# Flux Period, Spin Gap, and Pairing in the One-Dimensional $t$-$J$-$J'$ Model

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(Received 22 December 2003; published 21 July 2004)

Using the factorization of the wave function in the $t$-$J$-$J'$ model at small exchange couplings, we demonstrate the connection between the existence of a spin gap and an $hc/2e$ flux periodicity of the ground state energy. We conjecture that all spin-gapped SU(2)-invariant Luttinger liquids have $hc/2e$ flux periodicity, and that this is connected to the fact that a gapped spin-$\frac{1}{2}$ chain always breaks translational symmetry by doubling the unit cell.

DOI: 10.1103/PhysRevLett.93.046401 PACS numbers: 71.10.Pm, 71.10.Hf, 74.72.–h

Soon after the discovery of high-$T_c$ superconductivity, Anderson proposed that the basic physics of the cuprates is that of a doped two-dimensional Mott insulator [1]. In particular, the Cooper pairs of the superconducting state are viewed as the "liberated spin singlet pairs" of the insulating host material. While this picture is very attractive, it has been difficult to find an explicit model for which the proclaimed behavior can be shown to occur unequivocally.

Searching for models of Mott insulators that show superconductivity upon doping has been the motivation for many studies of one-dimensional systems [2–7]. Thanks to methods such as perturbative renormalization group and bosonization, considerable knowledge has been acquired on the weak coupling phase diagram of both strictly one-dimensional [8] and ladder systems [9]. The drawback of the weak coupling approach is that it often is only an instability analysis. The ultimate statement of the quantum phase still rests on certain assumptions about the "strong coupling fixed point" of the renormalization group flow.

Most strong coupling models cannot be solved analytically. A notable exception is the Luther-Emery action [10] which describes an electronic liquid with a spin gap and dominant singlet-superconducting (SS) correlations at large distances. Another interesting analytic method for analyzing strong coupling 1D models was introduced by Ogata and Shiba [11], and extended in Ref. [3]. This method is designed to treat the large $U$ Hubbard model (or the small $J$ $t$-$J$ model). It is based on two facts: (i) In the limit of $U \to \infty$ (or $J/t \to 0$) the ground state of the Hubbard ($t$-$J$ model) is infinitely degenerate, and (ii) each of the degenerate states is described by a wave function composed of a product of pure charge and spin components [11]. For large but finite $U$ (small $J/t$), one can apply degenerate perturbation theory to lift the degeneracy. After doing so, the ground state wave function remains factorized. Moreover, the spin wave function is given by that of the Heisenberg model on a "squeezed lattice" (i.e., the lattice where the unoccupied sites are omitted).

In superconductivity, the hallmark of electron pairing is the $\Phi_0/2 \equiv hc/2e$ flux period. In three dimensions, if one plots the ground state energy $E(\Phi)$ of a solid superconducting torus as a function of the Aharonov-Bohm (AB) flux $\Phi$ through the hole, one finds a periodic function with period $\Phi_0/2$. Moreover, the energy barrier separating the successive minima is extensive. In two and one dimensions, the flux period is the same. However, the energy barrier becomes intensive for two dimensions, and vanishes as the inverse circumference for one dimension.

In one dimension, the spin and charge degrees of freedom decouple in the low energy and long wavelength limit. According to common wisdom, the presence of a spin gap implies pairing. It is, thus, natural to draw a connection between the existence of a spin gap and a $\Phi_0/2$ flux period. However, since the vector potential enters only in the charge action, it is not obvious how the presence of a spin gap may affect the flux period. The purpose of this Letter is to clarify this issue in the context of a strongly correlated 1D system.

