数理解析研究所講究録 1364 巻 2004 年 108-117

Flux phase and Spin problem on the ring

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Abstract

This is a review of the author's recent work of the flux phase problem on the Hubbard ring, in which we derive the optimal flux phase which minimizes the ground state energy in the one-dimensional Hubbard model. Moreover, we study the relationship between the flux through the ring and the spin of the ground state.

1 Flux phase problem

The flux phase problem is to derive the optimal flux distribution which minimizes the ground state energy of the system of many fermions. In this paper, our system is the Hubbard Hamiltonian on the ring $\Lambda := \{1, 2, \cdots, L\}$ $(L + 1 \equiv 1)$ defined by

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

where $c_{x,\sigma}(c_{x,\sigma}^{\dagger})$ are the annihilation (creation) operator satisfying the canonical anticommutation relations :

$$\{c_{x,\sigma}, c_{y,\tau}^{\dagger}\} = \delta_{xy}\delta_{\sigma\tau}, \quad \{c_{x,\sigma}, c_{y,\tau}\} = \{c_{x,\sigma}^{\dagger}, c_{y,\tau}^{\dagger}\} = 0,$$

where $\{A, B\} := AB + BA$, and $n_{x,\sigma} := c_{x,\sigma}^{\dagger} c_{x,\sigma}$. $t_{x,x+1} \neq 0$ 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 is 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

$$B_N := \left\{ c_{x_1,\sigma_1}^{\dagger} c_{x_2,\sigma_2}^{\dagger} \cdots c_{x_N,\sigma_N}^{\dagger} |\text{vac} >: x_j \in \Lambda, \sigma_j = \uparrow, \downarrow, j = 1, 2, \cdots, N \right\}.$$

$|\text{vac} >$ is the vacuum state. Let $E_N(\varphi)$ be the ground state energy of $H(\varphi)$:

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

[1]partially supported by JSPS grant 15740049.

Our aim is to derive the optimal flux φ_{opt} which minimizes $E_N(\varphi)$: $E_N(\varphi_{opt}) = \min_{\varphi\in[0,2\pi)} E_N(\varphi)$. 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 [16].

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, 19], (2) In the study of the persistent current [4, 7, 20, 3], they discussed whether the response of the Hubbard ring to the magnetic flux is diamagnetic or paramagnetic, and the influence of the electron-electron interaction to this property, (3) In 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, becomes opposite in high electron density regime. This conjecture was rigorously proved by Lieb [9] at half filling. Macris-Nachtergaele [13] gave an improved proof of [9].

As for the rigorous study of the Hubbard ring (of even length), Lieb-Loss [10] considered free electron case ($U = V = 0$) at half filling ($N = |\Lambda|$), and computed φ_{opt} in general situation so that translation invariance is not assumed : T can be arbitrary. They also considered what have more complicated geometry such as tree of ring, ladder, etc. Lieb-Nachtergaele [12] computed φ_{opt} also at half filling when U is constant, and $V = 0$. In this paper, we obtain φ_{opt} when U, V and L are arbitrary (resp. $U = V = 0$, $N = L$) when N is even (resp. odd). Due to the hole-particle symmetry, it suffices to consider $N \leq L$. We first study the case where N is even [15].

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

The key ingredient of the proof of Theorem 1.1 is to regard $H(\varphi)$ as a hopping Hamiltonian on B_N and compute the flux through the circuit in B_N of "minimal" length[2]. 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 are no distinction. In fact, $E_N^{\infty}(\varphi) := \lim_{U\uparrow\infty} E_N(\varphi)$ has period $\frac{2\pi}{N}$ and $H_\infty(0)$ is

[2]We regard B_N as a graph on which the hopping Hamiltonian $H(\varphi)$ is defined.

gauge equivalent to $H_\infty(\pi)$ [3] This fact and its implications are discussed by Kusmartsev and Yu-Fowler[7, 20].

Remark 1.1

(1) We can derive the optimal flux in $S_z \neq 0$ subspaces.

(a) $U < +\infty$: the optimal flux takes 0 and π alternately as S_z varies. For instance, when $N = 4n$, and L is even, then $\varphi_{opt} = \pi$ ($S_z = 0, 2, 4, \cdots$), and $\varphi_{opt} = 0$ ($S_z = 1, 3, 5, \cdots$).

(b) $U = \infty$: the result is the same as Theorem 1.1(2).

