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Diamagnetic susceptibility of the ∞-U Hubbard model

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The diamagnetic susceptibility of the ∞-U Hubbard model is investigated in one and two dimensions. In one dimension, it is shown that the charge current flowing in the ground state of a ring threaded by a flux tube vanishes in the thermodynamic limit. Similar behavior is inferred for the single-hole problem on a two-dimensional square lattice, from exact-diagonalization results on small clusters. Effectively the applied field is *canceled* by an induced fictitious field and the susceptibility vanishes. Our results suggest that the Nagaoka ferromagnet is unstable with respect to a low-spin state, level crossing to a chiral spin state occurring at infinitesimally small diamagnetic coupling.

Unusual orbital response under Peierls coupling to an external magnetic field is a characteristic feature of doped Mott insulators. Several authors have drawn attention to this in the context of gauge theories,[1,2] and it can be understood as follows. Suppose we have a time-reversal symmetric ground state in the absence of the external field. When a field is applied, it is expected that a net spin chirality appears due to explicit breaking of time-reversal symmetry and the coupling of charge and spin degrees of freedom. It is known[3] that holons moving in a chiral spin state experience a fictitious magnetic field; thus holons experience the sum of applied and fictitious fields and the fictitious field must be included as part of the response. In the cases we examine this is a screening effect; the effective field seen by the charge degrees of freedom is smaller than the externally applied field. The results are of interest to diamagnetic susceptibility, Hall effect, magneto-oscillatory behavior, etc., of the strongly correlated states.

In this paper we study the ∞-U Hubbard model in a field

$$H=-\sum_{\langle i,j\rangle,\sigma} e^{i\theta_{ij}}(1-n_{i-\sigma})c_{i\sigma}^{\dagger}c_{j\sigma}(1-n_{j-\sigma})\,, \qquad (1)$$

subject to $\sum_\sigma n_{i\sigma}\le 1$ where the sum in the Hamiltonian is over nearest-neighbor lattice sites i and j and $n_{i\sigma}$ is the usual particle-number operator on site i. θ_{ij} is the Peierls phase for electron hopping in a uniform magnetic field. (Notice that we do not include a Zeeman coupling term. We comment on this later.) In the absence of external flux, Nagaoka[4] has shown that the ground state for one hole on a bipartite lattice is a maximal spin ferromagnet (the Nagaoka state) and Ioffe and Wiegmann[2] studied this model specifically using a gauge theory formulation. On the basis of exact diagonalization of small clusters and the analytic solution of the one-dimensional (1D) case, we assert that, in the presence of a magnetic field, it is energetically favorable to enter a chiral state where the external field is completely screened out, rather than remain in the Nagaoka state and pay a diamagnetic energy cost.

We first consider a ring of size L enclosing a magnetic flux ϕ, measured in units of the flux quantum and equivalent to a twisted boundary condition. In one dimension the Hamiltonian conserves spin ordering so we can characterize the solutions by an integer K ($\le N$, the number of electrons on the ring), representing the number of distinct spin configurations generated by a cyclic permutation of the spins. The Nagaoka state is sufficiently, but not necessarily, described by $K=1$. Consider first the simple case of one hole on the ring. To solve this, we define an operator R which moves the hole one site:

$$R=\sum_{i=1,\sigma}^{L}(1-n_{i+1-\sigma})c_{i+1\sigma}^{\dagger}c_{i\sigma}(1-n_{i-\sigma})\,. \qquad (2)$$

The Hamiltonian can be written as $H=-(e^{i2\pi\phi/L}R+\text{H.c.})$ and the charge current operator as $J=-i(e^{i2\pi\phi/L}R-\text{H.c.})$. The eigenstates $|\psi_p\rangle$ are

$$\sum_{n=0}^{LK}\exp(ik_pn)R^n|\{\sigma\}\{x\}\rangle\,,$$

where $|\{\sigma\}\{x\}\rangle=c_{x_1\sigma_1}^{\dagger}\cdots c_{x_N\sigma_N}^{\dagger}|0\rangle$. The hole momentum k_p is $2\pi p/LK$ for odd N and $\pi(2p+1)/LK$ for even N with p an integer. The energy eigenvalues are $E_p=-2\times\cos(2\pi\phi/L-k_p)$ with a corresponding current of $\langle J\rangle_p=2\sin(2\pi\phi/L-k_p)$. It is thus apparent that ensuring that K is maximal (i.e., $K=N\sim L$) enables the effect of the magnetic flux to be reduced to that of an effective flux $\le 1/N$. Thus in the large L limit, the diamagnetic current tends to zero as $(LK)^{-1}\sim L^{-2}$ compared to L^{-1} in the Nagaoka state. This reduced current is related to development of spin chirality in the ground state. For a single-spin flip state (which maximizes K), we find

