Haldane Gap and Fractional Oscillations in Gated Josephson Arrays

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An analogy between the twisted quantum *xxz* model and a gated Josephson junction array is used to predict sharp structure in the critical currents versus gate voltage, and fractional ac Josephson frequencies. We prove selection rules for level crossings which imply fractional periodicities of ground states with varying Aharonov-Bohm flux. Extrapolated numerical diagonalization on ladders indicates a Haldane gap at moderate easy-plane anisotropy, with vanishing superfluid stiffness. Physical parameters for experimental realization of these novel effects are proposed. [S0031-9007(98)07646-7]

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Quantum phase fluctuations in superconductors can drive zero temperature superconductor to insulator transitions [1], as observed, for example, in disordered films [2]. Their effects can be enhanced and studied in detail using a weakly coupled, low capacitance Josephson junction array (JJA) [3,4].

Theory of quantum phase fluctuations has used models of interacting bosons on a lattice [5], and quantum dynamics of vortices [6]. The latter approaches have proposed collective phases such as vortex Bose condensation [7] (for the insulator), and fractional quantum Hall phases (for JJAs in magnetic field [8]).

Lattice bosons map onto effective models of quantum spins. A popular approximation to the phase diagram is mean field theory on the classical (large S) spin model [9]. In the strongly quantum regime, the same mapping relates the Mott insulator (integer bosons per site) and the quantum disordered antiferromagnet [5].

In this paper we explore the quantum magnetism analogy further. We focus our attention to the effects of a *periodic* lattice on superconductivity. We study the quantum *xxz* model with twisted boundary conditions [i.e., an Aharonov-Bohm (AB) flux] both numerically and analytically. The many body spectrum, vortex tunneling rates, and superfluid stiffness are computed for different lattice dimensions and magnetization (Cooper-pair density). We prove general selection rules for symmetry protected level crossings. This rule imposes *fractional* periodicities of the ground state as a function of AB flux, and is closely related to the "fractionally quantized phases" found by Oshikawa, Yamanaka, and Affleck (OYA) in magnetized Heisenberg chains [10].

The following effects may be observed in JJAs of dimensions $L_x \times L_y$.

(i) Haldane gap.—Our numerical results for the *xxz* model on a two leg ladder find a Haldane gap, at least for weak easy plane anisotropy. The lowest gap remains finite, while the superfluid stiffness decays exponentially for $L_x \to \infty$. In a finite size system, the Haldane phase is indicated by a suppressed critical current (relative to its classical value) that decays exponentially with L_x. It is also characterized by a high ac Josephson frequency $f_Q = 2eV/h$, where the classical Josephson frequency of the array is $f_{\rm cl} = 2eV/hL_x$.

(ii) Fractional oscillations.—At fractional Cooper pair densities $n = p/(qL_y)$, p, q integers, selection rules derived below produce sharp dips in the critical current $I_{\rm cr}$ versus gate potential. In these states, ac Josephson oscillations appear at *subharmonic* frequencies $f_Q^q = f_Q/q$. For $q > 1$ the ground states are at least q-fold degenerate, and qualitatively different from the $q = 1$ Haldane phase.

We conclude by proposing physical parameters for experiments.

The short-range Bose-Hubbard (BH) model is given by

$$H^{\rm BH} = U\sum_i n_i^2 + \sum_{\langle ij\rangle}[Vn_in_j - 2J(e^{i\theta_{ij}}b_i^\dagger b_j + {\rm H.c})], \quad (1)$$

where $b_i^\dagger$ creates a boson (Cooper pair [11]) at site i on a square lattice with nearest neighbor bonds $\langle ij\rangle$, and $n_i = b_i^\dagger b_i$. The lattice is placed on a cylinder penetrated by an AB flux Φ, introduced via the gauge phases $\theta_{ij} = \delta_{j,i+\hat{x}}2\pi\phi/L_x$, where $\phi = \Phi/\Phi_0$, and $\Phi_0 = h/(2ec)$. The supercurrent in the x direction is given by $I_s = \frac{1}{h}\langle\frac{\partial H}{\partial\phi}\rangle$.

