Flux Quantization in the Two-Dimensional Repulsive and Attractive Hubbard Models

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In order to provide a numerical criterion for superconductivity, the ground state energy $E_0(\Phi)$ is calculated for the attractive and repulsive Hubbard models on a cylinder geometry threaded by a flux Φ. From the functional form of $E_0(\Phi)$, superconducting ground states may be identified without prior knowledge of the pairing symmetry. $E_0(\Phi)$ is calculated with Monte Carlo methods. For the attractive Hubbard model, our results confirm the existence of a superconducting ground state. In contrast, our results show that the quarter-filled repulsive Hubbard model is not superconducting and that a Hartree-Fock paramagnetic approximation fits the data very well.

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Since the discovery of high T_c superconductivity, a set of lattice models has been proposed to describe the physics of the underlying two-dimensional copper-oxide planes [1]. Apart from the difficulty to establish the existence (or nonexistence) of off-diagonal long-range order (ODLRO) by directly measuring the pair-pair correlations, the right symmetry channel has to be found. Here, we wish to detect superconducting ground states without knowledge of the symmetry of pair-pair correlation functions. Our method is based on flux quantization [2,3]. We thread a flux through a cylinder on which lies the electronic system. From the functional form of the ground state energy as a function of the threaded flux, $E_0(\Phi)$, one may distinguish between normal and superconducting ground states. In the case of a superconductor (i.e., ODLRO), Byers and Yang [2,3] have argued that $E_0(\Phi)$ is a periodic function of Φ with period Φ_0/n. Here, n stands (in Yang's notation [3]) for the sum of charges of the particles in the basic group ($n=2$ for Coopers pairs and $n=m$ for a Bose condensation of charge m bosons) and $\Phi_0 hc/e$. Furthermore, a nonvanishing energy barrier is to be found between the flux minima. This picture stands in close relationship to the existence of persistent currents [4] since supercurrents are trapped in metastable states corresponding to flux minima and thus cannot *dribble* away [5]. On the other hand, the curve $E_0(\Phi)$ is expected to be flat in the case of a crystal in its normal phase. Here, we emphasize that the above discussion is valid in the thermodynamic limit.

In this Letter, we present a new numerical approach to flux quantization. It is based on a finite-size scaling analysis of $E_0(\Phi)$ which is calculated with the projector quantum Monte Carlo (PQMC) [6] algorithm for the attractive and repulsive Hubbard models. Recently, Scalapino, White, and Zhang [7] have measured with quantum Monte Carlo (QMC) methods the linear response of the attractive and repulsive Hubbard models to a transverse magnetic field of wave vector $\mathbf{q}$. By taking the limit $\mathbf{q}\to 0$, which also requires a finite-size scaling study, they obtain the superfluid density. On the other hand, the superfluid density may be obtained from our $E_0(\Phi)$ data [3,7]. Thus, both methods are complementary, and as we shall see, yield similar results for the superfluid density.

In tight binding, the electron systems we consider are described by Hamiltonians of the type

$$H=-t\sum_{\langle \mathbf{i},\mathbf{j}\rangle,\sigma}\tilde{c}^{\dagger}_{\mathbf{i},\sigma}\tilde{c}_{\mathbf{j},\sigma}+H_V\,. \tag{1}$$

Here, $\tilde{c}^{\dagger}_{\mathbf{i},\sigma}$ creates an electron with z component of spin σ on lattice site $\mathbf{i}$, H_V is a density-density type interaction, and the sum runs over next neighbors. Since the wave function has to be single valued, a particle going once around the flux line acquires a phase $\exp(2\pi i\Phi/\Phi_0)$, where Φ_0 is the flux quantum and Φ the threaded flux [2]. Thus, the fermionic operators are submitted to the boundary conditions

$$\tilde{c}_{\mathbf{i}+L\mathbf{a}_x,\sigma}=\exp(2\pi i\Phi/\Phi_0)\tilde{c}_{\mathbf{i},\sigma},\quad \tilde{c}_{\mathbf{i}+L\mathbf{a}_y,\sigma}=\tilde{c}_{\mathbf{i},\sigma}\,. \tag{2}$$