In the following, we study the one-dimensional $t$-$J$-$J'$ model, making use of the degenerate perturbation approach introduced in Ref. [3]. The model is defined by the Hamiltonian

$$H = -t\sum_i \mathcal{P}(e^{[2\pi i/L]\Phi/\Phi_0} c^\dagger_{i,\sigma} c_{i+1,\sigma} + \text{H.c.})\mathcal{P} + J\sum_i \left( S_i \cdot S_{i+1} - \frac{1}{4} n_i n_{i+1} \right) + J'\sum_i \left( S_i \cdot S_{i+2} - \frac{1}{4} n_i n_{i+2} \right), \tag{1}$$

describing $N$ electrons on a ring of $L$ sites in the presence of an Aharonov-Bohm flux $\Phi$. Here, the projection operator $\mathcal{P}$ excludes states with doubly occupied sites, and the $S_i$ are spin-1/2 operators. At $J = J' = 0$, the model corresponds to the $U = \infty$ Hubbard model. As pointed out in Ref. [11], in this limit the eigenstates factorize into products of pure charge and spin states. This property has been used extensively to study the large (but finite) $U$ Hubbard model [11–13], which is related to the small $J$ $t$-$J$ model. Much less analytic work has been done on the $t$-$J$-$J'$ model with a finite $\alpha \equiv J'/J$, because the model is no longer integrable. In this case, however, the degenerate perturbation approach introduced in Ref. [3] still allows one to determine the ground state properties.

In the following, we will use this method to study the ground state energy of (1) as a function of the AB flux $\Phi$. We begin by defining the $N$-particle wave function of the system

$$\Psi(x_1, \sigma_1, \ldots, x_N, \sigma_N) = \langle 0| c_{x_1\sigma_1} \cdots c_{x_N\sigma_N} |\Psi\rangle, \tag{2}$$

on the domain

$$D := \{(x_1 \cdots x_N) \in \mathbb{Z}^N | x_1 < x_2 < \cdots x_N < x_1 + L\}.$$

Here $|\Psi\rangle$ and $|0\rangle$ are the state of the system and the vacuum of the fermionic operators $c_{x,\sigma} \equiv c_{x+L,\sigma}$, respectively. The fermion antisymmetry and the periodic boundary condition imply

$$\Psi(x_1, \sigma_1, \ldots, x_N, \sigma_N) = (-1)^{(N-1)} \Psi(x_2, \sigma_2, \ldots, x_N, \sigma_N, (x_1 + L), \sigma_1). \tag{3}$$

At $J = J' = 0$, each eigen wave function of (1) factorizes into a product of a charge and a spin wave function [11],

$$\Psi(x_1, \sigma_1, \ldots, x_N, \sigma_N) = f(x_1 \cdots x_N)\, g(\sigma_1 \cdots \sigma_N), \tag{4}$$

where

$$f(x_1 \cdots x_N) = \frac{1}{\sqrt{L^N}} \det[\exp(ik_i x_j)] \tag{5}$$

is a Slater determinant constructed from $N$ plane waves. It is of central importance here to observe that, for a finite ring with periodic boundary conditions, the spin part and the charge part of the wave function (4) are not completely independent. Specifically, if we quantize the $N$ momenta in (4) according to

$$k_j = \frac{2\pi}{L} q_j + \frac{K}{L}, \tag{6}$$

where $q_j \in \mathbb{Z}$ and $K \in [0, 2\pi)$; then the condition (3) requires the spin wave function to satisfy

$$g(\sigma_1 \cdots \sigma_N) = e^{iK} g(\sigma_2 \cdots \sigma_N, \sigma_1), \tag{7}$$

which implies that $K$ is the "spin momentum" on the squeezed lattice. Thus, by means of (6), the momentum $K$ of the spin wave function injects a twist into the charge wave function. For large but finite $U$, the exact ground state wave function of the Hubbard model remains of the form given by Eq. (4), and the same relation between charge twist and spin momentum is observed [11]. Within the degenerate perturbation approach introduced in Ref. [3], the same still applies to the ground state of (1) for any value of $\alpha = J'/J$ in the limit of vanishing exchange couplings. In this limit, all solutions of the form Eq. (4) are degenerate in the spin wave function, which is required only to have the spin momentum $K$ determined by the twist of the charge wave function.

