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Extended spin waves in aperiodic ferromagnetic chains

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Abstract. In this work, a one-dimensional quantum Heisenberg ferromagnet with aperiodic exchange couplings is considered. To produce an aperiodic distribution of exchange couplings, it is used a sinusoidal function whose phase ϕ varies as a power-law, $\phi \propto n^{\nu}$, where n labels the positions along the chain. By using exact diagonalization, the spin-wave participation number and the local density of states are computed. The numerical calculations indicate that for $0 < \nu < 1$, this ferromagnetic system displays a phase of extended spin waves in the low-energy region. For $\nu > 1$ all spin waves are localized except for the zero energy mode. By integrating the time-dependent Schrödinger equation, the temporal evolution of the mean-square displacement of the wave-packet was followed. Associated with the emergence of extended spin waves, it was observed that the wave-packet mean-square displacement displays a ballistic spread.

PACS. 75.30.Ds Spin waves – 73.23.Ad Ballistic transport – 73.20.Jc Delocalization processes – 72.15.Rn Localization effects (Anderson or weak localization)

1 Introduction

The dynamics of quantum noninteracting particles in disordered systems is one of the most intensively studied problems in condensed matter physics [1–6]. Within the point of view of noninteracting electrons in disordered solids, the Anderson's localization theory describes the overall behavior of the main pertinent physical quantities. In general lines, the Anderson theory predicts an electronic localization-delocalization transition (LDT) for weak disorder in three dimensional geometries. For low-dimensional systems with time-reversal symmetry, the localization of all one-electron eigenstates is anticipated at any disorder strength [1]. The localization of collective excitations by an uncorrelated random potential is a rather general phenomenon. It also applies to the study of magnon localization in random ferromagnets [7–9]. In fact, it is possible to map the Heisenberg Hamiltonian associated with one-magnon excitations onto an one-electron tight-binding model [7–9]. In general, it was demonstrated that the finite energy states are exponentially localized at any degree of disorder. However the typical localization length grows as one approaches the bottom of the band [7–9]. Moreover, it was shown that an initially localized spin excitation may exhibit a super-diffusive spread in the presence of disorder in contrast to the random oscillations on a finite segment displayed by an electronic wave-packet [9].

The above picture holds for systems with uncorrelated disorder distributions. Some years ago, it was reported that the presence of short [10–13] or long-range correlations [14–23] in disorder may induce the appearance of truly delocalized states in low-dimensional Anderson models. Within the context of noninteracting magnons, the one-dimensional quantum Heisenberg ferromagnet with exchange couplings exhibiting correlated long-range disorder was also studied in reference [24]. It was shown that extended states appear for sufficient strong correlations using a renormalization group approach, integration of the motion equations, as well as exact diagonalization. Another class of $1D$ models that can exhibit an Anderson-like localization-delocalization transition, involves a non-random, deterministic potential which is incommensurate with the underlying lattice [25]. This class of models depicts features that are in between those of the random Anderson model and the periodic Bloch model. The localized or extended nature of the eigenstates has been extensively investigated in the physics literature [26–29] and has been related to general characteristics of the aperiodic on-site distributions. However, the role played by aperiodic structures concerning the localization properties of magnons in quantum ferromagnetic chains have not been studied in detail. In reference [30], the authors studied the nature of noninteracting spin waves in a Thue-Morse ferromagntic chain. By using exact diagonalization, extended states for some specific high energies were found. This result, in contrast to what was found in the disordered case, suggests that Thue-Morse ferromagnetic chains can support resonances.

In fact, the role of disorder or aperiodicity on the electron, phonon, polariton and magnon modes, is still under

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some debate [31]. More recently, a very instructive paper by Macia [32] has shown the importance of aperiodicity in different domains of science. In this work, we report further progress along this line. We consider the one-dimensional quantum Heisenberg ferromagnet with aperiodic exchange couplings. In order to produce an aperiodic sequence of exchange couplings, the formalism used in reference [25] was considered. It consists in use a sinusoidal function whose phase ϕ varies as a power-law, $\phi \propto n^{\nu}$, where n labels the positions along the chain. The exponent ν controls the degree of aperiodicity in the sequence of exchange couplings. By using an exact diagonalization of finite sequences, we compute the spin-wave participation number and the local density of states. For $0 < \nu < 1$, the numerical calculations suggest that this system displays a phase of extended spin waves in the low-energy region. However, for $\nu > 1$ all spin waves are localized except for the zero energy mode. By integration of the time-dependent Schödinger equation, the mean-square displacement of the wave packet will be computed. A ballistic wave-packet spread will be shown to emerge associated with the presence of extended spin waves.

