Harper's equation for two-dimensional systems of antiferromagnetically correlated electrons

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Considering interacting (antiferromagnetically correlated) electrons, we derive a generalized Harper's equation in a mean-field approximation for a square lattice of infinite size. In the present study with the aid of a gap equation we explain the cause of the oscillatory behavior in staggered magnetization with the variation of an applied magnetic field for two-dimensional systems of antiferromagnetically correlated electrons. Exact diagonalization calculations on small clusters show additional evidence for the oscillatory behavior of staggered magnetization. We find that for systems of weakly correlated electrons both mean-field and exact diagonalization calculations yield an identical behavior in the propensity of diminishing staggered magnetization for even-denominator (but not for odd-denominator) values of q in the magnetic flux quanta per plaquette, i.e., p/q. [S0163-1829(99)15533-4]

I. INTRODUCTION

Since the discovery of high-temperature superconductors and related insulating materials, there has been enhanced interest in two-dimensional spin- $\frac{1}{2}$ magnetic or antiferromagnetically correlated electron systems.^{1,2} However, not much attention has been paid to the magnetic properties of these systems coupled to an external magnetic field.³⁻⁵ The original Harper's equation⁶⁻⁸ is concerned with the energy dispersion involving systems of noninteracting electrons due to an applied magnetic field. Hence it is of great interest to study how systems of interacting electrons behave under an external magnetic field. Earlier we paid attention to the dispersion of antiferromagnetically correlated electrons by considering a square lattice of finite size.⁹ In the present paper we derive a generalized Harper's equation which describes the dispersion of antiferromagnetically correlated electrons in a square lattice of infinite size. An analytic expression for the density of states is derived from the generalized Harper's equation. Earlier we found from numerical calculations the oscillatory behavior of staggered magnetization with a variation of the external magnetic field and its cause was unexplained.⁹ Here we explain the cause of the oscillatory behavior with the aid of an analytically derived density of states. Lanczos exact diagonalization calculations on small clusters also exhibit evidence for the oscillatory behavior of staggered magnetization. It is shown that below a critical electron correlation strength the staggered magnetization disappears at even-denominator values of q (but not at odd q) of given magnetic flux quanta per plaquette, p/q.

II. GENERALIZED HARPER'S EQUATION AND DENSITY OF STATES

We write the Hubbard model Hamiltonian describing the two-dimensional system of antiferromagnetically correlated electrons under an external magnetic field,⁸

$$H = -t \sum_{\langle ij \rangle \sigma} \left[\exp\left(-i \frac{2\pi}{\phi_0} \int_j^i \mathbf{A} \cdot d\mathbf{I} \right) c_{i\sigma}^{\dagger} c_{j\sigma} + \text{H.c.} \right]$$

+ $U \sum_i n_{i\uparrow} n_{i\downarrow} - \mu \sum_{i\sigma} c_{i\sigma}^{\dagger} c_{i\sigma}, \qquad (1)$

where *t* is the hopping integral, **A** the electromagnetic vector potential, $\phi_0 = hc/e$ the elementary flux quantum, *U* the onsite Coulomb repulsion energy, and μ the chemical potential. $\langle ij \rangle$ stands for summation over nearest-neighbor sites *i* and *j*. $c_{i\sigma}^{\dagger}$ ($c_{i\sigma}$) is the creation (annihilation) operator of an electron of spin σ at site *i*, and $n_{i\uparrow}$ ($n_{i\downarrow}$) the number operator of an up-spin (down-spin) electron at site *i*.

The staggered magnetization (antiferromagnetic order) at site *i* is written as $m_i = e^{i\mathbf{Q}\cdot\mathbf{r}_i}\Sigma_{\sigma}\sigma\langle c_{i\sigma}^{\dagger}c_{i\sigma}\rangle$, where $\mathbf{Q} = (\pi, \pi)$ and $\mathbf{r}_i = (i_x, i_y)$ with i_x and i_y being integers with the lattice spacing of unity. We allow a uniform staggered magnetization *m* and a uniform doping rate δ , i.e.,

$$m = \frac{1}{N} \sum_{i\sigma} e^{i\mathbf{Q}\cdot\mathbf{r}_i} \sigma \langle c_{i\sigma}^{\dagger} c_{i\sigma} \rangle, \qquad (2a)$$

$$\delta = 1 - \frac{1}{N} \sum_{i} \langle n_i \rangle, \qquad (2b)$$

with the number of lattice sites, *N*. By using the Landau gauge $\mathbf{A} = B(0,x,0)$, we obtain the mean-field (Hartree-Fock) Hamiltonian in the momentum space,