$$\frac{1}{L}\left\langle \sum_{i,j} \mathbf{S}_i\cdot\mathbf{S}_j\times\mathbf{S}_{j+1}\right\rangle_p = \left\langle \frac{i}{4L}(R^L - R^{\dagger L})\right\rangle_p = \tfrac{1}{2}\sin(Lk_p)\,. \quad (3)$$

Figure 1 illustrates these results for the case of a single-hole and single-spin flip on an eight-site ring.

The finite doping case can be solved similarly by Bethe's ansatz.[5] The ground state is of the form

$$|\psi\rangle = \sum_{\{x\}}\sum_P (-1)^P \exp\left[i\sum_{j=0}^{N} k_{P_j}x_j\right] \sum_{n=0}^{K-1} e^{i\alpha n}|C^n\{\sigma\}\{x\}\rangle\,, \quad (4)$$

where C permutes the spin arrangement

$$C\{\sigma\} = C\{\sigma_1\cdots\sigma_N\} = \{\sigma_2\sigma_3\cdots\sigma_N\sigma_1\}\,.$$

The sum over P is the usual sum over permutations. The periodic boundary conditions lead to $\alpha = 2\pi m/K$ and $k_i = 2\pi n_i/L - \alpha/L$ with n_i and m both integers.

With the occupied k values between n_0 and n_1 and writing $x_i = n_i - m/N + \phi$ so that $x_1 - x_0 = N-1$, we find in the large-L limit

$$E = -2\sum_{n=n_0}^{n_1}\cos\frac{2\pi}{L}\left[n - \frac{m}{N} + \phi\right] = -\frac{2L}{\pi}\sin\frac{\pi(N-1)}{L}\cos\frac{\pi(x_1+x_0)}{L}\,, \quad (5)$$

$$\langle J\rangle = 2\sum_{n=n_0}^{n_1}\sin\frac{2\pi}{L}\left[n - \frac{m}{N} + \phi\right] = -\frac{2L}{\pi}\sin\frac{\pi(N-1)}{L}\sin\frac{\pi(x_1+x_0)}{L}\,. \quad (6)$$

The lowest-energy state corresponds to a choice of n_1 and m such that the absolute value of $x_1 + x_0 = 2n_1 - N + 1 - 2(m/N - \phi)$ is minimized. We can always choose m and n_1 so that $|x_1 + x_0| \le 1/N$. Thus the ground-state energy and current behave as

$$E_0 = -\frac{2L}{\pi}\sin\frac{\pi(N-1)}{L} + O\left[\frac{1}{LN^2}\right]\,, \quad (7)$$

$$\langle J\rangle_0 = -\frac{2L}{\pi}\sin\frac{\pi(N-1)}{L}\,O\left[\frac{1}{LN}\right] \sim O\left[\frac{1}{N}\right]\,. \quad (8)$$

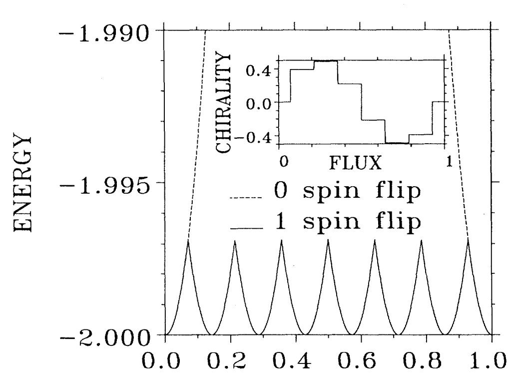

FIG. 1. Ground-state energy vs flux for an eight-site ring with one hole. The dotted line represents the ferromagnet state energy. Inset: Chirality vs flux. In the thermodynamic limit the chirality curve becomes sinusoidal. In the thermodynamic limit the curves evolve as described in the text.

Thus the energy is independent of flux and there is no diamagnetic current in the ground state. The effect of the magnetic field has been completely canceled by the chiral spin configuration. By contrast, for a spinless Fermi sea a macroscopic current flows in the presence of a flux.

