Coexistence of Antiferromagnetism and Dimerization in a Disordered Spin-Peierls Model: Exact Results

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(Received 21 January 1997)

A model of disordered spin-Peierls system is considered, where domain walls are randomly distributed as a telegraph noise. For this realization of the disorder in an *XX* spin chain, we calculate exactly the density of states as well as several thermodynamic quantities. The resulting physical behavior should be qualitatively unchanged even for an *XXZ* chain, up to the isotropic *XXX* point. For weak disorder, besides a high energy regime where the behavior of a pure spin-Peierls system is recovered, there is a crossover to a low energy regime with singular thermodynamic properties and enhanced antiferromagnetic fluctuations. These regimes are analyzed with the help of exact results, and the relevant energy scales determined. We discuss the possible relevance of such a disorder realization to the doped inorganic spin-Peierls compound $CuGeO_3$. [S0031-9007(97)03045-7]

PACS numbers: 75.10.Jm, 75.50.Ee

One dimensional quantum spin systems in the presence of randomness show unusual and intriguing properties (see, e.g., Ref. [1], and references therein). For instance, it has been shown [1–3] that the ground state of the Heisenberg antiferromagnet with random exchange constants can be interpreted as a random singlet state, where pairs of spins are coupled into singlets with an energy gap to the triplet configuration which is weaker for widely separated pairs. The uniform and staggered magnetic susceptibilities, χ and χ_s, have a (Griffith's-like) singular behavior at low temperature, $\chi \sim \chi_s \sim 1/(T \ln^2 T)$. Interestingly, in spite of the singlet nature of the ground state, the spin-spin correlation functions are still long ranged. In fact, $\langle S^i(r) S^i(0)\rangle \simeq 1/r^2$, for large r ($i = x, y, z$) [1]. These properties are not modified by spin anisotropy if, on average, $J_z \leq J_x = J_y$. Notice that spin anisotropy does not manifest itself in the spin-spin correlation function with different power law behavior of $i = z$ with respect to $i = x, y$, contrary to the case in the absence of disorder. The behavior of the random *XXZ* chain is, however, unstable towards a finite average dimerization, i.e., a finite average difference between the exchange constants of the even bonds and of the odd bonds. This case was recently analyzed by Hyman *et al.* [4] by means of a real space renormalization group approach. For a finite average dimerization ϕ, they find that the spin-spin correlation functions decay exponentially with a correlation length $\xi \sim |\phi|^{-2}$, but the Griffith singularities remain, even if weaker. In particular, singularities of the uniform susceptibility $\chi \sim T^{\alpha-1}$, and the specific heat $C_v \sim T^{\alpha}$, where $\alpha \propto |\phi|$, are found to persist [4].

The study of the role of disorder in a spin-Peierls system may be useful to understand the behavior upon doping of the inorganic spin-Peierls compound $CuGeO_3$. The pure compound is known to undergo a structural transition at 14 K [5], below which the CuO_2 chains dimerize and a spin gap opens. However, upon substitution of a few percent of Cu with magnetic (Ni [6]) or nonmagnetic (Zn [7,8]) impurities (as well as replacing Ge with Si [9]), besides the structural transition, which still occurs close to 14 K, an antiferromagnetically ordered phase appears below a lower temperature $T_N \sim 4$ K. Moreover, the estimated magnetic moment with 4% of Zn is as high as $0.2\mu_B$ [8]. This behavior is quite puzzling. First of all, heuristically, one would expect a Néel temperature exponentially small in the ratio of the average distance between the impurities to the spin-Peierls correlation length λ_{SP}. At 4% doping, this would imply $T_N/T_{SP} \simeq 0.04$, inconsistent with the experiment. In addition, one would also expect a magnetic moment of the order of the doping concentration, not almost an order of magnitude larger, as seen experimentally.

In this Letter, we study a particular realization of a disordered spin-Peierls system which does show a large enhancement of antiferromagnetic fluctuations, coexisting on a lower energy scale with an underlying dimerization. Moreover, this model permits an exact calculation of physical quantities for a wide range of temperature and energy.

The Hamiltonian of each chain in the absence of impurities is

$$\hat{H} = \sum_i [1 + \phi_0(-1)^i](S_i^x S_{i+1}^x + S_i^y S_{i+1}^y + \Delta S_i^z S_{i+1}^z), \tag{1}$$

where ϕ_0 is the strength of the dimerization. We assume that one impurity releases one spin-1/2 solitonic excitation, connecting regions of different dimerization parity.

