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The flux phase problem on the ring

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Abstract. We give a simple proof to derive the optimal flux which minimizes the ground state energy in the one-dimensional Hubbard model, provided the number of particles is even.

1. Introduction

We consider the Hubbard model on the ring (i.e. the one-dimensional system with periodic boundary condition), where the magnetic flux is threaded through the ring. Our problem is to obtain the optimal flux which minimizes the ground state energy.

To be precise, we define the Hubbard Hamiltonian as follows:

$$H := \sum_{\sigma=\uparrow,\downarrow} \sum_{x=1}^{L} t_{x,x+1} c^{\dagger}_{x+1,\sigma} c_{x,\sigma} + (\text{h.c.}) + \sum_{x=1}^{L} U_x n_{x,\uparrow} n_{x,\downarrow}$$

where L ($L \geqslant 3$) is the number of sites, the site $L + 1$ is equivalent to the site 1, $t_{x,x+1} \in \mathbb{C}$, $|t_{x,x+1}| \neq 0$, $U_x \in \mathbb{R}$, $c^{\dagger}_{x,\sigma}$ ($c_{x,\sigma}$) is the creation (annihilation) operator which satisfies the canonical anticommutation relations and $n_{x,\sigma} := c^{\dagger}_{x,\sigma} c_{x,\sigma}$.

We write $t_{x,x+1} = |t_{x,x+1}| \exp[\mathrm{i}\theta_{x,x+1}]$, $\theta_{x,x+1} \in [0, 2\pi)$. Then, the flux which penetrates the ring is defined to be $\varphi := \sum_{x=1}^{L} \theta_{x,x+1}$. The ground state energy E (in some fixed number of particles N_e) can be regarded as a function of φ (and hence we write $E = E(\varphi)$), because it does not depend on any choice of $\{\theta_{x,x+1}\}_{x=1}^{L}$ which satisfies $\sum_{x=1}^{L} \theta_{x,x+1} = \varphi$. Our aim is to obtain the flux $\varphi = \varphi_{\text{opt}}$ which attains $\min_{\varphi \in [0,2\pi)} E(\varphi)$. We call φ_{opt} the optimal flux. In general, φ_{opt} is not unique, and we will not discuss the uniqueness question in this paper.

There are some closely related problems in the literature (our problem is the same as mentioned in (3) below). (1) It appears in a theory of superconductivity [2,15]. (2) In the study of the persistent current [3,4,7,16], it was discussed whether the response of the Hubbard ring to the external field is diamagnetic or paramagnetic, and the influence of the electron–electron interaction on this property. (3) In a high-dimensional lattice, the flux phase conjecture [6] says that the optimal flux per plaquette is equal to the particle density per site. This implies that the diamagnetic feature, which widely holds in the one-particle system, is reversed in the high-electron density regime. This conjecture was rigorously proved by Lieb [8] at half filling. Macris–Nachtergaele [12] gave an improved proof of [8].

As for the rigorous study of the Hubbard ring (of even length), Lieb–Loss [9] considered the free electron case ($U_x \equiv 0$) at half filling, and computed φ_{opt} in a general situation so that translation invariance is not assumed. They also considered more complicated geometry such

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as a tree of rings, a ladder etc. Lieb–Nachtergaele [11] computed $\varphi_{\rm opt}$ also at half filling when $U_x \equiv U$ is any constant. In this paper, we obtain $\varphi_{\rm opt}$ when U_x and L are arbitrary, while N_e is even. Due to the hole–particle symmetry, it suffices to consider $N_e \leqslant L$.

Theorem. *Let $N_e (\leqslant L)$ be even.*

(1) Assume $U_x < +\infty$ for all x. $E(\varphi)$ is minimized if $\varphi \equiv (N_e/2 + 1)\pi$ (mod 2π) ($\varphi \equiv N_e\pi/2$) when L is even (L is odd).

(2) When $U_x = \infty$ for all x, $E(\varphi)$ is minimized if $\varphi = 0, \pi$.

Remarks. (1) We can derive the optimal flux in $S^z \neq 0$ subspaces.