2 Model and formalism

We consider a Hamiltonian model describing a spin-1/2 quantum ferromagnetic Heisenberg chain of N sites with nearest-neighbors isotropic exchange interaction:

$$H = -\sum_{n} J_{n,n+1} \boldsymbol{S_n}.\boldsymbol{S_{n+1}}. \tag{1}$$

The couplings $J_{n,n+1} = J_n$ will be considered to follow a deterministic rule given by

$$J_n = J_0 + W\cos(\alpha n^{\nu}), \tag{2}$$

with α being an arbitrary rational number and ν and W being tunable parameters [25]. From this sinusoidal form, one can control the degree of aperiodicity in the sequence of exchange couplings. In what follows, $J_0 > W$ will be taken in order to avoid negative or null exchange interactions. The ground state of the system contains all spins pointing in the same direction. If a spin deviation occurs at a site n, this excited state is described by:

$$\phi_n = S_n^{+}|0\rangle \tag{3}$$

where the operator S_n^{+} creates a spin deviation at site n and $|0\rangle$ denotes the ground state. The eigenstates of the Hamiltonian belonging to the sub-space of single flip excitations are, therefore, composed of a linear combination of ϕ_n, i.e., $\Phi(E) = \sum_n f_n\phi_n$. The coefficients f_n satisfy the equation [24]

$$(J_n + J_{n-1})f_n - J_n f_{n+1} - J_{n-1}f_{n-1} = 2Ef_n \tag{4}$$

where E is the excitation energy. The above equation for the eigenstate coefficients is similar to that for one-electron states in a tight-binding model with correlated hopping integrals. It is worth to mention here that the above procedure can not be extended to anti-ferromagnetic chains because the ground state does not correspond to a saturated anti-ferromagnetic order. In what follows, one can access the localization properties of all spin waves using exact diagonalization of finite chains to compute the participation number $P(E)$ and the local Density of states (LDOS). $P(E)$ is given by [19]

$$P(E) = \frac{1}{\sum_{n=1}^{N} f_n^4(E)} \tag{5}$$

and depends linearly of the chain size for extended states while being roughly size independent for exponentially localized states. We compute the average participation number defined by $\xi(E) = \frac{1}{N_E}\sum_{E=E-\Delta E}^{E=E+\delta E} P(E)$, where $\Delta E = 0.05$ and N_E is the number of eigenmodes within each interval $[E-\Delta E, E+\Delta E]$. LDOS is defined by [33,34]

$$\rho_i(E) = \sum_n |f_i(E_n)|^2 \delta(E - E_n). \tag{6}$$

For a given energy, the LDOS directly measures the local amplitude of the wave-function at site i. Averaging $\rho_i(E)$ arithmetically over N sites, we obtain the averaged density of states $\rho_{av}(E) = (1/N)\sum_{i=1}^{N}\rho_i(E)$. The geometric mean define the typical density of states $\rho_{ty}(E) = \exp\left[(1/N)\sum_{i=1}^{N}\log\rho_i(E)\right]$. For extended states, $\rho_{av}(E)$ and $\rho_{ty}(E)$ are almost equal, whereas for localized states $\rho_{ty}(E)$ vanishes and $\rho_{av}(E)$ remains finite [33,34]. This implies that the ratio of these two quantities,

$$R(E) = \frac{\rho_{ty}(E)}{\rho_{av}(E)}, \tag{7}$$

can serve to monitor extended states ($R(E) > 0$) and localized ones ($R(E) = 0$). In addition, we will investigate the time evolution of a wave-packet initially localized at site n_0. Using numerical methods to solve the time-dependent Schrödinger equation, we compute the second moment of the corresponding spatial probability distribution given by

$$\sigma = \sqrt{\sum_n (n - < n(t) >)^2 |f_n(t)|^2} \tag{8}$$

where $\langle n(t)\rangle = \sum_n n|f_n(t)|^2$ is the centroid of the wave-packet. From the mean-square displacement σ, we can estimate the wave-packet spread in space at time t.

