Anomalous Flux Quantization in a Hubbard Ring with Correlated Hopping

Liliana Arrachea,* A. A. Aligia, and E. Gagliano
Centro Atómico Bariloche and Instituto Balseiro, Comisión Nacional de Energía Atómica, 8400 Bariloche, Argentina
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We solve exactly a generalized Hubbard ring with twisted boundary conditions. The magnitude of the nearest-neighbor hopping depends on the occupations of the sites involved and the term which modifies the number of doubly occupied sites $t_{AB} = 0$. Although η-pairing states with off-diagonal long-range order are part of the degenerate ground state, the behavior of the energy as a function of the twist rules out superconductivity in this limit. A small t_{AB} breaks the degeneracy and for moderate repulsive U introduce superconducting correlations which lead to "anomalous" flux quantization. [S0031-9007(96)00300-6]

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One of the most interesting problems of the physics of highly correlated electronic systems is the characterization of the metallic, insulating, and superconducting phases, as well as the transitions among them. Kohn has shown that the Drude weight D_c is the adequate quantity to identify the metal-insulator transition (MIT) [1], while Yang introduced the concept of off-diagonal long-range order (ODLRO) to characterize the superconducting nature of a metallic phase [2]. ODLRO in *all* relevant low-energy eigenstates implies a periodicity of $h/2e$ in the free energy as a function of a magnetic flux threading a system with annular topology. This "anomalous" flux quantization (AFQ) [3,4] in the ground state (GS) means $E(\Phi + \pi) = E(\Phi)$, where E is the GS energy and Φ is the twist angle. It is a necessary but not sufficient condition for superconductivity. Since $D_c \sim \partial^2 E/\partial\Phi^2$, the function $E(\Phi)$ gives crucial information about the metallic and superconducting character of the system [1,4,5].

Exactly solvable highly correlated models displaying a MIT or ODLRO are good laboratories to investigate the nature of the MIT and electronic mechanisms of superconductivity. The Bethe ansatz solution with twisted boundary conditions of the one-dimensional (1D) Hubbard model [6] allowed application of Kohn's ideas to the MIT in this model [6,7]. In addition, the interest in electronic models exhibiting superconductivity (or dominant superconducting correlations at long distances in 1D), in particular, those with correlated hopping increases recently [8–12]. However, very few exact results exist. Several of them are related with the so-called η-pairing mechanism, which allows us to construct eigenstates with ODLRO [8–11]. In particular, the widely studied [13–15] effective model for cuprate superconductors,

$$H = H_U + H_t = U \sum_i n_{i\uparrow} n_{i\downarrow} + \sum_{\langle ij\rangle\sigma} (c^\dagger_{i\bar\sigma} c_{j\bar\sigma} + \text{H.c.}) \times \{t_{AA}(1 - n_{i\sigma})(1 - n_{j\sigma}) + t_{BB} n_{i\sigma} n_{j\sigma} + t_{AB}[n_{i\sigma}(1 - n_{j\sigma}) + n_{j\sigma}(1 - n_{i\sigma})]\}, \tag{1}$$

has been exactly solved recently in 1D in the limit $t_{AB} = 0$ for open [9] and periodic [10,11] boundary conditions. η-pairing states with ODLRO are part of the *degenerate* GS for moderate on-site repulsion U and arbitrary band filling. Unfortunately, the function $E(\Phi)$ has not been obtained and, then, the AFQ and D_c were not studied. Our main interest in this study is motivated by the following two facts: First, the superconducting character of the degenerate GS is not obvious, even when states with ODLRO are part of the GS manifold. Second, the GS was found to be a Mott insulator for $U > U_{\rm MI} = 2D(|t_{AA}| + |t_{BB}|)$ at half filling, in a simple cubic lattice in D dimensions, with a MIT for $D > 1$ [14,15]. Strictly in $D = 1$, however, we find that for $n = 1$, $D_c = 0\ \forall U$, *in spite of a vanishing charge gap* for $U < U_{\rm MI}$. The possibility of an insulating phase with this feature was first remarked by Kohn [1] and we think that this is, to our knowledge, the first nontrivial realization of that kind of insulators.