(a) $U_x < +\infty$: the optimal flux takes 0 and π alternatively as S^z varies. For instance, when $N_e = 4n$, and L is even, then $\varphi_{\rm opt} = \pi$ ($S^z = 0, 2, 4, \ldots$), and $\varphi_{\rm opt} = 0$ ($S^z = 1, 3, 5, \ldots$).

(b) $U_x \equiv \infty$: let $m := N_\uparrow/N_\downarrow$ ($N_\uparrow$ ($N_\downarrow$) is the number of up (down) spins). We suppose $N_\uparrow \geqslant N_\downarrow$ here. When $m \notin \mathbb{N}$, $\varphi_{\rm opt} = 2k\pi/N_e$, $k \in \mathbb{Z}$ (in this case, particles can also be regarded as hard-core bosons). When $m \in \mathbb{N}$, $\varphi_{\rm opt} = 2k\pi/(m+1) - (N_e - 1)\pi$ (if $(m+1)L$ is even), and $\varphi_{\rm opt} = (2k-1)\pi/(m+1) - (N_e - 1)\pi$ (if $(m+1)L$ is odd), $k \in \mathbb{Z}$.

(2) When $U_x \equiv +\infty$, the proof of the theorem tells us that the ground state energy is periodic w.r.t. φ with period π (when $S^z = 0$), and period $2\pi/N_e$ (when $m \notin \mathbb{Z}$). This fact and its implications are discussed by Kusmartsev and by Yu and Fowler [7, 16].

(3) When N_e is odd and $U_x \equiv +\infty$, we can still derive the optimal flux, and the result is the same as stated in remark (1).

On the other hand, when $U_x < +\infty$, and $N_e = L$ (half-filling), we believe $\varphi_{\rm opt} = \pi/2$, $3\pi/2$ as some examples imply (e.g. take $t_{x,x+1}$: constant and $U_x \equiv 0$). However, in general cases, $\varphi_{\rm opt}$ could be different depending on the value of U_x. For example, let $L = 4$, $N_e = 3$ and $t_{x,x+1} \equiv t$. When $U_x \equiv 0$, $E(\varphi)$ is minimized if and only if $\varphi = \pm 4 \arcsin(1/\sqrt{5})$, while in the case of $U_x \equiv +\infty$, $E(\varphi)$ is minimized if and only if $\varphi = 0, 2\pi/3, 4\pi/3$.

(4) $SU(2)$ invariance as well as translation invariance is not necessary to prove the theorem. We can let $t_{x,x+1} = t^\sigma_{x,x+1}$ ($\sigma = \uparrow, \downarrow$) also depend on the spin variable. In this case, our theorem mentions the optimal flux in the $S^z = 0$ subspace only. In addition, our Hamiltonian can include the one-body potential term as well.

(5) The argument in the proof, together with that in [10], yields that the ground state is unique and has spin zero: $S = 0$, provided the flux φ takes the value stated in the theorem. Moreover, if we let $E(S)$ denote the ground state energy in spin S subspace, then we have $E(S) < E(S+2)$.

(6) When $U_x = \infty$, not for all x, the argument of the proof says the following: if $\sharp\{x : U_x = \infty\} \leqslant L - N_e/2$, then the result is the same as in theorem (1). Otherwise, the result is the same as in theorem (2).

(7) When $U_x \equiv 0$, and $t_{x,x+1} \equiv t$, $E(\varphi)$ is maximized if and only if $\varphi \equiv N_e\pi/2$ ($\varphi \equiv (N_e/2 + 1)\pi$), if L is even (L is odd), which should be compared with the fact that $E(0) = E(\pi)$ when $U_x \equiv \infty$ (theorem (2)).

(8) When we let L be large, $|E(0) - E(\varphi)|$ will behave as $O(1/L)$ [11].

In section 2, we give the proof of the theorem, which is very simple. Our problem is reduced to considering a one-particle Hamiltonian $\mathcal{H}(\varphi)$ on the graph G which is composed of the basis of N_e-fermion Hilbert space. The theorem follows from obtaining the optimal flux of $\mathcal{H}(\varphi)$ on G, by the usual diamagnetic inequality argument.

