Exact Electron-Pairing Ground States of Tight-Binding Models with Local Attractive Interactions

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(Dated: March 22, 2022)

We present a class of exactly solvable models of correlated electrons. The models are defined in any dimension \( d \) and consist of electron-hopping terms and local attractive interactions between electrons. For each even number of electrons less than or equal to \( 1/(d+1) \)-filling, we find the exact ground state in which all electrons form pairs of a certain type, and thus the models exhibit an electron-pair condensation.

PACS numbers: 71.10.Fd, 74.20.-z

The origin of high-temperature superconductivity has attracted much interest and is still controversial. On the other hand, the properties of usual (low-temperature) superconductors are well explained by the celebrated Bardeen-Cooper-Schrieffer (BCS) theory [1]. On the basis of the BCS theory, one treats electron systems with effective electron-electron attraction arising from electron-phonon couplings and discusses a phase transition associated with an electron-pair condensation by using mean-field type approximations. However, whether attractive interactions between electrons really induce the formation of many electron pairs and their condensation is not at all trivial, and it is desirable to clarify this point without relying on approximation methods.

One of the results in this direction was obtained by Shen and Qiu [2], who proved the existence of off-diagonal long-range order, closely related to a condensation, in the Hubbard model with on-site attractive interactions on certain bipartite lattices. Another was obtained by Essler, Korepin, and Schoutens [3], who proposed solvable extended Hubbard models exhibiting a condensation at zero temperature \( \eta \)-pair [4, 5] which is a superposition of on-site pairs with momentum 0. There are some rigorous results related to these models, in particular, in one dimension where the models are exactly solvable by Bethe ansatz (see, for example, [6, 7, 8] and references therein). Results in higher dimensions are limited.

In this letter we introduce a new class of exactly solvable models exhibiting a condensation at zero temperature [9, 10]. The models are defined in arbitrary dimensions and consist of hopping terms of electrons and local attractive interactions between electrons. We show that the models have the ground states in which all electrons form pairs of a certain type. It is worth to note that our pair, unlike the \( \eta \)-pair used in the results mentioned above, is made up of spin-singlet pairs of electrons at different sites in addition to on-site pairs. We also show that, in the momentum space, the exact ground states are represented as superpositions of products of pairs formed from electrons with opposite wave vectors and spins.

As seen later, the present models are related to nearly-flat-band models, which are proved to exhibit ferromagnetism [11, 12, 13, 14]. Several authors [15, 16, 17] proposed possibilities of experimental realization of the nearly-flat-band ferromagnetism. Our results suggest that there is a chance of finding superconductivity or interesting phenomena caused by competition between magnetism and superconductivity as well as ferromagnetism in the proposed systems.

To simplify the discussion, we describe the results in the simplest version of the models. We can consider similar models on other lattices constructed by using the same methods as that by Mielke [11] and that by Tasaki [14], which were developed in the study of (nearly) flat-band ferromagnetism. Let \( V \) be a \( d \)-dimensional hypercubic lattice \( [1, L]^d \cap \mathbb{Z}^d \) with periodic boundary conditions, where \( L \) is an arbitrary integer. Let \( M \) be a collection of sites located at the mid-points of nearest-neighbor pairs in \( V \). Then we define decorated lattice \( \Lambda = V \cup M \). We denote by \( c_{i,\sigma} \) and \( c_{i,\sigma}^\dagger \) the annihilation and the creation operators, respectively, for an electron with spin \( \sigma = \uparrow, \downarrow \) at site \( i \in \Lambda \). These operators satisfy usual fermion anticommutation relations. The number operator \( n_{i,\sigma} \) is defined as \( n_{i,\sigma} = c_{i,\sigma}^\dagger c_{i,\sigma} \). We denote by \( N_0 \) the electron number and by \( \Phi_0 \) a state without electrons. We define fermion operators, which play an essential role in our model, as

\[
\begin{align*}
\alpha_x,\sigma &= c_x,\sigma - \alpha \sum_{u \in M \cap |u-x|=1/2} c_{u,\sigma} \\
\beta_u,\sigma &= c_{u,\sigma} + \alpha \sum_{x \in V \cap |x-u|=1/2} c_{x,\sigma}
\end{align*}
\]