$$H = -t \sum_{\mathbf{k}\sigma} \left[2 \cos k_x c^{\dagger}_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma} + e^{-ik_y} c^{\dagger}_{\mathbf{k}-\mathbf{g},\sigma} c_{\mathbf{k}\sigma} \right]$$
$$+ e^{ik_y} c^{\dagger}_{\mathbf{k}+\mathbf{g},\sigma} c_{\mathbf{k}\sigma} \left] - \frac{mU}{2} \sum_{\mathbf{k}\sigma} \sigma c^{\dagger}_{\mathbf{k}+\mathbf{Q},\sigma} c_{\mathbf{k}\sigma} \right]$$
$$+ \left[\frac{U}{2} (1-\delta) - \mu \right] \sum_{\mathbf{k}\sigma} c^{\dagger}_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma}, \qquad (3)$$

where $\mathbf{g} = (2 \pi \phi / \phi_0, 0) = (2 \pi p / q, 0)$ with p/q the number of flux quanta per plaquette. The first bracketed term in Eq. (3) represents electron hopping; the first term in the brackets represents the nearest-neighbor hopping in the *x* direction and the last two terms in the brackets the nearest-neighbor hopping in the *y* direction. Because of the choice of the Landau gauge $\mathbf{A} = B(0,x,0)$, the electron gains no phase when it hops in the *x* direction, while it acquires a phase when it hops in the *y* direction. The electromagnetic vector potential \mathbf{A}

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shifts the wave vector of electron in the k_x direction by $g \equiv |\mathbf{g}| = 2 \pi p/q$. The second term results from the antiferromagnetic spin order of correlated electrons, which causes the wave vector to shift by \mathbf{Q} . The last term represents the shift of the chemical potential by $U(1-\delta)/2$ as a result of hole doping.

The matrix form of the Hamiltonian (3) is written as

$$H = H_0 + H_1,$$

$$H_0 = \left[\frac{U}{2}(1-\delta) - \mu\right] \sum_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma}^{\dagger} c_{\mathbf{k}\sigma},$$

$$H_1 = \sum_{\mathbf{k}\sigma}' \mathbf{C}_{\mathbf{k}\sigma}^{\dagger} \mathbf{H}_{\mathbf{k}\sigma} \mathbf{C}_{\mathbf{k}\sigma},$$
(4a)

where

$$\mathbf{C}_{k\sigma} = \begin{bmatrix} c_{\mathbf{k}+\mathbf{g},\sigma} \\ \vdots \\ c_{\mathbf{k}+(q-1)\mathbf{g},\sigma} \\ c_{\mathbf{k}\sigma} \\ c_{\mathbf{k}\sigma} \\ c_{\mathbf{k}+\mathbf{g}+\mathbf{Q},\sigma} \\ \vdots \\ c_{\mathbf{k}+(q-1)\mathbf{g}+\mathbf{Q},\sigma} \\ c_{\mathbf{k}+\mathbf{Q},\sigma} \end{bmatrix}, \quad (4b)$$

$$\mathbf{H}_{k\sigma} = \begin{bmatrix} c | c \mathbf{T}_k & \mathbf{V}_{\sigma} \\ \mathbf{V}_{\sigma} & -\mathbf{T}_k \end{bmatrix}, \qquad (4c)$$

$$\mathbf{\Gamma}_{k} = -t \begin{bmatrix} M_{1} & e^{-ik_{y}} & 0 & 0 & e^{ik_{y}} \\ e^{ik_{y}} & M_{2} & \ddots & 0 & 0 \\ 0 & \ddots & \ddots & \ddots & 0 \\ 0 & 0 & \ddots & M_{q-1} & e^{-ik_{y}} \\ e^{-ik_{y}} & 0 & 0 & e^{ik_{y}} & M_{q} \end{bmatrix}, \quad (4d)$$

and

$$\mathbf{V}_{\sigma} = \begin{bmatrix} -\frac{\sigma m U}{2} & 0 & 0 & 0 & 0\\ 0 & -\frac{\sigma m U}{2} & 0 & 0 & 0\\ 0 & 0 & \ddots & 0 & 0\\ 0 & 0 & 0 & -\frac{\sigma m U}{2} & 0\\ 0 & 0 & 0 & 0 & -\frac{\sigma m U}{2} \end{bmatrix}_{(4e)}$$

with $M_n = 2 \cos(k_x + ng)$. The summation $\Sigma'_{\mathbf{k}}$ is over the reduced Brillouin zone, $\{(k_x, k_y) | -\pi/q \le k_x \le \pi/q, -\pi/2 \le k_y \le \pi/2\}$. The Brillouin zone is reduced by 1/q due to the presence of q plaquettes per magnetic unit cell, and is further reduced by 1/2 as a result of antiferromagnetic spin order. The diagonal matrix \mathbf{T}_k in Eq. (4c) represents electron hop-

ping and contains information on the phase modulation of hopping electrons due to the influence of the external field. The off-diagonal matrix V_{σ} in Eq. (4c) represents the anti-ferromagnetic electron correlation.