To first order in the exchange couplings, this degeneracy is lifted by an effective Hamiltonian acting in the "squeezed" space of $N$ spins [3]:

$$H_{\text{eff}} = \frac{L}{N}\left(J_{\text{eff}} \sum_{j=1}^{N} S_j \cdot S_{j+1} + J'_{\text{eff}} \sum_{j=1}^{N} S_j \cdot S_{j+2}\right),$$
$$J_{\text{eff}} = J\langle n_i n_{i+1}\rangle_f + J'\langle n_i(1 - n_{i+1}) n_{i+2}\rangle_f,$$
$$J'_{\text{eff}} = J'\langle n_i n_{i+1} n_{i+2}\rangle_f. \tag{8}$$

Here, $\langle\,\rangle_f$ denotes a spinless fermion expectation value with respect to the wave function $f$ displayed in (4).

We now focus on the case of constant $\alpha$, where $\alpha > \alpha_c \approx 0.241$ [14]. In this regime, numerical and analytical works suggest the phase diagram shown in Fig. 1. At zero doping, the spin chain corresponding to the model (1) at half filling ($N = L$) is gapped. The spin gap will survive for a finite range of doping $x = 1 - N/L < x_c$ (Fig. 1), and the effective spin Hamiltonian (8) may be used to calculate $x_c$ exactly in the limit $J/t \to 0$. This was first proposed by Ogata *et al.* [3] and has been confirmed numerically in Ref. [15]. Thus, the validity of degenerate perturbation theory is well established. [We will give a detailed discussion of the involved subtleties elsewhere [16] (see also [7])].

To first order in $J/t$ and $J'/t$, the ground state energy of Eq. (1) takes the form

$$E_{\text{tot}} = E_c + E_s, \tag{9}$$

where $E_c$ is the kinetic energy associated with the charge wave function $f_0$, and $E_s$ is the ground state energy of (8) with the spin momentum $K$. For any given AB flux, $f_0$ will be of the form given in (5), where the $N$ consecutively occupied momenta $k_j$ are given by (6) with

$$q_j = q_0 + j - 1, \qquad j = 1 \cdots N, \tag{10}$$

and $q_0$ is an integer. The kinetic energy is given by

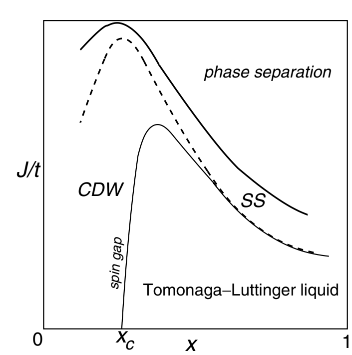


FIG. 1. Sketch of the zero temperature phase diagram of (1) as obtained in [3,15] for $\alpha = \frac{1}{2}$. The spin-gapped region is divided by a crossover (dashed line) between regions of dominant singlet superconducting (SS) and charge-density-wave (CDW) correlations.

$$E_c(q_0, K, \Phi) = -2t\sum_j \cos\left(k_j + \frac{2\pi}{L}\frac{\Phi}{\Phi_0}\right) = -2t\frac{\sin(k_f)}{\sin(\frac{\pi}{L})}\cos\left(k_f + \frac{2\pi}{L}q_0 + \frac{K-\pi}{L} + \frac{2\pi}{L}\frac{\Phi}{\Phi_0}\right). \quad (11)$$

In Eq. (11), $k_f$ is defined as $k_f \equiv \pi N/L$. Note that, for all charge wave functions characterized by Eqs. (6) and (10) with different $q_0$ and $K$, the effective couplings appearing in (8) are the same.

We will consider an even number of particles $N$ from now on. In the spin-gapped regime $0 < x < x_c$, the effective Hamiltonian (8) has two lowest-energy states with spin momenta $K = 0$ and $K = \pi$. These two states are separated from other spin states by an energy gap of the order of $J$ or $J'$. For a finite ring, the energy difference between these two lowest spin states vanishes exponentially with the circumference of the ring. Thus, in the thermodynamic limit these two states become degenerate.

