Level crossover and microscopic oscillations of persistent currents in the Hubbard model with attraction

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We show that when the number of uncoupled electrons is small or when the attraction constants are large, a Hubbard chain with N attractive electrons at the lattice sites placed in gauge nonforce magnetic and electric fields exhibits microscopic oscillations of persistent currents with fractional periods Φ_0/N and $F_0/(N-2M)$, where M is the number of pairs, Φ_0 is the "metallic" magnetic flux quantum, and F_0 is the electric flux quantum. These oscillations are related to the partitioning of the degrees of freedom of pairs and uncoupled electrons, and they occur in fields somewhat above the critical value for pair disruption. We study the role played by the crossover of energy levels in the change in period of mesoscopic oscillations of persistent currents, a change that is governed by the parameters of the system. © *1996 American Institute of Physics.* [S1063-7761(96)01801-8]

1. INTRODUCTION

In recent years there has been an upsurge of interest in studies of persistent currents in mesoscopic quantum rings, an interest related to the appearance of experiments that study oscillations of such currents in an external magnetic field.[1–3] The nonforce topological action of the electric and magnetic fields on charged particles with a magnetic moment manifests itself, for instance, in the Aharonov–Bohm (AB) and Aharonov–Casher (AC) quantum effects,[4,5] related to the fact that the wave functions acquire phases proportional, respectively, to the magnetic and electric fluxes. Systems of the greatest interest in this connection are those in which the nonforce topological effect of the electromagnetic field manifests itself along with the interactions of the particles comprising the systems, for instance, highly correlated electronic systems. The effect of the field fluxes may manifest itself in a special way in the low-temperature phases of such systems. For instance, in superconductors the magnetic flux becomes quantized.[6]

Quantum fluctuation effects are known to show themselves most vividly in low-dimensional systems, where they are enhanced by singularities in the density of states. Unfortunately, the approximate methods used in the theoretical description of low-dimensional systems, such as various mean-field approximation methods or variational methods, may even yield qualitatively incorrect results. Hence the particular interest in studying topological effects in exactly solvable quantum models of highly correlated electronic systems. In previous papers[7–9] effects of the AB and AC types were studied in one-dimensional quantum models of the Hubbard type with repulsion and attraction of the electrons at the lattice sites. Here we will continue examining persistent-current oscillations in a Hubbard chain with electron attraction,[9] which models the behavior of a "low-dimensional superconductor" (however, no real long-range order is present in such a superconductor). Earlier it was shown[9] that a Hubbard system with attraction may exhibit mesoscopic oscillations of charge and spin persistent currents, with the amplitude of such oscillations in the gapless phases being proportional to N_a^{-1} (N_a is the number of sites in the chain) and the period of, say, AB oscillations, depending on the system's magnetization, being either fundamentally metallic (Φ_0) or superconductive ($\Phi_0/2$). According to recent reports[10–12] concerning studies of persistent currents in a Hubbard chain with electron repulsion, in certain conditions the period of AB oscillations can be fractional, say, equal to $\Phi_0/2$, with N the number of electrons (these have become known as microscopic oscillations), or to $\Phi_0/2$ for a certain parity of the number of electrons (now known as the parity effect).

Here we show that if the magnetic field strength is somewhat higher than the first critical value (see below) and the occupation numbers are moderate (N is not very large) or if the attraction constants are large, the persistent currents in a Hubbard chain with electron attraction undergo microscopic oscillations with a fractional period of Φ_0/N. We therefore show that microscopic oscillations are unrelated to electron repulsion and that other systems with variable separation are possible (in the given case the local pair—uncoupled electrons system rather than the spin–charge system). We show how the periods of quantum topological effects vary for mesoscopic Hubbard chains with attraction due to crossover of the energy levels corresponding to different excitations in nonzero electromagnetic fluxes. In particular, in weak magnetic fields the persistent currents oscillate, owing to level crossover, with a period of $\Phi_0/2$, which agrees with the results reported in Ref. 9.