Here, $\mathbf{a}_{x,y}$ are the lattice vectors of unit length and L is the linear length of the square lattice. Through a canonical transformation, the Hamiltonian (1) may be written as

$$\begin{aligned}H(\Phi)=&-t\sum_{\mathbf{i},\sigma}\left[\exp\left(\frac{2\pi i\Phi}{L\Phi_0}\right)c^{\dagger}_{\mathbf{i},\sigma}c_{\mathbf{i}+\mathbf{a}_x,\sigma}+\exp\left(-\frac{2\pi i\Phi}{L\Phi_0}\right)c^{\dagger}_{\mathbf{i}+\mathbf{a}_x,\sigma}c_{\mathbf{i},\sigma}\right]\\&-t\sum_{\mathbf{i},\sigma}(c^{\dagger}_{\mathbf{i},\sigma}c_{\mathbf{i}+\mathbf{a}_y,\sigma}+c^{\dagger}_{\mathbf{i}+\mathbf{a}_y,\sigma}c_{\mathbf{i},\sigma})+H_V\,.\end{aligned} \tag{3}$$

The fermionic operators now satisfy periodic boundary conditions in both lattice directions.

In the free case [$H_V=0$ in Eq. (3)], the Hamiltonian (3) has a single particle spectrum of the form

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$$\epsilon(\mathbf{k},\Phi) = -2t\left\{\cos\left[\left(n_x + \frac{\Phi}{\Phi_0}\right)\frac{2\pi}{L}\right] + \cos\left(n_y \frac{2\pi}{L}\right)\right\}, \tag{4}$$

where $n_{x,y}$ are integers included in $-L/2,\ldots,L/2$. For free fermions or bosons of charge one, the total energy on a finite lattice has a periodicity $E_0(\Phi+\Phi_0) = E_0(\Phi)$. For bosons at $T=0$, the lowest single particle state is macroscopically occupied and thus ODLRO is present. In the thermodynamic limit one obtains

$$E_0\left(\frac{\Phi}{\Phi_0}\right) - E_0\left(\frac{\Phi}{\Phi_0}=1\right) = \begin{cases} 4t\pi^2\rho\left(\dfrac{\Phi}{\Phi_0}\right)^2, & 0 < \dfrac{\Phi}{\Phi_0} < \frac{1}{2}, \\ 4t\pi^2\rho\left(\dfrac{\Phi}{\Phi_0} - 1\right)^2, & \frac{1}{2} < \dfrac{\Phi}{\Phi_0} < 1. \end{cases} \tag{5}$$

Here, ρ denotes the density of particles. Thus, bosons show flux quantization at $T=0$. On the other hand, for free fermions, $E_0(\Phi)$ is given by the envelope of a series of energy levels which cross as Φ is varied. In the thermodynamic limit this envelope becomes flat and, thus, no flux quantization occurs. The curvature of this envelope at $\Phi=0$ may be identified with the superfluid density [3,7]. Figure 1 plots $E_0(\Phi)$ for free fermions and bosons on a 64×64 lattice. The $E_0(\Phi)$ curve for fermions is not flat due to finite-size effects.

The ground state energy $E_0(\Phi)$ is calculated with the PQMC algorithm [6] based on the equation

$$E_0(\Phi) = \lim_{\Theta\to\infty} \frac{\langle\Psi_T|e^{-\Theta H(\Phi)}H(\Phi)|\Psi_T\rangle}{\langle\Psi_T|e^{-\Theta H(\Phi)}|\Psi_T\rangle}, \tag{6}$$

where $|\Psi_T\rangle$ is a trial wave function which is required to be nonorthogonal to the ground state. Here, we consider the attractive and repulsive Hubbard models. For those models, one may carry out a discrete Hubbard-Stratonovich transformation so as to decouple the on-site Hubbard interaction [8]. For all presented calculations, we have taken $|\Psi_T\rangle$ to be the ground state of the noninteracting Hamiltonian [$H_V=0$ in Eq. (3)]. For this trial wave function, we have found $\Theta=10t$ to be sufficient to filter out the ground state within our statistical uncertainty. Because of the presence of the threaded flux, one has to work with complex numbers. The sign problem is thus replaced by a phase problem. Apart from adding a factor 3-4 in the CPU times, working with complex numbers does not increase the statistical uncertainty already involved in the usual PQMC algorithms. In fact, it adds a set of cross checks. For a given Hubbard-Stratonovich spin configuration, both the phase and the energy are complex numbers with nonvanishing imaginary parts. However, the expectation value of both quantities has to be real. Hence, the Monte Carlo sampling has to yield a cancellation, within statistical uncertainty, of the imaginary part of the phase and energy. This was the case for all our simulations. As in standard QMC algorithms, the real part of the average phase scales as $e^{-\Delta\Theta N}$ where N is the number of sites and Δ is a positive number. More details on the algorithm may be found in Ref. [9].

