Comments

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Comment on "Flux quantization in rings for Hubbard (attractive and repulsive) and t-J-like Hamiltonians"

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(Received 27 April 1992; revised manuscript received 25 June 1992)

It is shown for three models with strong correlations that the value of the total spin of the ground state of finite-size rings with two fermions (holes or electrons) can change as a function of magnetic flux Φ. It is concluded that the magnetic flux periodicity may be used as a test of binding only if one also checks for changes in spin quantum numbers.

In a recent paper[1] Ferretti, Kulik, and Lami have analyzed the ground-state energy as a function of magnetic flux for 10 and 16 site rings with 2 and 4 fermions for both positive- and negative-U Hubbard model and t-J model. They concluded, "In all cases the flux is found to be quantized in units $hc/2e$." However, we show in this comment that the ground-state wave function for the positive-U Hubbard model can change its total spin S as a function of flux. By contrast, the negative-U Hubbard model leads to total $S=0$ for all flux in the ground state. Therefore, despite the apparent flux quantization of $hc/2e$ for the energy, positive and negative-U Hubbard model may be distinguished as long as one also checks spin quantum numbers.

To begin our discussion, let us write the Hubbard model in momentum space in a d-dimensional hypercube of L^d sites:[2]

$$\hat{H}=\sum_{\mathbf{k},\sigma=\uparrow,\downarrow}\epsilon_{\mathbf{k},\Phi}c^{\dagger}_{\mathbf{k}\sigma}c_{\mathbf{k}\sigma}+\frac{U}{L^d}\sum_{\mathbf{pp'q}}c^{\dagger}_{\mathbf{p+q}\uparrow}c^{\dagger}_{\mathbf{p'-q}\downarrow}c_{\mathbf{p'}\downarrow}c_{\mathbf{p}\uparrow}\ , \tag{1}$$

where

$$\epsilon_{\mathbf{k},\Phi}=-2t\sum_{i=1}^{d}\cos\left[k_i a+\frac{2\pi}{L}\frac{\Phi_i}{\Phi_0}\right] .$$

a is the lattice spacing, k_i is the usual quantized wave vector $2\pi l_i/La$, $l_i\in(1,L)$, $\Phi_0=hc/e$ is the flux quantum, and Φ_i is equal to $A_i a$, where A_i is the ith component of the constant vector potential produced by the flux Φ enclosed by the system. A generic wave function[2] for two fermions is

$$|\Psi(\mathbf{P})\rangle=\sum_{\mathbf{q}}L(\mathbf{q})c^{\dagger}_{\mathbf{q}\uparrow}c^{\dagger}_{\mathbf{P-q}\downarrow}|0\rangle\ . \tag{2}$$

This function is an eigenvector with center-of-mass momentum $\mathbf{P}$ and energy eigenvalue E if the coefficients $L(\mathbf{q})$ satisfy the Schrödinger equation,

$$(E-\epsilon_{\mathbf{q},\Phi}-\epsilon_{\mathbf{P-q},\Phi})L(\mathbf{q})=\frac{U}{L^d}\sum_{\mathbf{p}}L(\mathbf{p})\ . \tag{3}$$

We call Υ the right-hand side of this equation, so that

$$L(\mathbf{q})=\frac{\Upsilon}{(E-\epsilon_{\mathbf{q},\Phi}-\epsilon_{\mathbf{P-q},\Phi})}\ . \tag{4}$$

By substituting this expression in that for Υ, it is easy to obtain a self-consistent equation of the usual type for the energy,[2] i.e.,

$$1=\frac{U}{L^d}\sum_{\mathbf{q}}\frac{1}{E_s-\epsilon_{\mathbf{q},\Phi}-\epsilon_{\mathbf{P-q},\Phi}}\ . \tag{5}$$

The solution E_s of this equation corresponds to a singlet, since, as one can easily show, $L(\mathbf{P-q})=L(\mathbf{q})$. The eigenvalues E_t for triplet $[S=1,\ L(\mathbf{P-q})=-L(\mathbf{q})]$ are obviously

$$E_t=\epsilon_{\mathbf{P-q},\Phi}+\epsilon_{\mathbf{q},\Phi} \tag{6}$$

with $(\mathbf{P-q})\mathrm{mod}(2\pi/a)$ different from $\mathbf{q}$. This completes the solution for two fermions on a d-dimensional hyper-