3 Results

The numerical diagonalization was performed using lattices up to $N = 16\,000$ sites. Integrations of the time-dependent Schrödinger equation were performed using fourth-order Runge-Kutta method with time step 10^{-3} and systems up to 16 000 sites. The norm conservation

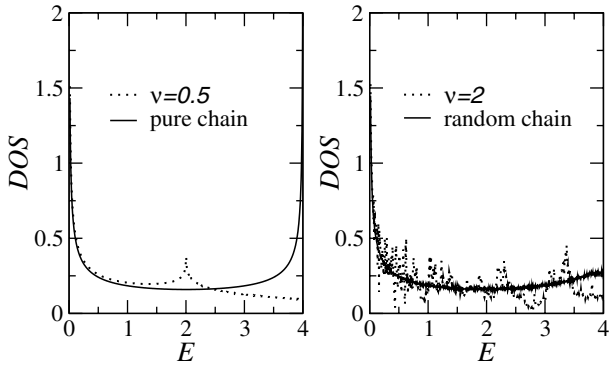

Fig. 1. The normalized spin-wave density of states (DOS) for chains with $N = 10^6$ sites using Dean's method. The DOS is smooth for aperiodic exchange couplings with $\nu = 0.5$ (dotted line at left panel). For $\nu < 1$, the nonfluctuating DOS can be compared with the one of the pure chain, $J_n = J_0$ (solid line at left panel). For $\nu > 1$ the DOS displays a roughness comparable to those obtained for uncorrelated random chains (solid and dotted lines at right panel).

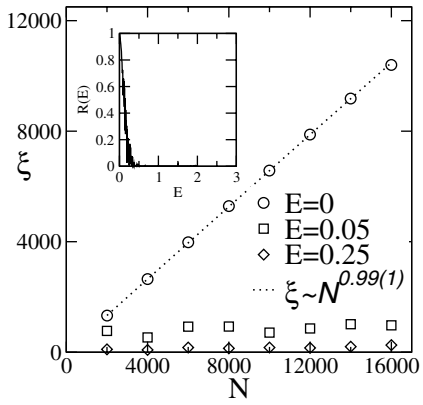

Fig. 2. Scaled average participation number ξ/N as a function of N for $\nu = 2$. For $E = 0$, the participation number scales proportional to the system size (the dotted line represents a power-law fitting $\xi \propto N^{0.99(1)}$). For $E > 0$, $\xi/N \to 0$ as N goes to infinity. Therefore, all magnon states with finite energy are localized. The ratio $R(E)$ vanishes for $E > 0$ and approaches 1 at the bottom of the band (see inset).

was checked at every time step to ensure the numerical convergence. In addition, the density of states (DOS) was calculated by using the numerical Dean's method [12,24]. The normalized DOS for chains with $N = 10^6$ sites is shown in Figure 1. One can see at the left panel of Figure 1 that the DOS is smooth for aperiodic exchange couplings with $\nu = 0.5$ (see dotted line). For $\nu < 1$, the nonfluctuating DOS can be compared with the one of the pure chain, $J_n = J_0$ (solid line at left panel). Previous studies have pointed out that the smoothing of the DOS is usually connected with the emergence of delocalized states [24]. For $\nu > 1$ the DOS displays a roughness compared to those obtained for a chain with uncorrelated random exchanges (solid and dotted lines at right panel of Fig. 1). The results for an uncorrelated random case were obtained using exchange couplings uniformly distributed in the interval range $[J_0 - W/2, J_0 + W/2]$ with $J_0 = 2$ and $W = 2$.