2. Proof of theorem

At first, we consider the case in which L is even and $N_e = 4n$. Due to the $SU(2)$ invariance, it is sufficient to work on the $S^z = 0$ subspace (i.e. $N_\uparrow = N_\downarrow = 2n$). We fix the basis of the Hilbert space of N_e-fermions:

$$\mathcal{B} := \{c^\dagger_{x_1,\sigma_1} c^\dagger_{x_2,\sigma_2}, \ldots, c^\dagger_{x_{N_e},\sigma_{N_e}} |\mathrm{vac}\rangle : x_1 \leqslant x_2 \leqslant \cdots \leqslant x_{N_e}, \sigma_i = \uparrow, \downarrow, i = 1, \ldots, N_e\}$$

that is, to arrange particles in increasing order w.r.t. the space coordinates. Our problem is equivalent to considering the one-particle Hamiltonian $\mathcal{H}(\varphi)$ on the graph G whose sites are composed of $\mathcal{B}$.

$$(\mathcal{H}(\varphi)u)(x) := \sum_{y \in \mathcal{B}} s_{xy}(\varphi) u(y)$$

where $s_{xy}(\varphi) := \langle x|H|y\rangle$, $x, y \in \mathcal{B}$. Two sites $x, y \in G$ are connected by a bond if and only if $s_{xy}(\varphi) \neq 0$ (we note $|s_{xy}(\varphi)|$ does not depend on φ). For given $\varphi \in [0, 2\pi)$, we fix some $\{\theta_{x,x+1}\}_{x=1}^L$ such that $\sum_{x=1}^L \theta_{x,x+1} = \varphi$, and thus we suppose $s_{xy}(\varphi)$, and hence $\mathcal{H}(\varphi)$, is determined by φ. Then, it is not hard to show that (1) every circuit in G has even length (because L is even), (2) the fluxes in these circuits are always integer multiples of $\psi := \varphi + 2n\pi + (4n-1)\pi$. In fact, let $\mathcal{C}$ be the set of circuits in G which have minimal length. Every element of $\mathcal{C}$ is given by fixing all particles which have down (up) spins and moving each up (down) spin all together until each spin comes to the next spin. To make this clear, we write down an element of $\mathcal{C}$ when $L = N_e = 4$:

$$\begin{array}{ccc}
c^\dagger_{1,\uparrow} c^\dagger_{2,\downarrow} c^\dagger_{3,\uparrow} c^\dagger_{4,\downarrow} |\mathrm{vac}\rangle & \leftarrow & c^\dagger_{2,\downarrow} c^\dagger_{3,\uparrow} c^\dagger_{4,\uparrow} c^\dagger_{4,\downarrow} |\mathrm{vac}\rangle \\
\downarrow & & \uparrow \\
c^\dagger_{2,\uparrow} c^\dagger_{2,\downarrow} c^\dagger_{3,\uparrow} c^\dagger_{4,\downarrow} |\mathrm{vac}\rangle & \rightarrow & c^\dagger_{2,\uparrow} c^\dagger_{2,\downarrow} c^\dagger_{4,\uparrow} c^\dagger_{4,\downarrow} |\mathrm{vac}\rangle.
\end{array}$$

The second term $2n\pi$ in the definition of ψ comes from the fact that up spins jump down spins $2n$ times in the above process, and each jump causes multiplication of (-1) to the corresponding $s_{xy}(\varphi)$. The third term $(4n-1)\pi$ in the definition of ψ arises from the fact that the $2n$th up spin jumps all the other $(4n-1)$ particles when it moves from site L to site 1, because we set the basis such that particles are arranged in increasing order.

On the other hand, because of the inequality $\sum_{x,y \in \mathcal{B}} s_{xy}(\varphi) \overline{u(x)} u(y) \geqslant -\sum_{x,y \in \mathcal{B}} |s_{xy}(\varphi)| |u(x)| |u(y)|$, we know that the ground state energy is minimized when all off-diagonal elements $s_{xy}(\varphi)$, $x \neq y$, are non-positive. Let $(\mathcal{H}_- u)(x) := -\sum_{y \in \mathcal{B}} |s_{xy}(\varphi)| u(y)$. When $\psi \equiv 0 \pmod{2\pi}$, $\mathcal{H}(\varphi)$ is unitarily equivalent to $\mathcal{H}_-$, because the fluxes of all circuits in G are all the same [9, lemma 2.1]. $\psi \equiv 0 \pmod{2\pi}$ yields $\varphi \equiv \pi \pmod{2\pi}$. This concludes the proof when L is even and $N_e = 4n$.

