Persistent current of a Hubbard ring threaded with a magnetic flux

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The persistent current in microscopic and mesoscopic Hubbard rings threaded with magnetic flux is studied as a function of the flux and the Coulomb repulsion parameter U. For microscopic rings having very large U, we find that as the flux is increased by one quantum, a magnon hole traverses the magnon sea, generating a periodicity of $1/N_c$ in the persistent current, but with no changes in the overall spin magnetization, in contrast to the earlier suggestion of Kusmartsev. For non-half-filled mesoscopic rings, we use methods developed by Woynarovich for the zero-flux case to build a rather complete picture of the variation of persistent current with magnetic flux. We find the periodicity to be a half flux quantum or a whole one, and show how the critical flux values at which the current reverses vary with system parameters. We show how the behavior characteristic of microscopic rings goes over to that of mesoscopic rings as N_c/U increases.

I. INTRODUCTION

Recently, several authors have examined the behavior of microscopic and mesoscopic Hubbard rings threaded by magnetic flux and, in particular, have examined the persistent currents generated in such rings by the flux.[1-5] The Hubbard ring is interesting as an example of a strongly-correlated-electron system that is solvable using the Bethe ansatz.[6] It has been argued to be a good model for the optical properties of such quasi-one-dimensional conductors as TTF-TCNQ,[7] various aromatic molecules, and systems of connected quantum dots.[4] It is also possible that understanding its properties might be helpful in analyzing the physics of the Aharonov-Bohm effect in mesoscopic metal rings.[8]

In this paper we map the persistent current as a function of magnetic flux for Hubbard rings over a wide range of ring sizes and values of the Hubbard Coulomb-repulsion parameter U. For convenience we usually plot the ground-state energy as a function of the threading magnetic flux; the persistent current is then just minus the slope of this curve. For a Hubbard ring, the effect of a small magnetic flux is to twist the boundary conditions on electronic eigenstates through an angle Φ proportional to the flux. A flux quantum corresponds to a twisting angle of 2π, and so $\Phi/2\pi$ measures the threading magnetic field in units of the flux quantum hc/e. Evidently, the ground-state energy $E_0(\Phi)$ of the electronic system is periodic in Φ with period 2π. (By "ground state" we mean the lowest-energy state of the system for a given angle of twist, which is in general not the state given by following adiabatically the quantum state lowest for zero twist as the angle is increased. A trivial counterexample is provided by a single noninteracting electron.)

Very recently, Kusmartsev[4] has pointed out that for microscopic Hubbard rings with very strong Coulomb repulsion U between electrons, that is, $U/N_c \gg 1$, where N_c is the number of electrons in the system, the ground-state energy varies with a surprisingly short period, $\Delta\Phi = 2\pi/N_c$. He states that this oscillation is driven by spin-flip processes, the number of spin-up electrons jumping by 1 for each period, so that the spin magnetization of the system varies over its maximum possible range as the flux increases by one flux unit. We examine these small Hubbard systems in Sec. III and confirm Kusmartsev's result that the ground-state energy (and hence, of course, the persistent current) does oscillate with the shorter period as Φ increases. However, we do not agree with his assertion that the spin magnetization varies over a wide range as the flux changes by one quantum. It is true that if U is actually infinite, the energy levels, including the ground state, become degenerate with respect to spin magnetization, and so Kusmartsev's choice of the successive ground states is as good as any other. Nevertheless, in the physically interesting situation of large but not infinite U, the degeneracy is broken, and we find that over the whole range of Φ, states having total spin 0, $\frac{1}{2}$, or 1 (depending on the number of particles present) have lower energies than the spin-magnetized states discussed by Kusmartsev.

To see what happens when an increasing magnetic flux threads these small Hubbard rings with large U, consider the Bethe-ansatz equations (2.3) (given below) for U going to infinity, giving (3.1) (following Kusmartsev). The point to note is that in this limit, the magnon sea contributes the same constant phase shift to each of the charge (or holon) momenta, so that its effect is the same as that of an added fractional flux proportional to the total momentum of the magnon sea. Now, on increasing the external twist angle Φ on the system (i.e., the magnetic flux) from zero, the lowest-energy state of the system for a particular Φ is given at large U by generating a compensating momentum in the magnon sea, that is to say, a momentum which will counterbalance as much as possible the extra holon phase shift Φ and, hence, minimize the increase in energy of the holon distribution. Of course, for finite U, there is some energy cost associated with creating momentum in the magnon sea. However, for large U, the spin degrees of freedom are equivalent to those of a Heisenberg antiferromagnetic chain with coupling of order N_c/NU. Thus, for large enough U, it is always worth creating momentum in the magnon sea, which costs energy of order N_c/NU, because the consequent lowering of energy of the charge Fermi sea is independent of U in leading order. It is of order $1/N$. As discussed in Sec. III, the energetically most economical way to create a given magnon momentum less than π is to create a single des Cloizeaux–Pearson excitation, that is, a single hole in the sea. As Φ is increased, this hole moves from one Fermi point to the other.

It should be noted that since the magnon momentum is itself quantized, it cannot perfectly compensate for the effect of a smoothly increasing twist angle Φ, and from (3.3) it is evident that this remaining imbalance leads to the energy oscillating with the short period $2\pi/N_c$. The picture is somewhat complicated by the parity requirements (integer or half odd integer) on the numbers of charges and spins. It is necessary to deal with the four possibilities separately, as they lead to different sets of ground-state configurations. A full analysis is presented in Sec. III.

Thus, for large enough U in a microscopic ring, the function $E_0(\Phi)$ has a sequence of N_c parabolic segments between zero and 2π. The analysis outlined above enables us to identify the states of the system corresponding to these curves However, it also suggests how $E_0(\Phi)$ will change as U becomes smaller or the size of the system increases. It is a good initial approximation just to add the appropriate magnon energy to each parabolic segment. This clearly means that, as U decreases, segments corresponding to higher magnon energies are raised and their share of the range in Φ shrinks and disappears. Beyond a certain point, only two segments remain: those corresponding to magnon momenta zero and π. By numerically solving the Bethe-ansatz equations, we have confirmed that this is indeed what happens, even when higher-order terms are included. For example, we find that for 16 electrons on a chain having 32 sites, there are only two segments remaining if U is less than 100. This means that for U below this value, there are *no holes* in the sequence of magnon quantum numbers in the lowest-energy state.