At large $U \gg J, V$ one can keep the two lowest energy Fock states at every site, say $|\bar{n}_i\rangle$ and $|\bar{n}_i + 1\rangle$, and project out all other occupations. In the projected subspace, $b_i^\dagger, b_i, n_i - \bar{n}_i$ are replaced by spin half operators S_i^+, S_i^-, and $S_i^z + \frac{1}{2}$, respectively. This transformation maps (1) onto the quantum $S = \frac{1}{2}$ *xxz* model [12]

$$H^{xxz} = \sum_{\langle ij\rangle}\left[\frac{J^z}{S^2}S_i^zS_j^z + \frac{J}{2S^2}(e^{i\theta_{ij}}S_i^+S_j^- + {\rm H.c.})\right], \quad (2)$$

where the Ising coupling is $J^z = V/4$, and we limit our discussion to easy plane anisotropy $J^z \leq J$, in order to avoid the charge density wave phases [9]. A pure gauge transformation $\phi \to \phi + 1$ on (1) or (2) leaves their spectrum invariant.

It is instructive to consider the classical (large S) ground state energies of (2) which are adiabatically connected to the ground states at $\phi = i$, $i = 0, 1, \ldots$. For lack of space we simplify the demonstration by setting $J^z = 0$ and neglecting charge density waves in the classical energy

$$E^i_{\rm cl}(\phi) = JL_yL_x\,\delta n(1 - \delta n)\cos\left(\frac{2\pi(\phi - i)}{L_x}\right), \quad (3)$$

where $\delta n \equiv n - \bar{n}$. At $\phi = q/2$, q integer, pairs of classical ground states of oppositely directed supercurrents become degenerate, as depicted in Fig. 1.

Tunneling paths between the two classical ground states can be constructed as histories of vortices traversing the lattice in the y direction, or nucleation and separation of a vortex-antivortex pairs up to the two edges. The tunneling matrix elements, *unless prohibited by selection rules*, open minigaps at the avoided level crossings. This allows their precise computation from the (many body) eigenenergies as a function of AB flux [14–16].

The Hamiltonian (2) was diagonalized using the Lanczos algorithm using lattice momentum and total magnetization to block diagonalize the matrix. For the two leg ladder at $S^z_{\rm tot} = 0$, we find a regime of $J^z < J$ where the minigaps at $\phi = 1/2$ remain finite as L_x increases, which indicates a Haldane gap phase in the thermodynamic limit. This phase has been previously established for isotropic integer spin chains [17], and half-odd-integer ladders [18] and chains at finite magnetic fields [10].

To establish this phase we plot in Fig. 2, the *magnon* gap [19] at $\phi = 1/2$ as a function of $1/L_x$, and extrapolate the results to $1/L_x \to 0$. However, for the extrapoltion to be justified, we must be certain that we have reached the asymptotic $L_x \gg \xi$ regime where ξ is the correlation length. ξ was calculated from the superfluid stiffness $K = \partial^2 E/\partial\phi^2$, which was found to fit to an exponential $K(L_x) \propto \exp(-L_x/\xi)$. We find that in the regime $J^z/J^x \in (0.5, 1)$, the correlation length is $\xi \in (4.26, 2.13)$ which is safely smaller than the larger system dimensions. For the pure xy model at $J^z = 0$, however, ξ reaches our largest system size. In this regime, therefore, an extrapolated finite gap at $1/L_x = 0$ is not credible.

An easy-plane Haldane phase is explained as follows. The path integral of an even leg ladder of $S = 1/2$ spins can be mapped onto a classical partition function of an O(2) relativistic field theory in two dimensions [13,17]. Its temperature $T^{\rm 2D}$ scales asymptotically as $\sim (SL_y)^{-1}$ [21]. This suggests that below a certain spin size and ladder width, a disordered phase with exponentially decaying correlations is possible, which translates into a finite gap for excitations and vanishing stiffness for long ladders. Above a critical width $L_y > L_y^{KT}$, correlations should decay as a power law with a finite (1D) superfluid density $4\pi^2\rho_s = \lim_{L_x\to\infty}(L_xK) > 0$.