When L is even and $N_e = 4n+2$, the only thing we have to do is to replace ψ in the above argument by $\psi' := \varphi + (2n+1)\pi + (4n+1)\pi$. When L is odd, then ψ (or ψ' in the case of $N_e = 4n+2$) should satisfy $\psi \equiv \pi \pmod{2\pi}$ having optimal flux, because the minimal length of the circuits in G is odd, and so the flux of $\mathcal{H}_-$ on every element of $\mathcal{C}$ is π. When $U_x \equiv \infty$, the minimal length of circuits in G is $2L$, whose flux is $2\varphi + 2(N_e - 1)\pi \equiv 2\varphi \pmod{2\pi}$.

Remarks. (1) As an alternative proof, one can compute the partition function $P(\varphi) := \mathrm{Tr}[\exp(-\beta H)]$ by using the path integral representation [1], and show that $P(\varphi)$ is maximized if φ takes the value stated in the theorem. This approach has been used by [5], where they derived the optimal flux in the Falicov–Kimball model.

(2) When the number of electrons is odd, the fluxes of elements of $\mathcal{C}$ are different from each other, depending on which spins move in the circuit. For example, let $L = N_e = 2n+1$, $N_\uparrow = n$, and $N_\downarrow = n+1$. By the hole–particle transformation only for down spins, we can

suppose $N_\uparrow = N_\downarrow = n$, but now the flux of down spins is $\pi - \varphi$ (this situation is similar to that discussed in [3]).

Our supposition is the following: the 'contributions' to the ground state energy from $\mathcal{C}$ would cancel each other, and an important contribution would arise from those circuits where up spins and down spins move together in the opposite direction, which has flux $\varphi - (\pi - \varphi) = 2\varphi - \pi$ and length $2n$ in G (the meaning of 'contribution' can be clear if we consider $\mathrm{Tr}[\exp(-\beta H)]$ instead of the ground state energy). $2\varphi - \pi \equiv 0$ would give the minimizing energy. However, this supposition would not be easy to prove.

(3) The proof above relies on the special nature of the ring geometry: there is always a fixed number of particles on only one loop, so that all circuits on the graph G favour the same flux 0 or π, depending on the case. However, on more complicated systems such as two-dimensional lattices, the graph G has so many different circuits which favour different fluxes that our argument does not work even if $U_x \equiv \infty$, except in the Nagaoka case ($N_e = |\Lambda| - 1$, $U_x \equiv \infty$ [13, 14]), where the optimal flux is zero everywhere.

3. Conclusion

In this paper, we derived the optimal flux φ_{opt} in the Hubbard model on the ring. Our result is true in the general situation so that the translation invariance is not necessary to assume, except that the number of particles must be even. In this section, we briefly discuss the physical interpretation of our result.

The result (1) of our theorem is consistent with that of [4], where it is shown that, at half filling, the current response is paramagnetic (resp. diamagnetic) when $N_e = 4n$ (resp. $4n+2$), by numerical computation. However, these are not equivalent especially when $N_e = 4n$. In fact, [4] showed, when $L = 6$, $N_e = 4$, and $U_x > 0$, the ground state is diamagnetic (this also implies why it would not be easy to seek φ which maximizes $E(\varphi)$). Therefore, our contribution may be that there would be no effects of spatial disorder.

The result (2) of our theorem and remark (2) after that has already been found and discussed [7, 16]. However, our proof gives a different picture: the graph G consists of rings of larger lengths, as $U = \infty$ prohibits the exchange of particles.

Finally, our argument gives a ring version of the Lieb–Mattis theorem [10] when $\varphi = \varphi_{\mathrm{opt}}$ (remark (5) after the theorem).

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