Since the relevant parameter in determining the number of segments is N_c/U from the discussion above, it certainly seems safe to conclude that for *mesoscopic* rings having U in the range of physical interest ($U \le 100$, say), there will be no holes in the magnon distribution in the ground state. This implies that we can construct $E_0(\Phi)$ for mesoscopic rings by extending some of the work of Woynarovich on the finite-size corrections to the ground-state energy of a Hubbard ring with the usual periodic-boundary conditions (no flux).[9] Among other things, Woynarovich found that the energy changes in these rings when the particle sea and/or the magnon sea is shifted over by discrete amounts (i.e., particles or spin quantum numbers are moved from one Fermi point to the other). But this is precisely what happens (for particles) when a magnetic flux is introduced through the ring, except that the flux gives a continuous shift rather than a discrete one. Woynarovich found the energy of the set of states generated in this way to vary as the square of the displacement, with a coefficient that could be expressed in terms of the Fermi velocities and the dressed charge. (The dressed charge, a renormalization factor, can be calculated from the Bethe-ansatz equations.[10]) Using his results, we can map out exactly the lowest-energy state of the system as a function of the magnetic flux. The graph is a sequence of parabolic segments, as it would be for noninteracting fermions, but the interaction changes both the curvature of the parabolas and their relative minima, so the segments are in general of different lengths. In fact, we find that the parabolic segment centered at the origin for a ring of $4n$ electrons disappears entirely near half filling. Another important difference from the noninteracting case is that the allowed quantum numbers for the particles can be either integer or half odd integer, depending on the numbers of excitations present, and this affects the ordering of energy levels at a given flux, as discussed in detail in Sec. IV.

It is instructive to compare the $E_0(\Phi)$ derived for mesoscopic rings using Woynarovich's approach with that following from our approximate analysis, and exact numerical work, on microscopic rings. The connection is clear. The mesoscopic $E_0(\Phi)$ given by (4.14) has two parabolic segments centered at zero and π. That at π is raised by $\pi v_s/N$, the magnon energy of a π magnon in a finite system. This is just what we found above on extrapolating the microscopic analysis. (It should be noted that in both microscopic and mesoscopic cases, what we refer to as the magnon energy here means the energy in the *spin* degrees of freedom. Introducing that same magnon into a system constrained by *periodic*-boundary conditions would cost more energy, because of the holon-phase shifting. That is the same effect, with opposite twist, as increasing Φ, which is what we have introduced the magnon to compensate.) However, the change in curvature of the parabolic segments, in other words, the dressed charge, is *not* given by our simple approximation of just adding the magnon energy, although it is a $1/U$ effect. This point is discussed in more detail in Sec. III.

Finally, we consider the exactly half-filled Hubbard ring. The curvature of the energy as a function of flux near the origin, which is essentially the Drude weight measuring the low-frequency optical response of the system, has been analyzed by Fye *et al.*[2] They find it to be negative (paramagnetic) for rings with $4n$ sites, positive for $4n+2$ sites, and exponentially vanishing with increasing system size. Stafford, Millis, and Shastry[3] emphasize what they term a rather peculiar property, namely, that for N electrons on a ring of $N=4n$ sites, the distribution of charge quantum numbers, which must be integers in this case, is necessarily not quite symmetric, going from $-N/2$ to $N/2-1$ or $-N/2+1$ to $N/2$, giving a ground-state momentum of $\pm\pi$. Unfortunately, our methods based on Woynarovich's results do not work for the half-filled case. This is because there is no headroom at the Fermi surface to insert extra particles—that is why the charge excitations have a gap. We did, however, note one unexpected point concerning the distribution of momenta in the ground state. Even though the distribution of quantum numbers may not be symmetric in the $4n$ ground state, as discussed above, the distribution of momenta is. The reason is that one of the momenta is exactly at π (for zero flux), well away from the others in a finite system. It is immediately apparent, on inspecting the Bethe-ansatz equations (2.3) below, that this is the momentum value corresponding to the quantum number $N/2$. When the flux moves away from zero, this particle rapidly descends, and the overall energy drops, although by a much smaller amount than the single-particle contribution as a result of backflow in the rest of the Fermi sea. For this system no level crossings take place as the flux varies. The $(4n+2)$-particle systems vary in a similar way, except that the maximum energy as a function of flux is now at π rather than at 0. This rapid movement of an isolated root as the twist angle varies through a symmetry point is closely related to that found by Sutherland and Shastry for the Heisenberg-Ising chain.[11]

II. BETHE-ANSATZ FORMALISM

We first review the standard Bethe-ansatz solution to the Hubbard ring. The Hamiltonian of the model is

$$\mathcal{H}=-\sum_{j=1}^{N}\sum_{\sigma}(e^{-ieA}\psi_{j+1,\sigma}^{\dagger}\psi_{j,\sigma}+e^{ieA}\psi_{j,\sigma}^{\dagger}\psi_{j+1,\sigma}) +U\sum_{j=1}^{N}n_{j\uparrow}n_{j\downarrow}\ . \tag{2.1}$$

Here N is the number of lattice sites of the ring, $n_{j,\sigma}=\psi_{j,\sigma}^{\dagger}\psi_{j,\sigma}$ is the number of spin-σ electrons at site j, and $U>0$ is the on-site Coulomb repulsion. $A=\Phi/N$ is the vector potential for the magnetic flux. We have neglected the interaction of the spin of the electrons with the magnetic field. We will study rings with a fixed number of electrons. The current in the ring at zero temperature is given by[12]

$$j=-\frac{\partial E_0(\Phi)}{\partial\Phi}\ , \tag{2.2}$$

where we used units $\hbar=1$ and $e=1$.