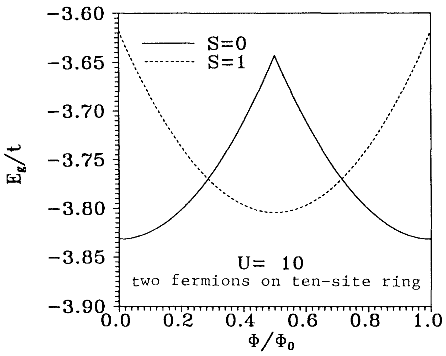

FIG. 1. The lowest energy of the Hubbard model with two fermions at $U=10$ in a 10-site ring for singlet and triplet states is plotted as a function of flux quantum. One can see that the minimum at $\Phi=\Phi_0/2$ is for the triplet.

cube for the Hubbard Hamiltonian.

In Fig. 1 we plot the lowest energy of the two-fermion singlet and triplet as a function of flux for the Hubbard model at $U=10$ for a 10-site ring. It is clear that the relative minimum discussed by FKL at $\Phi=\Phi_0/2$ is a triplet state. Also, this minimum value is not the same as that of the singlet at $\Phi=0$. In fact both become equal only in the limit[3] $U=+\infty$ or $L=\infty$. For the negative-U Hubbard model on the other hand, the lowest-energy triplet is consistently above the lowest-energy singlet, therefore the difference in spin-wave-function symmetry discussed for the positive-U Hubbard model above is absent. Furthermore, it is worth pointing out that, again, the ground-state energies at $\Phi=0$ and $\Phi_0/2$ are strictly identical only in the limiting case[3] $U=-\infty$ or $L=\infty$. This negative-U case is illustrated in Fig. 2 where we show the lowest-energy singlet as a function of the flux quantum. The lowest-energy triplet does not depend on U and is the same as the dashed curve in Fig. 1. The minimum at $\Phi=0$ is lower than that at $\Phi=\Phi_0/2$.

We conclude from the preceding results that the $\Phi_0/2$ periodicity discussed by FKL does not have the same physical significance in the positive and negative-U models. In the positive-U model, the difference in total-spin quantum number indicates that there is no pair, since the spin wave function, which is a characteristic of the pair, is different at $\Phi=0$ and $\Phi_0/2$. In the negative-U case, however, the center-of-mass wave function is different at $\Phi=0$ and at $\Phi_0/2$, but the spin of the relative wave function is identical at both values of the flux. In this sense the charge carriers could be described here as paired. Note that one cannot go adiabatically from the $\Phi=0$ ground state to the $\Phi=\Phi_0/2$ ground state since, in both models, there is a good quantum number which changes as a function of flux. Nevertheless, if the system is connected to a reservoir which allows symmetry breakings, the ground state would always be reached.

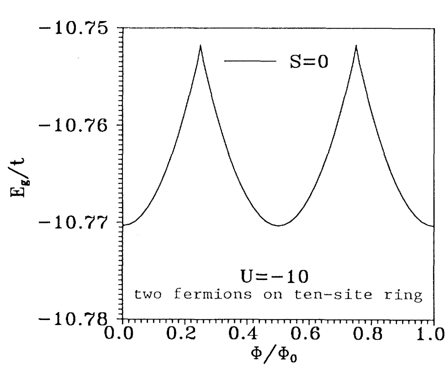

FIG. 2. The lowest-energy singlet of the Hubbard model with two fermions at $U=-10$ in a 10-site ring is plotted as a function of flux quantum. One can see that the values at $\Phi=0$ and $\Phi_0/2$ are not the same.

