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Localization and long-range order in magnetic chains

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We study quantum spin chains exhibiting long-range order in the presence of quasiperiodic interactions which are modulating functions of sites. The magnetic phase transition to long-range order is shown to accompany a transition from *critical* to *localized* states. The presence of more than one harmonic in the modulating interactions results in a cascade of transitions characterized by the vanishing of the gap and sharp peaks in the total bandwidth and free energy.

Recently, quasiperiodic (QP) magnetic chains undergoing a phase transition from (magnetically) disordered to ordered phase with long-range order (LRO) were investigated.[1,2] In these models, the nearest-neighbor (NN) exchange couplings were allowed two values in a Fibonacci sequence. In both ordered and disordered phases, the models were found to be *critical* where the scaling properties of the cantor spectrum exhibit distinct features in the two phases.

In this paper, we describe a zero-temperature study of quasiperiodic quantum chains with modulating interactions. The models under consideration include the Ising model in a transverse field,

$$H=\sum_n J_n\sigma_n^x\sigma_{n+1}^x+g_n\sigma_n^z\ , \quad (1)$$

and the anisotropic XY model,

$$H=\sum_n J_n\sigma_n^x\sigma_{n+1}^x+g_n\sigma_n^y\sigma_{n+1}^y\ , \quad (2)$$

where the σ_n^j are Pauli matrices associated with the site n. The models are made QP by choosing either J_n or g_n quasiperiodic. In the Ising model, the existence of a "duality" transformation between the bond and the link variables ensures that a similar role is played by the exchange and the field terms. We will set J_n equal to unity and choose the exchange interaction or magnetic field g_n as

$$g_n=\lambda\cos(2\pi\sigma n)\ , \quad (3)$$

where $\sigma=[\sqrt{5}-1]/2$ is the inverse golden mean.

Both the Ising and XY models, by Jordan-Wigner transformations,[3] can be mapped to fermion models, quadratic in fermion degrees of freedom,

$$H=\sum [c_n^\dagger A_{nm}c_m+\tfrac{1}{2}(c_nB_{nm}c_m+\text{H.c.})]\ . \quad (4)$$

Here, the c_n are anticommuting fermion operators. The matrices A and B are symmetric and antisymmetric matrices, respectively. The second term in Eq. (3) is responsible for the LRO in the spin systems and hence makes the study of the spin problem very different from previous studies[4] of tight-binding models describing an electron in an external potential. As discussed in Ref. 3, a unitary transformation reduces the model (4) to the tight-binding model which for the Ising and the XY models is respectively given by

$$g_n\psi_{n-1}+(1+g_n^2)\psi_n+g_{n+1}\psi_{n+1}=\frac{E^2}{4}\psi_n\ , \quad (5)$$

$$g_{n-1}\psi_{n-2}+(1+g_{n-1}^2)\psi_n+g_{n+1}\psi_{n+2}=\frac{E^2}{4}\psi_n\ . \quad (6)$$

Here, ψ_n represents the wave function of the free fermion at the site n.

The motivation for studying QP spin models with sinusoidally varying interaction is the resemblance of Eqs. (5) and (6) to the Harper equation[5]

$$\psi_{n-1}+\lambda\cos(2\pi\sigma n)\psi_n+\psi_{n-1}=E\psi_n\ . \quad (7)$$

This equation is a discrete Schrödinger equation for an electron moving in a potential given by Eq. (3) and constitutes a cornerstone for the analysis of QP models for electrons. Similarly, Eqs. (5) and (6) appear in spin models with sinusoidal external field or exchange interaction and hence will be referred to as "generalized Harper equations." Unlike the Harper equation, Eqs. (5) and (6) are not self-dual and have both the bond and on-site interaction quasiperiodic. It has been shown that for $\lambda<2$, all solutions of the Harper equation are extended while for $\lambda>2$, the states are localized. At the critical value $\lambda_c=2$, the metal-insulator transition, known as the Aubry-André (AA) transition takes place which is characterized by self-similar wave functions and a cantor spectrum. Such states have been referred to as the *critical* states.[4]

In this paper, we address the following questions: How do the order-disorder magnetic phase transition and the localization transition occur in the models (1) and (2)? What relationship exists between these two transitions? The magnetic transition is characterized by long-range correlations in the order phase while the localization transition is seen by studying the properties of the energy spectrum and wave function. We also investigate the effect of higher harmonics in g_n on the phase transitions in the spin models. In the case of the Harper equation, the presence of even one more harmonic to the cosine term is found[6] to change the picture dramatically: The system is found to exhibit not a single but a cascade of AA transitions with perhaps fractal phase boundaries. Similar questions have also been discussed in the related problem of the breakdown of Kol'ogorov-Arnol'd-Moser (KAM) tori in reversible area-preserving twist maps.[7] In this case, the addition of higher harmonics to the standard map is found to result in cascades of appearances and disappearances of the KAM trajectories.