These results should be contrasted with the "semiclassical" treatment of spin degrees of freedom sometimes used in this context.[6] Like the ferromagnet, the spin configuration forms a static background but the spins are now polarized with respect to a spin quantization axis which rotates from site to site. The problem maps to a spinless fermion problem on a lattice with effective hopping amplitudes t_{ij}:

$$H = -\sum_{\langle i,j\rangle} t_{ij}\exp(i\theta_{ij}^{\rm eff})c_i^\dagger c_j\,, \quad (9)$$

$t_{ij} = [(1+\mathbf{n}_i\cdot\mathbf{n}_j)/2]^{1/2}$, and $\theta_{ij}^{\rm eff} = \theta_{ij} + \Omega(\mathbf{n}_i,\mathbf{n}_j,\mathbf{z})/2$ with $\mathbf{n}_i$ and $\mathbf{n}_j$, the direction of the spinors on sites i and j, respectively, and $\Omega(\mathbf{n}_i,\mathbf{n}_j,\mathbf{z})$ the solid angle formed between the spinors on sites i, j, and the quantization axis z.[7] In this picture a static twisted spin configuration which cancels the applied field on average (but not strictly uniformly) can easily be obtained but always at a cost in the effective hopping amplitude, $|t_{ij}| < 1$. We have found through an extensive search of spin configurations that the cost in bandwidth is always larger than the diamagnetic energy gain through canceling the external magnetic field. Quite large two-dimensional systems were studied using Skyrmionic trial wave functions with null result.

The exact results in 1D show, however, not only that the ficticious gauge field can compensate for the applied magnetic field, but that there is *no bandwidth effect* in the thermodynamic limit. The inadequacy of the semiclassical-type approach may be associated with the failure to exploit the backflow of spin produced as the hole propagates. In the single hole on a 1D ring problem we can define an operator $\hat{\mathbf{L}}_c = R^L$ which moves the hole once around the ring and performs a single cyclic permutation of the spins through the spin backflow. We note that $\hat{\mathbf{L}}_c^K = (-1)^{N-1}$ so the eigenvalues of $\hat{\mathbf{L}}_c$ are the Kth roots of $(-1)^{N-1}$. For a given wave function $\langle\hat{\mathbf{L}}_c\rangle = a\exp(i2\pi\phi_{\rm fict})$ where $\phi_{\rm fict}$ is the ficticious flux seen by the moving hole and no bandwidth reduction is ensured if $a=1$. The degenerate energy minima in Fig. 1 show where $\phi_{\rm fict} = -\phi$. Only wave functions that are eigenstates of $\hat{\mathbf{L}}_c$ can have $a=1$ and $\phi_{\rm fict}\neq 0$. Wave functions, such as that used in the semiclassical approach, which do not couple the hole to the spin background will not be eigenstates of $\hat{\mathbf{L}}_c$ and will therefore be unable to generate ficticious flux without making $a<1$. Knopp, Ruckenstein, and Schmitt-Rink[8] have shown that Gutzwiller wave functions are also poor descriptions of one spin flip in the 1D and 2D ∞-U Hubbard model.

We now turn to the two-dimensional case with a single

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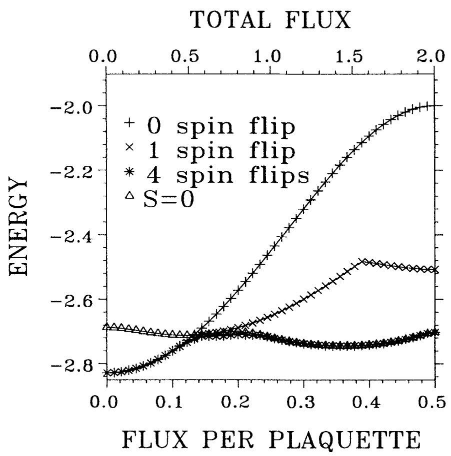

FIG. 2. Lowest energy vs flux for 3×3 square lattice, free boundary conditions, for 0, 1, and 4 spin flips and singlet spin states. The energies are symmetric about $\frac{1}{2}$ flux quanta per plaquette. Note the strong dispersion of the Nagaoka state curve in comparison with the low-spin case.