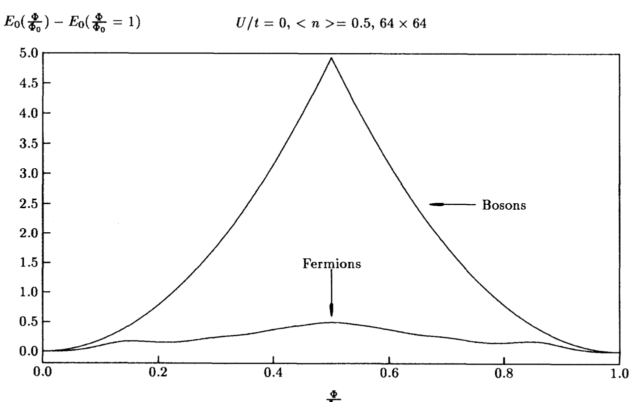

FIG. 1. $E_0(\Phi/\Phi_0) - E_0(\Phi/\Phi_0=1)$ for free bosons and fermions on a 64×64 lattice. The curve for free fermions scales to a flat curve in the thermodynamic limit.

Our analysis is based on a finite-size scaling study of the quantity

$$\Delta E_0(\Phi/\Phi_0) = E_0(\Phi/\Phi_0) - E_0(\Phi/\Phi_0 = R). \tag{7}$$

Here, we will use $R=0$ or $R=0.5$. Since $\Delta E_0(\Phi/\Phi_0) = \Delta E_0(1-\Phi/\Phi_0)$, we consider only $0<\Phi/\Phi_0<\frac{1}{2}$. We carried out our simulations on 4×4 to 10×10 clusters.

Figure 2(a) plots $\Delta E_0(\Phi/\Phi_0)$ for the attractive half-filled Hubbard model at $U/t=-4$. For our large lattice sizes, we were not able to carry simulations in the range $0<\Phi/\Phi_0<\frac{1}{4}$ due to severe phase problems. At strictly half band filling, the attractive Hubbard model shows both long-range superconducting and charge density wave correlations [10]. By carrying out a particle-hole transformation on say the up spin sector, the attractive, half-filled Hubbard model may be mapped onto the repulsive, half-filled, Hubbard model with down spins (up) submitted to a flux Φ ($-\Phi$). Such boundary conditions have been used by Shastry and Sutherland [11] to measure the spin stiffness of the one-dimensional Hubbard model. In Fig. 2(a), one notes that for values of $\frac{1}{4}<\Phi/\Phi_0<\frac{1}{2}$, $\Delta E_0(\Phi/\Phi_0)$ is very stable against growing lattice sizes. On the other hand, at $\Phi=0$, $\Delta E_0(\Phi/\Phi_0)$ decreases very rapidly with growing lattice sizes. The data suggest that $\Delta E_0(\Phi/\Phi_0)$ converges to a periodic function of period