The eigenstates of a chain with $N_c=N_\uparrow+N_\downarrow$ electrons and $N_s=N_\downarrow$ down spins are characterized by the momenta k_j of charges and the rapidities λ_α of spin waves. For a chain with twisted-boundary conditions, the Bethe-ansatz equations are[6,1]

$$\begin{aligned}Nkj&=2\pi I_j+\Phi-\sum_{\beta=1}^{N_s}2\arctan\left[\frac{4(\sin k_j-\lambda_\beta)}{U}\right],\\ \sum_{j=1}^{N_c}2\arctan\left[\frac{4(\lambda_\sigma-\sin k_j)}{U}\right]&=2\pi J_\alpha+\sum_{\beta=1}^{N_s}2\arctan\left[\frac{2(\lambda_\alpha-\lambda_\beta)}{U}\right].\end{aligned} \tag{2.3}$$

Here N is the number of sites in the ring. The quantum numbers I_j and J_α are either integers or half odd integers, depending on the parities of the numbers of down- and up-spin electrons, respectively:

$$I_j=\frac{N_s}{2}\ (\mathrm{mod}\ 1),\quad J_\alpha=\frac{N_c-N_s+1}{2}\ (\mathrm{mod}\ 1)\ . \tag{2.4}$$

The energy and momentum of the system in a state corresponding to a solution of (2.3) are given by

$$\begin{aligned}E&=-2\sum_{j=1}^{N_c}\cos k_j\ ,\\ P&=\sum_{j=1}^{N_c}\left[k_j-\frac{\Phi}{N}\right]=\frac{2\pi}{N}\left[\sum_j I_j+\sum_\alpha J_\alpha\right]\ .\end{aligned} \tag{2.5}$$

III. MICROSCOPIC RINGS

We study in this section a small chain with very strong on-site repulsion, $U/N_c\gg1$. As discussed by Kusmartsev,[4] in the limit $U/N_c\to\infty$, the $\sin k_j$ terms in (2.3) can be neglected, leading to

$$Nk_j=2\pi\left[I_j+\frac{1}{N_c}\sum_\alpha J_\alpha\right]+\Phi\ . \tag{3.1}$$

Equation (3.1) is identical to that describing a set of noninteracting spinless fermions on a ring threaded with a flux:

$$\Phi/2\pi+\frac{1}{N_c}\sum_\alpha J_\alpha\ . \tag{3.2}$$

If the I_j's are consecutive quantum numbers, the energy of the state is

$$E_0(\Phi)=-E_m\cos\left[\frac{2\pi}{N}\left[\frac{\Phi}{2\pi}+\frac{1}{N_c}\sum_\alpha^{N_s}J_\alpha+D_c\right]\right]\ , \tag{3.3}$$

where D_c is defined by $D_c=(I_{\max}+I_{\min})/2$, and E_m is a positive constant:

$$E_m=2\frac{\sin(\pi N_c/N)}{\sin(\pi/N)}\ . \tag{3.4}$$

We assume in the following that the system is not exactly half filled, for if it were, the above expression for E_m would be zero. The energy $E_0(\Phi)$ can be minimized for Φ by choosing the set J_α such that

$$\sum_{\alpha=1}^{N_s}J_\alpha=-p\quad\text{for}\quad\frac{2p-1}{2N_c}<\frac{\Phi}{2\pi}+D_c<\frac{2p+1}{2N_c}\ . \tag{3.5}$$

It is evident from (3.3) that, with these J_α, the graph of $E_0(\Phi)$ as a function of Φ is a sequence of identical parabolic segments (strictly, parabolic in the limit of large N), giving a function with period $1/N_c$ of a flux quantum. The problem is that this infinite-U system is highly degenerate. There are many ways of choosing sets of J_α's to give the same sum—one can adjust the total number of down spins, following Kusmartsev. There are, however, other possibilities. For example, gaps can be introduced in the magnon quantum-number distribution. The question to resolve is what states are the lowest-energy states when U is large but finite and the degeneracy is lifted. To find out we examine the leading-order $1/U$ corrections to the Bethe-ansatz equations for infinite U.

This $1/U$ expansion is actually quite tricky, as we shall discuss later. On examining the Bethe-ansatz equation (2.3), we note that, for large U, the λ_α's will be of order U, whereas the $\sin k_j$'s are, of course, of order unity; for a small system, the λ_α's will be widely scattered and, with one possible exception, will have $|\lambda| \gg 1$. With this picture in mind, we expand the arctangent functions to leading order in $\sin(k_j)/U$ and define scaled variables x_α by

$$x_\alpha = \lim_{U\to\infty} (2\lambda_\alpha/U) . \tag{3.6}$$

For large but finite U, the k_j's in (2.3) have leading $1/U$ corrections:

$$\delta k_j = -\frac{2\sin(k_j)}{NU} \sum_\alpha \frac{1}{\frac{1}{4}+x_\alpha^2} , \tag{3.7}$$

where the x_α satisfy the equations

$$2N_c \arctan(2x_\alpha) = 2\pi J_\alpha + \sum_{\beta=1}^{N_s} 2\arctan(x_\alpha - x_\beta) . \tag{3.8}$$

The corresponding correction to the energy is easily obtained from (2.5):

$$\begin{aligned} E_{\text{spin}} &= -\frac{4}{NU}\left[\sum_{j=1}^{N_c} \sin^2 k_j\right] \sum_{\alpha=1}^{N_s} \frac{1}{\frac{1}{4}+x_\alpha^2} \\ &= -J\sum_\alpha \frac{1}{\frac{1}{4}+x_\alpha^2} . \end{aligned} \tag{3.9}$$

We note that the energy E_{spin} and Eq. (3.8) are just the energy and Bethe-ansatz equations of an antiferromagnetic Heisenberg spin chain of exchange coupling J, with N_c sites and with N_s spins down.

