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Spin of the ground state and the flux phase problem on the ring

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Abstract
As a continuation of our previous work, we derive the optimal flux phase which minimizes the ground state energy in the one-dimensional many-particle systems, when the number of particles is odd in the absence of on-site interaction and external potential. Moreover, we study the relationship between the flux on the ring and the spin of the ground state through which we derive some information on the sum of the lowest eigenvalues of one-particle Hamiltonians.

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1. Introduction

The flux phase problem is to derive the optimal flux distribution which minimizes the ground state energy of the system of many fermions. There are a few physical significances of this problem, one of which is that the diamagnetic inequality, which widely holds for one-particle Hamiltonians, is sometimes reversed for many-particle ones. As for the mathematical results, we refer to [3, 4, 6] where many cases are studied at half-filling for bipartite rings, lattices, and ones with some particular geometry such as the tree of rings and hidden trees. Bethe-ansatz calculations are done in [10] where they study whether the current response to the variation of the magnetic flux is diamagnetic or paramagnetic. In this paper, we continue our study to derive the optimal flux of the Hubbard Hamiltonian on the ring $\Lambda := \{1, 2, \ldots, L\}$ $(L+1 \equiv 1)$ defined by

$$H := \sum_{\sigma=\uparrow,\downarrow} \sum_{x=1}^{L} t_{x,x+1} c^{\dagger}_{x+1,\sigma} c_{x,\sigma} + (\mathrm{hc}) + \sum_{\sigma=\uparrow,\downarrow} \sum_{x=1}^{L} V(x) n_{x,\sigma} + \sum_{x=1}^{L} U(x) n_{x,\uparrow} n_{x,\downarrow}$$

where $c_{x,\sigma}$ $\left(c^{\dagger}_{x,\sigma}\right)$ is the annihilation (creation) operator satisfying the canonical anticommutation relations and $n_{x,\sigma} := c^{\dagger}_{x,\sigma} c_{x,\sigma} \cdot t_{x,x+1} \neq 0$ and $\arg t_{x,x+1} = \theta_x \in [0, 2\pi)$ such that $\sum_{x=1}^{L} \theta_x = \varphi \pmod{2\pi}$. $U(x), V(x) \in \mathbf{R}$. Eigenvalues of H are independent of the choice of $\{\theta_x\}_{x=1}^L$ such that $\sum_{x=1}^L \theta_x = \varphi$ so that we write $H = H(\varphi)$. We consider $H(\varphi)$ on the spin-$\frac{1}{2}$ N-fermion Hilbert space $\mathcal{H}_N$ which is the span of

$$B_N := \left\{c^\dagger_{x_1,\sigma_1} c^\dagger_{x_2,\sigma_2} \cdots c^\dagger_{x_N,\sigma_N} |\mathrm{vac}\rangle : x_j \in \Lambda, \sigma_j = \uparrow, \downarrow, j = 1, 2, \ldots, N\right\}.$$

Let $E_N(\varphi)$ be the ground state energy of $H(\varphi)$:

$$E_N(\varphi) := \min\{\langle\Phi, H(\varphi)\Phi\rangle : \Phi \in \mathcal{H}_N, \langle\Phi, \Phi\rangle = 1\}.$$

Our aim is to derive the optimal flux φ_{opt} which minimizes $E_N(\varphi)$: $E_N(\varphi_{\mathrm{opt}}) = \min_{\varphi\in[0,2\pi)} E_N(\varphi)$. Uniqueness of φ_{opt}, which is not discussed in this paper, holds when $T := \{|t_{x,x+1}|\}_{x=1}^L$ has some periodicity, or T and V satisfy some particular relation [8]. In [7], we studied the case where N is even. The result there was

Theorem 1.1 (optimal flux on the ring: even case)**.** *Let $N \leqslant L$ be even:*
(1) $U < \infty$: $\varphi_{\mathrm{opt}} = \left(\frac{N}{2} + 1\right)\pi$ (L is even) $= \frac{N\pi}{2}$ (L is odd).
(2) $U = \infty$: $\varphi_{\mathrm{opt}} = \frac{2n}{N}\pi, n = 0, 1, \ldots, N-1$.

The key ingredient of the proof of theorem 1.1 was to regard $H(\varphi)$ as a hopping Hamiltonian on B_N and compute the flux through the circuit in B_N of 'minimal' length. The distinction between 0 and π comes from counting how many times a particle exchanges its location with others in these circuits. When $U = \infty$, such exchanges are not possible and hence there is no distinction. In fact, $E_N^\infty(\varphi) := \lim_{U\uparrow\infty} E_N(\varphi)$ has period[1] $\frac{2\pi}{N}$ and $H_\infty(0)$ is gauge equivalent to $H_\infty(\pi)$.[2]

We turn to the case where N is odd and $U = 0$. Some computations of examples imply that φ_{opt} depends on U in general and there seems to be no general rule except the half-filling case.