2. THE BASIC EQUATIONS

The Hamiltonian of a ring-shaped Hubbard chain with mutual attraction of the site electrons in external electric and magnetic fields has the following form:[9,13]

$$H=-\sum_{j,\sigma}\left\{a^{+}_{j,\sigma}a_{j+1,\sigma}\exp\left\{\frac{i\alpha_\sigma}{N_a}\right\}+\text{H.c.}\right\}$$
$$-4U\sum_j n_{j,1}n_{j,-1}-\frac{h_e}{2}\sum_j(n_{j,1}-n_{j,-1})$$
$$-A\sum_{j,\sigma}n_{j,\sigma}, \qquad (1)$$

where $U>0$ is the Hubbard attraction constant (the hopping constant is set to unity), h_e is the external magnetic field, A is a Lagrange multiplier equivalent to the chemical potential, $a^{+}_{j,\sigma}$ ($a_{j,\sigma}$) is the operator of creation (annihilation) of an electron with spin σ ($\sigma=\pm1$) at site j, N_a is the number of sites, $n_{j,\sigma}=a^{+}_{j,\sigma}a_{j,\sigma}$, and α_σ is the phase acquired by the wave function of the system because of the nonforce effect of the magnetic flux Φ through the plane bounded by the ring (the Aharonov–Bohm effect) and/or the flux F of the radially directed electric field generated by a charged string in the middle of the ring (the Aharonov–Casher effect), with $F=4\pi\tau$, where τ is the linear density of the charge on the string, and

$$4\pi\frac{\Phi}{\Phi_0}=\alpha_1+\alpha_{-1},\quad 4\pi\frac{F}{F_0}=\alpha_1-\alpha_{-1}, \qquad (2)$$

where $\Phi_0=ch/e$ is the "metallic" magnetic flux quantum, and $F_0=ch/\mu$ is the electric flux quantum, with μ the Bohr magneton.

The persistent current in a ring in the ground state is

$$j=-\frac{\partial E_0(\Phi)}{\partial\Phi}, \qquad (3)$$

where here and in what follows we use the system of units in which $h=c=e=1$, i.e., $\Phi_0=2$ and $F_0=2\pi/\mu$. The eigenfunctions and the low-lying eigenvalues of the Hamiltonian of a chain with N electrons (M is the number of electrons with spin "down") are parametrized by the quasimomenta k_j and rates λ_α, which can be found from the equations of Bethe's ansatz:[9]

$$N_ak_j=2\pi(I_j+\alpha_1)+2\sum_{\alpha=1}^{M}\tan^{-1}\left(\frac{\sin k_j-\lambda_\alpha}{U}\right),$$
$$2N_a\,\mathrm{Re}\{\sin^{-1}(\lambda_\alpha-iU)\}=2\pi(J_\alpha+\alpha_1+\alpha_{-1})$$
$$+2\sum_{j=1}^{N-2M}\tan^{-1}\frac{\lambda_\alpha-\sin k_j}{U}+2\sum_{\substack{\beta=1\\\beta\neq\alpha}}^{M}\tan^{-1}\frac{\lambda_\alpha-\lambda_\beta}{2U}, \qquad (4)$$

where the I_j and J_α are integers or half-integers, depending on the parities of N and $N-M$, and M the number of electrons bound in local pairs. Note that in contrast to the wrong "minus" in Ref. 9, in the AB effect the phase in the second equation has a "plus" (the results obtained in Ref. 9 are independent of this sign, but it could play an important part in parity effects and microscopic oscillations). Depending on the occupation number $\nu=N/N_a$ and the magnitude of the external magnetic field h_e, the ground state of the chain form "Dirac seas" of free electrons, characterized by the quasimomenta k_j, and bound states of two electrons at the sites (local pairs), characterized by the rates λ_α. Equations (4) clearly show that only the fractional parts $\{\alpha_1\}$ and $\{\alpha_1+\alpha_{-1}\}$ of the phases of the AB and AC effects are important, since the integer parts only renormalize the sets of numbers I_j and J_α. In the ground state, the quantum numbers are symmetric with respect to zero:[14]

$$I_j=\tfrac{1}{2}(1-N+2M)+j-1,\quad J_\alpha=\tfrac{1}{2}(1-M)+\alpha-1. \qquad (5)$$