In this Letter, we solve exactly the 1D model (1) with $t_{AB} = 0$, for twisted boundary conditions $\Phi_\uparrow$ ($\Phi_\downarrow$) for spin up (down) fermions. This allows us to calculate the Drude weight D_c and the spin stiffness D_s and to discuss the nature of the MIT as the particle density $n \to 1$. The behavior of $E(\Phi_\uparrow, \Phi_\downarrow)$ rules out superconductivity in the model for $t_{AB} = 0$. In addition, we show how the GS degeneracy is broken in favor of a state with dominant superconducting correlations when a finite t_{AB} is allowed, for moderate repulsive U.

We first consider the Hamiltonian (1) with $-t_{AA} = t_{BB} = t > 0, t_{AB} = 0$. The other possible choices of the sign of t_{AA} and t_{BB} lead to an equivalent model [16]. At each site i, we introduce two fermions $f_{i\sigma}$ and two bosons $b_{i\sigma'}$ where $b_{i+} \equiv e$ (empty) and $b_{i-} \equiv d$ (doublon). In this representation, H_t of (1) in a ring of L sites with twists Φ_σ for particles with spin σ reads

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$$H_t = \sum_{i=1} H_{i,i+1} + H_{L,1} = -t \sum_{i=1,\sigma\sigma'}^{L-1} (f_{i+1\sigma}^\dagger f_{i\sigma} b_{i\sigma'}^\dagger b_{i+1\sigma'} + \text{H.c.})$$
$$- t \sum_{\sigma} [f_{1\sigma}^\dagger f_{L\sigma}(e^{i\Phi_\sigma} b_{1+}^\dagger b_{L+} + e^{-i\Phi_{-\sigma}} b_{1-}^\dagger b_{L-}) + \text{H.c.}]. \quad (2)$$

The numbers $N_\sigma = \sum_i f_{i\sigma}^\dagger f_{i\sigma}$, $N_e = \sum_i e_{i\sigma}^\dagger e_{i\sigma}$, $N_d = \sum_i d_{i\sigma}^\dagger d_{i\sigma}$ are all conserved. In each subspace with fixed $N_\uparrow, N_\downarrow, N_e, N_d$, any state has the form $\prod_{m=1}^{N_b} b_{i(m)\sigma'(m)}^\dagger \prod_{j=1}^{N_f} f_{i(j)\sigma(j)}^\dagger |0\rangle$, where j labels the $N_f = N_\uparrow + N_\downarrow$ fermions from left to right and $i(j)$, $\sigma(j)$ denote the position and the spin of the jth fermion. Similarly $i(m), \sigma'(m)$ [with $i(m+1) > i(m)$] are the position and the pseudospin [9] of the mth boson. The number of bosons is $N_b = N_e + N_d = L - N_f$. For the periodic case ($\Phi_\sigma = 0$), the Hamiltonian is invariant under cyclic permutations of the fermions and bosons and it is convenient to work in the basis of the irreducible representations of the direct product group $C_{N_f} \otimes C_{N_b}$ [11]. Our idea is to use appropriate weighted representations to cancel out the difference in phases in $H_{1,L}$ in order to map the problem into one of spinless fermions with twisted boundary conditions. We think of the ring as a periodic system in which $f_{i+L\uparrow}^\dagger = f_{i\uparrow}^\dagger$, $e_{i+L}^\dagger = e_i^\dagger$, but $f_{i+L\downarrow}^\dagger = e^{-i(\Phi_\uparrow - \Phi_\downarrow)} f_{i\downarrow}^\dagger, d_{i+L}^\dagger = e^{-i(\Phi_\uparrow + \Phi_\downarrow)} d_i^\dagger$. Thus $H_{L,1} = e^{i\Phi_\uparrow} \sum_{\sigma\sigma'} f_{1+L\sigma}^\dagger f_{L\sigma} b_{1+L\sigma'}^\dagger b_{L\sigma'}$.