Selection rules for avoided level crossings.—Vortex tunneling is enabled by the lattice since it breaks continuos translational symmetry. However, the remaining discrete translational symmetry imposes selection rules which are given by the following theorem.

Theorem: For the Hamiltonian (2), at $\phi = q/2$, for integer q, any eigenstate $|S^z_{\rm tot}, k_x, \alpha\rangle$ where k_x is the lattice momentum in the x direction, and $S^z_{\rm tot}$ is the total magnetization, is at least twofold degenerate *unless* the following condition is satisfied:

$$\frac{S^z_{\rm tot}}{L_x} + \frac{k_x}{\pi} + SL_y = p/q \qquad (p, q \text{ integers}). \quad (4)$$

The theorem is similar to the Lieb, Shultz, and Mattis (LSM) theorem [20] for half-odd-integer spin chains, and its extension to finite magnetizations by OYA [10]. Here,

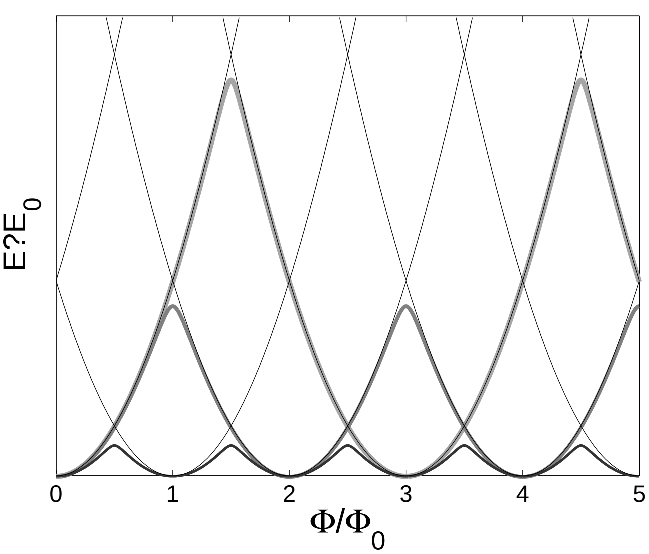

FIG. 1. Schematic adiabatic ground state energies as a function of Aharonov-Bohm flux $E(\Phi)$, where $E_0 = E(0)$. Thin lines: Classical energies $E^i_{\rm cl}$ (3). Thick lines: Quantum adiabats of periods $q\Phi_0$, for $q = 1, 2, 3$. Notice the level crossings for $q \neq 1$, which are protected by the selection rules (4).

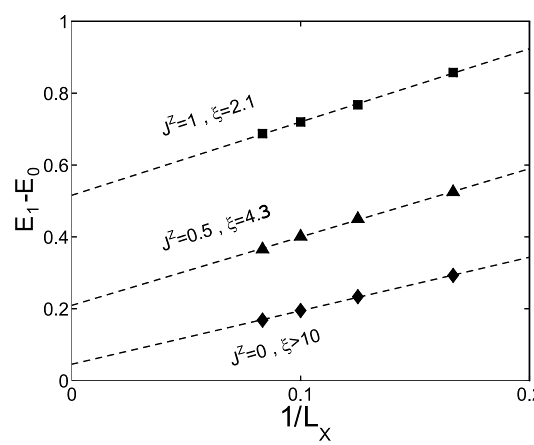

FIG. 2. Haldane gaps: Magnon excitation energies for two leg Josephson ladders for different anisotropy J^z/J. Here $J = 1$ and E_m is the lowest eigenenergy of magnetization m at flux $\Phi = \Phi_0/2$. ξ is the stiffness correlation length given by finite size scaling of ladder lengths up to $L_x = 12$.

however, we prove *exact* degeneracies of the twisted *xxz* model on *finite* lattices, while previous work concerned gaplessness in the thermodynamic limit at zero external gauge field.

