\Sigma_{y\in\Lambda\setminus\{0\}}(U_\theta)_{y,x_0}\tilde{a}'_{y,\sigma}$. From this and the anticommutation relation $\{b'^{\dagger}_{\theta,x,\sigma},a_{x_0,\sigma}\}=\{b^{\dagger}_{\theta,x,\sigma},a_{x_0,\sigma}\}=(U_\theta)_{x,x_0}$ for $x\in\Lambda\setminus\{0\}$, we deduce

$$\sum_{A\subset\Lambda\setminus\{0\}}\ \sum_{y,y'\in\Lambda\setminus\{0\}}\chi[y\notin A, y'\in A]\mathbf{sgn}[y,y';A] \times F^{x_0}_{y,y'}\phi_A\Phi^{\uparrow}_{(A\cup\{y\},A\setminus\{y'\})}=0, \qquad (22)$$

where $F^{x_0}_{y,y'}=(U_\theta)_{x_0,y}(U_\theta)_{y',x_0}$, and $\mathbf{sgn}[\cdots]$ is a fermion sign factor. Let us choose a subset A that 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, and y' are in the same axis.) For this set of sites, $F^{x_0}_{y,y'}$ is nonzero. By checking the coefficient of $\Phi^{\uparrow}_{(A\cup\{y\},A\setminus\{y'\})}$, we then have $(\mathbf{sgn}[y,y';A]\phi_A+\mathbf{sgn}[y',y;A_{y'\to y}]\phi_{A_{y'\to y}})=0$ where $A_{x\to y}$ is defined for $x\in A$ and $y\notin A$ by $A_{x\to y}=(A\setminus\{x\})\cup\{y\}$. Since $\mathbf{sgn}[y,y';A]=-\mathbf{sgn}[y',y;A_{y'\to y}]$, we obtain $\phi_A=\phi_{A_{y'\to y}}$.

Repeating the same argument for all $x\in\Lambda\setminus\{0\}$, 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 furthermore assume that $v_\theta=0$ for all θ and that L_1 and L_2 are even integers. In this case the Hamiltonian becomes $H^{\lambda=0}_{\theta,U}=W\Sigma_x\Sigma_\sigma c^{\dagger}_{x,\sigma}b_{\theta,x,-\sigma}b^{\dagger}_{\theta,x,-\sigma}c_{x,\sigma}+U\Sigma_x c^{\dagger}_{x,\uparrow}c^{\dagger}_{x,\downarrow}c_{x,\downarrow}c_{x,\uparrow}$ with $U>0$, which is still positive semidefinite. At half-filling, zero-energy states of on-site repulsion term are given by $(\Pi_{x\in\Lambda}c^{\dagger}_{x,\sigma_x})\Phi_0$ with $\sigma_x=\uparrow,\downarrow$. Considering the zero-energy condition for the first term in the Hamiltonian, we then conclude that the ground states of $H^{\lambda=0}_{\theta,U}$ are twofold degenerate and given by the Néel states, exhibiting antiferromagnetism.

One can readily find that the Hamiltonian H_θ does not possess spin rotational symmetry. In the case of $\theta=\alpha,\beta$, however, we can construct an isotropic model with the ground state (9) as follows. Let us define $H'_{\mathrm{int},\theta}=(W/2)\Sigma_x(a^{\dagger}_{x,\uparrow}b_{\theta,x,\uparrow}-a^{\dagger}_{x,\downarrow}b_{\theta,x,\downarrow})(b^{\dagger}_{\theta,x,\uparrow}a_{x,\uparrow}-b^{\dagger}_{\theta,x,\downarrow}a_{x,\downarrow})$ for $\theta=\alpha,\beta$. A straightforward calculation yields that $(b^{\dagger}_{\theta,x,\uparrow}a_{x,\uparrow}-b^{\dagger}_{\theta,x,\downarrow}a_{x,\downarrow})\zeta^{\dagger}_\theta=\zeta^{\dagger}_\theta(b^{\dagger}_{\theta,x,\uparrow}a_{x,\uparrow}-b^{\dagger}_{\theta,x,\downarrow}a_{x,\downarrow})$,[12] and, since $H'_{\mathrm{int},\theta}$ is positive semidefinite, (9) remains the ground state of $H_\theta+H'_{\mathrm{int},\theta}$ with $W=t/4$ for $\theta=\alpha,\beta$. Furthermore, $H_\theta+H'_{\mathrm{int},\theta}$ is isotropic since it commutes with $S^{(3)}_{\mathrm{tot}}=\Sigma_x(c^{\dagger}_{x,\uparrow}c_{x,\uparrow}-c^{\dagger}_{x,\downarrow}c_{x,\downarrow})/2$ and $S^{+}_{\mathrm{tot}}=\Sigma_x c^{\dagger}_{x,\uparrow}c_{x,\downarrow}$.[13] 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.