Finding the lowest-energy state of a Hubbard chain with sufficiently large U in a magnetic field is thus reduced to finding the state of lowest energy of a Heisenberg spin chain with a certain momentum $q = 2\pi\sum J_\alpha/N_c$. This problem has been studied by des Cloizeaux and Pearson.[13] For zero momentum the state of lowest energy of the Heisenberg chain is the singlet state. However, for a given nonzero momentum, the lowest-energy state is the des Cloizeaux–Pearson spin-wave excitation, a triplet state described by real $\{x_\alpha\}$, with a hole in the distribution of the quantum numbers $\{J_\alpha\}$. Creating a single-hole excitation of this kind is the most energy-efficient way of generating a given total magnon momentum, because the spin-wave energy plotted as a function of its momentum curves downward below its low-energy linear form, so it would cost more energy to produce the same momentum using several excitations. In particular, we find that for finite U, the states in Ref. 4, where the total spin magnetization undergoes large fluctuations as Φ increases, have higher energies than the single-hole states with the same magnon momentum. States with complex λ_α are also found to have higher energies than these states (compare the remarks of Woynarovich in Ref. 9). For large U this follows from a consideration of the corresponding states of the equivalent finite antiferromagnetic Heisenberg chain. Translating the quantum numbers back to the Hubbard model, we find that, for $U \gg 1$, the states minimizing the energy for nonzero flux depend on the values of N_c, N_s (mod 4).

A. $N_c = 4n+2$, $N_s = 2n+1$

In this case, from (2.4), the I_j's are half odd integers and the J_α's are integers. For zero flux, the quantum numbers I_j's and J_α's are both distributed symmetrically about the origin. For nonzero flux, the new ground state has a hole in the J_α distribution. The ground state for a chain with flux

$$(2p-1)/2N_c < \Phi/2\pi < (2p+1)/2N_c$$

is

$$\begin{aligned} &I_1, \ldots, I_{N_c} = -(N_c-1)/2, \ldots, (N_c-1)/2 , \\ &J_1, \ldots, J_{N_s} = -(N_s+1)/2, -(N_s-1)/2, \ldots, -(N_s-2p+1)/2, -(N_s-2p-3)/2, \ldots, (N_s-1)/2 . \end{aligned} \tag{3.10}$$

The J_α from the hole at $-(N_s-2p-1)/2$ has been moved to the left Fermi surface. This is a state with a magnon excitation of momentum $-2\pi p/N$ and is the lowest-energy state from approximately $\Phi/2\pi = (2p-1)/2N_c$ to $\Phi/2\pi = (2p+1)/2N_c$. We say "approximately," because different parabolic segments have had their bottoms raised by different amounts of order $1/U$, so the points of intersection will have shifted to this order.

B. $N_c = 4n$, $N_s = 2n$

The I_j's must be integers, and all the J_α's must be half odd integers. The energy at zero flux is minimized by taking

$$I_j = -N_c/2, -(N_c-2)/2, \ldots, (N_c-2)/2 , \tag{3.11}$$

$$J_\alpha = -(N_s-3)/2, -(N_s-5)/2, \ldots, (N_s+1)/2 . \tag{3.12}$$

We note that one of the J_α's has been moved from the left Fermi surface to the right one and the state has momentum $P = 2\pi N_s/N$. For nonzero flux, $(2p-1)/2N_c < \Phi/2\pi < (2p+1)/2N_c$ (approximately, as discussed above), the ground state is the one with the pth J_α from the left moved to the left Fermi surface.

C. $N_c = 4n+1$, $N_s = 2n$

For this case the I_j's and J_α's all have to be integers. At zero flux the quantum numbers are

$$I_j = -(N_c-1)/2, \ldots, (N_c-1)/2 ,$$
$$J_\alpha = -N_s/2, \ldots, -1, 1, \ldots, N_s/2 . \quad (3.13)$$

There is a hole at $J_\alpha = 0$. This state has momentum zero. For $(2p-1)/2N_c < \Phi/2\pi < (2p+1)/2N_c$, the ground state will be the one with $J_\alpha = p$ moved to 0. We note in particular that for $\Phi = \pi/2$, the J_α's are consecutive integers.

D. $N_c = 4n-1, N_s = 2n-1$

In this case all the I_j's and J_α's must be half odd integers. For zero flux the ground-state quantum numbers are

$$I_j = -N_c/2, \ldots, (N_c-2)/2 ,$$
$$J_\alpha = -(N_s-2)/2, \ldots, -\tfrac{1}{2}, \tfrac{3}{2}, \ldots, (N_s+2)/2 . \quad (3.14)$$

We note that there is a hole between $-\frac{1}{2}$ and $\frac{3}{2}$. As the flux increases, the hole will move to the right. For

$$(2p-1)/2N_c < \Phi/2\pi < (2p+1)/2N_c ,$$

the hole is at $J_\alpha = (2p+1)/2$. At Φ equal to half a flux quantum, the J_α quantum numbers all consecutive half odd integers. Beyond that the I_k quantum numbers will all shift to the right by 1, and the hole in the J_α distribution will move to the negative side.

What we have done in the above analysis is to find, by evaluating the leading term in $1/U$ for a small system, just which of the many degenerate (at infinite U) states has lowest energy at finite but large U. At the same time, we have determined approximately what the energy splitting is and how the parabolic segments are moved up and down relative to each other by amounts equal to the appropriate magnon-energy differences. We wish to examine the range of validity of this picture as we go to smaller U or to larger systems. From (3.9) we see that the energy cost of creating the magnon has order of magnitude N_c/NU. From (3.3) the untwisting of the boundary angle made possible by creating the magnon lowers the energy of the k distribution by an amount of order $1/N$. Thus the relevant parameter in assessing the reliability of our picture is N_c/U. It is also clear from our remarks before Eq. (3.7) why this is so. For mesoscopic systems, $N_c \gg U$, and many λ_α's are of order unity. In this case, taking only the leading-order term in the Taylor expansion for each of them and adding is clearly not a reliable approximation.

Despite these limitations the analysis gives a picture of $E_0(\Phi)$ as a function of Φ, in good agreement with numerical results from infinite U down to U of order 50. The main point is that the sequence of parabola bottoms—and for infinite U there are N_c of them per period—are raised by amounts of order $1/U$, reflecting the magnon energy at the appropriate momentum. Those parabolic sectors raised least therefore become the lowest-energy states over larger and larger intervals in Φ. Thus sectors corresponding to large spin-wave energies disappear from the $E_0(\Phi)$ curve, until finally only two sectors remain: those corresponding to magnon momentum zero and π.