We look for a basis of many particle states transforming as irreducible representations of $C_{N_f} \otimes C_{N_b}$ under the above mentioned boundary conditions. The part of these states which describes the singly occupied sites can be constructed using the operators

$$F^\dagger(\{i(j)\},\{k_l\}) = \prod_{\tilde{k}_l\uparrow}^{N_\uparrow} \tilde{f}_{\tilde{k}_l\uparrow}^\dagger \prod_{l=1}^{N_\downarrow} f_{k_l\downarrow}^\dagger, \quad f_{k\downarrow}^\dagger = \frac{1}{\sqrt{N_f}} \sum_{j=1}^{N_f} e^{-ikj} f_{i(j)\downarrow}^\dagger, \quad k_l = \frac{2\pi\nu_l - (\Phi_\uparrow - \Phi_\downarrow)}{N_f},$$
$$\tilde{f}_{\tilde{k}\uparrow}^\dagger = \frac{1}{\sqrt{N_f}} \sum_{j=1}^{N_f} e^{-i\tilde{k}j} f_{i(j)\uparrow}^\dagger (1 - f_{i(j)\downarrow}^\dagger f_{i(j)\downarrow}), \quad (3)$$

where in contrast to the wave numbers k_l, the $\tilde{k}_l$ are not shifted ($\tilde{k}_l N_f/2\pi$ is integer), and are chosen in such a way that $\sum_l \tilde{k}_l = 0(\pi)$ for N_f odd (even). The ν_l are $N_\downarrow$ different integers lying in the interval $[0, N_f - 1]$, and each of the $N_f!/N_\uparrow!N_\downarrow!$ possible choices of the set of ν_l define a spin configuration. It is easy to see that under cyclic permutation C_{N_f}, which carries each fermionic position to the right $C_{N_f} F^\dagger = -(-1)^{N_f} \exp(i \sum_l k_l) F^\dagger$. In a similar way, using a transformation that interchanges spin and pseudospin [17], the pseudospin configuration can be described by an operator $B^\dagger(\{i(m)\},\{k_l'\})$, such that $C_{N_b} B^\dagger = \exp(i \sum_l k_l') B^\dagger$, with the N_d different $k_l' = [2\pi\nu' - (\Phi_\uparrow + \Phi_\downarrow)]/N_b$. The (nonorthonormal) basis states that we use are denoted by $|\psi\{i(j)\},\{k\},\{k'\}\rangle = B^\dagger F^\dagger |0\rangle$.

H_t permutes a fermion and a nearest-neighbor boson. The cyclic orders of fermions and bosons are conserved. Thus the numbers $\{k\}$ and $\{k'\}$ are conserved. We drop these indices for simplicity. $H_{l,l+1}|\psi\{i(j)\}\rangle = 0$ unless one and only one of the sites l and $l+1$ is contained in $\{i(j)\}$. We restrict ourselves to these states in the following discussion. It can be seen that for $l < L$, $H_{l,l+1}|\Psi(\{i(j)\})\rangle = -t|\Psi(\{i'(j)\})\rangle$, where $\{i'(l)\}$ differs from $\{i(j)\}$ in the position of one fermion only, which is shifted from site l to $l+1$ or conversely. If $i(N_f) = L$, then $H_{L,1}|\Psi(\{i(j)\})\rangle = -te^{i\Phi_\uparrow} C_{N_f} C_{N_b}^{-1} |\psi\{i'(j)\}\rangle = t(-1)^{N_f} \exp[i(\sum_{l=1}^{N_\downarrow} k_l - \sum_{l=1}^{N_d} k_l' + \Phi_\uparrow)] |\psi\{i'(j)\}\rangle$, where $i'(1) = 1$, and for $j < N_f, i'(j+1) = i(j)$. When $N_\downarrow = N_d = 0$, H_t takes the form of a problem of spinless fermions with flux $\Phi_\uparrow$. The above equations show that in the general case the problem takes the same form, with an effective flux:

$$\Phi_{\text{eff}} = \Phi_\uparrow + \sum_{l=1}^{N_\downarrow} k_l - \sum_{l=1}^{N_b} k_l' = \left(\frac{N_\uparrow}{N_f} - \frac{N_d}{N_b}\right)\Phi_\uparrow + \left(\frac{N_\downarrow}{N_f} - \frac{N_d}{N_b}\right)\Phi_\downarrow + \frac{2\pi}{N_f}\sum_{l=1}^{N_\downarrow} \nu_l - \frac{2\pi}{N_b}\sum_{l=1}^{N_d} \nu_l'. \quad (4)$$

The energy of the system is given by

$$E = -2t \sum_{j=1}^{N_f} \cos\left(\frac{2\pi\nu_j'' + \Phi_{\text{eff}}}{L}\right) + UN_d, \quad (5)$$

where the N_f integer numbers ν_j'' should be different and can be chosen in the interval $[-L/2 + 1, L/2]$.