Theorem 1.2 (optimal flux on the ring: odd case)**.** *Let $N = L$ be odd and $U = V = 0$. Then $E_N(\varphi)$ has period π and is minimized if $\varphi = \frac{\pi}{2}, \frac{3\pi}{2}$.*

Remark 1.1. The same result is deduced in [9] by a different argument. For the translation invariant case ($t_{x,x+1}, U_x$ are constant), Bethe-ansatz calculation has been done [10] and the result of theorem 1.2 is the same as they obtained. Since we set $U = 0$, only the free particle case is considered in theorem 1.2. So our contribution is that the hopping coefficients $T = \{t_{x,x+1}\}_{x=1}^L$ can be arbitrary which is not covered by the Bethe-ansatz solutions. Therefore, in the free case, the hopping disorder has no effect on the optimal flux.

Remark 1.2. If $U = \infty$ and N $(<L)$ is odd, the argument of the proof of theorem 1.1.(2) proves that $E(\varphi)$ has period $\frac{2\pi}{N}$ and $\varphi_{\mathrm{opt}} = \frac{2n}{N}\pi$ (L even), $\frac{2n+1}{N}\pi$ (L odd), $n = 0, 1, \ldots, N-1$.

Remark 1.3. The following example implies that the conclusion of theorem 1.2 is not true in general if $V \neq 0$ so that the potential disorder may have some effect on the optimal flux. Let $N = L = 5$ and let

$$|t_{x,x+1}| = \begin{cases} 1 & (x = 1, 4) \\ t & (x = 3) \\ \sqrt{2} & (x = 2, 4) \end{cases} \qquad V(x) = \begin{cases} 0 & (x \neq 3, 4) \\ t & (x = 3, 4) \end{cases} \qquad t > 0.$$

[1] This fact and its implications are discussed in [1, 10].

[2] $H_\infty(\varphi) := PH(\varphi)P$ and $P := \prod_{x\in\Lambda}(1 - n_{x,\uparrow}n_{x,\downarrow})$ is the orthogonal projection onto the space of states with no doubly occupied sites.

Since the Hamiltonian $H(\varphi)$ contains terms of the form $t\big(c_{3,\sigma}^{\dagger} + c_{4,\sigma}^{\dagger}\big)(c_{3,\sigma} + c_{4,\sigma})$, when t is sufficiently large, eigenvalues of $H(\varphi)$ approach to that of $H'(\varphi + \pi)$ in which $N = 5$, $L = 4$ and $|t_{x,x+1}| = 1$ for any x. The ground state energy of $H'(\varphi + \pi)$ is minimized if and only if $\varphi = \pi \pm 4 \arcsin \frac{1}{\sqrt{5}}$. On the other hand, we believe theorem 1.2 is true when $U \neq 0$ as the computations in translation invariant cases imply [10].

Remark 1.4. At finite temperature, optimal flux is different from $\frac{\pi}{2}, \frac{3\pi}{2}$ in general. In fact, in the canonical ensemble, the partition function $P(\varphi) := \mathrm{Tr}[\mathrm{e}^{-\beta H(\varphi)}]$ (restricted on $S_z = 1/2$ subspace for simplicity) is a complicated function of φ if β is large, and $\varphi = \frac{\pi}{2}, \frac{3\pi}{2}$ do not necessarily maximize it, although they are always the critical points. This is different from the case of an even number of particles where $P(\varphi)$ is maximized for any $\beta > 0$ by the optimal flux given in theorem 1.1 [7]. In the grand canonical ensemble, the average particle number depends on φ, β and the absolute ground state does not lie at half-filling unless $\varphi = \frac{\pi}{2}, \frac{3\pi}{2}$. In [4], it is shown that the grand canonical partition function with zero chemical potential is maximized if $\varphi = 0, \pi$.

Next, we study the spin of the ground state. In what follow, we assume L is even for simplicity; the results for odd L follow by exchanging 0 and π in each statement of the theorems given below. The proof of theorem 1.1, together with the Lieb–Mattis argument [5], proves the following fact[3].

Theorem 1.3 (ground state is unique with spin zero)**.** *Let $U < \infty$, N even and $\varphi = \left(\frac{N}{2} + 1\right)\pi$ (mod 2π). Then the ground state of $H(\varphi)$ is unique and $S = 0$.*

Remark 1.5. If $\varphi = \frac{N\pi}{2}$ (mod 2π) and $|t_{x,x+1}| = 1$, $U = V = 0$, then the ground state of $H(\varphi)$ is not unique and $S = 0, 1$. This contrasts with the Lieb–Mattis theorem [5] which states that the ground state is always unique and $S = 0$ in the one-dimensional chain with open boundary condition (and thus no flux is present so that one can freely adjust the sign of the matrix elements). The example above shows, if φ is not optimal, that the boundary effect is not negligible in general. We also remark that such a 'non-unique' situation is not stable under the variation of T, V and U. For instance, once $U_x < 0$ for any x, then the ground state is again unique and $S = 0$ [2]. On the other hand, theorem 1.3 states, if φ is optimal, that this uniqueness property is stable which holds for any T, V and U.