Before providing the proof, let us review three important classes to which the theorem for $S = 1/2$ applies.

(1) Odd ladders; $q = 1$, $k_x = 0$, $S^z_{\rm tot} = 0$.—The selection rules (4) cannot be satisfied, implying exact ground-state degeneracy at $\phi = 1/2$. This is closely related to the existence of gapless excitations in the thermodynamic limit of *short-range* half-odd-integer spin chains [20].

(2) Even ladders with integer magnetization per rung.—The selection rule is obeyed for $q = 1$, which implies a minigap at the first avoided crossing of the ground states. If this minigap survives the $L_x \to \infty$ limit, the system is in the Haldane gap phase.

(3) Even ladders with rational magnetization per rung.—The selection rule is obeyed only for some $q > 1$. This gives rise to a *fractional* AB periodicity of the ground state.

Proof: The twist operator is defined as

$$\hat{O}(\phi) \equiv \exp\left(-i\,\frac{2\pi}{L_x}\,\phi \sum_{\mathbf{r}} S^z(\mathbf{r})x\right). \quad (5)$$

In addition, an x-inversion operator I_x is defined $I_x S^\alpha_{x,y} I_x = S^\alpha_{-x,y}$. For any state $\psi_0 = |S^z_{\rm tot}, k_x, \alpha\rangle$, we define the "$q$-conjugated" state ψ_q as

$$|\psi_q\rangle = \hat{O}(-q) I_x |\psi_0\rangle\,. \quad (6)$$

Lemma (degeneracy):

$$\langle\psi_q|H(q/2)|\psi_q\rangle = \langle\psi_0|H(q/2)|\psi_0\rangle\,. \quad (7)$$

The lemma is proved by a direct substitution of (6) in (7) noting that $O(\phi)$ is the explicit gauge transformation on H,

$$H(\phi) = \hat{O}(-\phi) H(0) \hat{O}(\phi)\,, \quad (8)$$

and using the identities $I_x O(\phi) I_x = O(-\phi)$, and $[H(0), I_x] = 0$.

The theorem is proved by showing that ψ_0 will be transformed by "q conjugation" into an orthogonal state $\langle\psi_q \,|\, \psi_0\rangle = 0$ unless the selection rule (4) is obeyed. The unit lattice translation in the x direction is T_x. We make use of the two identities

$$T_x \hat{O}(-q) T_x^{-1} = \exp\!\left(i2\pi q S^z_{\rm tot}/L_x + i2\pi q S L_y\right) \times O(-q)\,, \quad (9)$$

$$I_x T_x I_x = T_x^{-1}.$$

The lattice momentum of ψ_q is given by

$$T_x|\psi_q\rangle = \exp\left(-i\,\frac{2\pi q}{L_x}\,S^z_{\rm tot} + i2\pi q S L_y + i k_x\right)|\psi_q\rangle\,. \quad (10)$$

It follows that $\langle\psi_q \,|\, \psi_0\rangle = 0$ unless the momentum difference $\delta k_x = 2\pi(q S^z_{\rm tot}/L_x - q S L_y) + 2k_x$ is an integer multiple of 2π, which proves selection rules (4). Q.E.D.

Translating back into the boson language, we consider the ground state at $\phi = 0$, with $k_x = 0$, and excess Bose density $\delta n = \frac{p}{qL_y}$. The selection rule implies that as ϕ is increased, the adiabatic ground state passes $q - 1$ exact level crossings before reaching the first minigap allowed by (4). Hence it is clear that the ground state adiabatic periodicity in AB flux is $q\Phi_0$. Figure 1 depicts the ground-state evolution for the cases $q = 1, 2, 3$. The critical current is bounded by

$$I_{\rm cr}(q) \le (J/\hbar) L_y \delta n (1 - \delta n) \sin\left(\frac{\pi}{L_x}\,q\right), \quad (11)$$

which holds up to $q = L_x/2$ where the bound coincides with the classical critical current $I^{\rm cl}_{\rm cr} = (J/\hbar) \times L_y \delta n (1 - \delta n)$.