The energy and momentum of the system in a state with $N-2M$ free electrons and M local pairs are

$$\frac{E}{N_a}=-\sum_{j=1}^{N-2M}\left(2\cos k_j+A+\frac{h_e}{2}\right)$$
$$-\sum_{\alpha=1}^{M}(4\,\mathrm{Re}\sqrt{1-(\lambda_\alpha-iU)^2}+2A),$$
$$P=\sum_{j=1}^{N-2M}(k_j-2\pi\alpha_1)$$
$$+\sum_{\alpha=1}^{M}[2\,\mathrm{Re}\sqrt{1-(\lambda_\alpha iU)^2}-2\pi(\alpha_1+\alpha_1)]. \qquad (6)$$

3. MICROSCOPIC OSCILLATIONS

The ground state of a Hubbard chain with attraction between electrons at the lattice sites is formed by Dirac seas of electrons and localized pairs. The ground state of the system depends on the magnitude of the external field. If $h_e<h_c$ (here we employ, for example, the notation used in Ref. 9, with h_c the field strength at which pairs are ruptured; see also Refs. 14–19), only local pairs form the ground state, while excitations of the free-electron type have a gap in the spectrum. Here we are interested in the field-strength interval $h_c<h_e<h_s$ (h_s is the field strength at which the system becomes ferromagnetic) in which excitation spectra of the free-electron type and the coupled-pair type are gapless.

When $U\gg1$ and λ_α (note that although h_c is naturally related to U but is smaller than U—see, e.g., Ref. 19—the conditions that $U\gg1$ and $h_e>h_c$ can be met simultaneously), in Eqs. (4) we can ignore the term $\sin k_j$ in comparison to λ_α. The system of equations (4) leads to the following:

$$N_ak_j=2\pi\left(I_j+\alpha_1+\frac{1}{N-2M}\sum_{\alpha=1}^{M}(J_\alpha+\alpha_1+\alpha_{-1})\right)$$
$$-\frac{N_a}{N-2M}\sum_{\alpha=1}^{M}2\mathrm{Re}\,\sin^{-1}(\lambda_\alpha-iU). \qquad (7)$$

Equation (7) describes the behavior of a system of noninteracting spinless fermions in a ring with the following effective "topological" flux:

$$\alpha_1+\frac{1}{N-2M}\sum_{\alpha=1}^{M}(J_\alpha+\alpha_1+\alpha_{-1}).$$

If I_j is a sequence of integers or half-integers,

$$\frac{E_0(\Phi,F)}{N_a}=-E_m\cos\left[\frac{2\pi}{N_a}\left(\alpha_1+\frac{1}{N-2M}\sum_{\alpha=1}^{M}(J_\alpha+\alpha_1+\alpha_{-1})+D_f\right)\right]-(N-2M)\left(A+\frac{h_e}{2}\right)-2M(2U+A),$$

where $2D_f=I_{\max}+I_{\min}$, and

$$E_m=2\,\frac{\sin[\pi(N-2M)/N_a]}{\sin(\pi/N_a)}.$$

The energy $E_0(\Phi,F)$ can be minimized with respect to Φ and F by selecting a set of values of J_α that partially balances the external electromagnetic fluxes by creating local pairs with oppositely directed quasimomenta (or by changing the local-pair rates):

$$\sum_{\alpha=1}^{M}J_\alpha=-p$$

for

$$p-\tfrac{1}{2}<(N-2M)(\alpha_1+D_f)-M(\alpha_1+\alpha_{-1})<p+\tfrac{1}{2}.$$

Clearly, the energy of the ground state of a Hubbard chain with electron attraction for $h_c<h_e<h_s$ is a function of the magnetic flux with a period $(2\pi N)^{-1}$ or of the electric flux with a period $\mu[2\pi(N-2M)]^{-1}$. Thus, in a microscopic Hubbard chain with a fairly strong attraction between the electrons at the lattice sites ($U\gg 1$) or with low occupation numbers, when both M and N are not very large, there are microscopic oscillations (with a fractional period related to the number of electrons) of the ground-state energy and hence the persistent currents. These microscopic oscillations, in contrast to the case of a Hubbard chain with electron repulsion,[11,12] occur only in a mixed state with a fairly high magnetic moment of the system. There are no such microscopic oscillations in fields weaker than h_c or stronger than h_s, since in such fields even virtual creation of excitations of the free-states type caused by the nonforce action of an electromagnetic field is unprofitable. In contrast to ordinary mesoscopic oscillations,[9] related to the virtual motion of a single excitation (quasiparticle), microscopic oscillations are related to the motion of the electronic system as a whole, which, naturally, has an effect on the charge that enters the expression for the period of oscillations of these persistent currents.