The above picture can be verified for small chains by direct diagonalization of the Hamiltonian for various flux values. Figure 1 gives the ground-state energy of a ring of eight sites and four electrons, calculated by both direct diagonalization and minimization of energy of states within the sector of real λ using the Bethe ansatz, with the same result. As can be seen, for very large U ($U=200$ in the figure), there are four cusps and four parabolic segments in the energy-versus-flux curve in one flux quantum, as many as the number of electrons in the ring. However, for smaller U, the width of some of the segments gets smaller and smaller, until at some U they are taken over by others.

The assumption that only real λ appear in the ground state for any flux thus proves to be correct for large U, where a map to the Heisenberg model is possible, and for small chains, where direct diagonalization of the Hamiltonian is possible. As will be seen in the next section, the assumption is also correct for large systems, in which case the energy of various states can be analytically calculated up to $1/N$. We therefore assume it to be true for any chain size and U and minimize the energy of the system by using only real λ for various sizes of the chain. This is, of course, much more feasible than allowing general complex λ. Figure 2 is the ground-state energy $E(\Phi)$ calculated for chains with $U=100$ and density $n_c=0.5$. The energy for the chain with four sites has four pronounced cusps. For the chain with eight electrons, the energy has eight parabolic segments in a period, but some become very narrow, while the segments around $\Phi=0$ and π widen. For 16 electrons, these two branches take over the whole period.

As mentioned above, these two sectors correspond to the singlet ground state of the spin chain and the spin-wave state with momentum $q=\pi$, respectively. These two states have the same energy in the thermodynamic limit, as indicated by the spin-wave dispersion relation. However, for finite chains, the spin-wave state has an excitation energy proportional to $1/N_c$. For large yet finite chains, this spin-wave excitation energy scales as a function of the chain size N the same way as the energy

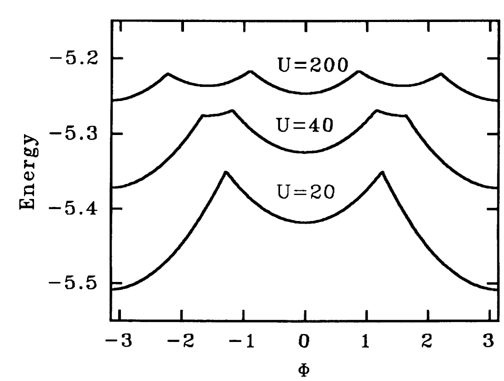

FIG. 1. Ground-state energy $E(\Phi)$ for a chain of eight sites and two spin-up and two spin-down electrons for the Hubbard repulsion $U=20$, 40, and 200.

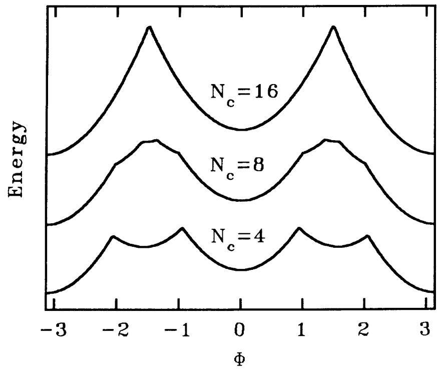

FIG. 2. Ground-state energy $E(\Phi)$ for chains with $U=100$ and density $n_c=0.5$. For the chain with 4 electrons, the energy has 4 pronounced cusps in one period. For 8 electrons there are 8 parabolic segments, but some are very narrow. For 16 electrons there are only two segments. Larger chains also have two level crossings. Note that the energies have been scaled.

reduction achieved in E_0 by the partial flux cancellation. As a result, for large chains, the widths of the two sectors at $\Phi=0$ and π approach values independent of the size of the chain. However, the width of the two sectors is dependent on the on-site repulsion U and the density of electrons.

Again, for chains with $U \gg 1$, this relative width is easy to find, at least in certain limits. For very large U, the magnon energy is negligible, and the two sectors should have almost the same width. However, for chains with density close to half filling, E_m in Eq. (3.4) is proportional to the hole density and is very small. The magnon energy in this case becomes dominant, and the sector with a magnon of $q=\pi$ will not be the ground state for any flux value. In this case the ground-state energy will have only one parabolic sector in the whole period.

In the next section, we will discuss mesoscopic chains with $N \gg 1$ and $N/U \gg 1$. In this case the k_j and λ_α become continuously distributed on the real axis. We can analytically discuss the flux dependence of the ground-state energy without resorting to the $1/U$ expansion. We will find that any chain with $N/U \gg 1$ has qualitatively the same behavior as chains with $N/U \gg 1$ and $U \gg 1$, independent of the value of U.

IV. MESOSCOPIC RINGS

In the thermodynamic limit, the momenta k_j of the electrons and rapidities λ_α of the magnons are continuously distributed on the real axis, and the Bethe-ansatz equations can be reduced to a set of integral equations, making them much easier to solve. This is the standard approach for finding the ground-state energy of a large system, for example. However, it has to be used carefully for the problem we are considering. The persistent current has an order of magnitude equivalent to that generated by a single electron at the Fermi level. In other words, for a noninteracting gas, this would be the current resulting from moving all the electrons to the right in momentum space by just one quantum state—a $1/N$ effect. In fact, the change in the ground-state energy arising from such a shift is down by a factor $1/N^2$ from the total ground-state energy, since to leading order the energy gained in the shift at one Fermi point is lost at the other. This implies that simply replacing the sum over momenta in the Bethe-ansatz equations by an integral will miss the effect we are looking for, since that introduces an error of order $1/N^2$.