(2) $SU(2)$ invariance as well as translation invariance is not necessary to prove Theorem 1.1. We can let $t_{x,x+1} = t^\sigma_{x,x+1}$ ($\sigma =\uparrow, \downarrow$) depend also on spin variable. In this case, our theorem mentions the optimal flux in the $S_z = 0$ subspace only.

(3) When $U = 0$, and $t_{x,x+1}$ is constant, $E(\varphi)$ is maximized if and only if $\varphi = N\pi/2$ (resp. $\varphi = (N/2 + 1)\pi$), if L is even (resp. L is odd), which should be compared with the fact that $E(0) = E(\pi)$ when $U = \infty$ (Theorem 1.1(2)).

(4) When we let L large, $|E(0) - E(\varphi)|$ will behave as $O(1/L)$ [12].

(5) As an alternative proof, one can compute the partition function $P(\varphi) := Tr[\exp(-\beta H)]$ by using the path integral representation [1], and show that $P(\varphi)$ is maximized (for any $\beta > 0$) if φ takes the value stated in Theorem 1.1. This approach has been done by [5], where they derived the optimal flux in the Falicov-Kimball model.

(6) The proof above relies on the special nature of the ring geometry: there is always fixed number of particles on only one loop Λ, so that all circuits on B_N favor the same flux 0 or π, depending on cases. However, on more complicated systems such as two dimensional lattice, B_N has so many different circuits which favor different fluxes so that our argument does not work even if $U = \infty$, except the Nagaoka-case ($N = |\Lambda| - 1$, $U = \infty$ [15, 18]), where the optimal flux is zero everywhere.

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

[3] $H_\infty(\varphi) := PH(\varphi)P$ 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.

If we try to apply the method of proof of Theorem 1.1, the fluxes of minimal circuits are different from each other, depending on which spins move in the circuit. For instance, let $L = N = 2n+1$, $N_\uparrow = n$, 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 "contribution" to the ground state energy from minimal circuits would cancel each other, and an important contribution would come 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 has length $2n$ in B_N (the meaning of "contribution" could be clear if we consider $P(\varphi)$ instead of the ground state energy). $2\varphi - \pi = 0$ would give the minimizing energy. However, this supposition would be hard to prove(Remark 1.2(3)).

Nevertheless, if $U = V = 0$, we have

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 $\varphi = \frac{\pi}{2}, \frac{3\pi}{2}$.

Theorem 1.2 is proved by reducing the problem to the case of even number of particles using the ideas of Floquet analysis.

Remark 1.2
(1) 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 $\varphi_{opt} = \frac{2n}{N}\pi$ (L even), $\frac{2n+1}{N}\pi$ (L odd), $n = 0, 1, \cdots, N-1$.
(2) The same result is deduced in [17] by a different argument. However, the following example implies the conclusion of Theorem 1.2 is not true in general if $V \neq 0$. Let $N = L = 5$ and let

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

where $t > 0$. Since the Hamiltonian $H(\varphi)$ contains terms of the form $t(c_{3,\sigma}^\dagger + c_{4,\sigma}^\dagger)(c_{3,\sigma} + c_{4,\sigma})$, 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 [20].*
(3) 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* $P(\varphi) := Tr\,[e^{-\beta H(\varphi)}]$ *(restricted on* $S_z = \frac{1}{2}$ *subspace for simplicity) is a complicated function of* φ *if* β *is large, and* $\varphi = \frac{\pi}{2}, \frac{3\pi}{2}$ *does not necessarily maximize it, although they are always the critical point. We note that, when* N *is even,* $P(\varphi)$ *is maximized for any* $\beta > 0$ *by the optimal flux given in Theorem 1.1(Remark 1.1(5)). 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 [10], it is shown that the grand canonical partition function with zero chemical potential is maximized if* $\varphi = 0, \pi$.