4. MESOSCOPIC OSCILLATIONS

To calculate the finite-size corrections we use the method developed in Ref. 15. The correction, due to magnetic and electric fluxes to the energy of the ground state of a Hubbard chain with attractive electrons at the sites is

$$\frac{\Delta E_0(\Phi,F)}{N_a}=\frac{2\pi v_f}{N_a^2}\left\{\left[\zeta_{ff}(k_0)\left(\frac{\alpha_1}{2\pi}+D_f\right)+\zeta_{fb}(\lambda_0)\left(D_b-\frac{\alpha_s}{2\pi}\right)\right]^2\right\}+\frac{2\pi v_b}{N_a^2}\left\{\left[\zeta_{bf}(\lambda_0)\left(D_f+\frac{\alpha_1}{2\pi}\right)+\zeta_{bb}(\lambda_0)\left(D_b-\frac{\alpha_s}{2\pi}\right)\right]^2\right\},\qquad(8)$$

where $\alpha_s=\alpha_1+\alpha_{-1}$, v_f and v_b are the Fermi velocities of the free electrons and local pairs, and ζ_{ik} $(i,k=f,b)$ are the excitation charges "dressed" because of the interaction (electrons and pairs), which are found by solving a system of integral equations.[9] (Note that, in contrast to Ref. 9, here we explicitly allow for the initial phases related to excitation creation, $D_{f,b}$), which in the case of a Hubbard ring with electron repulsion lead to a parity effect and to a decrease by a factor of two of the period of oscillations of persistent current owing to level crossover.[11] Clearly, such a mesoscopic correction is present only in excitations without a gap in the spectrum. The quantum numbers of the free electrons and local pairs are distributed in such a manner as to minimize the energy of the system:[14]

$$I_{\max}-I_{\min}+1=N-2M,\quad 2D_f=I_{\max}+I_{\min},$$

$$J_{\max}+J_{\min}+1=M,\quad 2D_b=J_{\max}+J_{\min}.$$

The corrections to the ground-state energy due to the nonforce topological effect of electromagnetic fields on the considered Hubbard chain and resulting from the gaps $\Delta_{f,b}$ in the excitations spectrum are proportional to $\exp\{-N_a\Delta_{f,b}/v_{f,b}\}$.

We also note that superconductivity correlators decrease in a power-like manner as the distance grows,[16,17] though more slowly than the spin correlators and free-electron correlators do. Hence because of a nonforce topological electromagnetic field, even at absolute zero the system manifests mesoscopic oscillations of the charge and spin current, rather than quantization of the external field fluxes, as in superconductors, although the Hubbard model with attraction can be taken as a model of type II superconductors.

The electromagnetic fluxes α_1 and $\alpha_1+\alpha_{-1}$ determine, as Eqs. (4) demonstrate, the fraction of quantum numbers that transfer, owing to the gauge fields, from one edge of the Fermi bands of electrons and local pairs to the other edge, i.e., they are related to the number of virtual excitations of the free-electron and local-pair types existing above the ground state because of the nonforce effect of magnetic fluxes (the AB effect) and electric fluxes (the AC effect).