At $q = 1$ when conditions for the Haldane phase are met, a finite gap opens, and the stiffness constant vanishes exponentially with L_x. Hence $I_{\rm cr}$ would similarly vanish in the thermodynamic limit.

In Fig. 3 the schematic structure of the critical current is plotted against the Cooper pairs density for a Josephson ladder with $L_x = 20$. Notice the sharp dips in the critical current at rational densities which obey the selection rule. For weak easy plane anisotropy, these minima are expected to vanish in the thermodynamic limit, reflecting vanishing stiffness and gapped excitations at these points.

The classical Josephson frequency of an array of length L_x array is $f_{\rm cl} = 2eV/hL_x$, where V is the *total* voltage drop in the x direction. However, at rational densities $n_q = p/qL_y$, for bias current slightly above $I_{\rm cr}(n_q)$, an ac Josephson effect should be observed with frequency $f_q = 2eV/qh$. This could be pictured as current oscillations caused by moving on the adiabatic curves of Fig. 1. Alternatively, this effect could perhaps be better detected as fractional Shapiro steps in an external high frequency electromagnetic field [22].

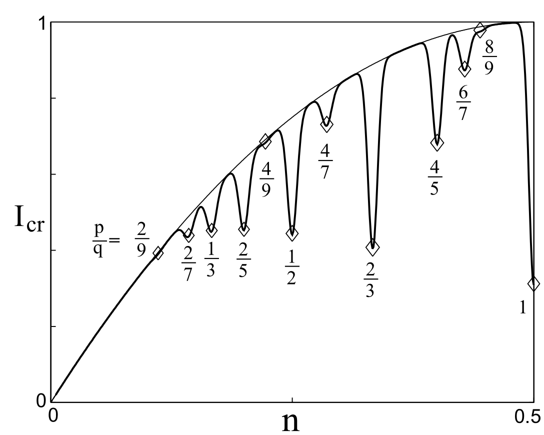

FIG. 3. Schematic diagram of critical currents versus Cooper pair density n for an array of size $L_x = 20$ and $L_y = 2$. Rational numbers $p/q = n_q L_y$, which label the dips at n_q, are indicated. The classical critical current is depicted by a thin line. Above the critical currents at n_q, fractional ac Josephson frequencies are expected at $2eV/hq$. Spatial disorder and finite temperature are introduced qualitatively by broadening of the dips.

Experimental realization.—One of the experimental setups described in Ref. [4], has individual gate voltage probes which control the Cooper pair density at each island to high accuracy. The short-range Bose Hubbard model for this type of JJA can be justified if the ratio of interisland capacitance to gate capacitance obeys $\epsilon = C/C_0 \ll 1$. The junction parameters reported in Ref. [4] were $C_0 = 0.64$ fF, and $C = 1.0$ fF, and $J = 0.63$ K where J is the Josephson coupling between islands. This implies $\epsilon = 1.56$. To reach the desired regime, JJA parameters should be pushed to obey $C/C_0 \leq 0.1$. To lowest order in ϵ, the interactions of Eq. (1) are given by $U \approx 2e^2(1 - 4\epsilon)/C_0$ and $V \approx \epsilon 4e^2/C_0$, respectively. The demand $U \gg V$ is automatically satisfied.

In order to map (1) to (2), we must demand that $U \gg J$. The easy-plane anisotropy regime is given by $V \leq 4J$, i.e., $\epsilon e^2/C_0 \leq J \ll 2e^2(1 - 4\epsilon)/C_0$. As emphasized earlier, these bounds are crucial for eliminating charge density phases, that also exhibit critical currents dips at commensurate fillings.

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