Remark 1.6. When $N = L$ is odd, $U = V = 0$, and $\varphi = \frac{\pi}{2}, \frac{3\pi}{2}$, then the ground state is unique with $S = 1/2$ apart from the $(2S + 1)$-degeneracy.

When $U = \infty$, there is some relationship between the flux φ and the spin of the ground state. Let $\{e_j(\varphi)\}_{j=1}^{L}$ be the eigenvalues (in increasing order) of the one-particle Hamiltonian $h(\varphi)$ corresponding to $H(\varphi)$ (that is, $H(\varphi)$ is an operator on $\mathcal{H}_1$).

Theorem 1.4 (spin and flux are related)**.** *Let $N (< L)$ be even and $U = \infty$:*
(1) $H_\infty(0)$ does not have the ground state with $S = \frac{N}{2}$ if and only if $\sum_{j=1}^{N} e_j(\pi) < \sum_{j=1}^{N} e_j(0)$.
(2) $H_\infty(0)$ does not have the ground state with $S = \frac{N}{2}$.

Remark 1.7. Theorem 1.4 implies that the spin of the ground state changes when the flux changes. For instance, let $N = 4n + 2$. Then $H_\infty(\pi)$ has a ground state with $S = \frac{N}{2}$ while $H_\infty(0)$ does not, but has one with $S = 0$.

[3] Theorem 1.3 is pointed out by Professor E Lieb to whom the author is grateful.

Remark 1.8. The inequality $\sum_{j=1}^{N} e_j(\pi) \leqslant \sum_{j=1}^{N} e_j(0)$ follows from theorem 1.1. So the statement $\sum_{j=1}^{N} e_j(\pi) < \sum_{j=1}^{N} e_j(0)$ has something to do with the uniqueness question of the optimal flux. Theorem 1.4 states that an 'analytical' statement $\sum_{j=1}^{N} e_j(\pi) < \sum_{j=1}^{N} e_j(0)$ is equivalent to a property of the spin of the ground state, which is robust under the variation of T, V and U.

Finally, we discuss a connection between the ferromagnetic ($S = \frac{N}{2}$) ground state of $H_\infty(\pi)$ and the singlet ($S = 0$) one of $H_\infty(0)$. Since $H_\infty(\pi)$ is gauge equivalent to $H_\infty(0)$, there is a gauge transformation g under which $H_\infty(\pi)$ is transformed to $H_\infty(0)$.[4] Because the ground state of $H_\infty(\pi)$ is degenerate (it has at least all even (odd) spins for $N = 4n(4n+2)$), it is not clear how each ground state of $H_\infty(\pi)$ is transformed under g. In fact, when $N = 4n$, the ground states of $H_\infty(0)$ can have all spins such that $S < \frac{N}{2}$ and $g\Psi_f^{\pi,\infty}$ does not have fixed spin. However, if $N = 4n + 2$, we have the following theorem, which states that the ferromagnetic ground state of $H_\infty(\pi)$ is directly connected to the singlet ground state of $H_\infty(0)$ via the gauge transformation mentioned above.

Theorem 1.5 (a connection between ferromagnetic and singlet states)**.** *Let $N = 4n + 2$ and let $\Psi_f^{\pi,\infty}$ be the ferromagnetic ground state of $H_\infty(\pi)$. Then there is a gauge transformation g_∞ under which $H_\infty(\pi)$ is transformed to $H_\infty(0)$ and $g_\infty\Psi_f^{\pi,\infty}$ is a singlet ground state of $H_\infty(0)$.*

The singlet state $g_\infty\Psi_f^{\pi,\infty}$ is described as follows. If we write $\Psi_f^{\pi,\infty}$ as a linear combination of elements of B_N, the coefficients are the same for every configuration of spins for each fixed location of particles. The gauge transformation g_∞ then puts (-1) alternately on every cyclic permutation of spins. Therefore, the singlet ground state of $H_\infty(0)$ is a sort of 'spiral' state in the configuration space B_N produced from the ferromagnetic one.

