Undulatory variation of antiferromagnetic strength with magnetic field based on the Hubbard-model Hamiltonian

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(Received 30 May 1996; revised manuscript received 27 January 1997)

Using the Hubbard model Hamiltonian for the two-dimensional system of antiferromagnetically correlated electrons, we examine the undulatory variation of antiferromagnetic order (strength) with applied magnetic field. The marked reduction (or local minimum) of antiferromagnetic strength is predicted to occur only at the even integer denominator values of the rational number of magnetic flux quanta per plaquette. The predicted change of the antiferromagnetic order with the external magnetic field is explained in terms of electronic structure (band gap) and Wigner-Jordan transformation. [S0163-1829(97)01222-8]

I. INTRODUCTION

For the studies of interacting electron systems, one of the most widely used theoretical methods is the Hubbard model Hamiltonian[1] for various investigations of physical properties.[2–4] Earlier, by considering the system of uncorrelated electrons Hasegawa *et al.*[5] reported the total kinetic energy of the spinless noninteracting electrons in two-dimensional lattices as a function of magnetic flux per plaquette and found an absolute minimum for the case of one flux quantum per particle for a square lattice. However, to the best of our knowledge, for the system of antiferromagnetically correlated electrons there exists no systematic study on the variation of antiferromagnetic order (strength), band gap, and total energy with applied magnetic field. Unlike our earlier preliminary studies,[7] here we present a systematic examination on the variation of antiferromagnetic strength (Fig. 1) with Coulomb repulsion (electron correlation) and the variation of the band gap with magnetic field. In addition, we present an interpretation of the unexplained undulatory variation of the antiferromagnetic order with applied magnetic field.

II. VARIATION OF ANTIFERROMAGNETIC STRENGTH, TOTAL ENERGY, AND BAND GAP WITH EXTERNAL MAGNETIC FIELD

With the external magnetic field, the one-band Hubbard Hamiltonian is written

$$H=-t\sum_{\langle i,j\rangle\sigma}\exp\left[(-i2\pi/\phi_0)\int_j^i A\ dl\right]C_{i\sigma}^{\dagger}C_{j\sigma}+U\sum_j n_{j\uparrow}n_{j\downarrow}-\mu\sum_j (n_{j\uparrow}+n_{j\downarrow}). \tag{1}$$

Here t and U are the hopping integral and the Coulomb repulsion energy, respectively. μ is the chemical potential. $\langle i,j\rangle$ stands for summation only over the nearest neighbors. $n_{j\sigma}$ is the number operator for an electron of spin σ at site j, $n_{j\sigma}=C_{j\sigma}^{\dagger}C_{j\sigma}$ with $C_{j\sigma}^{\dagger}$ $(C_{j\sigma})$, the creation (annihilation) operator for an electron at site j. ϕ_0 is the magnetic flux quantum, $\phi_0=hc/e$. The electromagnetic vector potential in the Landau gauge is $A=B(0,x,0)$ with $x=j_x a$ for the jth site along the x direction with the lattice spacing a. Thus $\int A\ dl=j_x Ba^2=j_x\phi$, with $\phi=Ba^2$.

Applying the mean-field (Hartree-Fock) approximation[6] to the Hubbard model Hamiltonian with the use of the two-component spinor

$$\psi_j=\begin{pmatrix}C_{j\uparrow}\\ C_{j\downarrow}\end{pmatrix}$$

and the spin operators

$$S_z(j)=\tfrac{1}{2}(C_{j\uparrow}^{\dagger}C_{j\uparrow}-C_{j\downarrow}^{\dagger}C_{j\downarrow})$$

and

$$S_+(j)=C_{j\uparrow}^{\dagger}C_{j_\downarrow},\quad S_-(j)=C_{j\downarrow}^{\dagger}C_{j\uparrow},$$

and using the relation $\int A\ dl=j_x\phi$ in Eq. (1) above, one readily obtains