This assumption is, in fact, more appropriate to describe the effect of Cu substitution by Zn or Ni doping. An analysis of a model for Si doping has been given in Ref. [10], leading to results similar to those we are going

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to present here [11]. The role of the interchain coupling is to provide a confining potential to the soliton, which will be trapped within some distance from the impurity [12]. Moreover, the weak link connecting the impurity nearest neighbors (which would be, for instance, generated by a next-nearest-neighbor exchange) is approximated to be equal to the weak bonds in (1). Therefore, the effective Hamiltonian, defined now on a chain of one site less, remains the same apart from the presence of a domain wall. For a finite number $n_{\rm imp}$ of randomly distributed impurities, the effective model will therefore be assumed to consist of a chain with $n_{\rm imp}$ sites less, described by the same Hamiltonian Eq. (1), but in the presence of randomly distributed domain walls. This amounts to take a site dependent $\phi(i)$, which takes alternatively two values $\pm\phi_0$, jumping from one to the other at the (random) position of the antiphase walls. We will show that it is possible to calculate many physical properties of the soliton band which is created by disorder inside the spin-Peierls gap, without the precise knowledge of the soliton wave functions. In Eq. (1), $\Delta = 0$ corresponds to the XX chain, while $\Delta = 1$ is the isotropic XXX model. On the basis of the analyses of Refs. [1,3,4], we expect that the behavior at $0 < \Delta \leq 1$ should be similar to that at $\Delta = 0$, therefore we will only study the latter case, which is much simpler. We believe that this approximation gives qualitatively good results for all the range $0 \leq \Delta \leq 1$, especially in view of our particular choice of the disorder. By means of a Jordan-Wigner transformation, the model can be mapped onto a model of disordered spinless fermions. By linearizing the spectrum around the Fermi energy, introducing the right and left moving components of the fermion field, and then taking the continuum limit, the diagonalization of the Hamiltonian amounts to solve the following coupled differential equations:

$$\mp i\partial_x \chi_{R(L)\epsilon}(x) + [\phi(x) \pm ih_s]\chi_{L(R)\epsilon}(x) = \epsilon\chi_{R(L)\epsilon}(x),$$

where $\chi_{R(L)\epsilon}(x)$ is the eigenfunction of energy ϵ on the right (left) moving field, and we have also considered for later convenience a uniform staggered magnetic field h_s in the z direction. The dimerization field $\phi(x)$ corresponds to that introduced in Eq. (1), apart from an appropriate normalization factor. The equations can be decoupled by the following transformation:

$$u_{+(-)\epsilon}(x) = \pm\chi_{R(L)\epsilon}(x) + i\chi_{L(R)\epsilon}(x).$$

These two functions are solutions of the Schroedinger-like equations

$$[-\partial_x^2 + \phi^2(x) + (-)\phi'(x)]u_{+(-)\epsilon}(x) = Eu_{+(-)\epsilon}(x),$$

where $E = \epsilon^2 - h_s^2$ should be greater than zero. In the following, we will often use the integrated density of states as a function of E, which we will define as $N(E)$. In terms of this function, the density of states of the fermionic model is

$$\rho(\epsilon) = 2\epsilon \left.\frac{\partial N(E)}{\partial E}\right|_{E=\epsilon^2-h_s^2}. \quad (2)$$

In the case in which $\phi(x)$ is a white noise, these equations have been analyzed quite in detail in the context of disordered one-dimensional Fermi systems [13,14], or classical diffusion of a particle in a random medium (for a review see, e.g., Ref. [15]). An interesting anomaly of this problem is that, for a zero-average white noise, the $E = 0$ state is extended [14,16,17], and both the localization length and the density of states diverge as $\epsilon \to 0$. Quite recently, Comtet, Desbois, and Monthus (CDM) [18] specialized those equations for a particular disorder, for which they have been able to calculate exactly the integrated density of states $N(E)$ and the localization length $\lambda(E)$. Specifically, they assumed a random potential $\phi(x)$ which takes alternatively two values ϕ_0 and ϕ_1 at intervals whose lengths $l \geq 0$ are randomly distributed according to the probability densities $f_0(l) = n_0 \exp(-n_0 l)$ and $f_1(l) = n_1 \exp(-n_1 l)$ (see also Ref. [16]). This choice of $\phi(x)$ is particularly suited for studying our problem of randomly distributed domain walls. In particular, our case corresponds to $\phi_1 = -\phi_0 < 0$, and $n_0 = n_1$, i.e., to an average dimerization $\phi = (\phi_0 n_1 + \phi_1 n_0)/(n_0 + n_1) = 0$. Nevertheless, we will also discuss the more general situation $n_0 \neq n_1$, in which case ϕ is finite. Moreover, we start by taking $h_s = 0$. In the model there are three relevant length scales, $\lambda_{\rm SP} = 1/\phi_0$, $l_0 = 1/n_0$, and $l_1 = 1/n_1$. $\lambda_{\rm SP}$ is the correlation length of the system in the absence of disorder, which is the case if, for instance, $l_0/l_1 \to \infty$. In this case, the spectrum of the single-particle excitations (which is symmetric around zero energy) shows a gap $2\phi_0$, and the density of states $\rho(\epsilon)$ has an inverse square root singularity at $\epsilon = \pm\phi_0$. For generic l_0 and l_1, the density of states can still be exactly calculated within the phase formalism approach [18], and expressed in terms of integrals which have to be numerically evaluated. Essentially, the method consists in writing the master equation for the joint probability distribution of the phase of the wave function and $\phi(x)$, and solving for the stationary x-independent solution. In particular, if l_0 and l_1 are much longer than $\lambda_{\rm SP}$, i.e., if the gap has the time to develop in a region of constant $\phi(x)$, the density of states still shows a peak at $\pm\phi_0$, even though states are created inside the gap. These states accumulate, in a singular manner, as $\epsilon \to 0$. In particular, the density of states around zero energy goes like $\rho(\epsilon) \sim \epsilon^{2\mu-1}$, where $\mu = (n_1 - n_0)/(2\phi_0)$ is finite. In Fig. 1, we draw $\rho(\epsilon)$ for $\epsilon > 0$, $\phi_0 = 1$, and various n_0 and n_1. For $\mu = 0$, $\rho(\epsilon) \sim 1/|\epsilon \ln^3 \epsilon|$. The key feature of our choice for the random potential is that, even if the average dimerization $\phi = 0$, i.e., if $n_0 = n_1 = n$, the density of states shows a pseudogap if $\phi_0 \gg n$ (see Fig. 1), totally absent for a white noise process [19].