In Figure 2, one shows the scaled average participation number ξ/N as a function of N for $E = 0.00$, 0.05, and 0.25, with $\nu = 2$ and $W = 1$. For $E = 0$, the participation number scales with the system size (the dotted line in Fig. 2 represents a power-law fitting $\xi \propto N^{0.99(1)}$). This feature is a clear signature of extended spin waves. For finite energies, $\xi/N \to 0$ as N goes to infinity. Therefore, all magnon states with $E > 0$ are localized. The ratio $R(E)$ (see Eq. (7)) versus energy E for $N = 16\,000$ sites is shown in the inset of Figure 2. The delta function in equation (6) was computed as $\delta(\Delta E) \approx 1/\Delta E$ with $\Delta E = 0.005$. The ratio vanishes for $E > 0$ and approaches 1 at the bottom of the band. Therefore, for $\nu > 1$, we obtain a behavior similar to that found in an uncorrelated random ferromagnetic chain: extended states only at the bottom of the band. In fact, the limit $\nu > 1$ was called the "pseudorandom limit" at reference [27]. The authors have shown that one-electron states becomes localized at the presence of an aperiodic potential at this limit [27]. The ratio $R(E)$ versus energy E is plotted in Figure 3, with $N = 16\,000$ sites

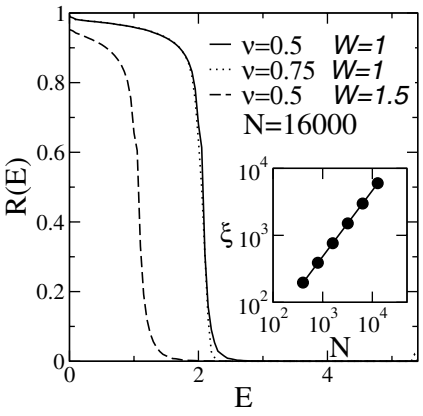

Fig. 3. Ratio $R(E)$ versus energy E with $N = 16\,000$ sites and $\nu = 0.5, W = 1$ (solid line), $\nu = 0.75, W = 1$ (dotted-line) and $\nu = 0.5, W = 1.5$ (dashed-line). $R(E)$ becomes larger than zero within a low-energy region $[E < E_c]$. The mean participation number for this low-energy region $\xi = \sum_{E<E_c} P(E)/N_E$ displays a linear dependence with the system size $[\xi \propto N^{0.99(1)}]$ (inset).

and $\nu = 0.5, W = 1$ (solid line), $\nu = 0.75, W = 1$ (dotted-line) and $\nu = 0.5, W = 1.5$ (dashed-line). One can see from these calculations that the function $R(E)$ becomes larger than zero within a low-energy region $[R(E < E_c) > 0]$. This is a signature of extended states in this region. In fact, analyzing the mean participation number for this low-energy region $\xi = \sum_{E<E_c} P(E)/N_E$ we can see a linear dependence with system size $[\xi \propto N^{0.99(1)}]$ (see inset in Fig. 3). For fixed W, the critical energy separating extended from localized modes does not depend on the exponent ν (see solid and dotted-line in Fig. 3). In fact, the critical energy depends only on the width W of the exchange distribution (see dashed-line in Fig. 3). We have also investigated the dependence of the mobility edge on the width W. In Figure 4, the complete phase

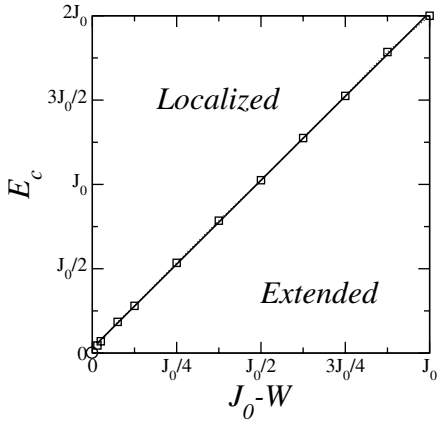

Fig. 4. Phase diagram for $\nu < 1$ on the $(E_c, (J_0 - W))$ plane. Calculations were performed for $(J_0 - W) > 0$. The width of the extended band E_c was found to be proportional to $(J_0 - W)$ within our numerical precision.

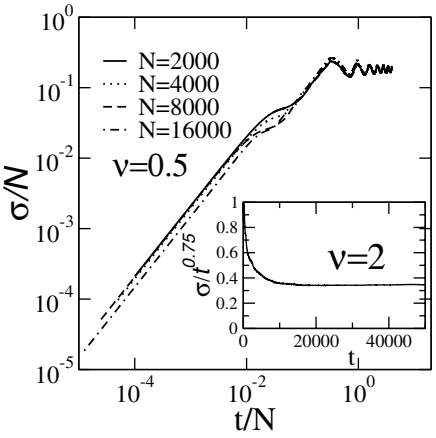

Fig. 5. Scaled mean-square displacement $\sigma(t)/N$ versus scaled time t/N computed from lattices with $N = 2000, 4000, 8000, 16\,000$ and $\nu = 0.5$. A fine data collapse for long times is found thus implying that, for $\nu = 0.5$, $\sigma \propto t$, i.e. the wave-packet presents a ballistic spread before reaching the chain boundaries. For $\nu > 1$ (see inset), $\sigma \propto t^{0.75}$ in perfect agreement with reference [9].