In section 2, we give proof of theorems. Theorem 1.2 is proved by reducing the problem to the case of an even number of particles using the ideas of Floquet analysis. We remark that a simple adaptation of the method of proof of theorem 1.1 would lead us to a complicated computation of the partition function $P(\varphi)$ of $H(\varphi)$. Theorem 1.3 is proved by putting the arguments in [5, 7] together. The key fact is that the ground states of $H_{U\neq 0}$ and of $H_{U=0}$ are both unique and not orthogonal to each other. The ground state of $H_{U=0}$ has spin zero because it is unique. To prove theorem 1.4 (1), we use the Perron–Frobenius theorem which implies that $H_\infty(\pi)$ has the ferromagnetic state which makes it possible to derive the ground state energy of $E_N(\pi)$, which is equal to $E_N(0)$ since $H_\infty(0)$ and $H_\infty(\pi)$ are gauge equivalent. Then the equivalence follows from comparing ferromagnetic energies of $H_\infty(0)$ and $H_\infty(\pi)$. Theorem 1.4 (2) follows from comparing the spin of the ground state of $H_\infty(0)$ with that of $H_\infty^0(0)$ where $|t_{x,x+1}| = 1$ and $V = 0$. To prove theorem 1.5, we note that for $U < \infty$, $H(0)$ is gauge equivalent to H_{PF} whose matrix elements (B_N as its basis) are non-positive. The ground states of both are unique and that of $H(0)$ has $S = 0$ while that of H_{PF} is positive[5]. When U goes to infinity, the ground state of $H(0)$ tends to the singlet one of $H_\infty(0)$ while the ground state of H_{PF} tends to the ferromagnetic one of $H_\infty(\pi)$.

Section 3 is devoted to the discussion, and in the appendix, we prove a simple lemma which appears in the proof of theorem 1.1 (2).

[4] g is not unique, since $H_\infty(\varphi)$ is not irreducible.

[5] A state Ψ is positive (non-negative) means that Ψ is expanded as $\Psi = \sum_j a_j\psi_j$, $\psi_j \in B_N$ with $a_j > 0$ ($a_j \geqslant 0$) for all j.

2. Proof of theorems

First of all, we provide the proof of theorem 1.1(2) for the sake of completeness, because in [7], we only asserted $\varphi_{\mathrm{opt}} = 0, \pi$.

Proof of theorem 1.1(2). We assume L is even; the proof for odd L follows similarly. We always work on $S_z = 0$ subspace of $\mathcal{H}_N$ and let $\mathcal{G} = \mathrm{Range}\, P$ be the space of states with no doubly occupied sites. Let $\mathcal{G} = \mathcal{G}_1 \oplus \mathcal{G}_2 \oplus \cdots \oplus \mathcal{G}_K$ be the decomposition of $\mathcal{G}$ such that $H_j(\varphi) := H(\varphi)|_{\mathcal{G}_j}$ is irreducible. We choose the basis B_j of $\mathcal{G}_j$ as

$$B_j := \left\{ c^\dagger_{x_1,\sigma_1} c^\dagger_{x_2,\sigma_2} \cdots c^\dagger_{x_N,\sigma_N} |\mathrm{vac}\rangle : x_1 < x_2 < \cdots < x_N, \sigma_j = \uparrow, \downarrow \right\}. \tag{2.1}$$

Since $U = \infty$, exchange of particles is not allowed so that for each $c^\dagger_{x_1,\sigma_1} c^\dagger_{x_2,\sigma_2} \cdots c^\dagger_{x_N,\sigma_N} |\mathrm{vac}\rangle \in B_j$, the spin configuration $(\sigma_1, \sigma_2, \ldots, \sigma_N)$ of that can be obtained by the cyclic permutation[6] of a fixed spin configuration $(\tau_1, \tau_2, \ldots, \tau_N)$. There exists $p\,(= 2, \ldots, N)$ such that $(\tau_1, \tau_2, \ldots, \tau_N)$ is invariant under the cyclic permutations of p-times. Because we are working in $S_z = 0$ subspaces, p must be even. In this case, we say $\mathcal{G}_j$ has period p. We rearrange $\mathcal{G}_j$ w.r.t. their period and rewrite, $\mathcal{G} = \oplus_{p=2}^{N} \oplus_{j=1}^{J_p} \mathcal{G}_j^p$, where $\mathcal{G}_j^p$ has period p with B_j^p as its basis which is chosen like (2.1). Let $H_j^p(\varphi) := H(\varphi)|_{\mathcal{G}_j^p}$ which we regard as a hopping Hamiltonian on B_j^p. The flux Φ_j^p of these circuits in B_j^p with 'minimal' length[7] is given by

$$\Phi_j^p = p\varphi + p(N-1)\pi \equiv p\varphi \pmod{2\pi}.$$

The first term comes from the hopping of particles and the second one comes from the fact that if a particle hops from site L to site 1, we have to add π to the flux (as discussed in the proof of theorem in [7]). Therefore the lowest eigenvalue $E_j^p(\varphi)$ of $H_j^p(\varphi)$ is minimized if $\varphi_j^p = \frac{2\pi n}{p}$, $n = 0, 1, \ldots, p-1$. Since p is even, they always include $0, \pi$. Hence

$$E_j^p(\pi) = E_j^p\left(\frac{2\pi n}{p}\right) \qquad n = 0, 1, \ldots, p-1. \tag{2.2}$$