In fairly strong magnetic fields $h_c\leqslant h_e\leqslant h_s$, the dressed-charge matrix is[14]

$$\hat{\zeta}=\begin{pmatrix}1+\kappa k_0/2 & -1/2-\kappa k_0\\ 0 & (1+U/\lambda_0 2\pi)/\sqrt{2}\end{pmatrix},$$

where

$$\kappa=\frac{\ln 2}{2U},\quad k_0=\sqrt{\frac{h-h_c}{\eta}},$$

$$\eta=1-2\int_0^\infty\omega\,d\omega\,\frac{J_1(\omega)}{1+\exp(2U\omega)}>0,$$

$$\lambda_0=\frac{2U}{\pi}\ln\frac{C}{1-D},\quad C=\sqrt{\frac{8}{\pi e}}\,I_0\left(\frac{\pi}{2U}\right).$$

Here $J_n(x)$ and $I_n(x)$ are the Bessel functions of a real and imaginary argument, and e is the base of natural logarithms. Note that for a fixed number of particles the chemical potential is related to the occupation-number density by

$$-A-2U=4\exp\left(-\frac{\lambda_0\pi}{2U}\right)\sqrt{\frac{\pi}{2e}}\,I_1\left(\frac{\pi}{2U}\right),$$

i.e., it depends on the coupling constant U. Note that the coefficients of the dressed-charge matrix, defined at the Fermi points, have singularities at the points corresponding to infinite limits in the integrals of the integral equations for the dressed charges.[9] Solutions of the system of integral equations differ considerably if, say, we immediately set infinite limits and solve these equations by the Fourier method, or we solve it by the Wiener–Hopf method and then send the number of free electrons to zero (see, e.g., Refs. 14, 16, and 17). One of the reasons is that the system considered has a fixed number of particles rather than a fixed chemical potential, and dressed charges are strongly related to the way in which chemical potential is defined.[14] The same situation occurs in other exactly solvable models when finite-size corrections are being determined.

Equation (8) shows, as reported in Ref. 9, that for $h_e \leqslant h_c$ a Hubbard chain with attractive electrons at the sites exhibits, in the ground state, mesoscopic oscillations of the charge persistent current and the related diamagnetic moment with a "superconducting flux quantum" Φ_s. At $h_e=h_s$ the spin current in the chain oscillates with the electric flux F, the period of oscillations being "metallic," F_0 (see Ref. 8). This assumption is supported by experiments in the AC effect involving a superconducting ring in the quasi-one-dimensional geometry of the experiment conducted by Elien *et al.*[20] In the intermediate state with $h_c \leqslant h_e \leqslant h_s$, there may occur both oscillations of the spin current with the "metallic" period and oscillations of the charge current with the period Φ_s (these are due to the combination of "superconducting" and "metallic" oscillations with periods Φ_s and Φ_0, respectively). The amplitudes of the other oscillations in the ground state ("metallic" oscillations of the charge and spin currents for $h_e<h_c$ and all oscillations for $h_e>h_s$) are much smaller and are proportional to $\exp\{-N_a\}$.

However, because of crossover of the energy levels corresponding to different excitations in finite electromagnetic fluxes,[11,12] there may be a change in the effective period of mesoscopic oscillations in a Hubbard chain with electron attraction. This is reflected in the variation of the numbers I_j and J_α, i.e., in the variation of the $D_{f,b}$, defined by (mod 1), which corresponds to effective creation of excitations in the system, similar to the tower structure of excitations in conformal field theory.[14,16] If level crossover is taken into account (levels corresponding to different types of excitation depend differently on the magnetic and electric fluxes), one can see that the period dependence on, say, the magnetic flux is determined by the electric flux, the magnetization of the system, and band population. This conjecture also refers to mesoscopic oscillations of the AC type in an electric flux.

As the electromagnetic fluxes increase starting at zero, at certain values of Φ and F the set of quantum numbers, $\{J_\alpha\}$ and $\{I_j\}$, minimizing the energy changes. The Fermi velocities of both subsystems, the electronic and the local-pair, and the dressed-charge matrix can be calculated if one knows the occupation-number density, the coupling constants U, and the system's magnetization. Obviously, the system's energy at zero fluxes is minimized if $D_f=0$ and $D_b=0$. We denote the minimum value by $E_{00}(0,0)$. Then for finite fluxes the energy $E_{00}(\Phi,F)$ will change by

$$\frac{\Delta E_{(00)}(\Phi,F)}{N_a}=\frac{2\pi v_f}{N_a^2}\left[\zeta_{ff}(k_0)\frac{\alpha_1}{2\pi}-\zeta_{fb}(\lambda_0)\frac{\alpha_s}{2\pi}\right]^2+\frac{2\pi v_b}{N_a^2}\left(\zeta_{bb}(\lambda_0)\frac{\alpha_s}{2\pi}\right)^2$$