for \( x \in V \) and

\[
\begin{align*}
\alpha_x,\sigma &= c_{x,\sigma} - \alpha \sum_{u \in M \cap |u-x|=1/2} c_{u,\sigma} \\
\beta_u,\sigma &= c_{u,\sigma} + \alpha \sum_{x \in V \cap |x-u|=1/2} c_{x,\sigma}
\end{align*}
\]

for \( u \in M \), where \( \alpha \) is a real number. We note that localized single-electron states corresponding to \( \alpha \)-operator and \( \beta \)-operator are orthogonal because

\[
\{ \beta_u,\sigma, a_x,\sigma^\dagger \} = 0
\]

for any \( x \in V \) and any \( u \in M \).

We consider the tight-binding model of electrons with local attractive interactions described by the Hamilto-
The operator $H^a$ creates an electron in the band with the dispersion relation $\varepsilon_a(k) = s + 2a^2t(1 + \cos k)$ and $b^\dagger_{i,\sigma}$ creates an electron in the band with $\varepsilon_{b,i}(k) = t + 2a^2t(1 + \cos k)$.

$$H = H^a_{\text{hop}} + H^b_{\text{hop}} + H_{\text{int}} \quad \text{with}$$

$$H^a_{\text{hop}} = s \sum_{x \in V} \sum_{\sigma = \uparrow, \downarrow} a^\dagger_{x,\sigma} a_{x,\sigma},$$

$$H^b_{\text{hop}} = t \sum_{u \in M} \sum_{\sigma = \uparrow, \downarrow} b^\dagger_{u,\sigma} b_{u,\sigma},$$

$$H_{\text{int}} = -W \sum_{x \in V} a^\dagger_{x,\uparrow} a^\dagger_{x,\downarrow} a_{x,\uparrow} a_{x,\downarrow},$$

where $s, t$ and $W$ are positive parameters. It is noted that $H$ conserves the electron number $N_e$ and possesses the spin SU(2) symmetry.

The sum of $H^a_{\text{hop}}$ and $H^b_{\text{hop}}$ can be reduced to a standard tight-binding Hamiltonian $\sum_{i,j \in \Lambda} \sum_{\alpha} t_{ij} \Phi^\dagger_{i,\alpha} \Phi_{j,\alpha}$, describing quantum mechanical motion of electrons in $\Lambda$. It follows from \ref{18} that the dispersion relations of the model are classified into two types; one corresponds to single-electron states $(a^\dagger_{x,\sigma}\Phi_0)_{x \in V}$, and the others correspond to $(b^\dagger_{u,\sigma}\Phi_0)_{u \in M}$. More precisely, the dispersion relations are given by $\varepsilon_a(k) = s + 2a^2t(1 + \cos k_l)$, $\varepsilon_{b,i}(k) = t + 2a^2t \sum_{l=1}^d (1 + \cos k_l)$, and $\varepsilon_{b,m}(k) = t$ with $m = 2, \ldots, d$ (see Fig. 1 for an example in one dimension). Here, $k$ is the wave vector in the set $\mathcal{K}$.

$$\mathcal{K} = \{(2\pi n_1/L, \ldots, 2\pi n_d/L)|n_l = 0, \pm 1, \ldots, \pm (L-1)/2\}.\quad \text{(7)}$$

The energy eigenstate with eigenvalue $\varepsilon_a(k)$ is given by

$$a^\dagger_{k,\sigma} \Phi_0 \text{ with \ref{19}}$$

$$a^\dagger_{k,\sigma} = \sqrt{\frac{s}{\varepsilon_a(k)|V|^2}} \sum_{x \in V} e^{ik\cdot x} a^\dagger_{x,\sigma}.$$

The many-electron ground state of $H^a_{\text{hop}} + H^b_{\text{hop}}$ is usually the Fermi sea \ref{21}.