$$H=-t\sum_{\langle ij\rangle}\exp\left(-i2\pi j_x\frac{p}{q}\right)\psi_i^{\dagger}\psi_j+U\sum_j \psi_j^{\dagger}[\tfrac{1}{2}\langle n(j)\rangle-\langle S(j)\rangle]\psi_j+U\sum_j\{\langle S_z(j)\rangle^2+\langle S_+(j)\rangle\langle S_-(j)\rangle-\tfrac{1}{4}\langle n(j)\rangle^2\}-\mu\sum_j (n_{j\uparrow}+n_{j\downarrow}), \tag{2}$$

where

$$\frac{p}{q}=\frac{\phi}{\phi_0},$$

$$n(j)=C_{j\uparrow}^{\dagger}C_{j\uparrow}+C_{j\downarrow}^{\dagger}C_{j\downarrow},$$

and

$$S(j)=\begin{pmatrix}S_z(j) & S_-(j)\\ S_+(j) & -S_z(j)\end{pmatrix},$$

where $\langle S_z(j)\rangle$, $\langle S_+(j)\rangle$, and $\langle S_-(j)\rangle$ denote the average values of S_z, S_+, and S_-, respectively, in the ground state. The phase angle $2\pi j_x p/q$ in the first term Eq. (2) above can

TABLE I. Variation of the total electronic energy per site with magnetic flux per plaquette, $\phi = (p/q)\phi_0$, for the 24×24 square lattice of a half-filled band for various strengths of electron correlation, U.

$U \backslash \phi$	0	$\frac{1}{8}$	$\frac{1}{4}$	$\frac{1}{3}$	$\frac{3}{8}$	$\frac{1}{2}$
0.0	−1.617	−1.650	−1.717	−1.712	−1.758	−1.915
0.5	−1.743	−1.775	−1.842	−1.838	−1.883	−2.040
1.0	−1.870	−1.900	−1.967	−1.965	−2.009	−2.165
1.5	−2.001	−2.027	−2.092	−2.097	−2.139	−2.290
2.0	−2.139	−2.160	−2.218	−2.235	−2.275	−2.415
3.0	−2.447	−2.462	−2.500	−2.533	−2.565	−2.666
4.0	−2.797	−2.808	−2.836	−2.865	−2.886	−2.935
20.0	−10.198	−10.198	−10.198	−10.199	−10.199	−10.200

be interpreted as an acquired phase as a result of electron (fermion) hopping by absorbing the external magnetic flux. Obviously, the hopping term in Eq. (1) or Eq. (2) remains completely fermionic in nature if there exists no external magnetic field. With this view, such a gain of statistical phase during electron (fermion) hopping can be regarded to affect the antiferromagnetic order (strength).

For the sake of comparison with the exact results of Hasegawa *et al.*,[5] we performed numerical calculations of the total kinetic energies per site at various values of both electron filling factor ν and magnetic flux per plaquette, $\phi = (p/q)\phi_0$, for a finite-size square lattice of 24×24. Encouragingly, our calculations[7] yielded excellent agreement with the exact calculations of Hasegawa *et al.*[5] for a square lattice of infinite size. In Table I we show the variation of the total electronic energy at half-filling with the flux quantum per plaquette at various values of Coulomb repulsion energy. Our computed total kinetic energies for the noninteracting electrons agree extremely well with the exact results of Hasegawa *et al.* The computed total energy at $\phi = \frac{1}{2}\phi_0$ is exactly twice the value for the case of the integer quantum Hall effect (IQHE) with quantum number 1,[5] as expected. In terms of filling fraction, it corresponds to the IQHE with quantum number 2 for the present case of a half-filled band. It is of note that the predicted absolute minima of the total energies are found at the half-integer flux value of $\phi = \frac{1}{2}\phi_0$, whether electron correlation is present ($U \neq 0$) or not ($U = 0$). The total electronic ground-state energy for nonzero external magnetic field is found to be always smaller than the case of zero magnetic field. The total energy difference between zero and nonzero magnetic fields was found to decrease with an increase of electron correlation (or Coulomb repulsion U), as expected.