From the eigenvalue equation of the Hamiltonian matrix $\mathbf{H}_{k\sigma}$,

$$\det(\mathbf{H}_{k\sigma} - E_k \mathbf{I}) = 0, \tag{5}$$

with **I** the identity matrix, we obtain the quasiparticle energy dispersion E_k of the antiferromagnetically correlated electrons in the presence of a magnetic field. In the limiting case of noninteracting electrons (U=0) the "generalized" Harper's equation (5) above is reduced to the original Harper's equation derived by Hasegawa *et al.*,⁸ that is,

$$\det(\mathbf{T}_k - \varepsilon_k \mathbf{I}) = 0, \tag{6}$$

where ε_k is the energy dispersion of noninteracting electrons in the presence of a magnetic field.

Following Hasegawa *et al.*,⁸ Eq. (6) can be rewritten in a simplified form

$$\gamma(\varepsilon) = \cos(qk_x) + \cos(qk_y), \tag{7}$$

where $\gamma(\varepsilon)$ is given in Table I for various values of p/qwhich are not presented in the study of Hasegawa *et al.*⁸ Now for the case of antiferromagnetically correlated electrons we obtain, from the diagonalization of the Hamiltonian matrix $\mathbf{H}_{k\sigma}$ in Eq. (4c) above,

$$E_k = \sqrt{\varepsilon_k^2 + \Delta^2},\tag{8}$$

with $2\Delta = mU$ the band gap. Thus the band gap is linearly dependent on both the staggered magnetization *m* and the electron correlation strength (Coulomb repulsion) *U*. It is of great interest how such a linear dependence obtained from the mean-field approximation is modified with accurate calculations.

From the use of the energy dispersion relation (8), we obtain an analytic form of the density of states,

$$g(E) = 2 \int \frac{d^2k}{(2\pi)^2} \delta(E - E_k)$$
$$= \frac{2}{q\pi^2} \left| \frac{d\gamma(\varepsilon)}{d\varepsilon} \right| K \left[\sqrt{1 - \left(\frac{\gamma(\varepsilon)}{2}\right)^2} \right] \left| \frac{E}{\varepsilon} \right|, \qquad (9)$$

where $|\varepsilon| = \sqrt{E^2 - (mU/2)^2}$ and *K* is a complete elliptic integral of the first kind,¹⁰

$$K(\alpha) = \int_0^{\pi/2} \frac{d\phi}{\sqrt{1 - \alpha^2 \sin^2 \phi}}.$$

Equation (9) above represents the density of states for the systems of correlated electrons in the presence of a magnetic field. In the limiting case of U=0, it correctly reproduces the results of Hasegawa *et al.*⁸ for noninteracting electrons. Although not shown here, the analytic result of Eq. (9) for U=0 is in excellent agreement with the numerical results obtained by Hasegawa *et al.*⁸ In the presence of a magnetic field with the flux quanta per plaquette p/q, a single band splits into q subbands. This is analogous to the energy level

TABLE I. $\gamma(\varepsilon)$ for various values of magnetic flux quanta per plaquette, p/q. The energy dispersion of noninteracting electrons at a given p/q is determined from the Harper's equation $\gamma(\varepsilon) = \cos(qk_x) + \cos(qk_y)$. For other values of p/q the reader is referred to the results of Hasegawa *et al.* (Ref. 8).