By rewriting each term in $H_{\text{int}}$ as

$$-W\|a\|^4 + W\|a\|^2 a^\dagger_{x,\uparrow} x^\dagger_{x,\downarrow} + W a^\dagger_{x,\downarrow} x^\dagger_{x,\uparrow} a^\dagger_{x,\downarrow}$$

with $\|a\|^2 = (1 + 2a^2t)$, one finds that this is bounded below by $-W\|a\|^4$, which is attained by states in the form of $a^\dagger_{x,\uparrow} a^\dagger_{x,\downarrow} \cdots \Phi_0$. The terms in $H_{\text{int}}$ are thus interpreted as attractive interactions between electrons in localized single-electron states corresponding to $a$-operator. In the $k$-space, $H_{\text{int}}$ is represented as

$$H_{\text{int}} = -\frac{1}{|V|} \sum_{k,k',q \in \mathcal{K}} W_{k,k',q} a^\dagger_{k,q} a^\dagger_{k'+q,\uparrow} a_{k'-q,\downarrow} a_{k,\uparrow},$$

which has a similar form to the BCS interaction Hamiltonian \ref{21}, although there is a difference in the dependence of the amplitudes on the wave vectors. It is noted that interaction $H_{\text{int}}$ contains scattering processes of electron pairs with non-zero total momentum, which are usually dropped in the BCS theory. Nevertheless, our theorem below establishes that the ground state of $H$ with fixed even $N_e$ consists of electron pairs having total momentum $0$ (see \ref{15} and \ref{16}).

Before stating our main result, we need to introduce further notation. Let $G$ be the $|V| \times |V|$ Gram matrix for $a$-operator, whose matrix elements are defined by $(G)_{xy} = \langle a^\dagger_{x,\sigma} a_{y,\sigma} \rangle$ for $x, y \in V$. Since $(a^\dagger_{x,\sigma}\Phi_0)_{x \in V}$ is linearly independent, $G$ is regular and has its inverse matrix $G^{-1}$. Then we introduce the dual operators of $a$-operator as $\tilde{a}_{x,\sigma} = \sum_{y \in V} (G^{-1})_{xy} a^\dagger_{y,\sigma}$ and the anti-commutation relations

$$\{\tilde{a}_{x,\sigma}, a^\dagger_{y,\tau}\} = \{a^\dagger_{x,\sigma}, \tilde{a}^\dagger_{y,\tau}\} = \delta_{xy}\delta_{\sigma\tau},$$

for $x, y \in V$ and $\sigma, \tau = \uparrow, \downarrow$. Let us define

$$\zeta^\dagger = \sum_{x,y \in V} (G)_{xy} \tilde{a}_{x,\uparrow}^\dagger \tilde{a}_{y,\downarrow}^\dagger,$$

which creates two electrons in a spin-singlet pairing state. We note that $\zeta^\dagger$ is rewritten as

$$\zeta^\dagger = \sum_{x \in V} \tilde{a}_{x,\uparrow}^\dagger \tilde{a}_{x,\downarrow}^\dagger = \sum_{x \in V} a^\dagger_{x,\uparrow} a^\dagger_{x,\downarrow} = \sum_{x,y \in V} (G^{-1})_{xy} a^\dagger_{x,\uparrow} a^\dagger_{y,\downarrow},$$

since $G$ and $G^{-1}$ are real symmetric matrices. Our main result in this letter is summarized as follows:
Theorem. Consider Hamiltonian $H$ with $W = 2s/|a|^2$ and fixed electron number $N_e$ in $N_e \leq 2|V|$. For even $N_e$, the ground state $\Phi_{G,N_e}$ is unique, has zero energy, and is expressed as

$$\Phi_{G,N_e} = (\zeta)^{\Delta} \Phi_0.$$ (15)

When $N_e$ is odd, the ground state has positive energy.

It is noted that the ground state energy for odd $N_e$ may converge to zero as $L \to \infty$. Whether this is the case or not should be clarified in a future study.

If we set $s = 1$ and $W = 0$, Hamiltonian $H = H_{\text{hop}}^u + H_{\text{int}}^b$ is equal to the hopping term of the nearly-flat-band model studied in Ref. [12]. Thus, in this case, the model has saturated ferromagnetic ground states for $N_e = |V|$ when sufficiently large on-site repulsion is added. We note that the ferromagnetic ground states found in the above situation survive for all $W$ and also for sufficiently small positive values of $W$ [22]. The present model with the on-site repulsion is expected to describe a quantum phase transition between magnetic states and electron-pairing states.