For two-dimensional systems of antiferromagnetically correlated electrons at half-filling, we define

$$m \equiv 2 \left| \sum_{i_x, i_y}^{N} (-1)^{i_x + i_y} \langle S_z(i_x, i_y) \rangle \right| \Big/ N$$

as antiferromagnetic strength (order) or staggered magnetization. Here N is the total number of lattice sites. i_x and i_y are the integers corresponding to the x and y coordinates of site i, respectively, for the two-dimensional (2D) square lattice of present interest. We report the variation of m with the applied magnetic field. In Fig. 1 we show the computed results of the antiferromagnetic strength m for finite-size square lattices for both cases of zero and nonzero magnetic fields corresponding to $p/q = 0$ and $\frac{1}{2}$, respectively. Encouragingly, we find that they are in excellent agreement with the values for the infinite-size lattice particularly for relatively large U values (say, $U \gtrsim 3t$ for the case of $p/q = \frac{1}{2}$). As can be readily seen from this figure, the difference in m between the zero magnetic field and the nonzero magnetic field indicates the reduction of antiferromagnetic strength. Such a reduction tends to disappear for substantially strong correlations, e.g., $U \gtrsim 10t$.

In Fig. 2 we show the variation of m with magnetic flux $\phi = (p/q)\phi_0$ for various selected values of U. The solid lines indicate the computed results for a 20×20 square lattice. Symbols other than the solid line represent computed results for various chosen sizes of square lattices up to the size of 36×36 by satisfying the necessary periodic boundary conditions. However, even in the case of failure in meeting the periodic boundary conditions with the odd-integer denominator values of $q = 3,5,7$ in the rational number p/q, it was found that the 20×20 square lattice yielded reasonably good agreement with the results obtained from the lattice sizes which satisfied the periodic boundary conditions.[7] The undulatory variation of antiferromagnetic order m with magnetic field tends to disappear at extremely high values of U, e.g., $U = 20t$. $m = 1$ corresponds to the maximum antiferromagnetic (spin) order which means the ''perfectly'' antisymmetric states of electrons. However, the degree of such perfect

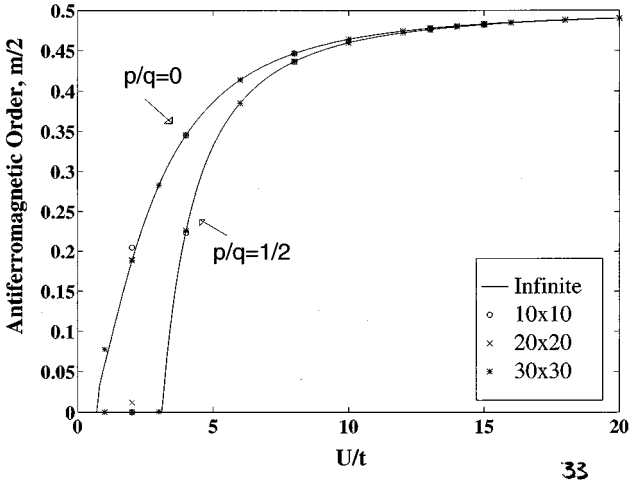

FIG. 1. Dependence of the antiferromagnetic order (strength) on lattice size with zero and nonzero magnetic fields corresponding to $p/q = 0$ and $p/q = \frac{1}{2}$, respectively.