We now summarize the results of the paper. For QP exchange interaction of field, equal to $\lambda\cos(2\pi\sigma)$, the spin systems (1) and (2) undergo a phase transition at $\lambda_c=2$ where the long-range correlation in the x direction characterized by the correlation function $C_x(n) =\langle 0|\sigma_n^x\sigma_{n+N/2}^x|0\rangle$ vanishes. (Here N is the size of the spin chain.) Our numerical results indicate that at the same critical coupling, a transition from *critical* to *localized* states takes place. The addition of even one more harmonic to the exchange interaction results in a cascade of transitions signaled by the vanishing of the gap and sharp peaks in the total bandwidth and free energy at the critical points.

In our numerically exact study of the QP models, the system is approximated by a sequence of periodic models with progressively larger unit cells of size equal to the Fibonacci sequences and is studied with periodic boundary conditions. With use of the method of Lieb, Schultz, and Mattis,[3] the eigenspectrum was computed, from which the free energy and the correlation lengths were obtained. The critical value λ_c for the onset of LRO corresponding to the vanishing of the gap in the spectrum can be analytically obtained from the following equation:[8]

$$\prod_{n=1}^{N} g_n=\prod_{n=1}^{N}\lambda\cos(2\pi\sigma n)=1\,. \tag{8}$$

This equation has a unique solution at $\lambda=\lambda_c=2$ as $N\to\infty$. Figure 1 shows the x correlation $C_x(1)$ for the Ising model. For $\lambda<\lambda_c$, the system is ordered along the x direction with nonzero x correlation and makes a phase transition at λ equal to λ_c beyond which it has zero correlation along the x direction. Figure 2 shows analogous plots for the x and y correlations in the XY model.

Figures 3 and 4 show the numerical results of total bandwidth for a finite cyclic chain for the Ising and XY models, respectively. Identical results are obtained if $J_n=\lambda\cos(2\pi\sigma n)$ and $g_n=1$. This computation involves

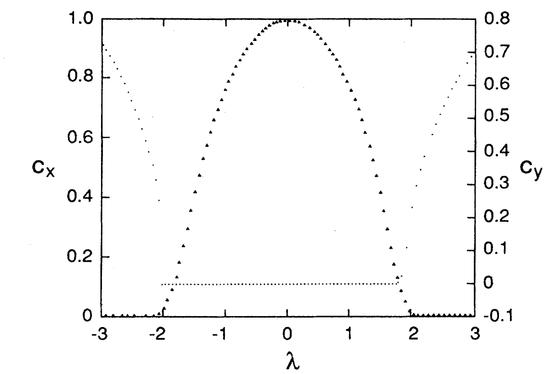

FIG. 2. The long-range correlations $C_x(1)$ (triangles) and $C_y(1)$ (dotted line) for the XY chain of 89 sites. The first vanishes outside the region $(-2,2)$ while the latter vanishes within these boundaries.

calculating the bandwidth associated with each of the energy levels and then summing them as the Bloch index is varied in the first Brillouin zone.[9] The total bandwidth, although finite for a finite-size cyclic chain for $\lambda<\lambda_c$, goes to zero as $N^{-\delta}$. This implies that the eigenspectrum is a cantor set and that the states are *critical.* The scaling exponent δ was found to exhibit a very mild dependence on λ for $\lambda<\lambda_c$, which we believe is due to finite-size effects and is equal to 1.0 ± 0.1 for the Ising and 1.3 ± 0.1 for the XY model. For $\lambda>\lambda_c$, the δ diverges to infinity, thereby implying that we have a point spectrum. The "tails" in the total bandwidth, corresponding to its rapid falloff for $\lambda>\lambda_c$, are longer than the corresponding tails in the spin correlations. However, as shown in Fig. 3, they are found to become shorter as the number of sites in the chain is increased. Apart from looking at the total bandwidth, the nature of the states both above and below λ_c was also confirmed by looking at the scaling properties of various individual states. The individual bandwidth is also found to decay algebraically for $\lambda<\lambda_c$ and exhibits exponential decay above λ_c.

For the pure models, the states are always extended and in the previously studied QP models,[1,2] the states were always critical and hence the transition to LRO is not ac-

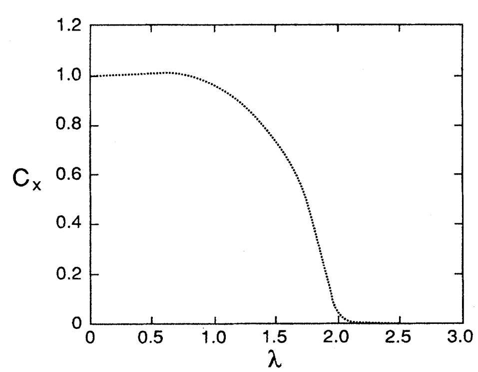

FIG. 1. The long-range correlation $C_x(1)$ vs λ for an Ising spin chain of 89 sites.