If $\varphi = \pi$, by taking the gauge such that $t_{x,x+1} < 0$ $(x = 1, 2, \ldots, N-1)$, and $t_{N,1} > 0$, the matrix elements of $H_j^p(\varphi)$ in terms of the basis B_j^p are non-positive. Hence, by the Perron–Frobenius theorem, we have a ferromagnetic ground state Ψ_f of $H_\infty(\pi)$ so that for some $\left\{a_j^p\right\}_{j,p}$, it is written as

$$\Psi_f = \sum_{j,p}^{K} a_j^p \psi_j^p \tag{2.3}$$

where ψ_j^p is the lowest eigenvector of $H_j^p(\pi)$. Since it has maximal spin, it can also be written as

$$\Psi_f = \sum_{x_1,\ldots,x_N} b_{x_1,\ldots,x_N} \sum_{\sigma_1,\ldots,\sigma_N} c^\dagger_{x_1,\sigma_1} c^\dagger_{x_2,\sigma_2} \cdots c^\dagger_{x_N,\sigma_N} |\mathrm{vac}\rangle$$

with $b_{x_1,\ldots,x_N} > 0$. Therefore for any fixed $x_1, x_2, \ldots, x_N$, every spin configuration $(\sigma_1, \sigma_2, \ldots, \sigma_N)$ appears in (2.3), so that $a_j^p \neq 0$ for any j, p. Hence the lowest eigenvalue $E_j^p(\pi)$ are the same for any j, p:

$$E_j^p(\pi) = E_N^\infty(\pi). \tag{2.4}$$

[6] The one-time cyclic permutation of a configuration $(\tau_1, \tau_2, \ldots, \tau_N)$ is defined by $(\tau_2, \tau_3, \ldots, \tau_N, \tau_1)$.

[7] 'Minimal' means circuits having least length whose flux depends on φ. If $L \geqslant 4$, the length of circuits of least length is always 4, but fluxes there are always zero and do not affect the discussion here.

By the diamagnetic inequality, we have

$$E_j^p(\pi) \leqslant E_j^p(\varphi) \qquad \varphi \in [0, 2\pi]. \tag{2.5}$$

The assertion $\varphi_{\text{opt}} = \frac{2\pi n}{N}$ then follows from (2.2), (2.4), (2.5).

The claim that $E(\varphi)$ has period $\frac{2\pi}{N}$ is proved by the following lemma.

Lemma 2.1. *$E_k^N(\varphi) \leqslant E_j^p(\varphi)$ for any $p = 2, \ldots, N$ and $j = 1, 2, \ldots, J_p$.*

The proof of lemma 2.1 is given in the appendix for completeness, which is a simple proof of the fact 'the hard core boson has the lowest energy'. Lemma 2.1 also gives an alternative and simpler proof of theorem 1.1(2), for $E_j^N(\varphi)$ has period $\frac{2\pi}{N}$. □

Proof of theorem 1.2. Let $\{e_j(\varphi)\}_{j=1}^L$ be the eigenvalue (in increasing order) of $H(\varphi)$ on $\mathcal{H}_1$, that is, eigenvalues of the corresponding one-particle Hamiltonian $h(\varphi)$, and let $F_K(\varphi) := \sum_{j=1}^K e_j(\varphi)$ be the sum of the K lowest eigenvalues. Let $N = 2n + 1$. By hole–particle transformation for down spins and by the assumption that $V = 0$, we have $E_N(\varphi) = F_n(\varphi) + F_{n+1}(\varphi) = F_n(\varphi) + F_n(\varphi + \pi)$. In what follows we show

$$F_n(\varphi) + F_n(\varphi + \pi) = F_{2n}^{2L}(2\varphi) \tag{2.6}$$

where $F_K^{2L}(\varphi)$ is the sum of the K lowest eigenvalues of the Hamiltonian $\hat{H}^{2L}(\varphi)$ given by extending $H(\varphi)$ to $\hat{\Lambda} := \{1, 2, \ldots, 2L\}$ periodically, i.e.

$$\hat{t}_{x,x+1} = \begin{cases} t_{x,x+1} & (x = 1, \ldots, L) \\ t_{x-L,x+1-L} & (x = L+1, \ldots, 2L) \end{cases} \qquad \hat{V} = \hat{U} = 0.$$

Once (2.6) is proved, theorem 1.1 leads us to the conclusion[8].

Proof of equation (2.6). By choosing the gauge, we assume $\theta_x = 0$ $(x \neq L), = \varphi$ $(x = L)$. Let $\left\{\psi_j^\varphi\right\}_{j=1}^L$ be the eigenvector of $h(\varphi)$ and set

$$\hat{\psi}_j^\varphi(x) := \begin{cases} \psi_j^\varphi(x) & (x = 1, 2, \ldots, L) \\ \mathrm{e}^{\mathrm{i}\varphi}\psi_j^\varphi(x) & (x = L+1, \ldots, 2L). \end{cases}$$

$\left\{\hat{\psi}_j^\varphi, \hat{\psi}_j^{\varphi+\pi}\right\}_{j=1}^L$ are linearly independent and are eigenvectors of $\hat{H}^{2L}(2\varphi)$ with eigenvalues $\{e_j(\varphi), e_j(\varphi+\pi)\}_{j=1}^L$. Then (2.6) follows from the fact that the ground state can be chosen from the $S_z = \frac{1}{2}$ subspace of $\mathcal{H}_N$, or alternatively, from the theory of one-dimensional periodic Schrödinger operators. □

Remark 2.1. The argument of the above proof shows $\frac{F_n(0)+F_n(\pi)}{2} \geqslant F_n\left(\frac{\pi}{2}\right)$ in general.