For fixed $\Phi$, we choose $K$ and $q_0$ so that the total energy is minimized. This minimization can be achieved by first minimizing $E_c$ by varying $q_0$ for fixed $K$, then minimizing $E_s + E_c$ with respect to $K$. When the first minimization is achieved, the argument of the cosine is always of order $1/L$ regardless of the values of $K$. Hence, the effect of varying $K$ in the second minimization can result only in $O(t/L)$ modulations in $E_c$. We consider the limit $t/L \ll J$ here. It then follows that the value of $K$ must be either 0 or $\pi$. Other choices of $K$ would increase $E_s$ by the spin gap of order $J$, which cannot be compensated by the possible lowering of $E_c$.

After substituting the optimum value of $q_0$ for $K = 0$ or $K = \pi$ back into Eq. (11), we obtain two branches of energy versus $\Phi$ curves shown in Fig. 2(a). The lower envelope of these curves is the ground state energy as a function of $\Phi$ for small $J/t$ and $J'/t$. One observes that this function does indeed show a period of $\Phi_0/2$, owing to the existence of two different types of branches corresponding to $K = 0$ and $K = \pi$, respectively. This structure is resemblant of that proposed for the dimer model [17,18]. It is also interesting to note that $K = \pi$ is the analogy of the "vison" flux [19] in 1D.

The situation is fundamentally different in the regime $x > x_c$ (Fig. 1), where the spin gap vanishes. Here the ground state of the effective spin Hamiltonian (8) has $K = 0$ or $K = \pi$ depending on whether $N = 4m$ or $N = 4m + 2$ (see, e.g., [20]). For a finite chain of length $N = O(L)$, the first spin excited states at $K = \pi$ or $K = 0$ (i.e., whose momenta differ by $\pi$ from that of the respective ground state) have excitation energies of the order of $J/L$. This energy gives rise to the relative shift between the $K = 0$ and $K = \pi$ branches shown in Fig. 2(b) for $N = 4m$. The resulting lower envelope is illustrated for a small but finite $J/t$, where the flux period is now $\Phi_0$. For $N = 4m + 2$, the shift between the $K = 0$ and $K = \pi$ branches is opposite in sign. This behavior is well demonstrated in the large repulsive $U$ Hubbard model [21], where no spin gap is present.

It is sometimes felt that the existence of metastable minima of $E(\Phi)$ at $\Phi_0/2$ intervals is the sign of a pairing tendency, even though $\Phi_0/2$ is strictly not the flux period. Figure 2(b) presents a clear counterexample of this type of reasoning. Indeed according to Fig. 2(b) this can happen in a regime of the phase diagram where the ground state is neither spin-gapped nor features a dominance of superconducting pairing correlations.

On the other hand, for $x < x_c$, there is a spin gap but no charge gap, and the ground state energy is a periodic function of $\Phi$ with period $\Phi_0/2$. It has, thus, all the characteristics of a superconductor. However, for $J/t \ll 1$ the superconducting correlations (SS) are weaker than the charge density wave (CDW) correlations (Fig. 1). In this regime, we can think of the system as being close to a superconductor-(Cooper pair) insulator transition due to strong quantum fluctuations of the phase of the superconducting order parameter. Here, a weak external perturbation such as disorder can easily localize the Cooper pairs and drive the system insulating. As the system crosses the crossover line in (Fig. 1), the phase fluctuations become much less severe so that the SS correlations become dominant over the CDW correlations. We expect the appearance of a $\Phi_0/2$ flux period to hold in the entire spin-gapped regime. Indeed, more detailed considerations show that the arguments given

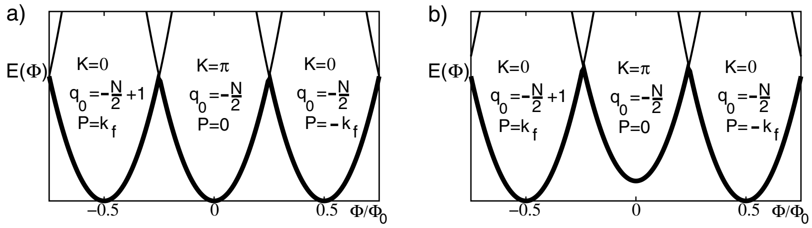


FIG. 2. Ground state energy according to (9) and (11) for $x < x_c$ and $x > x_c$. The energy scale is $t/L$. (a) $x < x_c$ (spin-gapped case). Periodic pattern of branches with $K = 0$ and $K = \pi$ separated by half a flux quantum. The thick line represents the ground state energy at given $\Phi$. The ground state momentum $P$ changes by $k_f$ between adjacent branches. (b) $x > x_c$ (no spin gap). The $\frac{1}{2}\Phi_0$ periodicity is destroyed by a relative shift of order $J/L$ between $K = 0$ and $K = \pi$ branches.