р	q	$2\gamma(\varepsilon)$
2	5	$-\varepsilon^{5}+10\varepsilon^{3}+\varepsilon\left[-20-10\cos\left(\frac{2\pi}{5}\right)\right]$
1	7	$-\varepsilon^{7}+14\varepsilon^{5}+\left[-49+14\cos\left(\frac{2\pi}{7}\right)\right]\varepsilon^{3}+\left[42-28\cos\left(\frac{2\pi}{7}\right)-28\cos\left(\frac{3\pi}{7}\right)\right]\varepsilon^{3}+\left[42-28\cos\left(\frac{2\pi}{7}\right)-28\cos\left(\frac{3\pi}{7}\right)\right]\varepsilon^{3}+\left[42-28\cos\left(\frac{2\pi}{7}\right)-28\cos\left(\frac{3\pi}{7}\right)\right]\varepsilon^{3}+\left[42-28\cos\left(\frac{2\pi}{7}\right)-28\cos\left(\frac{3\pi}{7}\right)\right]\varepsilon^{3}+\left[42-28\cos\left(\frac{2\pi}{7}\right)-28\cos\left(\frac{3\pi}{7}\right)\right]\varepsilon^{3}+\left[42-28\cos\left(\frac{2\pi}{7}\right)-28\cos\left(\frac{3\pi}{7}\right)\right]\varepsilon^{3}+\left[42-28\cos\left(\frac{2\pi}{7}\right)-28\cos\left(\frac{3\pi}{7}\right)\right]\varepsilon^{3}+\left[42-28\cos\left(\frac{2\pi}{7}\right)-28\cos\left(\frac{3\pi}{7}\right)\right]\varepsilon^{3}+\left[42-28\cos\left(\frac{2\pi}{7}\right)-28\cos\left(\frac{3\pi}{7}\right)\right]\varepsilon^{3}+\left[42-28\cos\left(\frac{2\pi}{7}\right)-28\cos\left(\frac{3\pi}{7}\right)\right]\varepsilon^{3}+\left[42-28\cos\left(\frac{2\pi}{7}\right)-28\cos\left(\frac{3\pi}{7}\right)\right]\varepsilon^{3}+\left[42-28\cos\left(\frac{2\pi}{7}\right)-28\cos\left(\frac{3\pi}{7}\right)\right]\varepsilon^{3}+\left[42-28\cos\left(\frac{2\pi}{7}\right)-28\cos\left(\frac{3\pi}{7}\right)\right]\varepsilon^{3}+\left[42-28\cos\left(\frac{2\pi}{7}\right)-28\cos\left(\frac{3\pi}{7}\right)\right]\varepsilon^{3}+\left[42-28\cos\left(\frac{3\pi}{7}\right)-28\cos\left(\frac{3\pi}{7}\right)\right]\varepsilon^{3}+\left[42-28\cos\left(\frac{3\pi}{7}\right)-28\cos\left(\frac{3\pi}{7}\right)\right]\varepsilon^{3}+\left[42-28\cos\left(\frac{3\pi}{7}\right)-28\cos\left(\frac{3\pi}{7}\right)\right]\varepsilon^{3}+\left[42-28\cos\left(\frac{3\pi}{7}\right)-28\cos\left(\frac{3\pi}{7}\right)\right]\varepsilon^{3}+\left[42-28\cos\left(\frac{3\pi}{7}\right)-28\cos\left(\frac{3\pi}{7}\right)\right]\varepsilon^{3}+\left[42-28\cos\left(\frac{3\pi}{7}\right)-28\cos\left(\frac{3\pi}{7}\right)\right]\varepsilon^{3}+\left[42-28\cos\left(\frac{3\pi}{7}\right)-28\cos\left(\frac{3\pi}{7}\right)\right]\varepsilon^{3}+\left[42-28\cos\left(\frac{3\pi}{7}\right)-28\cos\left(\frac{3\pi}{7}\right)\right]\varepsilon^{3}+\left[42-28\cos\left(\frac{3\pi}{7}\right)-28\cos\left(\frac{3\pi}{7}\right)\right]\varepsilon^{3}+\left[42-28\cos\left(\frac{3\pi}{7}\right)-28\cos\left(\frac{3\pi}{7}\right)\right]\varepsilon^{3}+\left[42-28\cos\left(\frac{3\pi}{7}\right)-28\cos\left(\frac{3\pi}{7}\right)\right]\varepsilon^{3}+\left[42-28\cos\left(\frac{3\pi}{7}\right)-28\cos\left(\frac{3\pi}{7}\right)\right]\varepsilon^{3}+\left[42-28\cos\left(\frac{3\pi}{7}\right)-28\cos\left(\frac{3\pi}{7}\right)\right]\varepsilon^{3}+\left[42-28\cos\left(\frac{3\pi}{7}\right)-28\cos\left(\frac{3\pi}{7}\right)\right]\varepsilon^{3}+\left[42-28\cos\left(\frac{3\pi}{7}\right)-28\cos\left(\frac{3\pi}{7}\right)\right]\varepsilon^{3}+\left[42-28\cos\left(\frac{3\pi}{7}\right)-28\cos\left(\frac{3\pi}{7}\right)\right]\varepsilon^{3}+\left[42-28\cos\left(\frac{3\pi}{7}\right)-28\cos\left(\frac{3\pi}{7}\right)\right]\varepsilon^{3}+\left[42-28\cos\left(\frac{3\pi}{7}\right)-28\cos\left(\frac{3\pi}{7}\right)\right]\varepsilon^{3}+\left[42-28\cos\left(\frac{3\pi}{7}\right)-28\cos\left(\frac{3\pi}{7}\right)\right]\varepsilon^{3}+\left[42-28\cos\left(\frac{3\pi}{7}\right)-28\cos\left(\frac{3\pi}{7}\right)\right]\varepsilon^{3}+\left[42-28\cos\left(\frac{3\pi}{7}\right)-28\cos\left(\frac{3\pi}{7}\right)\right]\varepsilon^{3}+\left[42-28\cos\left(\frac{3\pi}{7}\right)-28\cos\left(\frac{3\pi}{7}\right)\right]\varepsilon^{3}+\left[42-28\cos\left