Fortunately, a complete analysis of these finite-size corrections for the usual periodic-boundary conditions has been carried out by Woynarovich,[9] and it is not difficult to adapt his work to the case of twisted-boundary conditions. Woynarovich succeeded in calculating the energies of those states which resemble the ground state in that both momentum and spin quantum numbers form consecutive sets; that is to say, there are no holes in the distributions. (He later went on to add low-energy excitations, but these are not relevant to our present considerations.) These hole-free states differ from the standard half-filled nonmagnetic Hubbard ground state in that they may have different total numbers of particles, N_c, and of down spins, N_s, and they also may be shifted off center, by displacements D_c and D_s, respectively. It is easy to see that for the states under consideration these quantum numbers can be written in terms of the maximum and minimum occupied single-particle and -magnon quantum numbers $I_{\max}$, $I_{\min}$, $J_{\max}$, and $J_{\min}$ as follows;[9]

$$\begin{aligned} I_{\max}-I_{\min}+1=N_c, \quad I_{\max}+I_{\min}=2D_c\ , \\ J_{\max}-J_{\min}+1=N_s, \quad J_{\max}+J_{\min}=2D_s\ . \end{aligned} \tag{4.1}$$

Woynarovich found that, to order $1/N$, the energy of a hole-free distribution defined as above is

$$\begin{aligned} E=N\varepsilon_\infty+\frac{2\pi v_c}{N}\left[\frac{(N_c-n_cN)^2}{4\xi^2}+\xi^2\left[D_c+\frac{D_s}{2}\right]^2-\frac{1}{12}\right] \\ +\frac{2\pi v_s}{N}\left[\frac{1}{2}\left[\frac{N_c}{2}-N_s\right]^2+\tfrac{1}{2}D_s^2-\frac{1}{12}\right]\ . \end{aligned} \tag{4.2}$$

Here v_c and v_s are the so-called holon and spinon velocities, that is to say, the speeds of excitations near the Fermi points in the charge and spin distributions, ξ is the dressed charge, and n_c is the ground-state density in the thermodynamic limit. These parameters can all be found as functions of the electron density and on-site repulsion strength by solving some integral equations, as has been shown by Woynarovich.

The important thing to note in Eq. (4.2) is that the energy has a simple quadratic dependence on the four parameters N_c, D_c, N_s, and D_s.

Now adding a phase twist Φ to the boundary conditions in the Bethe-ansatz equations is equivalent to a uniform shift in the quantum numbers $I_j \rightarrow I_j+\Phi/2\pi$. Evidently, then, the generalization of (4.2) to twisted-boundary conditions is just to replace D_c by $D_c+\Phi/2\pi$, giving

$$E=N\varepsilon_\infty+\frac{2\pi v_c}{N}\left[\frac{(N_c-n_cN)^2}{4\xi^2}+\xi^2\left[D_c+\frac{\Phi}{2\pi}+\frac{D_s}{2}\right]^2-\frac{1}{12}\right]+\frac{2\pi v_s}{N}\left[\frac{1}{2}\left[\frac{N_c}{2}-N_s\right]^2+\tfrac{1}{2}D_s^2-\frac{1}{12}\right]. \quad (4.3)$$

It is clear from this equation that the curvature constant, the coefficient of Φ^2, is just the charge-stiffness constant discussed in Refs. 1–3. That is, we define the charge-stiffness constant by

$$\mathcal{D}_c=\frac{v_c\xi^2}{2\pi}. \quad (4.4)$$

The analogous spin-stiffness constant $\mathcal{D}_s$ is defined by

$$\mathcal{D}_s=\frac{v_s}{2\pi}, \quad (4.5)$$

for the systems that we consider. (For systems having finite spin magnetization, the dressing factors are more complicated.) The spin stiffness becomes relevant when the lowest-energy state for a given flux has a shifted magnon sea.

It is now straightforward to find how the ground-state energy of the Hubbard ring varies with the magnetic flux enclosed. For a given total number of electrons, N_c, and given magnetic flux Φ threading the system, the expression for the energy in (4.3) is minimized by appropriate choice of the other quantum numbers. Obviously, as Φ is increased from zero, at certain values the best choice of these other quantum numbers will change, and so the graph of ground-state energy as a function of Φ will be a sequence of parabolic segments.

The only other complication in this analysis is a bookkeeping one—the quantum numbers I_j and J_α, and hence the displacements D_c and D_s, are integer or half odd integer, depending on the parities of the numbers of electrons and of down spins, so one must consider separately the different possible total numbers of electrons *modulo 4*.

The physics of the problem is contained in the curvature of the parabolic segments, that is to say, the second derivative of total energy as a function of Φ, and the switch points, or level crossings, the values of Φ at which the lowest-energy state moves from one parabolic segment to another one defined by a different set of quantum numbers. These determine the periodicity of the energy, and hence of the persistent current, as a function of the threading magnetic field. It is evident from (4.3) above that these points are determined by the Fermi-point velocities and the dressed charge, which in turn can be calculated from the total electron density and on-site Coulomb-repulsion parameter U.

For the convenience of the reader, we summarize here the equations derived by Woynarovich for computing the Fermi-point velocities and dressed charge (for the case of no net macroscopic spin magnetization) and solve them analytically in some simple limits.

The dressed charge ξ is given by

$$\xi=\xi(k_0), \quad (4.6)$$

where $\xi(x)$ satisfies the integral equation

$$\xi(x)=1+\frac{1}{2\pi}\int_{-\sin k_0}^{\sin k_0}\bar{K}(x-x')\xi(x')dx',$$
$$\bar{K}(x)=\int_{-\infty}^{\infty}\frac{\exp(-|\omega|U/4)}{2\cosh(\omega U/4)}\exp(i\omega x)d\omega. \quad (4.7)$$

The holon and spinon velocities are given by

$$2\pi v_c=\varepsilon_c'(k_0)/\rho_c(k_0),$$
$$2\pi v_s=\left[\int_{-k_0}^{k_0}\exp\left[\frac{2\pi\sin k}{U}\right]\varepsilon_c'(k)dk\right]\times\left[\int_{-k_0}^{k_0}\exp\left[\frac{2\pi\sin k}{U}\right]\rho_c(k)dk\right]^{-1}. \quad (4.8)$$

Here $\rho_c(k)$ and $\varepsilon_c'(k)$ satisfy the integral equations

$$\rho_c(k)=\frac{1}{2\pi}+\frac{1}{2\pi}\cos k\int_{-k_0}^{k_0}\bar{K}(\sin k-\sin k')\rho_c(k')dk' \quad (4.9)$$

and

$$\varepsilon_c'(k)=2\sin k+\frac{1}{2\pi}\cos k\int_{-k_0}^{k_0}\bar{K}(\sin k-\sin k')\varepsilon_c'(k')dk'. \quad (4.10)$$

These equations can be solved analytically in the following limits.