Proof of theorem 1.3. As usual, we work on $S_z = 0$ subspace. We fix $\varphi = \left(\frac{N}{2} + 1\right)\pi$ and write $H = H(U)$ to specify the U-dependence of H. For $x, y \in \mathcal{B}_N$, let $s_{xy} := \langle x|H(U)|y\rangle$. We regard $H(U)$ as a hopping Hamiltonian on $\mathcal{B}_N$: $(H(U)\psi)(x) = \sum_{y\in\mathcal{B}_N} s_{xy}\psi(y)$. Let $(H_-(U)\psi)(x) = -\sum_{y\in\mathcal{B}_N} |s_{xy}|\psi(y)$. Then by the argument in the proof of theorem in [7], $H(U)$ and $H_-(U)$ have same fluxes on each circuit in $\mathcal{B}_N$ so that they are gauge equivalent: there exists a gauge transformation g on $\mathcal{B}_N$ such that $H(U) = g^{-1}H_-(U)g$. Since s_{xy} does not depend on U for $x \neq y$, g is independent of U. By the Perron–Frobenius theorem, the ground state $\Psi_-(U)$ of $H_-(U)$ is unique and so is the ground state $\Psi(U)$ of $H(U)$. Since $\Psi_-(U)$ and $\Psi_-(0)$ are both positive and thus not orthogonal to each other, and since $\Psi(U)$

[8] Equation (2.6) and theorem 1.3 show that the ground state is unique if $\varphi = \frac{\pi}{2}, \frac{3\pi}{2}$ which proves the statement in remark 1.6.

and $\Psi_-(U)$ are related via the U-independent gauge transformation, $\Psi(U)$ and $\Psi(0)$ have the same spin and thus it suffices to derive the spin of $\Psi(0)$.

Now we regard $H(0)$ as an operator on $\mathcal{H}_N$ and let $e_1 \leqslant e_2 \leqslant \cdots \leqslant e_L, \psi_1, \psi_2, \ldots, \psi_L$ $(\in \mathbf{C}^L)$ be eigenvalues and corresponding eigenvectors of one-particle Hamiltonian of H (that is, $H(0)$ as an operator on $\mathcal{B}_1$). Since the ground state $\Psi(0)$ of $H(0)$ is unique, it is written by

$$\Psi(0) = \prod_{j=1,\sigma=\uparrow,\downarrow}^{L} \Psi_{j,\sigma}|\text{vac}\rangle \qquad \text{where} \quad \Psi_{j,\sigma} = \sum_{x=1}^{L} \psi_{j,\sigma}(x) c^\dagger_{x,\sigma}$$

which has spin zero. □

Proof of theorem 1.4. (1) By theorem 1.1(2), $E_N^\infty(0) = E_N^\infty(\pi)$. The matrix elements of $H_\infty(\pi)$ in terms of the basis B_N are non-positive so that the Perron–Frobenius theorem shows that $H_\infty(\pi)$ has a ground state with $S = \frac{N}{2}$. Hence $E_N^\infty(0) = E_N^\infty(\pi) = \sum_{j=1}^N e_j(\pi)$. Therefore the statement that $H_\infty(0)$ does not have a ground state with $S = \frac{N}{2}$ is equivalent to $\sum_{j=1}^N e_j(\pi) < \sum_{j=1}^N e_j(0)$.

(2) The essential ingredient of the proof is that the gauge transformation g, which transforms $H_\infty(\pi)$ to $H_\infty(0)$, transforms the ferromagnetic ground state $\Psi_f^{\pi,\infty}$ of $H_\infty(\pi)$ to those with $S < \frac{N}{2}$. In fact, g transforms $\Psi_f^{\pi,\infty}$ into that which is antisymmetric under the cyclic permutations. Let $\mathcal{G} :=$ Range$P$ be the subspace of $\mathcal{H}_N$ of states with no doubly occupied sites and let $\mathcal{G} = \oplus_{j=1}^K \mathcal{G}_j$ be the decomposition of $\mathcal{G}$ such that $H_j(\pi) := H_\infty(\pi)|_{\mathcal{G}_j}$ is irreducible as in the proof of theorem 1.1 (2). Since the matrix element of $H_j(\pi)$ is non-positive, the Perron–Frobenius theorem shows that the lowest eigenvector $\psi_j(\pi)$ is unique and positive. Moreover, $H_\infty(\pi)$ has a ground state Ψ with $S = \frac{N}{2}$. That is, there exists $\{a_j\}_{j=1}^K$ such that $\Psi = \sum_{j=1}^K a_j \psi_j(\pi)$ is a ground state of $H_\infty(\pi)$ with $S = \frac{N}{2}$. Fix distinct points $x_1, x_2, \ldots, x_N \in \Lambda$. Let