The elements of Gram matrix $G$ are explicitly given by $(G)_{xy} = 1 + 2d \rho^2$ if $x = y$, $(G)_{xy} = \alpha^2$ if $|x - y| = 1$, and $(G)_{xy} = 0$ otherwise, and a standard Fourier analysis yields $(G^{-1})_{xy} = |V|^{-1} \sum_{k \in \mathbb{K}} \frac{e^{i k (x-y)}}{2} \Delta_k$. From this, we find that the pair creation operator $\zeta$ is written as

$$\zeta = \sum_{k \in \mathbb{K}} a_{k,\uparrow}^\dagger a_{-k,\downarrow}.$$ (16)

Substituting this expression into (14), one finds that the ground state is a superposition of products of pairs $a_{k,\uparrow}^\dagger a_{-k,\downarrow}$. To see the representation of $\zeta$ in terms of $c$-operator, we substitute $a_{k,\sigma}^\dagger = \sum_{i \in \Lambda} \varphi_{xi} c_{i,\sigma}^\dagger$ into the final expression in (14), where $\varphi_{xi} = \{a_{x,\sigma}^\dagger, c_{i,\sigma}^\dagger\}$. Then we obtain

$$\zeta = \sum_{i \in \Lambda} w_i c_{i,\uparrow}^\dagger c_{i,\downarrow} + \sum_{i, j \in \Lambda; i < j} w_{ij} (c_{i,\uparrow}^\dagger c_{j,\downarrow}^\dagger + c_{i,\downarrow}^\dagger c_{j,\uparrow}^\dagger)$$ (17)

with $w_{ij} = \sum_{x,y \in V} (G^{-1})_{xy} \varphi_{xi} \varphi_{yj}$. Each term in the second sum in (17) corresponds to a spin-singlet pair of electrons at different sites. In the case of $x, y \in V$, the weight $w_{xy}$ of a pair reduces to $(G^{-1})_{xy}$, which has the Ornstein-Zernicke behavior for $|x - y| \gg 1$.

By making a linear combination of $\Phi_{G,N_e}$ with different electron numbers, we can construct an explicit electron-number symmetry breaking ground state. To see this, let us introduce order parameter $\Delta = \zeta/|V|$. A straightforward calculation yields

$$\langle \Delta_{\Lambda} \Delta_{\Lambda}^\dagger \rangle_{A,N_e} = \frac{(\Phi_{G,N_e}, \Delta_{\Lambda}^\dagger \Phi_{G,N_e})}{(\Phi_{G,N_e}, \Phi_{G,N_e})} = \mu_{\Lambda,N_e}.$$ (18)

with $\mu_{\Lambda,N_e} = (N_e/(2|V|) + 1/|V|)(1 - N_e/(2|V|))$. Taking a limit $L, N_e \to \infty$ so that the electron density $N_e/(2|\Lambda|)$ will converge to $\nu$, we conclude that $\langle \Delta_{\Lambda} \Delta_{\Lambda}^\dagger \rangle_{A,N_e} \to \mu_{\nu}$ with $\mu_{\nu} = (d+1)\nu(1-(d+1)\nu)$. Then, we define $\Phi_{G,N_e} = \left(1 + \Delta_{\Lambda}^\dagger/\sqrt{\langle \Delta_{\Lambda} \Delta_{\Lambda}^\dagger \rangle_{A,N_e}}\right) \Phi_{G,N_e}$, which is also a zero-energy state of $H$. It is easy to see that

$$\langle \Delta_{\Lambda} \rangle_{A,N_e} = \frac{(\Phi_{G,N_e}, \Delta_{\Lambda} \Phi_{G,N_e})}{(\Phi_{G,N_e}, \Phi_{G,N_e})} \to \sqrt{\mu_{\nu}}/2,$$ (19)

which implies the explicit electron-number symmetry breaking for $0 < \nu < 1/(d+1)$.

Proof of the theorem. By using $W = 2s/|a|^2$, we rewrite $H$ as $H = H_{\text{hop}}^b + H_{\text{int}}^b$ with

$$H_{\text{int}}^b = \frac{W}{2} \sum_{x \in V} \sum_{\sigma = \uparrow, \downarrow} a_{x,\sigma}^\dagger a_{x,\sigma} - \sum_{x \in V} a_{x,\uparrow}^\dagger a_{x,\downarrow}.$$ (20)