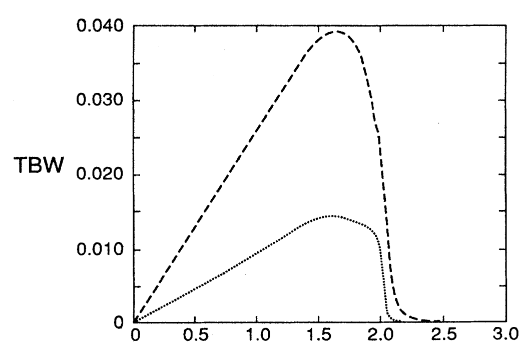

FIG. 3. The total bandwidth (TBW) vs λ for an Ising chain for 233 (dotted line) and 89 sites (dashed lines).

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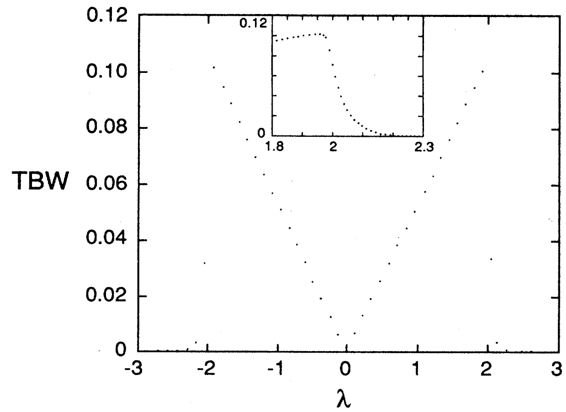

FIG. 4. The total bandwidth vs λ for an XY chain for 89 sites. The inset shows the blowup of the critical regime.

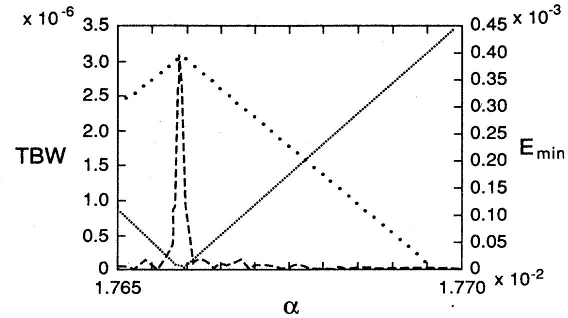

FIG. 5. The total bandwidth (dashed line), the free energy (dots), and the energy gap (dotted line) for a fixed $\lambda=6$ for 89 sites in the neighborhood of one of the critical points. Similar behavior is seen at other critical points.

companied by any transition in the spectral properties. The isotropic XY model with $J_n=g_n=\lambda\cos(2\pi\sigma n)$ can be reduced to the Harper equation (7) which undergoes the AA transition. However, this metal-insulator transition does not correspond to any magnetic phase transition as the isotropic XY model does not exhibit any transition to LRO. In the study of systems with two competing interactions, to the best of our knowledge, the QP spin systems studied here provided the first example where the magnetic and spectral transitions occur simultaneously.

We examine next the effect of adding higher harmonics to the modulating interaction,

$$g_n=\frac{\lambda}{(1+\alpha^2)^{1/2}}[\cos(2\pi\sigma n)+\alpha\cos(4\pi\sigma n)]\,. \tag{9}$$

For α nonzero, the critical equation (8) has no solution for $\lambda<2$ for any value of α. Therefore, in this parameter regime, the gap remains finite. Furthermore, the total bandwidth retains its character, i.e., corresponds to the critical states in this regime. For $\lambda>2$, where the unperturbed system is localized, the critical equation has N solutions $\alpha_c(k), k=1,\dots,N$, as $N\to\infty$, corresponding to $g_k=0$,

$$\alpha_c(k)=-\frac{\cos(2\pi\sigma k)}{\cos(4\pi\sigma k)}\,. \tag{10}$$

The cascades of transitions in the Ising and XY models correspond to the vanishing of the gap in the spectrum. We observe that at these critical points where the theory becomes gapless, the free energy and the total bandwidth exhibit local maxima (see Fig. 5). Therefore, an addition of higher harmonic in g_n results in the models becoming gapless at certain critical values of α for fixed $\lambda>2$ where the total bandwidth shows an enhancement. We point out that unlike the AA cascades in the Harper equation, where the extended states are intermingled with the localized states with fractal boundaries,[6] the cascades in the generalized Harper equation alter the nature of localized states only at the critical points. This distinction is due to the complex nature of transition in spin models where the magnetic phase transition is forced to occur simultaneously with the transition to localization. Unlike the cascades of the Harper equation, the cascades in spin models have to satisfy an additional constraint; namely, the critical points have to satisfy Eq. (8). Therefore, the cascades of the transition that we see in spin models with LRO are more restrictive and the deeper understanding of their nature requires more detailed investigation.

In conclusion, in both Ising and XY chains with QP modulating exchange interaction or magnetic field, the vanishing of the gap not only signals the onset of LRO but also corresponds to a transition in spectral properties. We hope that the future studies of the generalized Harper equation will provide deeper understanding of its rich and complex behavior.

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