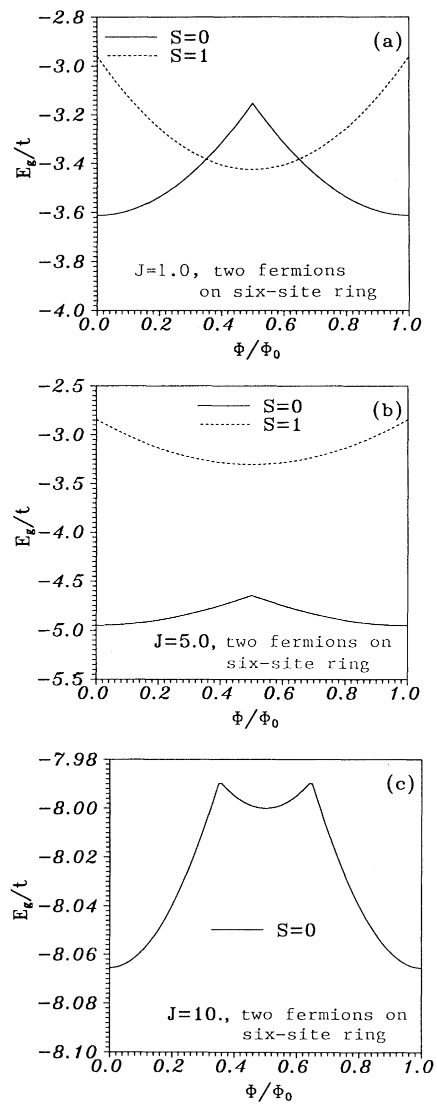

FIG. 3. (a) The lowest energy of the t-J model for two fermions at $J=1$ in six-site ring for singlet and triplet states is plotted as a function of flux quantum. One can see that the minimum at $\Phi=\Phi_0/2$ is a triplet in this parameter range. (b) Same as that of (a) for $J=5$. One sees that the minimum at $\Phi=\Phi_0/2$ disappears. (c) Lowest energy for $S=0$ is shown for $J=10$. It is seen that the minimum at $\Phi=\Phi_0/2$ reappears and is similar to the negative-U Hubbard model.

Finally we discuss the t-J model with the Hamiltonian

$$\hat{H} = -t \sum_{\langle ij \rangle \sigma = \uparrow,\downarrow} (c_{i\sigma}^{\dagger} c_{j\sigma} e^{i\phi} + \text{H.c.}) + J \sum_{\langle ij \rangle} \mathbf{S}_i \cdot \mathbf{S}_j \; , \qquad (7)$$

with the constraint of no doubly occupied sites and $\phi = (2\pi/L)(\Phi/\Phi_0)$. In Fig. 3(a) we plot the lowest energy of the two-fermion singlet and triplet as a function of flux in a six-site ring. As one can see, at $\Phi = \Phi_0/2$ the minimum energy for $J=1$ corresponds to a triplet just as in the case of the positive-U Hubbard model. However, as one increases the value of J, the minimum at $\Phi_0/2$ first disappears as can be seen in Fig. 3(b) for $J=5$. The ground state is a singlet for all flux values. The minimum then reappears when J increases even further, as shown for $J=10$ in Fig. 3(c). This case is similar to the negative-U Hubbard model.

In conclusion we have shown that it is important to know the spin symmetry of the ground-state wave function as a function of the flux when one uses flux as a probe of pairing in a strongly correlated system. From such studies then, one can conclude that two fermions are not paired in the positive-U Hubbard model, while they are for the negative-U Hubbard model. The t-J model when J is small, behaves as the positive-U Hubbard model, but as one increases J it behaves like the negative-U Hubbard model, though J has to be quite large for this to happen. For large J there is a known phase separation instability,[4] so the pairing discussed here cannot be taken as a necessary sign of superconductivity, even in the many-body case. The same analysis has been done for two-dimensional systems. This will be described in another publication.[5]

We would like to thank the authors of Ref. 1 for useful comments on the original manuscript. We gratefully acknowledge the support of the Natural Sciences and Engineering Research Council of Canada (NSERC), the Fonds pour la Formation de Chercheurs et l'Aide à la Recherche (FCAR) of the Government of Québec, and (A.-M.S.T.) the Canadian Institute of Advanced Research (C.I.A.R.).

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