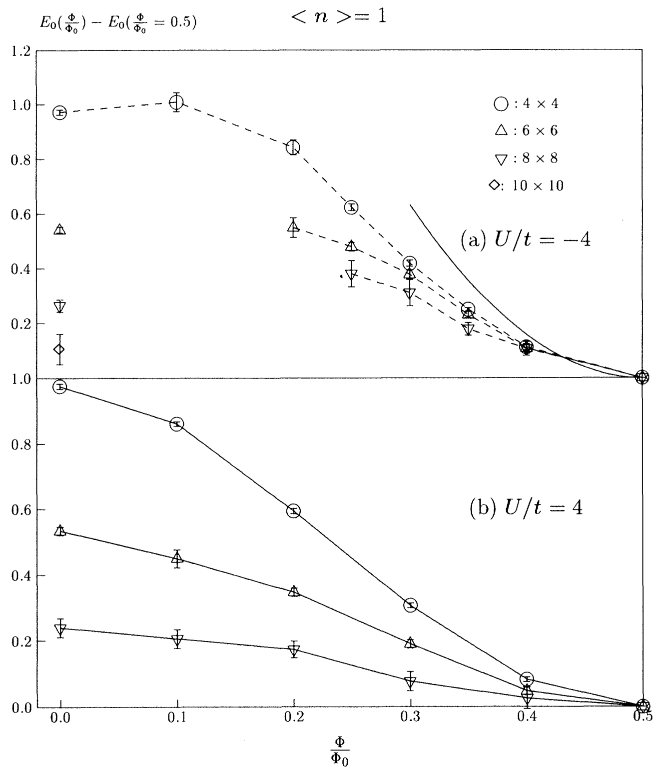

FIG. 2. (a) $E_0(\Phi/\Phi_0) - E_0(\Phi/\Phi_0 = 0.5)$ for the half-filled attractive Hubbard model at $U/t = -4$. The curvature of the plotted parabola (solid line) at $\Phi/\Phi_0 = 0.5$ is obtained from the estimated value of the superfluid density of Ref. [7]. The dashed lines are guides to the eye. (b) Same as (a) but for the repulsive Hubbard model at $U/t = 4$.

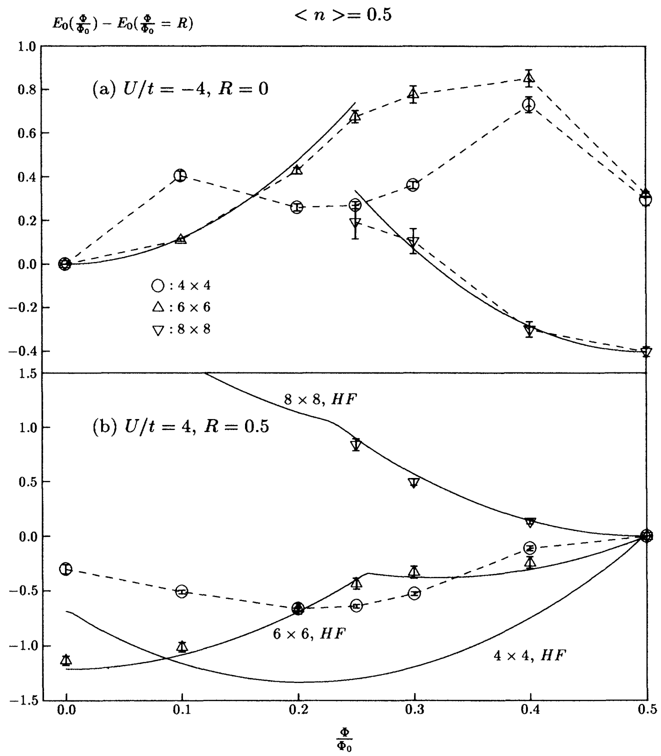

FIG. 3. (a) $E_0(\Phi/\Phi_0) - E_0(\Phi/\Phi_0 = 0)$ for the quarter-filled attractive Hubbard model at $U/t = -4$. Again, the curvature of the plotted parabolas (solid lines) at $\Phi/\Phi_0 = 0$ and 0.5 are obtained from the estimate of the superfluid density of Ref. [7]. The dashed lines are guides to the eye. (b) $E_0(\Phi/\Phi_0) - E_0(\Phi/\Phi_0 = 0.5)$ for the quarter-filled repulsive Hubbard model at $U/t = 4$. The solid lines denote the paramagnetic HF results for the three considered lattice sizes at $T = 0$. The plot symbols represent the QMC data. The dashed line is a guide to the eye.