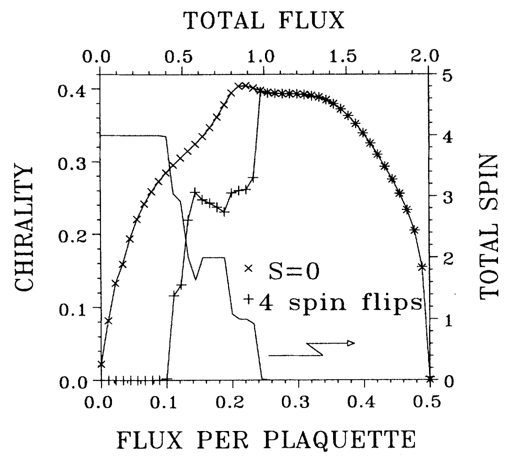

FIG. 3. Chirality in the singlet state and in the ground state and the expectation value of total spin vs flux for 3×3 lattice. The chirality is antisymmetric about $\frac{1}{2}$ flux quanta per plaquette. Also shown is the total spin quantum number S measured in the Lanczos ground state; convergence to expected values is excellent away from the level crossings of Fig. 2.

hole. Although we failed to find a static spin configuration which had a lower energy than the Nagaoka state in a field, the one-dimensional results suggest that a more complete solution of the problem is required. However, the difference between one and two dimensions is the number of closed loops enclosing a finite amount of magnetic flux around which the hole may propagate. In one dimension there is only one such loop and the above discussion shows how we can generate a canceling fictitious flux on such a single loop with no loss in bandwidth. The presence of many closed loops in two dimensions means there is a macroscopic energy to be gained by screening the applied field even in the single-hole case but it is much more difficult to construct the screening fictitious field. We therefore performed Lanczos diagonalization of 3×3 and 4×4 square lattices with free boundary conditions as a function of applied flux per plaquette ϕ. We work in the Landau gauge.

The results are shown in Figs. 2–4. Only fluxes up to $\frac{1}{2}$ flux quanta per plaquette are shown since the energy is symmetric about this value and the chirality is antisymmetric. First, notice that the Nagaoka state energy versus flux curves $E_{\rm Nag}[\phi]$ shows strong finite-size effects. For small systems, if the magnetic length is much smaller than the system size (or, equivalently, the total flux through the systems is much less than a flux quantum), first-order perturbation theory gives a diamagnetic energy shift proportional to ϕ^2. The infinite system Landau-level energy is of course proportional to ϕ for small ϕ; the crossover behavior is most clearly seen in Fig. 4. Also notice that, due to finite size, the Nagaoka state curves are smeared out with respect to the Hofstadter band minimum;[9] but in Fig. 4 there is a maximum in $E_{\rm Nag}[\phi]$ which reflects the maximum energy reached on an infinite lattice at a flux of ~0.4.

While the results are clearly distinct from those seen in one dimension (e.g., there is no additional periodicity in the energy as a function of flux and the flux is never totally canceled as it is for certain fields in one dimension) there are some similarities. The most striking feature of the results is the very weak dependence of energy on flux in the lowest-energy singlet state on 3×3 or lowest-energy spin-$\frac{1}{2}$ state on 4×4. Consequently, the magnetization $\partial E/\partial\Phi_{\rm tot}$ of the system is small. The remarkable flatness of $E[\phi]$ thus provides strong evidence that an internally generated field cancels the applied field in these states. Note that the flux per plaquette at which the low spin state becomes the ground state is roughly when the total flux is one flux quantum on 3×3.

The internal field should be signaled by the presence of a net spin chirality. The average chirality $\langle \mathbf{S}_i \cdot \mathbf{S}_{i+\hat{x}} \times \mathbf{S}_{i+\hat{x}+\hat{y}} \rangle$ is plotted in Figs. 3 and 4. The chirality was