diagram on the $(E_c, J_0 - W)$ plane is shown. The width of the extended band E_c was found to be proportional to $J_0 - W$ within our numerical precision. We can understand this behavior following simple heuristic arguments similar to those used in reference [25]. For large n, J_n is very slowly varying and can be regarded as a constant $J^\star$ locally. Therefore, the spin wave equation becomes $f_{n-1} + f_{n+1} = (2 - 2E/J^\star)f_n = C_n f_n$, where $C_n \approx C$ is a constant locally. The condition for a complex solution to this equation is $|C_n| < 2$. Since $(J^\star)^{min} = J_0 - W$, we found that extended states exist for $0 < E < 2(J_0 - W)$. This result agrees with our numerical calculations of the mobility edge (see Fig. 4). We further collected in Figure 5 results for the wave-packet scaled mean-square displacement $\sigma(t)/N$ versus scaled time t/N computed from lattices with $N = 2000, 4000, 8000, 16\,000$ and $\nu = 0.5$. We numerically integrate the wave-equation until a stationary state can be reached after multiple reflections of the wave-packet on the chain boundaries. Therefore, the mean-square displacement saturates at a value $\propto N$ due to finite size effects. A fine data collapse for long time is found implying that, for $\nu = 0.5$, $\sigma \propto t$, i.e. the wave-packet presents a ballistic spread before reaching the chain boundaries. Similar results are also found in the range of exponents $0 < \nu < 1$. For $\nu > 1$, due to the pseudo-random character of the exchange interaction distribution, we obtain the well known super-diffusive spread in perfect agreement with reference [9] $\sigma \propto t^{0.75}$ (see inset in Fig. 5). The initial site n_0 was varied around the center of the chain and no qualitative change in the physical properties was found.

4 Summary

A key question in solid state physics is the relationship between the atomic topological order and the physical properties stemming from their structure. In this paper, we addressed the problem of spin waves in aperiodic ferromagnetic chains. We considered finite chains of $S = 1/2$ spins coupled via a nearest neighbor isotropic Heisenberg exchange interaction. To introduce aperiodicity the couplings were distributed according a deterministic rule $J_n = J_0 + W\cos(\alpha n^\nu)$, where α is an arbitrary rational number and ν and W are tunable parameters [25]. The exponent ν controls the degree of aperiodicity in the exchange couplings sequence. The density of states (DOS) was calculated by using the Dean's method. The DOS was found to be smooth for aperiodic exchange couplings sequences with $\nu < 1$. For $\nu > 1$ the DOS displays a roughness comparable to those obtained for uncorrelated random chains. The smoothing of the DOS is usually connected with the emergence of delocalized states. Using exact diagonalization on finite chains, we computed the participation number and the ratio $R(E)$ between the typical local density of states ρ_{ty} and the averaged local density of states ρ_{av} within the band of allowed energies. We observe that, for $\nu < 1$, the ratio $R(E)$ approaches 1 and the participation number diverges linearly with N in the low-energy region. Therefore, there is a new phase of extended spin waves in this aperiodic ferromagnetic model. The phase diagram showing the dependence of the mobility edge on the width of the exchange coupling distribution W was also obtained. For $\nu < 1$, we have also shown that the wave-packet mean-square displacement displays a ballistic behavior. For $\nu > 1$ the pseudo-random character of the exchange interaction distribution induces a behavior similar to that found in a disordered quantum Heisenberg model. Therefore, we reported the existence of an Anderson transition in aperiodic Heisenberg ferromagnetic chains. In contrast with the results of reference [30] where few extended states were found for some energy values, the model studied here has showed the existence of a phase of extended spin waves. We expect that the present work will stimulate further theoretical and experimental

investigations of spin-wave dynamics on nonperiodic ferromagnetic models or superlattices.

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