For fixed $N_f = n_f L$ and total number of particles $N = nL = N_f + 2N_d$, minimization of (5) leads to

$$E_g(\Phi_\uparrow, \Phi_\downarrow) = UN_d - 2t[\sin(n_f\pi)/\sin(\pi/L)]\cos(\varphi), \quad (6)$$

where $\varphi = \Phi_{\text{eff}}/L$ for N_f odd and $\varphi = (\Phi_{\text{eff}} - \pi)/L$ for N_f even. The value of U determines N_d for the GS. For each $\Phi_\uparrow, \Phi_\downarrow$, the numbers $N_\uparrow, N_\downarrow$ as well as $\{\nu\}, \{\nu'\}$ should be chosen to minimize $|\varphi|$ (mod 2π). It can be easily seen that in the simplest case $\Phi_\uparrow = \Phi_\downarrow = 0$ and $U = 0$ that the GS is highly degenerate (many choices of quantum numbers lead to $\varphi/2\pi$ integer). For $U > U_c = -4t\cos(\pi n)$, $N_d = 0$ [9–11], and we recover the solution of the $U = +\infty$ Hubbard model with twisted boundary conditions. In this case $E(\Phi_\uparrow + 2\pi/N, \Phi_\downarrow + 2\pi/N) = E(\Phi_\uparrow, \Phi_\downarrow)$, since the shift in Φ_σ can be absorbed decreasing one of the ν by 1, what is always possible if $0 \neq N_\downarrow \neq N_f$. For $\Phi_\uparrow = \Phi_\downarrow$, this result has been obtained previously [18]. When $N_d \neq 0$, a change in both Φ_σ by $2\pi/|N_b - N_e|$ can be counterbalanced by a change in the $\{\nu'\}$, leading to

$$E_g\left(\Phi_\uparrow + \frac{2\pi}{|L - N|}, \Phi_\downarrow + \frac{2\pi}{|L - N|}\right) = E_g(\Phi_\uparrow, \Phi_\downarrow), \tag{7}$$

for $L \neq N$, whereas for a half-filled system E_g depends only on the *difference* $\Phi_\uparrow - \Phi_\downarrow$, a behavior typical of an insulator. For $U < -4\cos(\pi n)$, $N_d > 0$ and η-pairing states with ODLRO are present in the GS [9–11]. However, we do not find AFQ, but a periodicity which depends on the particle density *n*. An example for finite chains is shown in Figs. 1(a) and 1(b). The number of peaks of $E_g(\Phi_\uparrow = \Phi_\downarrow = \Phi)$ for $0 \leq \Phi \leq 2\pi$ is *at least* $L|n - 1|$, diverging in the thermodynamic limit, while the height of each peak decreases as $1/L^3$, as in the $U = +\infty$ Hubbard model. The response of the system to the flux is like that of a single particle with charge $L - N$ or larger. One might ask whether a collection of weakly coupled chains behaves like a superfluid of these particles. However, since the compressibility diverges in the interesting regime [9], charge can be transferred between chains without cost of energy, and the response to the flux of different chains does not add coherently. Thus the system does not show the Meissner effect [2–4]. We should also note that the SU(2) η symmetry which allows for the construction of eigenstates with ODLRO is broken in the presence of a flux. Thus the η-pairing states do not necessarily give rise to superconducting currents in the presence of an external flux. The physics in the region with $U < -4t$, where $n_f = 0$ [9–11] is more obvious. In this case, there are also η-paired states with ODLRO in the degenerate GS. However, these states are static, and from Eq. (6) $E(\Phi_\uparrow, \Phi_\downarrow) = UN_d$ for all Φ_σ. This demonstrates that the ODLRO of the η-paired states *is not a sufficient condition for the existence of superconductivity*.