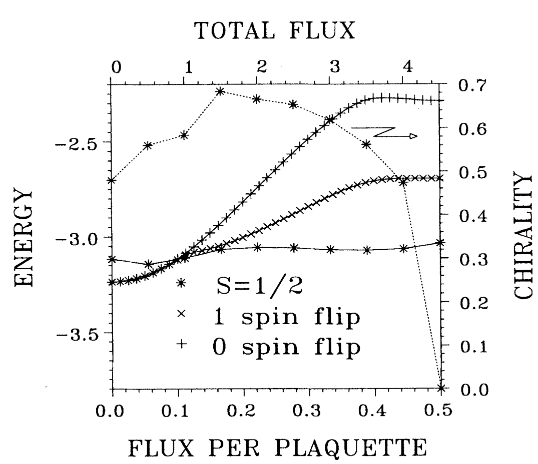

FIG. 4. Energy and chirality vs flux on 4×4 lattice with free boundary conditions. Note that the spin-$\frac{1}{2}$ state energy at $\frac{1}{2}$ flux quantum per plaquette is already lower than $-2\sqrt{2}$, the infinite lattice Nagaoka state energy, despite finite-size effects.

found to be uniform over the cluster. The chirality should vanish at $\phi=0,\pi$ if these states are time-reversal symmetric. In the spin-$\frac{1}{2}$ case it is finite at $\phi=0$ in our calculation. However, the chirality has a very sharp variation near this point for spin $\frac{1}{2}$ so the finite value obtained is influenced by use of the adjacent finite flux states as seed states for the zero flux Lanczos run. Figure 3 shows clearly the relation between the evolution of chirality and applied flux.

What conclusions can be drawn for the infinite system? Rigorous variational bounds on the stability of the Nagaoka state in a field can be extracted. A trial state for the infinite lattice can be constructed by embedding the finite system wave function in a ferromagnetic background. The energy of this state on the infinite lattice is the same as its cluster energy. Above a critical flux, $\phi_c \sim 0.17$, the energies obtained from the finite cluster low-spin states are already lower than the energy of the Nagaoka state on an infinite lattice in the same magnetic field, providing that the ferromagnet is unstable. Of course, this is not unexpected, since the magnetic field produces a frustrated lattice.

These trial wave functions are, of course, poor upper bounds on the energy of the ground state since they do not allow the hole to properly delocalize. From the independence of the singlet wave function energy of the applied field in the small cluster diagonalizations and the one-dimensional results, we make the following conjecture concerning the infinite system. There exist singlet states with infinitesimally higher energy than the Nagaoka state in the absence of a magnetic field.[10] Thus, as the lattice size L increases, the low-spin state of Fig. 4 approaches the band minimum at -4. If the flatness of $E[\phi]$ which we observe here is preserved then level crossing of Nagaoka and low-spin states must occur at zero flux. Thus we conjecture that the diamagnetic susceptibility vanishes in the thermodynamic limit[11] as in the one-dimensional ∞-U model.

We also want to comment on the application of the results to the problem of the stability of Nagaoka ferromagnetism under finite hole doping. At present the Nagaoka ferromagnet is known to be unstable beyond a doping $x \sim 0.29$.[12] Douçot and Rammal[13] considered semiclassical skyrmionic (flux) states, their idea being to take advantage of the special stability of hole fermions in a fictitious field of one flux quantum per hole. However, they did not find an appreciable energy gain over Nagaoka for fillings greater than $\frac{1}{4}$, because of the loss of bandwidth within the semiclassical framework. The present results suggest that the bandwidth problem can be overcome; however at the same time the spinless Fermi sea prescription for holes is lost. It is not clear what firm conclusions can be drawn.

Two final remarks. First we note that finite Hubbard U leads to finite spin stiffness. It is, therefore, expected that $E[\phi]$ is no longer strictly flat since generation of the necessary chirality will lead to an unfavorable exchange energy. Nevertheless the diamagnetic susceptibility is strongly suppressed in the large U limit. (This was confirmed on a small ring.) Second, the addition of a Zeeman term favors ferromagnetism and so suppresses the diamagnetic response discussed here. Nevertheless Zeeman and antiferromagnetic interactions are in competition and some fictitious field effects should survive. Further work on this important problem is planned.

To conclude, we have calculated the ground-state energy of a ∞-U Hubbard model, as a function of Peierls coupled magnetic field, analytically in 1D and by exact diagonalization for one hole in small 2D clusters. We find that the energy is remarkably independent of applied flux. An induced ficticious field is effectively canceling the applied field, the susceptibility vanishes, and there is a corresponding development of chirality in the ground state. We expect these features to persist in the thermodynamic limit. We suggest that, under infinitesimally small diamagnetically coupled fields, a level crossing occurs from the Nagaoka ferromagnet to a low spin, chiral state.

Note added in proof. After submitting this paper we became aware of work similar to our 1D calculation by Kusmartsev.[14]

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