$\Phi/\Phi_0 = \frac{1}{2}$ with a nonvanishing energy barrier at $\Phi = \Phi_0/4$ as appropriate for the condensation of electron pairs. To confirm the above interpretation of the data, we considered the quantities $E_0(\Phi = \Phi_0/4) - E_0(\Phi = 0)$ and $E_0(\Phi = \Phi_0/4) - E_0(\Phi = \Phi_0/2)$. To a first approximation, both quantities scale as $1/L^2$ to the same nonvanishing value in the thermodynamic limit. Hence, we expect in the thermodynamic limit, $E_0(\Phi = 0) = E_0(\Phi = \Phi_0/2)$ and $E_0(\Phi = \Phi_0/4) > E_0(\Phi = 0)$. The superfluid density is related to the curvature of the $\Delta E_0(\Phi/\Phi_0)$ at $\Phi/\Phi_0 = \frac{1}{2}$ [12]. We may compare our results with those of Scalapino, White, and Zhang [7]. The curvature of the parabola plotted in Fig. 2(a) is obtained from Ref. [7] and, as may be seen, the agreement to our $\Delta E_0(\Phi/\Phi_0)$ data is quite good.

Figure 2(b) plots $\Delta E_0(\Phi/\Phi_0)$ for the half-filled repulsive Hubbard model at $U/t = 4$. Here, no phase problem occurs so that the full $\Delta E_0(\Phi/\Phi_0)$ curve may be plotted for the three considered lattice sizes. The ground state of the half-filled repulsive Hubbard model is believed to be a Mott insulator with long-range antiferromagnetic spin correlations [13]. Thus, no flux quantization is expected. Figure 2(b) confirms this since $\Delta E_0(\Phi/\Phi_0)$ vanishes with growing lattice sizes for all values of the threaded flux.

We now consider the quarter-filled attractive Hubbard model at $U/t = -4$. Away from half band filling, the attractive Hubbard model shows long-range superconducting correlations. The charge density wave correlations present at half band filling are now short range [10]. Our results are plotted in Fig. 3(a). Here, the finite-size scaling is irregular. However, for each considered lattice size, clear local flux minima may be found at $\Phi/\Phi_0 = 0$ and 0.5, as expected for a superconducting ground state. Again, the signature of a superconducting ground state requires (1) $\Delta E_0(\Phi/\Phi_0)$ to scale to a periodic function of period $\Phi/\Phi_0 = 0.5$ and (2) the existence of a finite energy barrier between $\Phi/\Phi_0 = 0$ and $\Phi/\Phi_0 = 0.5$. Both above-mentioned points are hard to detect from the available data due to the large finite-size effects. As in Fig. 2(a), we have used the data of Ref. [7] for the superfluid density to obtain the curvature of the plotted parabolas. Both the 6×6 and 8×8 lattices show the right curvature at, respectively, $\Phi/\Phi_0=0$ and $\Phi/\Phi_0=0.5$. Clearly, the weak point of the method lies in establishing the existence of a finite energy barrier between flux minima in the thermodynamic limit due to large finite-size effects.

Finally, we turn to the quarter-filled repulsive Hubbard model at $U/t=4$. At the above filling, a phase problem occurs so that only partial results were obtained for the 8×8 lattice. Our results are plotted in Fig. 3(b). The finite-size scaling of $\Delta E_0(\Phi/\Phi_0)$ is again irregular. However, when one compares the QMC data to a paramagnetic Hartree-Fock (HF) calculation, one clearly sees that for the two largest lattice sizes (6×6 and 8×8) the QMC data compare extremely well with the paramagnetic HF prediction of $\Delta E_0(\Phi/\Phi_0)$. Thus, the data give numerical evidence that the quarter-filled repulsive Hubbard model has no ODLRO, and that a paramagnetic HF approximation reproduces the QMC data very well.

In conclusion, we have introduced and tested a new numerical approach so as to detect superconducting ground states via flux quantization. For the repulsive Hubbard model, and at the two considered band fillings, our results clearly show the absence of superconductivity. The data for the quarter-filled Hubbard model are very well reproduced by a paramagnetic HF approximation and thus provide numerical evidence for a nonsuperconducting ground state. On the other hand, the data for the attractive Hubbard model are less clear-cut but nonetheless point to superconducting ground states especially for the half-filled band case. Our $E_0(\Phi)$ data provide an independent check of the superfluid density measurements (QMC) of Scalapino, White, and Zhang [7] and good agreement is found.

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