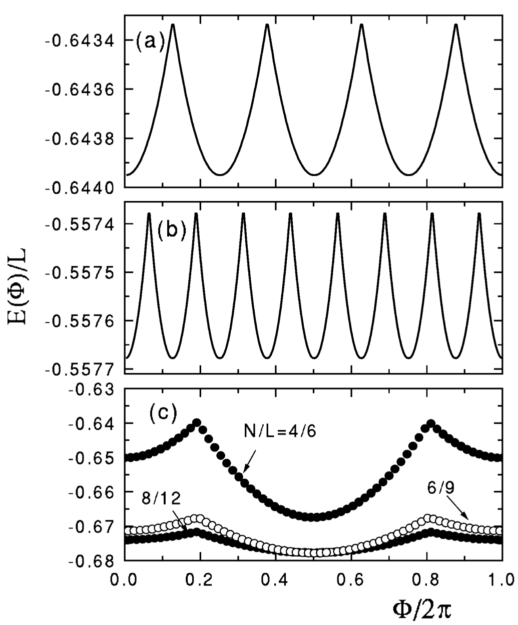

FIG. 1. Ground state energy as a function of twist angle (a) for $|t_{AA}| = |t_{BB}| = 1$, $t_{AB} = 0$, density $n = 2/3$, $U = 0$, and ring length $L = 12$, (b) same as (a) with $U > 4$; (c) for $t_{AA} = t_{BB} = -1$, $t_{AB} = -0.2$, $U = 0$, $n = 2/3$.

The GS Drude weight and spin stiffness are

$$D_c = \frac{L}{2}\,\frac{\partial^2 E(\Phi,\Phi)}{\partial\Phi^2}\Big|_{\varphi=0} = \frac{t}{\pi}\left(\frac{1-n}{1-n_f}\right)^2 \sin(\pi n_f),$$
$$D_s = \frac{L}{2}\,\frac{\partial^2 E_g(\Phi,-\Phi)}{\partial\Phi^2}\Big|_{\varphi=0} = \frac{t}{\pi}\left(\frac{n_\uparrow - n_\downarrow}{n_f}\right)^2 \sin(\pi n_f), \tag{8}$$

where n_f is a function of U/t and n [9,11]. For half-filling, $D_c = 0$, $\forall U$. The result is not surprising for $|U| > 4t$, where the system is a Mott insulator, but rather unexpected for $|U| < 4t$, where the charge gap vanishes. The behavior of the Drude weight for $n \to 1$ is the same as that of a system of n_f carriers with effective mass diverging as $(1 - n_f)^2/(1 - n)^2$.

The ground state is highly degenerate as a consequence of the rich symmetry structure of Eq. (1) when $|t_{AA}| - |t_{BB}| = t_{AB} = 0$. In particular, for an open chain there is a local spin and pseudospin symmetry at each site [9]. Since $t_{AB} = 0$ is an accident rather than a generic feature, it is very important to discuss the effect of a finite t_{AB}, particularly taking into account that this term lifts the GS degeneracy. When $t_{AB} \neq 0$, the sign of t_{AB} or those of t_{AA} and t_{BB} simultaneously, can be changed using symmetry properties [15], but models with different $t_{AA}t_{BB}$ are not equivalent. In the following, we consider the case $t_{AA} = t_{BB} = -t$, which interpolates between two exactly solvable cases: the one considered above and the Hubbard model. This case preserves the SU(2) pseudospin symmetry when $t_{AB} \neq 0$ [15]. We have studied numerically $E(\Phi_\uparrow = \Phi_\downarrow = \Phi)$ for finite systems with fixed densities $n \neq 1$, $n_e, n_d \neq 0$ at $t_{AB} \neq 0$. An example is shown in Fig. 1(c). We find that a small t_{AB} gives rise to an $E(\Phi)$ with two well-defined local energy minima which strongly suggests AFQ in the thermodynamic limit [the fact that there is a small difference between $E(\Phi + \pi)$ and $E(\Phi)$ is a finite-size effect [19]]. Study of the correlation exponent K_ρ [9] confirms the dominance of superconducting correlations at large distances.