here are not limited to first order perturbation theory [16]. In particular, we find that second order contributions to the ground state energy may be incorporated into the effective spin Hamiltonian. The latter will then also depend on the twist of the zeroth order wave function and on flux, yet $H_{\mathrm{eff}}(K, \Phi) = H_{\mathrm{eff}}(K - \pi, \Phi + \Phi_0/2)$ continues to hold. Furthermore, we have shown that all the results presented here also follow from a weak coupling/bosonization procedure [22].

The analysis presented here can be applied to a wide class of models of the form of Eq. (1), where the second line is replaced by a more general spin-chain type of Hamiltonian. Most features of the phase diagram shown in Fig. 1 will likely survive as long as the spin chain at half filling is gapped. In particular, the spin gap will survive for a range of doping, and phase separation will occur at sufficiently large values of $J/t$, where $J$ is an appropriate energy scale for the spin couplings. As the phase separation line is approached, the charge compressibility diverges, and Luttinger liquid physics then implies a regime of dominant SS correlations. Our analysis on flux period will then carry over to this more generic case, provided that the gapped spin state at $x = 0$ also breaks translational symmetry by doubling of the unit cell, analogous to the dimerization that occurs in the $J$-$J'$ model at half filling. Such an example is given by the $t$-$J_z$ model studied in Ref. [23]. Although in Ref. [23] the possibility of $\Phi_0/n$ flux periods ($n \geq 2$) has been postulated for models of the type considered here, only the case $n = 2$ has been found for the $t$-$J_z$ model. This follows easily along the line of arguments given here, and we believe that only $n = 1$ and $n = 2$ are found in generic models.

If, on the other hand, a gapped spin-$\frac{1}{2}$ chain exists that does not break translational symmetry, it appears that a doped model with a spin gap could be constructed which does not feature $\Phi_0/2$ flux quantization as displayed in Fig. 2(a). However, such a state would violate the Lieb-Schultz-Mattis theorem [24]. For SU(2)-invariant spin-$\frac{1}{2}$ chains in one dimension, we are aware of only one way to create a spin gap, i.e., breaking the translational symmetry by doubling the unit cell. Hence, there seems to be an intimate relation between this fact and the possible universality of the $\Phi_0/2$ flux period which we postulate below.

We note that a $\Phi_0/2$ flux period associated with a spin gap has also been observed in numerical studies of a two-leg ladder [25]. This suggests that our main conclusion may be generalized beyond the purely one-dimensional case. However, a two-leg ladder has an even number of sites per unit cell. Here the undoped system may have a spin gap due to the formation of singlet pairs located on the rungs, which does not require symmetry breaking. These singlet pairs become mobile upon doping, and the above notion of symmetry breaking in some internal spin space is not required to explain the $\Phi_0/2$ period.

In conclusion, we have demonstrated the relation between a $\Phi_0/2$ periodicity in the ground state energy and the existence of a spin gap in the small exchange limit of the $t$-$J$-$J'$ model. Based on these findings, we conjecture that the observed $\Phi_0/2$ flux period is a universal property of spin-gapped SU(2) invariant one-dimensional systems of spin-$\frac{1}{2}$ particles with gapless charge degrees of freedom. In particular, the value of the charge Luttinger parameter is not a determining factor of the flux periodicity, as our result did not require the predominance of singlet superconducting correlations. Our findings further suggest an intimate relation between the proposed universality of the $\Phi_0/2$ flux period and the fact that all gapped SU(2)-invariant spin-$\frac{1}{2}$ chains feature broken translational symmetry with a doubling of the unit cell.

This work has been supported by DOE Grant No. DE-AC03-76SF00098.


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