(Here $-\sigma$ denotes spin opposite to $\sigma$.) This expression is crucial in our proof. Since both $H_{\text{hop}}^b$ and $H_{\text{int}}^b$ are positive semidefinite operators, one can conclude that a zero-energy state of both of these terms is a ground state. We first show that $\Phi_{G,N_e}$ in (15) is in fact a zero-energy state of $H$. From (19) and $a_{x,\sigma}^\dagger = 0$, one finds that

$$a_{x,\uparrow}^\dagger a_{x,\uparrow}^\dagger = \zeta a_{x,\uparrow}^\dagger a_{x,\uparrow}^\dagger + a_{x,\uparrow}^\dagger a_{x,\downarrow}^\dagger = \zeta a_{x,\uparrow}^\dagger a_{x,\uparrow}^\dagger.$$ (21)

Similarly, we have $a_{x,\uparrow}^\dagger a_{x,\downarrow}^\dagger = \zeta a_{x,\uparrow}^\dagger a_{x,\downarrow}^\dagger x$. These two relations imply that $H_{\text{int}}^b \Phi_{G,N_e} = 0$. Furthermore it immediately follows from (20) that $H_{\text{hop}}^b \Phi_{G,N_e} = 0$. Therefore $\Phi_{G,N_e}$ is a ground state having zero energy.

To prove the other statement in the theorem, we use the following lemma, which will be proved later.

Lemma. Any zero-energy state $\Phi$ of $H$ with $N_e \leq 2|V|$ (where $N_e$ is not fixed) is written as

$$\Phi = \sum_{A \in \mathcal{V}} \phi_A \left( \prod_{x \in A} a_{x,\uparrow}^\dagger \right) \left( \prod_{x \in A} a_{x,\downarrow}^\dagger \right) \Phi_0,$$ (22)

where coefficients $\phi_A$ satisfy $\phi_A = \phi_{A'}$ if $|A| = |A'|$.

This lemma implies that the ground state energy for fixed odd $N_e$ is positive. Let us prove the uniqueness of the ground state for fixed even $N_e$. Now suppose that there are two zero-energy states. Then any linear combination of these states is also a zero-energy state, which must satisfy the statement in the lemma. However, this implies that all the coefficients are vanishing, since we can make a suitable linear combination such that a coefficient $\phi_A$ for a subset $A_0$ is zero. This is contradicting with the assumption, and thus the ground state, which must have zero energy, is unique. This completes the proof of the theorem.

Proof of the lemma. Let $\Phi$ be an arbitrary zero-energy state of $H$ with $N_e \leq 2|V|$. Since each term $tb_{u,\sigma} b_{u,\sigma}$ in $H_{\text{hop}}^b$ is positive semidefinite, $\Phi$ should satisfy $b_{u,\sigma} \Phi = 0$.
for any \( u \in M \) and \( \sigma = \uparrow, \downarrow \). Thus \( \Phi \) must be of the form

\[
\Phi = \sum_{A, A_x \subset V} \phi_{(A, A_x)} \left( \prod_{x \in A} a_{x, \uparrow}^\dagger \right) \left( \prod_{x \in A} a_{x, \downarrow}^\dagger \right) \Phi_0,
\]

where \( \phi_{(A, A_x)} \) are suitable coefficients. To be a zero-energy state, \( \Phi \) must furthermore satisfy

\( H'_{\text{int}} \Phi = 0 \), i.e., \( a_{x, \sigma}^\dagger \phi_{(A, A_x)} = 0 \) for any \( x \in V \) and \( \sigma = \uparrow, \downarrow \). By using

\[
\tilde{\Phi}_{(A, A_x)} = \left( \prod_{x \in A_x} a_{x, \uparrow} \right) \left( \prod_{x \in A_x} a_{x, \downarrow} \right) \Phi_0,
\]

we obtain \( \tilde{\Phi}_{(A, A_x)} \) and take \( \Phi \) as

\[
\Phi = \sum_{A, A_x \subset V} \phi_{(A, A_x)} \tilde{\Phi}_{(A, A_x)},
\]

where \( \phi_{(A, A_x)} \) are new coefficients, and operate \( a_{x, \uparrow}^\dagger a_{x, \uparrow} \) on \( \Phi \) in this form. Then, by using \( (12) \), we have

\[
\sum_{A, A_x \subset V} \chi[\{x \in A_\uparrow, x \notin A_\downarrow\}\text{sgn}[x; A_\uparrow, A_\downarrow]}
\]