[1] M. Sigrist and K. Ueda, Rev. Mod. Phys. **63**, 239 (1991).

[2] C. C. Tsuei and J. R. Kirtley, Rev. Mod. Phys. **72**, 969 (2000).

[3] Y. Maeno, T. M. Rice, and M. Sigrist, Phys. Today **54**(1), 42 (2001).

[4] K. Kanoda, Physica C **282–287**, 299 (1997), and references therein.

[5] The uniqueness of the ground state excludes an appearance of physically less interesting phenomena such as the paramagnetism and the translational symmetry breaking in a finite system. It guarantees that one can discuss the physical properties of the model by analyzing the exact ground states.

[6] Related models were studied in A. Tanaka, J. Phys. A **37**, 1559 (2004); A. Tanaka, J. Phys. Soc. Jpn. **73**, 1107 (2004).

[7] Here $|\cdot|$ denotes the Euclidean norm. The same symbol $|X|$ is used to denote the number of elements in a set X.

[8] From the wave-space representation of $\zeta^{\dagger}_{\gamma,\sigma}$, one finds that the states $\Phi_{\gamma,N_{\mathrm{e},\uparrow},N_{\mathrm{e},\downarrow}}$ are nonvanishing. Unfortunately, the uniqueness of the ground state for fixed values of $N_{\mathrm{e},\uparrow}$ and $N_{\mathrm{e},\downarrow}$ is not proved at present.

[9] S. S. Saxena *et al.*, Nature (London) **406**, 587 (2000).

[10] D. Aoki, A. Huxley, E. Ressouche, D. Braithwaite, J. Flouquet, J. P. Brison, E. Lhotel, and C. Paulsen, Nature (London) **413**, 613 (2001).

[11] The linear independence of $\{b^{\dagger}_{\theta,x,\sigma}\Phi_0\}_{x\in\Lambda\setminus\{0\}}$ with $\theta=\beta,\gamma$ is proved as follows. Let G_θ be the Gram matrices of b-operators whose matrix elements are given by $(G_\theta)_{x,y}=\{b^{\dagger}_{\theta,x,\sigma},b_{\theta,y,\sigma}\}$. The eigenvalues of G_θ are $g^2_\theta(k)$ 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_θ with $\theta=\beta,\gamma$ is 1. This together with (17) proves the linear independence. In the case of $\theta=\alpha$, all $g_\alpha(k)$ are nonzero, so that $\{b^{\dagger}_{\alpha,x,\sigma}\Phi_0\}_{x\in\Lambda}$ is linearly independent.

[12] Recall $\zeta^{\dagger}_\theta=\Sigma_x\tilde{a}^{\dagger}_{x,\uparrow}b^{\dagger}_{\theta,x,\downarrow}=\Sigma_x b^{\dagger}_{\theta,x,\uparrow}\tilde{a}^{\dagger}_{x,\downarrow}$, and use (6).

[13] We note that $H_{\mathrm{int},\theta}+H'_{\mathrm{int},\theta}$ is rewritten as $(2W/t)H_{\mathrm{hop}}+W\Sigma_x\{\boldsymbol{S}^a_x\cdot\boldsymbol{S}^b_x-\frac{3}{4}n^a_x n^b_x\}$, where $n^a_x=\Sigma_\sigma a^{\dagger}_{x,\sigma}a_{x,\sigma}$, $(S^a_x)^{(l)}=\Sigma_{\sigma,\tau}a^{\dagger}_{x,\sigma}(p^{(l)}_{\sigma,\tau}/2)a_{x,\tau}$ with the Pauli matrices $p^{(l)}$, and n^b_x etc. are defined similarly for the b-operator.