(\frac{3\pi}{7}\right)-28\cos\left(\frac{3\pi}{7}\right)\right]\varepsilon^{3}+\left[42-28\cos\left(\frac{3\pi}{7}\right)-28\cos\left(\frac{3\pi}{7}\right)\right]\varepsilon^{3}+\left[42-28\cos\left(\frac{3\pi}{7}\right)-28\cos\left(\frac{3\pi}{7}\right)\right]\varepsilon^{3}+\left[42-28\cos\left(\frac{3\pi}{7}\right)-28\cos\left(\frac{3\pi}{7}\right)\right]\varepsilon^{3}+\left[42-28\cos\left(\frac{3\pi}{7}\right)-28\cos\left(\frac{3\pi}{7}\right)\right]\varepsilon^{3}+\left[42-28\cos\left(\frac{3\pi}{7}\right)-28\cos\left(\frac{3\pi}{7}\right)\right]\varepsilon^{3}+\left[42-28\cos\left(\frac{3\pi}{7}\right)-28\cos\left(\frac{3\pi}{7}\right)\right]\varepsilon^{3}+\left[42-28\cos\left(\frac{3\pi}{7}\right)-28\cos\left(\frac{3\pi}{7}\right)\right]\varepsilon^{3}+\left[42-28\cos\left(\frac{3\pi}{7}\right)-28\cos\left(\frac{3\pi}{7}\right)\right]\varepsilon^{3}+\left[42-28\cos\left(\frac{3\pi}{7}\right)$
2	7	$-\varepsilon^{7}+14\varepsilon^{5}+\left[-49-14\cos\left(\frac{3\pi}{7}\right)\right]\varepsilon^{3}+\left[28-28\cos\left(\frac{2\pi}{7}\right)+56\cos\left(\frac{3\pi}{7}\right)\right]\varepsilon^{3}$
3	7	$-\varepsilon^{7}+14\varepsilon^{5}+\left[-56-14\cos\left(\frac{2\pi}{7}\right)+14\cos\left(\frac{3\pi}{7}\right)\right]\varepsilon^{3}+\left[56+56\cos\left(\frac{2\pi}{7}\right)-28\cos\left(\frac{3\pi}{7}\right)\right]\varepsilon^{3}+\left[56+56\cos\left(\frac{2\pi}{7}\right)-28\cos\left(\frac{3\pi}{7}\right)\right]\varepsilon^{3}+\left[56+56\cos\left(\frac{2\pi}{7}\right)-28\cos\left(\frac{3\pi}{7}\right)\right]\varepsilon^{3}+\left[56+56\cos\left(\frac{2\pi}{7}\right)-28\cos\left(\frac{3\pi}{7}\right)\right]\varepsilon^{3}+\left[56+56\cos\left(\frac{2\pi}{7}\right)-28\cos\left(\frac{3\pi}{7}\right)\right]\varepsilon^{3}+\left[56+56\cos\left(\frac{2\pi}{7}\right)-28\cos\left(\frac{3\pi}{7}\right)\right]\varepsilon^{3}+\left[56+56\cos\left(\frac{2\pi}{7}\right)-28\cos\left(\frac{3\pi}{7}\right)\right]\varepsilon^{3}+\left[56+56\cos\left(\frac{2\pi}{7}\right)-28\cos\left(\frac{3\pi}{7}\right)\right]\varepsilon^{3}+\left[56+56\cos\left(\frac{2\pi}{7}\right)-28\cos\left(\frac{3\pi}{7}\right)\right]\varepsilon^{3}+\left[56+56\cos\left(\frac{2\pi}{7}\right)-28\cos\left(\frac{3\pi}{7}\right)\right]\varepsilon^{3}+\left[56+56\cos\left(\frac{2\pi}{7}\right)-28\cos\left(\frac{3\pi}{7}\right)\right]\varepsilon^{3}+\left[56+56\cos\left(\frac{2\pi}{7}\right)-28\cos\left(\frac{3\pi}{7}\right)\right]\varepsilon^{3}+\left[56+56\cos\left(\frac{2\pi}{7}\right)-28\cos\left(\frac{3\pi}{7}\right)\right]\varepsilon^{3}+\left[56+56\cos\left(\frac{2\pi}{7}\right)-28\cos\left(\frac{3\pi}{7}\right)\right]\varepsilon^{3}+\left[56+56\cos\left(\frac{2\pi}{7}\right)-28\cos\left(\frac{3\pi}{7}\right)\right]\varepsilon^{3}+\left[56+56\cos\left(\frac{2\pi}{7}\right)-28\cos\left(\frac{3\pi}{7}\right)\right]\varepsilon^{3}+\left[56+56\cos\left(\frac{2\pi}{7}\right)-28\cos\left(\frac{3\pi}{7}\right)\right]\varepsilon^{3}+\left[56+56\cos\left(\frac{2\pi}{7}\right)-28\cos\left(\frac{3\pi}{7}\right)\right]\varepsilon^{3}+\left[56+56\cos\left(\frac{2\pi}{7}\right)-28\cos\left(\frac{3\pi}{7}\right)\right]\varepsilon^{3}+\left[56+56\cos\left(\frac{2\pi}{7}\right)-28\cos\left(\frac{3\pi}{7}\right)\right]\varepsilon^{3}+\left[56+56\cos\left(\frac{2\pi}{7}\right)-28\cos\left(\frac{3\pi}{7}\right)\right]\varepsilon^{3}+\left[56+56\cos\left(\frac{2\pi}{7}\right)-28\cos\left(\frac{3\pi}{7}\right)\right]\varepsilon^{3}+\left[56+56\cos\left(\frac{2\pi}{7}\right)-28\cos\left(\frac{3\pi}{7}\right)\right]\varepsilon^{3}+\left[56+56\cos\left(\frac{2\pi}{7}\right)-28\cos\left(\frac{3\pi}{7}\right)\right]\varepsilon^{3}+\left[56+56\cos\left(\frac{2\pi}{7}\right)-28\cos\left(\frac{3\pi}{7}\right)\right]\varepsilon^{3}+\left[56+56\cos\left(\frac{2\pi}{7}\right)-28\cos\left(\frac{2\pi}{7}\right)\right