2 Spin problem

Next, we study the spin of the ground state. Spin operators are defined by

$$S_+ := \sum_{x=1}^{L} c_{x,\uparrow}^\dagger c_{x,\downarrow}, \quad S_- := (S_+)^*, \quad S_z := \frac{1}{2}\sum_{x=1}^{L}(n_{x,\uparrow} - n_{x,\downarrow}),$$
$$\mathbf{S}^2 := \frac{1}{2}(S_+S_- + S_-S_+) + (S_z)^2.$$

$\mathbf{S}^2$ has eigenvalues of the form $S(S+1)$, $S = 0, 1, \cdots, \frac{N}{2}$ (resp. $S = \frac{1}{2}, \frac{3}{2}, \cdots, \frac{N}{2}$) when N is even (resp. odd). An eigenvector of $\mathbf{S}^2$ with eigenvalue $S(S+1)$ is called to have spin S. Because $[H(\varphi), \mathbf{S}^2] = 0$, $H(\varphi)$ and $\mathbf{S}^2$ can be simultaneously diagonalized.

In what follows, we assume L is even for simplicity; the results for odd L follows by exchanging 0 and π in each statement of theorems given below. The proof of Theorem 1.1, together with the Lieb-Mattis argument [11] proves the following fact.

Theorem 2.1 (Ground state is unique with spin zero)
Let N *be even and* $\varphi = \left(\frac{N}{2} + 1\right)\pi$ *(mod* 2π*). Then the ground state of* $H(\varphi)$ *is unique with* $S = 0$.

Remark 2.1
(1) 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 Lieb-Mattis theorem [11] which states 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, the boundary effect is not negligible in general. We also remark that such "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* $S = 0$ *[8]. On the other hand, Theorem 2.1 says, if* φ *is optimal, this uniqueness property is stable which holds for any* T, V *and* U.
(2) When $N = L$ *is odd,* $U = V = 0$, *and* $\varphi = \frac{\pi}{2}, \frac{3\pi}{2}$, *then the ground state is unique with* $S = \frac{1}{2}$ *apart from the* $(2S+1)$*-degeneracy.*
(3) The proof of Theorem 2.1 also implies the following. Let $E(S)$ *denote the ground state energy in spin* S *subspace, then we have* $E(S) < E(S+2)$. *It becomes equality when* $U = \infty$, $\varphi = \pi$ *(resp.* $\varphi = 0$*), and* L*: even (resp.* L*: odd).*

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

Theorem 2.2 (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* $S = \frac{N}{2}$.

To prove Theorem 2.2(1), we use Perron-Frobenius theorem which implies that $H_\infty(\pi)$ has the ferromagnetic ($S = \frac{N}{2}$) 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 2.2(2) follows from comparing the spin of the ground state of $H_\infty(0)$ with that of $H^0_\infty(0)$ where $|t_{x,x+1}| = 1$ and $V = 0$.

Remark 2.2
(1) Theorem 2.2 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 have one with $S = 0$.
(2) The inequality $\sum_{j=1}^N e_j(\pi) \leq \sum_{j=1}^N e_j(0)$ 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 2.2 says 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 an 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 states of $H_\infty(\pi)$ are 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 says 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 2.3 (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 $H_\infty(0)$.

To prove Theorem 2.3, 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. Ground states of both are unique and that of $H(0)$ has $S = 0$ while one 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 $H_\infty(\pi)$. 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, coefficients are the same for every configurations of spins for each fixed locations of particles. The gauge transformation g_∞ then puts (-1) alternately on every cyclic permutation of

[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 $a_j > 0 (a_j \geq 0)$ for all j.

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.

3 Discussion

We derived the optimal flux φ_{opt} in the Hubbard model on the ring. Our result is true in general situation so that the translation invariance is not necessary to assume, except that we need the absence of on-site interaction and the external potential, if the number of particles is odd.

The result (1) of Theorem 1.1 is consistent with that of [4], where it is shown that, at half-filling, the current response of the ground state is paramagnetic (resp. diamagnetic) when $N = 4n$ (resp. $4n + 2$) by numerical computation. However, these are not equivalent, especially when $N = 4n$. In fact, [4] showed, when $L = 6$, $N = 4$, and $U(x) > 0$, the ground state is diamagnetic (this also implies why it is not 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 Theorem 1.1 is already found and discussed by [7, 20]. However, our proof gives a different picture: B_N consists of rings of larger lengths, for $U = \infty$ prohibits the exchange of particles.

Theorem 1.2 gives simple proof of results in [20] found by the Bethe ansatz calculation, and thus our contribution is to show that this is also true even if the hopping coefficients are not constant. However, our proof requires the condition that the external potential is zero which seems to be important.

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 it is not stable. It also implies the conclusion of 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 seems to show interesting connection between the flux threading the system and the spin of the ground state.

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