$$A := \left\{c^\dagger_{y_1,\sigma_1} \cdots c^\dagger_{y_N,\sigma_N}|\text{vac}\rangle \in \mathcal{G} : y_i = x_1, \ldots, x_N, \sigma = \uparrow, \downarrow\right\} \qquad A_j := A \cap B_j$$

and let P_A be the orthogonal projection onto the subspace of $\mathcal{G}$ spanned by A. Since Ψ has $S = \frac{N}{2}$, $P_A\Psi = a\sum_k \rho_k$, $\rho_k \in A$ for some $a > 0$ which implies that $P_A\psi_j(\pi) = b_j \sum_k \nu_{jk}$, $\nu_{jk} \in A_j$ for some $b_j > 0$. We normalize $\psi_j(\pi)$ such that $b_j = 1$. Since $H_\infty(\pi)$ and $H_\infty(0)$ are gauge equivalent, there exists a gauge transformation g such that $\psi_j(0) = g\psi_j(\pi)$. Suppose $H_\infty(0)$ has a ground state $\tilde{\Psi}$ with $S = \frac{N}{2}$. Then $\tilde{\Psi} = \sum_{j=1}^K c_j \psi_j(0)$ for some $\{b_j\}_{j=1}^K$ and

$$\mathbf{S}^2(P_A\tilde{\Psi}) = \frac{N}{2}\left(\frac{N}{2} + 1\right)(P_A\tilde{\Psi}). \tag{2.7}$$

Let $H_\infty^0(\varphi)$ be the Hamiltonian with $|t_{x,x+1}| = 1$ and $V = 0$. Let $\psi_j^0(\pi)$ be the corresponding lowest eigenvector of $H_\infty^0(\pi)|_{\mathcal{G}_j}$. Normalize $\psi_j^0(\pi)$ by the same procedure as above. Since $H_\infty^0(\pi)$ is transformed to $H_\infty^0(0)$ by the same gauge transformation g,

$$P_A\psi_j^0(0) = P_A\psi_j(0). \tag{2.8}$$

On the other hand, $\tilde{\Psi}_0 := \sum_{j=1}^K c_j \psi_j^0(0)$ is a ground state of $H(0)$ which satisfies

$$\mathbf{S}^2(P_A\tilde{\Psi}_0) = \frac{N}{2}\left(\frac{N}{2} + 1\right)(P_A\tilde{\Psi}_0) \tag{2.9}$$

by (2.7), (2.8). Equation (2.9) contradicts the fact that $H_\infty^0(0)$ has no ground state with $S = \frac{N}{2}$, since we have $\sum_{j=1}^N e_j(\pi) < \sum_{j=1}^N e_j(0)$ in this case. □

Proof of theorem 1.5. Let $U < \infty$. Then there is a gauge transformation g which is independent of U such that $H(0) = gH_{\text{PF}}\,g^{-1}$. H_{PF} is the Hamiltonian whose matrix elements (in terms of B_N) are non-positive and have the same absolute values as those of $H(0)$. The ground states Ψ_s^0, Ψ_{PF} of $H(0)$, H_{PF} satisfy

$$\Psi_s^0 = g\Psi_{\mathrm{PF}} \tag{2.10}$$

and Ψ_s^0 has $S = 0$ while Ψ_{PF} is positive. When U goes to infinity, $\lim_{U\uparrow\infty}\Psi_s^0 = \Psi_s^{0,\infty}$ which is a singlet ground state of $H_\infty(0)$. On the other hand, $\lim_{U\uparrow\infty} H_{\mathrm{PF}} = H_\infty(\pi)$ and moreover, $\lim_{U\uparrow\infty}\Psi_{\mathrm{PF}} = \Psi_f^{\pi,\infty}$ where $\Psi_f^{\pi,\infty}$ is the ferromagnetic ground state of $H_\infty(\pi)$. This follows from the observation that both Ψ_{PF} and $\Psi_f^{\pi,\infty}$ are positive and the other ground states of $H_\infty(\pi)$ are not non-negative. Letting $U \to \infty$ in (2.10), we have

$$\Psi_s^{0,\infty} = g_\infty \Psi_f^{\pi,\infty} \qquad g_\infty = g|_{\mathcal{G}}$$

which is the desired conclusion. □

3. Discussion

In this paper, we study the flux phase problem, that is, to minimize the ground state energy w.r.t. the flux, in the one-dimensional many-particle systems. In particular, we studied the case in which the particle number is odd at half-filling, and deduced that the optimal flux is $\frac{\pi}{2}$, $\frac{3\pi}{2}$, in the absence of on-site interaction. Such results are already derived by the Bethe-ansatz calculation [10], and thus our contribution is to show that this is also true even if the hopping coefficients are not constant, namely the hopping disorder has no effect on the optimal flux. Moreover, unlike the case of even number of particles, we find that something unusual happens: theorem 1.2 is not necessarily true if $V \neq 0$, implying that the potential disorder may have some effect on the optimal flux, or if the temperature is nonzero (remarks 1.3 and 1.4). This also implies that the method of proof of theorem in [7] may not apply to the case of odd numbers of particles in general.