]\varepsilon^{3}+\left[56+56\cos\left(\frac{2\pi}{7}\right)-28\cos\left(\frac{2\pi}{7}\right)\right]\varepsilon^{3}+\left[56+56\cos\left(\frac{2\pi}{7}\right)-28\cos\left(\frac{2\pi}{7}\right)\right]\varepsilon^{3}+\left[56+56\cos\left(\frac{2\pi}{7}\right)-28\cos\left(\frac{2\pi}{7}\right)\right]\varepsilon^{3}+\left[56+56\cos\left(\frac{2\pi}{7}\right)-28\cos\left(\frac{2\pi}{7}\right)\right]\varepsilon^{3}+\left[56+56\cos\left(\frac{2\pi}{7}\right)-28\cos\left(\frac{2\pi}{7}\right)\right]\varepsilon^{3}+\left[56+56\cos\left(\frac{2\pi}{7}\right)-28\cos\left(\frac{2\pi}{7}\right)\right]\varepsilon^{3}+\left[56+56\cos\left(\frac{2\pi}{7}\right)-28\cos\left(\frac{2\pi}{7}\right)\right]\varepsilon^{3}+\left[56+56\cos\left(\frac{2\pi}{7}\right)-28\cos\left(\frac{2\pi}{7}\right)\right]\varepsilon^{3}+\left[56+56\cos\left(\frac{2\pi}{7}\right)-28\cos\left(\frac{2\pi}{7}\right)\right]\varepsilon^{3}+\left[56+56\cos\left(\frac{2\pi}{7}\right)-28\cos\left(\frac{2\pi}{7}\right)\right]\varepsilon^{3}+\left[56+56\cos\left(\frac{2\pi}{7}\right)-28\cos\left(\frac{2\pi}{7}\right)\right]\varepsilon^{3}+\left[56+56\cos\left(\frac{2\pi}{7}\right)-28\cos\left(\frac{2\pi}{7}\right)\right]\varepsilon^{3}+\left[56+56\cos\left(\frac{2\pi}{7}\right)-28\cos\left(\frac{2\pi}{7}\right)\right]\varepsilon^{3}+\left[56+56\cos\left(\frac{2\pi}{7}\right)-28\cos\left(\frac{2\pi}{7}\right)\right]\varepsilon^{3}+\left[56+56\cos\left(\frac{2\pi}{7}\right)-28\cos\left(\frac{2\pi}{7}\right)\right]\varepsilon^{3}+\left[56+56\cos\left(\frac{2\pi}{7}\right)-28\cos\left(\frac{2\pi}{7}\right)\right]\varepsilon^{3}+\left[56+56\cos\left(\frac{2\pi}{7}\right)-28\cos\left(\frac{2\pi}{7}\right)\right]\varepsilon^{3}+\left[56+56\cos\left(\frac{2\pi}{7}\right)-28\cos\left(\frac{2\pi}{7}\right)\right]\varepsilon^{3}+\left[56+56\cos\left(\frac{2\pi}{7}\right)-28\cos\left(\frac{2\pi}{7}\right)\right]\varepsilon^{3}+\left[56$
1	9	$-\varepsilon^9 + 18\varepsilon^7 + \left[-99 + 4\sqrt{3}\cos\left(\frac{\pi}{18}\right) + 6\cos\left(\frac{2\pi}{9}\right) + 4\sqrt{3}\cos\left(\frac{7\pi}{18}\right)\right]\varepsilon^5$
		$+ \left[186 - 24\sqrt{3}\cos\left(\frac{\pi}{18}\right) - 36\cos\left(\frac{2\pi}{9}\right) + 4\sqrt{3}\cos\left(\frac{5\pi}{18}\right) - 28\sqrt{3}\cos\left(\frac{7\pi}{18}\right) + 24\cos\left(\frac{4\pi}{9}\right)\right]\varepsilon^{3}$
		$+\left[-126+36\sqrt{3}\cos\left(\frac{\pi}{18}\right)+36\cos\left(\frac{2\pi}{9}\right)+36\sqrt{3}\cos\left(\frac{7\pi}{18}\right)-54\cos\left(\frac{4\pi}{9}\right)\right]\varepsilon$
2	9	$-\varepsilon^9 + 18\varepsilon^7 + \left[-99 + 4\sqrt{3}\cos\left(\frac{5\pi}{18}\right) - 4\sqrt{3}\cos\left(\frac{7\pi}{18}\right) + 6\cos\left(\frac{4\pi}{9}\right)\right]\varepsilon^5$
		$+ \left[186 - 4\sqrt{3}\cos\left(\frac{\pi}{18}\right) - 24\cos\left(\frac{2\pi}{9}\right) - 28\sqrt{3}\cos\left(\frac{5\pi}{18}\right) + 24\sqrt{3}\cos\left(\frac{7\pi}{18}\right) - 60\cos\left(\frac{4\pi}{9}\right)\right]\varepsilon^{3}$
		$+\left[-126+54\cos\left(\frac{2\pi}{9}\right)+36\sqrt{3}\cos\left(\frac{5\pi}{18}\right)-36\sqrt{3}\cos\left(\frac{7\pi}{18}\right)+90\cos\left(\frac{4\pi}{9}\right)\right]\varepsilon$
4	9	$-\varepsilon^9 + 18\varepsilon^7 + \left[-99 - 4\sqrt{3}\cos\left(\frac{\pi}{18}\right) - 6\cos\left(\frac{2\pi}{9}\right) - 4\sqrt{3}\cos\left(\frac{5\pi}{18}\right) - 6\cos\left(\frac{4\pi}{9}\right)\right]\varepsilon^5$
		$+\left[186+28\sqrt{3}\cos\left(\frac{\pi}{18}\right)+60\cos\left(\frac{2\pi}{9}\right)+24\sqrt{3}\cos\left(\frac{5\pi}{18}\right)+4\sqrt{3}\cos\left(\frac{7\pi}{18}\right)+36\cos\left(\frac{4\pi}{9}\right)\right]\varepsilon^{3}$
		$+ \left[-126 - 36\sqrt{3}\cos\left(\frac{\pi}{18}\right) - 90\cos\left(\frac{2\pi}{9}\right) - 36\sqrt{3}\cos\left(\frac{5\pi}{18}\right) - 36\cos\left(\frac{4\pi}{9}\right)\right]\varepsilon$