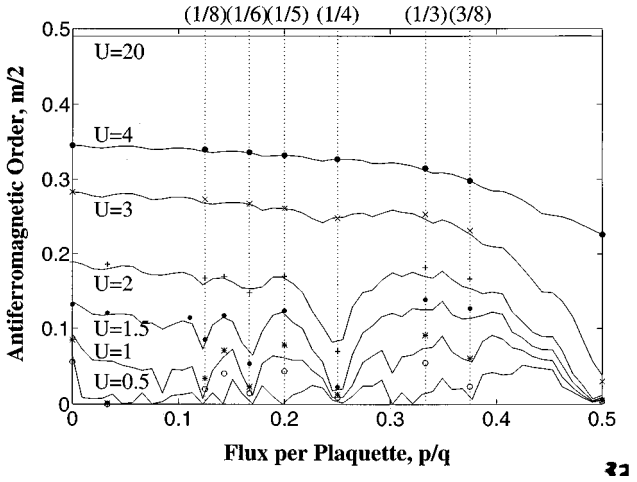

FIG. 2. Change of antiferromagnetic order (strength), m, with magnetic flux per plaquette, ϕ, for various strengths of electron correlation U.

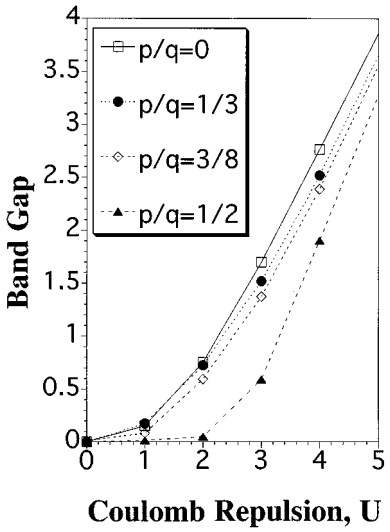

FIG. 3. Band gap vs Coulomb repulsion energy U as a function of magnetic flux per plaquette, ϕ.

antisymmetrization may be subject to change due to the variation of phase in Eq. (2) with applied magnetic field. Indeed, it is quite interesting to note from Fig. 2 that there exists a strong tendency of losing the antiferromagnetic strength particularly at $\phi=\frac{1}{2}\phi_0$, with $U\lesssim 3t$. Unless the correlation (Coulomb repulsion U) is exceedingly strong, the predicted absolute minima invariably occur at $\phi=\frac{1}{2}\phi_0$, showing an undulatory variation of the antiferromagnetic strength with magnetic field. Interestingly, the local minima are found only at the even-integer denominator values of q in the rational number p/q of magnetic flux quanta per plaquette, $\phi=(p/q)\phi_0$, e.g., $\frac{1}{2}$, $\frac{3}{8}$, $\frac{1}{4}$, $\frac{1}{6}$, and $\frac{1}{8}$, while at the odd-integer value of q such local minima tend to disappear. To explore the cause of such differences in antiferromagnetic strength between the even- and odd-integer values of q, we computed the band gap as a function of magnetic field. The computed band gap also showed local minima at the even integer values of q, although not displayed here. Consequently, easier electron hopping at the even-integer denominator values for the flux p/q tends to destroy the antiferromagnetic order. A noticeable band gap opening begins to occur at $U\sim 2t$ for $p/q=\frac{1}{2}$, as shown in Fig. 3. At all values of Coulomb repulsion energy U, the lower values of band gaps are predicted to occur with $\phi=\frac{1}{2}\phi_0$. Accordingly, the locations of the absolute minima in antiferromagnetic strength m are found to occur only at this half-integer value of the magnetic flux per plaquette, $p/q=\frac{1}{2}$, for values of $U\lesssim 2t$.