Next, we study the spin of the ground state and showed that it is zero when the flux is optimal. When it is not optimal, the spin is not zero and changes its value depending on the hopping coefficients T, the on-site interaction U and the external potential V, implying that it is not stable. It also implies that the conclusion of the Lieb–Mattis theorem is not true for such cases so that the boundary effect is not negligible. Nevertheless, if the flux is optimal, the spin is always zero for any T, U and V, implying that it is always stable under the perturbation.

Moreover, we study the case in which $U = \infty$ and found a relation between the spin of the ground state and the sum of the lowest eigenvalues of the one-particle Hamiltonian. Since the spin is a 'robust' property, we can derive some information on the sum of lowest eigenvalues which holds for any T, U and V. We also discussed the 'spiral state': a singlet ground state of $H_\infty(0)$ which is obtained by a simple gauge transformation of a ferromagnetic state of $H_\infty(\pi)$. These results seem to reveal interesting connection between the flux threading the system and spin of the ground state.

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Appendix. Proof of lemma 2.1

Let Ψ_1 be the eigenvector of H_j^p with eigenvalue E. It suffices to construct the eigenvector Ψ_0 of H_k^N with the same eigenvalue E. We write Ψ_1, Ψ_0 in terms of the linear combination of their basis:

$$\Psi_1 = \sum_{x_1,\ldots,x_N,\sigma_1,\ldots,\sigma_N} a(x_1,\sigma_1;x_2,\sigma_2;\ldots;x_N,\sigma_N) c^\dagger_{x_1,\sigma_1} c^\dagger_{x_2,\sigma_2}\cdots c^\dagger_{x_N,\sigma_N}|\mathrm{vac}\rangle$$

$$\Psi_0 = \sum_{x_1,\ldots,x_N,\sigma_1,\ldots,\sigma_N} b(x_1,\sigma_1;x_2,\sigma_2;\ldots;x_N,\sigma_N) c^\dagger_{x_1,\sigma_1} c^\dagger_{x_2,\sigma_2}\cdots c^\dagger_{x_N,\sigma_N}|\mathrm{vac}\rangle$$

where in Ψ_1, $c^\dagger_{x_1,\sigma_1} c^\dagger_{x_2,\sigma_2}\cdots c^\dagger_{x_N,\sigma_N}|\mathrm{vac}\rangle \in B^p_j$ and similarly for Ψ_0. Fix $x_1 < x_2 < \cdots < x_N$. Pick any spin configuration $(\sigma_1,\sigma_2,\ldots,\sigma_N)$ and we determine $b(x_1,\sigma_1;x_2,\sigma_2;\ldots;x_N,\sigma_N)$ by the following steps. Pick any fixed element $c^\dagger_{x_1,\tau_1} c^\dagger_{x_2,\tau_2}\cdots c^\dagger_{x_N,\tau_N}|\mathrm{vac}\rangle \in B^N_k$. Then for any other elements $c^\dagger_{x_1,\sigma_1} c^\dagger_{x_2,\sigma_2}\cdots c^\dagger_{x_N,\sigma_N}|\mathrm{vac}\rangle \in B^N_k$, $(\sigma_1,\sigma_2,\ldots,\sigma_N)$ is the cyclic permutation of $(\tau_1,\tau_2,\ldots,\tau_N)$ and since B^N_k has period N, we can find k $(1 \leqslant k \leqslant N)$ uniquely such that $(\sigma_1,\sigma_2,\ldots,\sigma_N) = (\tau_k,\tau_{k+1},\ldots,\tau_N,\tau_1,\tau_2,\ldots,\tau_{k-1})$. Pick and fix any element $c^\dagger_{x_1,\tau'_1} c^\dagger_{x_2,\tau'_2}\cdots c^\dagger_{x_N,\tau'_N}|\mathrm{vac}\rangle \in B^p_j$. We define $b(x_1,\sigma_1;x_2,\sigma_2;\ldots;x_N,\sigma_N)$ as

$$b(x_1,\sigma_1;x_2,\sigma_2;\ldots;x_N,\sigma_N) := a(x_1,\tau'_k;x_2,\tau'_{k+1};\ldots;x_N,\tau'_{k-1}).$$

It is straightforward to check that Ψ_0 is the eigenvector of H^N_j with eigenvalue E. Lemma 2.1 is proved.

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