splitting into Landau levels for electrons embedded in a continuum state under a magnetic field.

III. STAGGERED MAGNETIZATION AT ZERO TEMPERATURE AND AT HALF FILLING IN EXTERNAL MAGNETIC FIELDS

Now we investigate the staggered magnetization at half filling (δ =0) and at zero temperature in a magnetic field. The chemical potential is given by $\mu = U/2$. The selfconsistent equation (2a) for the staggered magnetization *m* can be expressed as

$$\frac{1}{U} = \int_{-\infty}^{0} d\varepsilon \frac{g_0(\varepsilon)}{2} \frac{1}{\sqrt{\varepsilon^2 + (mU/2)^2}}.$$
 (10)

Here $g_0(\varepsilon)$ is the density of states of noninteracting electrons in the presence of a magnetic field. It is readily obtained from Eq. (9). It is of interest to note that the "gap equation" above [Eq. (10)] is in a form similar to the one that appears in the spin density wave theory of cuprate materials.^{11,12} It will be used for the determination of the staggered magnetization *m* varying with the external mag-

netic field for the system of weakly correlated electrons, i.e., small U values. In Fig. 1 the oscillatory behavior of staggered magnetization is predicted particularly for small values of correlation strength $U \leq 1$. It is of note that the Hartree-Fock results are not reliable for large values of U. Thus its reliability at high U values is diminished. Various symbols represent the results obtained from the use of the newly derived analytic gap equation above for the square lattice of infinite size. They are in good agreement with the selfconsistent numerical calculations for a 20×20 finite square lattice.⁹

In the following with the aid of the gap equation [Eq. (10)] we explain the cause of the oscillatory behavior of the staggered magnetization for the case of weakly correlated electrons. At even-denominator values of q in p/q the staggered magnetization is predicted to disappear (e.g., see the case of p/q=1/2). This feature is well depicted in Fig. 1. We now define the critical electron correlation strength (Coulomb repulsion) $U_{p/q}$ to be a value below which the staggered magnetization rom Eq. (10) vanishes at even q values below a critical value $U_{p/q}$, i.e., $U < U_{p/q}$. On the other



FIG. 1. Staggered magnetization (antiferromagnetic order) at zero temperature as a function of p/q, the magnetic flux quanta per plaquette. Various symbols represent the results calculated from the analytic gap equation [Eq. (10)] for a square lattice of infinite size. The interpolating lines are guides to the eye.

hand, in the absence of the magnetic field the staggered magnetization tends to appear even at small values of U.¹² The critical correlation strength $U_{p/q}$ is obtained by substituting m=0 in Eq. (10), and is shown for various values of p/q in Table II. For odd q in p/q, the integral in Eq. (10) is logarithmically divergent, and thus the critical correlation strength $U_{p/q}$ does not exist. Although not numerically precise for the case of our earlier finite-size calculations (solid lines),⁹ a propensity of vanishing staggered magnetization for the even-denominator values of q in p/q is correctly observed below $U_{p/q}$ as shown in Fig. 1. The oscillatory behavior is found to occur owing to the disappearance of staggered magnetization distinctively at the even-denominator values of q in p/q below the critical value of $U_{p/q}$.