By introducing a statistical phase interpretation,[3] we now examine the even-odd differences (associated with the denominator value q in the rational number p/q) in antiferromagnetic strength. The generalized equal-time commutation relation for anyons with a hard core condition on a square lattice is given by

$$a_i a_j^\dagger = \delta_{ij} - e^{i\gamma} a_j^\dagger a_i \tag{3}$$

in connection with the Jordan-Wigner transformation.[3] Here $a_i^\dagger$ and a_j are the anyon creation and annihilation operators at the sites i and j, respectively, on the square lattice. The phase angle γ in Eq. (3) above represents a possible statistical transmutation of particles as a result of coupling to a statistical (Chern-Simons) gauge field.[3] For example, a Heisenberg antiferromagnet is equivalent to a system of spinless electrons coupled to a statistical (Chern-Simons) gauge field[3] when such coupling results in the statistical phase angle of $\gamma=n\pi$ with n zero or even integers, thus satisfying the fermion commutation relation. On the other hand, with n odd integers (or γ, odd multiple of π) the operators a_i satisfy the boson commutation relation and a hard core condition. The antiferromagnetic order comes originally from the statistically (Fermi-Dirac statistics) antisymmetric state (exchange symmetry) of electrons (fermions). Bosonic statistical transmutation corresponding to the odd multiple of π in the phase angle γ above will result in the disappearance of antiferromagnetic order m. As well known,[3] such bosonic transmutation arises when an even (odd) integer number of flux quanta is attached to each spinless electron (fermion). Electron (i.e., fermion) hopping strength in Eq. (1) or Eq. (2) is modulated by the ''statistical'' phase factor in $t_{ij}=t\exp(-i2\pi j_x p/q)$ as a result of the applied magnetic field. As can be inferred from the phase factor that appears in Eq. (2), such bosonic statistical transmutation is possible for the even integer denominator values of q in p/q. However, for the odd-integer denominator values of q, such antiferromagnetic order is not likely to disappear. Indeed, such even- and odd-integer differences are well predicted from our calculations as shown in Fig. 2. Indeed, for the case of relatively weak electron correlation, say, $U\lesssim 2t$, the predicted antiferromagnetic strength tends to disappear at the half-integer value ($q=2$, i.e., an even denominator value) of $\phi=\frac{1}{2}\phi_0$, which is clearly equivalent to the phase angle of an odd-integer multiple of π for the spinless electron considered in Eq. (3), thus satisfying the bosonic commutation relation. On the other hand, such a tendency is not found with odd denominator values, e.g., $p/q=\frac{1}{3}$ and $\frac{1}{5}$ as shown in Fig. 2. Finally, bosonic statistical transmutation is difficult to occur at sufficiently large U values due to the persistence of antiferromagnetic order. Indeed, this feature is well predicted as shown in Fig. 2.

III. CONCLUSION

By considering the two-dimensional systems of antiferromagnetically correlated electrons, we have systematically examined the variations of the total electronic ground-state energy, band gap, and antiferromagnetic order with applied magnetic field. The absolute minima of antiferromagnetic strength, total electronic energy, and band gap were found to invariably occur at the half-integer value of magnetic flux per plaquette, $\phi=\frac{1}{2}\phi_0$. For the case of the total energy, the absolute minima were shown to occur, also, at $\phi=\frac{1}{2}\phi_0$, whether there exists electron correlation (electron repulsion U) or not. For $U\neq 0$, the local minima of the antiferromagnetic strength were found to invariably occur at the even- (but not odd-) integer denominators of the magnetic flux per plaquette, that is, $p/q=\frac{1}{2}$, $\frac{3}{8}$, $\frac{1}{4}$, and $\frac{1}{8}$. Unless electron correlation is sufficiently strong, the undulatory variation of antiferromagnetic strength with magnetic field of the even-odd difference in the denominator of q in p/q was found to correlate well not only with electronic structure (band gap), but also with the statistical phase, which results from the coupling of fermions to the fictitious (statistical or Chern-Simons) gauge field, which tends to screen out the electromagnetic gauge field.

ACKNOWLEDGMENTS

One of us (S.H.S.S.) was supported by the Korean Ministry of Education BSRI program, POSTECH BSRI special fund, and the Center for Molecular Science at the Korea Advanced Institute of Science and Technology. We are grateful to Professor H. Y. Choi at Sung Kyun Kwan University for his computational assistance.

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