What is the origin of the superconducting correlations? Is it related with the η pairing? Note that the (nondegenerate) GS for $t_{AB} \to 0$ is exactly known in two cases. For $U > -4t\cos(\pi n)$ and $U > 0$, $N_e N_b = 0$ [9–11] and the low energy physics of the model becomes equivalent to that of a Hubbard model with interaction $U_H = t^2 U/t_{AB}^2 \to \infty$. In this limit Ogata and Shiba [20] have shown that the GS wave function can be factorized in two parts: one describing the position and the other the spin of the N_f fermions. This GS wave function can be mapped into the corresponding one for $U < 0$ and a magnetic field high enough to ensure $N_\uparrow N_\downarrow = 0$ using the transformation that interchanges spin and pseudospin [17]. It is natural to expect that the effect of a small t_{AB} is to introduce antiferromagnetic correlations between spins and pseudospins in the general case. This fact led us to propose an *ansatz* for the GS in the limit $t_{AB} \to 0$ consisting of *three* factors, describing the positions of fermions and bosons and the spin and pseudospin variables. The first two factors are those of the GS Bethe ansatz solution of the $U = +\infty$ Hubbard model. The last one is the GS of a Heisenberg model for the pseudospin variables, which is also the GS of the large negative-U Hubbard model in a system with N_b sites and $2N_d$ particles. We have computed the overlap of our ansatz with the exact GS obtained from exact diagonalization in different chains (up to $L = 12$ sites), and we found that it is equal to $(1 - \alpha^2 t_{AB}^2)^{1/2}$, with $\alpha \sim 2 - 4$, for $0 \neq t_{AB} < 0.1$, confirming our conjecture for $t_{AB} \to 0$. It is easy to verify with our ansatz that in the thermodynamic limit, for $L \to \infty$, the pair correlation function $C(l) = \langle c^\dagger_{i+l\uparrow} c^\dagger_{i+l\downarrow} c_{i\downarrow} c_{i\uparrow} \rangle$ can be expressed in terms of the corresponding correlation function of the large $|U|$ attractive Hubbard model $C_H(l)$ for density $(n - n_f)/(1 - n_f)$ as $C_H(l) = (1 - n_f)[C_H(l')]_{\rm av}$, where the average l' is centered around $L(1 - n_f)$. Thus the superconducting properties of the system are essentially those of the large U attractive Hubbard model with dilute superfluid density. The superconducting properties of the model are not related with the η pairing. For $t_{AA} = t_{BB}$, the generators of the total pseudospin algebra are $\eta' = \sum_i (-1)^i c^\dagger_{i\uparrow} c^\dagger_{i\downarrow}$, $\eta^+ = (\eta^-)^\dagger$, and $\eta^z = (1/2) \sum_i (1 - \sum_\sigma n_{i\sigma})$. The η-pairing mechanism applies η^- to an eigenstate with $\eta \neq 0$ to obtain eigenstates with $\eta^z < \eta$ which possess ODLRO [8–11]. However, since by construction, our ansatz for the GS has $\eta^z = \eta$, and the true (nondegenerate) ground state has the same quantum numbers, it cannot be the result of applying η^- to any eigenstate. Exact diagonalization results show that this is also the case in 2D, even for $t_{AB} = 0$ [15].

In summary, we have shown that at least in the 1D generalized Hubbard model (1) for $|t_{AA}| - |t_{BB}| = t_{AB} = 0$, the η pairing does not lead to superconductivity. The possibility of constructing eigenstates with ODLRO using the SU(2) symmetry does not guarantee the existence of superconducting currents giving rise to anomalous flux quantization and Meissner effect. The ODLRO must be analyzed in the presence of a finite magnetic flux threading the ring. This fundamental fact is in the spirit of the proposals of Refs. [2–4]. We have also examined the character of the metal-insulator transition near half filling and we have presented strong evidence that the GS degeneracy is broken in favor of a GS with dominant superconducting correlations in 1D when a small t_{AB} is turned on.

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*Permanent address: Departamento de Física, Universidad Nacional de La Plata, 1900 La Plata, Argentina.

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