A. Strong coupling limit

In the limit $U\gg1$, the kernel of the integral equations $\bar{K}\to4\pi\ln2/U$. The Fermi velocities and ξ can be explicitly obtained:

$$v_c=2\sin(\pi n_c)\left[1-\frac{4\pi\ln2}{U}n_c[2+\cos(\pi n_c)]\right],$$
$$v_s=\frac{4}{\pi U}[2\pi n_c-\sin(2\pi n_c)], \quad (4.11)$$
$$\xi=1+\frac{4\ln2}{\pi U}\sin(\pi n_c).$$

We note that the charge-stiffness constant approaches the finite value corresponding to free spinless fermions, while the spin-stiffness constant goes to zero.

B. Close to half-filled chain

As is well known, a half-filled repulsive chain is an insulator, and the charge stiffness $\mathcal{D}_c$ is zero. Close to the half-filled limit, the charge stiffness is proportional to the hole density:[14]

$$\mathcal{D}_c=\frac{v_c\xi^2}{2\pi}=4n_c(1-n_c)b/a^2, \quad (4.12)$$

where b and a are two functions of U introduced in Ref. 14. On the other hand, the spin-stiffness constant is related to the magnetic susceptibility, which has been obtained by Shiba in Ref. 15:

$$2\pi\mathcal{D}_s = v_s = \frac{1}{2\pi\chi} = 2\frac{I_0(2\pi/U)}{I_1(2\pi/U)} , \tag{4.13}$$

where I_ν is the Bessel function of imaginary argument of order ν. We see that in this limit the spin stiffness is a nonzero constant, while the charge-stiffness constant goes to zero as the density approaches the half-filled limit. In general, the two stiffness constants are of comparable value and have to be calculated numerically.

We now discuss the possible level crossings as the flux through the ring changes. As always, the ground state of an individual ring depends crucially on the parities of the numbers of up- and down-spin electrons. Below we give the ground state and its energy as a function of flux for each of the four possible cases. Note that because $E(-\Phi)=E(\Phi)$, we only give the ground-state energy for $0<\Phi<\pi$.

C. $N_c = 4n+2$

In this case, $N_s = 2n+1$. There are odd numbers of spin-up and spin-down electrons in the ground state. The quantum numbers I_j must be half odd integers, and the J_α are integers. From (2.4) this gives $D_c = 0$ (mod 1) and $D_s = 0$ (mod 1). For Φ close to zero, the ground state is the state with $D_c = D_s = 0$. We will call this state (0,0). However, for Φ close to π, the state $(0,-1)$ with $D_c = 0$, $D_s = -1$ may have lower energy. The energies of the two states are

$$\begin{aligned} E_{0,0}(\Phi) - E(0) &= \frac{v_c}{2\pi N}\xi^2\Phi^2 , \\ E_{0,-1}(\Phi) - E(0) &= \frac{v_c}{2\pi N}\xi^2(\pi-\Phi)^2 + \frac{\pi v_s}{N} . \end{aligned} \tag{4.14}$$

Here $E(0)$ is the ground-state energy at $\Phi=0$. These two energy levels will cross at

$$\Phi_c = \frac{\pi}{2} + \frac{\pi v_s}{v_c \xi^2} . \tag{4.15}$$

We first discuss the current for Φ close to the origin. The current is diamagnetic and is proportional to the flux. Its magnitude is particularly easy to find in the two limits discussed above. In the strongly repulsive case, differentiating (4.14) with respect to Φ and using (4.11), we find

$$j = \frac{2}{N}\sin(\pi n_c)\left\{1 - \frac{4\ln 2}{\pi U}[2n_c\pi^2 + n_c\pi^2\cos(\pi n_c) + 2\sin(\pi n_c)]\right\}\Phi . \tag{4.16}$$

The first-order term is actually the current of a spinless fermion ring with density n_c. We see that for low density the current is proportional to the electron density, while close to half filling the current is proportional to $(1-n_c)$. In fact, close to half filling, the current is always proportional to $(1-n_c)$ for any nonzero U, as can be seen from (4.12). The current is maximum for quarter-filled rings. Now we discuss where these levels cross.

In the strong-coupling limit, the spin stiffness is very small, and these two levels cross at the point $\Phi_c = \pi/2$. The energy is close to periodic in the flux with period half a flux quantum. At the level crossing, the current changes from a diamagnetic one to an paramagnetic one. We emphasize that here the period halving is caused by level crossing; none of the usual averaging has been introduced.

Near half filling, on the other hand, from (4.12) and (4.13), the charge-stiffness constant is very small and the spin stiffness is not small. It follows that, close enough to half filling, the two levels in (4.14) will cross at some point *beyond* $\Phi=\pi$, and in this case the state (0,0) will first intersect $(-1,0)$, which then becomes the lowest-energy state, and $(0,-1)$ is never the lowest-energy state. In this case the period of the current is one flux quantum.

For general U and filling, we have numerically calculated the level-crossing point Φ_c. Figure 3 is a contour graph of the width of the branch of the parabola centered at $\Phi=\pi$ as a function of U and the filling. We note that, close to half filling, there is a region in the (U, n_c) plane where the width is zero; in other words, the level crossing mentioned above does not happen at all, whereas for large U and away from half filling the level crossing occurs somewhere near $\frac{1}{4}$ of the flux quantum.