\[
\times \phi_{(A, A_x)} \tilde{\Phi}_{(A, A_x)} \Psi_{\{x \in A_\downarrow \}, A \setminus \{x\}}(\{y\}) = 0,
\]

where \( \text{sgn}[\cdot \cdot \cdot] \) is a sign factor arising from exchanges of fermion operators, and \( \chi[\text{event}] \) takes 1 if “event” is true and 0 otherwise. Since all the terms in the left hand side in the above equation are linearly independent, we obtain \( \phi_{(A, A_x)} = 0 \) if both \( x \in A_\uparrow \) and \( x \notin A_\downarrow \). Since this must hold for all \( x \in V \), we find that the sum in \( (24) \) is restricted to subsets \( A_\uparrow, A_\downarrow \) such that \( A_\uparrow \subset A_\downarrow \).

By using \( \tilde{\Phi}_{(A, A_x)} = \left( \prod_{x \in A_x} a_{x, \uparrow} \right) \left( \prod_{x \in A_x} a_{x, \downarrow} \right) \Phi_0 \), and by taking account of the above result, we again rewrite \( \Phi \) as

\[
\Phi = \sum_{A, A_x \subset V \mid |A_\downarrow| \leq |A_\uparrow|} \phi_{(A, A_x)} \tilde{\Phi}_{(A, A_x)}
\]

with new coefficients \( \phi_{(A, A_x)} \). Operating \( a_{x_1, \uparrow}^\dagger a_{x_\uparrow, \downarrow} \) on \( \Phi \) in expression \( (26) \) and repeating a similar argument to the above, we find that \( \phi_{(A, A_x)} \) must be zero if \( A_\downarrow \neq A_\uparrow \).

Thus we have shown that \( \Phi \) must be written as

\[
\Phi = \sum_{A \subset V} \phi_A \tilde{\Phi}_A
\]

where \( \phi_A = \phi_{(A, A)} \). Now we again operate \( a_{x, \uparrow}^\dagger a_{x, \uparrow} \) on \( \Phi \) in expression \( (27) \) and derive conditions on \( \phi_A \). The resulting equation is

\[
\sum_{A \subset V} \sum_{y, y' \in V} \chi[y \notin A, y' \in A] \text{sgn}[y, y'; A]
\]

\[
\times F_{y y'}^{x x} \phi_A \tilde{\Phi}_A (A \setminus \{y\}, A \cup \{y\}) = 0,
\]

where \( F_{y y'}^{x x} = (G)_{y y'} (G)_{x x'} \) and \( \text{sgn}[\cdot \cdot \cdot] \) is a fermion-sign factor. Let us choose a subset \( A \) which contains site \( x \) and does not contain a site \( y \) with \( |y - x| = 1 \). By checking the coefficient of \( \tilde{\Phi}_A (A \setminus \{x\}, A \cup \{y\}) \), we have

\[
F_{y y'}^{x x} \phi_A \tilde{\Phi}_A (A \setminus \{x\}, A \cup \{y\}) (\{y\}) = 0,
\]

where \( A \cup \{y\} = (A \setminus \{x\}) \cup \{y\} \). Since \( F_{y y'}^{x x} \) for \( |y - x| = 1 \) is non-zero by definition and \( \text{sgn}[y, x; A] = -\text{sgn}[x, y; A] \), we find that the coefficients satisfy \( \phi_A = \phi_{A'} \). Repeating the same argument for all \( x \in V \), we conclude that \( \phi_A = \phi_{A'} \) whenever \( |A| = |A'| \). This completes the proof of the lemma.  

I would like to thank Masanori Yamanaka for useful discussions.

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[18] We assume that \( L \) is an odd integer here.
[19] For a set \( X \), \( |X| \) means the number of elements in \( X \).
[20] The dispersion relations for \( d \geq 2 \) contain a flat band, and thus the ground states in the non-interacting case are highly degenerate when the Fermi energy equals the flat-band energy.
[21] Note that \( (a_{k, \sigma}^\dagger \Phi_0)_{k \in K} \) is orthonormal.
[22] When \( s < 0 \), the model with \( N_0 = |V| \) is proved to exhibit saturated ferromagnetism for sufficiently large negative values of \( W \) even in the absence of on-site repulsion.