if one allows for the fact that $\zeta_{bf}(\lambda_0)=0$. In what follows the quantities ζ_{ik} $(i,k=f,b)$ denote the values of the dressed-charge matrix elements at the edge of the Fermi band. But if Φ (or F) is close to Φ_0 (or F_0), the state $(0,\mp 1)$ could prove to be a low-energy one:

$$E_{(0,\mp 1)}(\Phi,F)-E_{(0,0)}(0,0)=\pm\frac{2v_f}{N_a}(\zeta_{ff}\alpha_1\pm\pi\zeta_{fb}-\zeta_{fb}\alpha_s)\times\zeta_{fb}+\frac{2v_b}{N_a}(\pi\mp\alpha_s)\zeta_{bb}^2.$$

Crossover is realized in magnetic fluxes Φ or electric fluxes F satisfying the following relationship:

$$\frac{\Phi}{\Phi_0}[\varepsilon\zeta_{ff}\zeta_{fb}-2(\varepsilon\zeta_{fb}^2+\zeta_{bb}^2)]+\frac{F}{F_0}\varepsilon\zeta_{ff}\zeta_{fb}=\pm\frac{1}{2}(\varepsilon\zeta_{fb}^2+\zeta_{bb}^2),$$

where $\varepsilon=v_f/v_b$. Without an electric flux F, the period of AB oscillations is

$$\frac{\Phi}{\Phi_0}=\mp\frac{1}{2}\,\frac{\varepsilon\zeta_{fb}^2+\zeta_{bb}^2}{\varepsilon\zeta_{ff}\zeta_{fb}-2(\varepsilon\zeta_{fb}^2+\zeta_{bb}^2)}.$$

In weak magnetic fields $(h_e<h_c)$,

$$v_f=0,\quad \frac{\Phi}{\Phi_0}=\pm\frac{1}{4},$$

i.e., oscillations with a period of $\Phi_0/2=hc/2e$ are observed.

Without a magnetic flux Φ, the period of AC oscillations is

$$\frac{F}{F_0}=\mp\frac{1}{2}\,\frac{\varepsilon\zeta_{fb}^2+\zeta_{bb}^2}{\varepsilon\zeta_{ff}\zeta_{fb}}.$$

If the set of the quantum numbers J_α becomes such that D_f changes by ± 1, the energy of the system in fluxes of electromagnetic "topological" fields changes by

$$E_{(\pm 1,0)}(\Phi,F)-E_{(0,0)}(0,0)=\pm\frac{2v_f}{N_a}(\zeta_{ff}\alpha_1\pm\pi\zeta_{ff}-\zeta_{fb}\alpha_s)\zeta_{ff}$$

at $F=0$, while level crossover occurs at

$$\Phi=\pm\frac{\Phi_0\zeta_{ff}}{2\zeta_{fb}-\zeta_{ff}}.$$

In the absence of a magnetic flux Φ, the period of AC oscillations is $\mp F_0/2$. Hence allowing for the possible excitations (the parity effect) in a Hubbard ring with attraction between the electrons at the sites does not lead, in contrast to the case of repulsion,[11,12] to a further decrease by a factor of two of the oscillations as a function of the electron number density, while the period $\Phi_0/2$ of AB oscillations is related to the charge of the local pairs forming the system's ground state. This corresponds to the results of the computer simulation for a Hubbard chain with attraction conducted by Ferreti *et al.*[21]

5. CONCLUSION

We have shown that in a Hubbard chain with attraction between the electrons at the lattice sites, a model of a type II superconductor, there can be microscopic oscillations of the charge and spin persistent currents with fractional oscillation periods $\Phi_0/2$ and $F_0/(N-2M)$. These oscillations are related to variable separation in the system and occur in a magnetic field somewhat higher than the field strength of pair rupture, h_c, i.e., in a mixed state. We have analyzed the role of level crossover in the mesoscopic currents of pairs and free electrons. It leads to a change in the period of the persistent currents of pairs and free electrons.

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