D. $N_c = 4n$ with n integer

The ground state should have $N_s = 2n$. According to (2.4), all the I_j's must be integers and all the J_α's must be half odd integers. We have

$$D_c = \tfrac{1}{2} \text{ (mod 1)} \quad \text{and} \quad D_s = 0 \text{ (mod 1)} . \tag{4.17}$$

For Φ around 0, the ground state should have $D_c = -\frac{1}{2}$ and $D_s = 1$. The energy of this state is

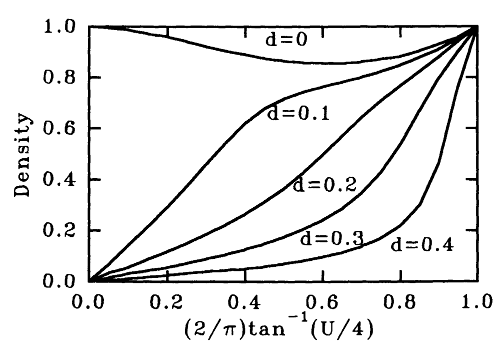

FIG. 3. Width d of the local minimum centered at $\Phi=0$ for a chain with $4n$ electrons. Close to the top of the graph (close to half filling) is a region where the width is zero; this minimum is never the real ground state, and the current is paramagnetic. As the density is decreased and/or the repulsion gets stronger, the width of that local minimum gets bigger. On the lines shown in the figure, the width of the minimum is constant. From top to bottom: $d=0$, 0.1, 0.2, 0.3, and 0.4 flux quantum.

$$E(\Phi)-E(0)=\frac{v_c}{2\pi N}\xi^2\Phi^2+\frac{\pi v_s}{N}\ , \tag{4.18}$$

while for Φ around π, the ground state should have $D_c=-\frac{1}{2}$ and $D_s=0$. The energy of this state is

$$E(\Phi)-E(0)=\frac{v_c}{2\pi N}\xi^2(\pi-\Phi)^2\ . \tag{4.19}$$

These two energy levels cross at

$$\Phi=\pi-\Phi_c\ , \tag{4.20}$$

where Φ_c is given by (4.15). We note that the spectrum is same as in Sec. IV C shifted by half a flux quantum.

E. $N_c=4n+1$

In this case we assumed $N_s=2n$ ($N_s=2n+1$ will give the same result). Then we have $D_c=0$ (mod 1) and $D_s=\frac{1}{2}$ (mod 1). The ground state for Φ between zero and π is the state with $D_c=0$ and $D_s=-\frac{1}{2}$. The energy is

$$E(\Phi)-E(0)=\frac{v_c}{2\pi N}\xi^2(\Phi-\pi/2)^2+\frac{\pi v_s}{4N}\ . \tag{4.21}$$

Extending the above formula to $\Phi<0$, we find that level crossing occurs at $\Phi=0$ and $\Phi=\pm\pi$. Unlike the level crossings for chains with even numbers of electrons, these level crossings are caused by the electron statistics and also occur for free electrons.

F. $N_c=4n+3$

The ground state in this case is $D_c=-\frac{1}{2}$ and $D_s=\frac{1}{2}$. The ground-state energy is the same as in Sec. IV E.

Let us now summarize our findings concerning the persistent current in mesoscopic Hubbard rings. For rings with an *odd* number of electrons, the period of the current is a half a flux quantum, independent of the interaction strength. The current is *paramagnetic* around $\Phi=0$:

$$j=B(\pi/2-|\Phi|)\mathrm{sgn}(\Phi),\quad B=v_c\xi^2/\pi N\ , \tag{4.22}$$

where $\mathrm{sgn}(x)$ is the signum function of x. There is a renormalization of the magnitude of the current due to the interaction, but the periodicity and sign of the current are the same as those of rings of odd numbers of free electrons.

For rings with an *even* numbers of electrons, the current is *diamagnetic* around $\Phi=0$ [except rings whose density is very close to half filling, in which case the current may be paramagnetic for a ring whose electron number is 0 (mod 4)]. For a chain whose numbers of spin-up and -down electrons are both odd, the current will become paramagnetic at $\Phi_c, \pi/2<\Phi_c<\pi$,

$$j=\begin{cases}-B\Phi, & |\Phi|<\Phi_c\\ -B(\pi-|\Phi|), & \Phi_c<|\Phi|<\pi\ ,\end{cases} \tag{4.23}$$

whereas for a chain in which the numbers of spin-up and -down electrons are both even, the switch occurs at $\pi-\Phi_c$,

$$j=\begin{cases}-B\Phi, & |\Phi|<\pi-\Phi_c\\ -B(\pi-|\Phi|), & \pi-\Phi_c<|\Phi|<\pi\ .\end{cases} \tag{4.24}$$

An interesting observation is that for chains with strong repulsion $U\gg 1$, the switch occurs at $\Phi_c\simeq\pi/2$. For such chains the period of the persistent current of each individual ring is half a flux quantum. A comparison with the persistent current of free-electron rings[16] shows that in this case the current is drastically different from the free-electron case. The current for a ring with $4n$ electrons for small Φ is, e.g., changed from a paramagnetic one into a diamagnetic one.

For rings with not very strong interactions or with a density close to half filling, the period of the persistent current of an individual ring is still one flux quantum. However, just as demonstrated by Loss and Goldbart, and by Kusmartsev[16] for free-electron rings, the average current of a collection of rings with random numbers of electrons has a period of half a flux quantum. Assuming there are equal numbers of rings with even and odd numbers of electrons, a simple average of the current yields

$$j_{\mathrm{av}}=\begin{cases}B(\mathrm{sgn}\Phi-4\Phi), & |\Phi|<\pi-\Phi_c\\ B(2\pi\,\mathrm{sgn}\Phi-4\Phi), & \pi-\Phi_c<|\Phi|<\Phi_c\\ B(3\pi\,\mathrm{sgn}\Phi-4\Phi), & \Phi_c<|\Phi|<\pi\ .\end{cases} \tag{4.25}$$

The period of the average current is half a flux quantum, and the current is paramagnetic. The periodicity and sign of the average current are the same as those of free-electron rings.

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