We now investigate the oscillatory behavior of staggered magnetization in the Lanczos exact diagonalization scheme. To incorporate the Aharonov-Bohm phase $[\exp(-i2\pi\int_{j}^{i}\mathbf{A}\cdot d\mathbf{V}/\phi_{0})]$ it is necessary to choose a sufficiently large size of square lattice to meet the periodic boundary conditions of magnetic unit cells for various values of magnetic fields corresponding to p/q. The exact diagonalization calculations are not presently able to treat such a large-size square lattice for a system of antiferromagnetically correlated electrons. The only allowed value of magnetic flux quanta to satisfy the periodic boundary conditions with the above square lattice is p/q = 1/2. For the choice of Landau gauge $\mathbf{A} = B(0,x,0)$, the electron gains no phase when it hops in the x direction and it acquires a phase

TABLE II. Critical correlation strength $U_{p/q}$ as a function of magnetic flux quanta per plaquette, p/q.

$\frac{p}{q}$	$\frac{1}{8}$	$\frac{1}{6}$	$\frac{1}{4}$	$\frac{3}{8}$	$\frac{1}{2}$
$U_{p/q}$	1.29	1.49	1.87	0.897	3.11



FIG. 2. Staggered magnetization as a function of magnetic flux quanta per plaquette on a tilted $\sqrt{8} \times \sqrt{8}$ square lattice. The inset indicates the appropriateness of the magnetic flux quanta per plaquette, p/q = 1/2, by satisfying the periodic boundary condition for the magnetic unit cell. The + and - signs represent the acquired Aharonov-Bohm phase. The thick solid box denotes a unit cell of the $\sqrt{8} \times \sqrt{8}$ lattice and the dotted box is a magnetic unit cell for p/q = 1/2.

of $\exp[-i2\pi(p/q)i_x]$ when it hops in the y direction. The acquired phase is +1 or -1 for p/q = 1/2. It is indicated by + for +1 and - for -1 in the inset of Fig. 2. The thick solid square represents a unit cell of the $\sqrt{8} \times \sqrt{8}$ square lattice and the dotted box in the solid square denotes a magnetic unit cell. The magnetic unit cell satisfies the periodic boundary conditions. Hopping of an electron from site A to site B is equivalent to hopping from site A' to site B'. In the exact diagonalization treatment, the staggered magnetization is defined by¹³

$$\langle \mathbf{M}^2 \rangle = \left\langle \left(\frac{1}{N} \sum_i e^{i\mathbf{Q} \cdot \mathbf{r}_i} \mathbf{S}_i \right)^2 \right\rangle, \tag{11}$$

with $\mathbf{Q} = (\pi, \pi)$. We show the predicted staggered magnetization in Fig. 2. In agreement with the mean-field result, the staggered magnetization is found to be reduced at the evendenominator value of p/q = 1/2. It is noted that the nonvanishing value of staggered magnetization for small values of U is due to the finite-size effect.

In order to study the behavior of staggered magnetization for additional values of magnetic flux quanta, we are led to consider a 2×6 ladder system owing to a difficulty of meeting satisfactory periodic boundary conditions with computationally accessible small-size square lattices. The values of magnetic flux quanta satisfying the periodic boundary conditions are p/q=1/6, 1/3, and 1/2. In Fig. 3 the oscillatory behavior of staggered magnetization is satisfactorily predicted for the above chosen values of correlation strength. This trend is in agreement with the mean-field result shown in Fig. 1, by showing a propensity of vanishing staggered magnetization only for the even-denominator values of q in p/q.

IV. CONCLUSION

We derived a generalized Harper's equation for the energy dispersion relation of interacting (antiferromagnetically correlated) electrons in an external magnetic field. Unlike the



FIG. 3. Staggered magnetization as a function of magnetic flux quanta per plaquette on a 2×6 ladder system.

original Harper's equation which deals only with noninteracting electron systems, the generalized Harper's equation derived in Eq. (5) [with Eq. (4c)] has the definite merit of studying the physical properties of correlated electron systems in the presence of the external magnetic field. From this Harper's equation we derived an analytic expression for the density of states of antiferromagnetically correlated electrons in a magnetic field. For the limiting case of noninteracting electrons, the analytic density of states is found to reproduce the numerical results of Hasegawa et al.⁸ For the case of half filling, we derived a gap equation for the determination of staggered magnetization for antiferromagnetically correlated electron systems in the presence of a magnetic field. As a comprehensive and improved version over our earlier preliminary study,⁹ we were able to find from the gap equation the cause of the oscillatory behavior in staggered magnetization under a varying external magnetic field for systems of weakly correlated electrons, that is, small U values. We demonstrated that below a critical electron correlation strength (Coulomb repulsion) the staggered magnetization in the presence of a magnetic field vanishes at even-denominator q values (but not at odd q) of magnetic flux quanta per plaquette, p/q. We find that for systems of weakly correlated electrons both mean-field and exact diagonalization calculations yield an identical behavior in the propensity of diminishing staggered magnetization for the even-denominator (but not for the odd-denominator) values of q in the magnetic flux quanta per plaquette, i.e., p/q.

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