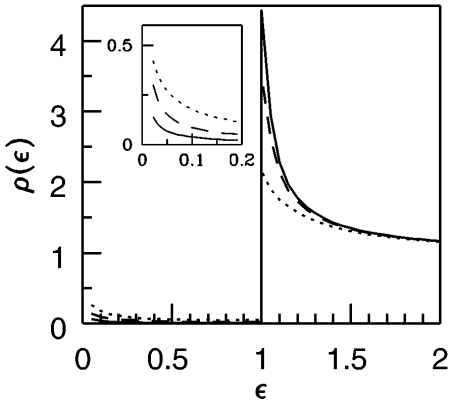

FIG. 1. Density of states for $\phi_0 = 1$ and $n_0 = n_1 = 0.3$ (dotted line), $n_0 = n_1 = 0.1$ (full line), $n_0 = 0.1$, $n_1 = 0.3$ (dashed line). Also shown in the inset is the low energy behavior.

To be more precise, from our numerical results we find, similarly to CDM, that the integrated density of states $N(E)$ for weak disorder (i.e., both n_0 and n_1 much smaller than ϕ_0) saturates below the pseudogap ϕ_0 to a value $N_* \sim n_0 n_1/(n_0 + n_1)$, which is of the order of half the average number per unit length of steps of the random potential. The saturation occurs at an energy scale E_* which can be identified as the typical effective bandwidth of those midgap excitations. This result physically implies that, for weak disorder, the number of states generated inside the gap is of the order of the average number of domain walls. From the analytical expression of $N(E)$, we obtain that $\ln(E_*/\phi_0^2) \sim -2\phi_0/(n_0 + n_1)$, i.e., E_* is exponentially small in the inverse of the disorder strength. In addition, it is also possible to calculate the localization length $\lambda(E)$. In particular, for $\phi \neq 0$, $\lambda(0) = 1/\phi$, which implies that the localized wave functions inside the gap have a much longer localization length than the spin-Peierls correlation length λ_{SP}. More interesting, for $\phi = 0$, which is relevant for our disorder modelization, $\lambda(E) \sim |\ln E|$, so that the states close to $E = 0$ are almost delocalized.

More generally, our model at low temperature and energy is equivalent to the models analyzed in Ref. [1] and in Ref. [4], for $\phi = 0$ and $\phi \neq 0$, respectively. The analogy can be expected by the following arguments. For $\epsilon \leq \phi_0$ and $n_0 = n_1 \ll \phi_0$, the problem reduces to a model of weakly coupled spins localized close to each domain wall. As a first approximation, only the exchange coupling between two successive spins can be retained, which is given by $J(r) \simeq \phi_0 \exp(-r\phi_0)$, r being the random distance between two domain walls distributed according to $n \exp(-rn)$. Thus the model is indeed equivalent to an Heisenberg chain with randomly distributed exchange constants. The probability distribution of J at energy scales $\leq \phi_0$ can be readily found to be

$$P(J) = \theta(\phi_0 - J)\left(\frac{n}{\phi_0^2}\right)\left(\frac{\phi_0}{J}\right)^{1-n/\phi_0},$$

and it has to be used as the starting point of the renormalization group flow equations of Ref. [1]. In this way, it is possible to recover the same results that we obtain by exploiting the exact solvability of our model, thus showing not only that the two models are equivalent, but also that spin anisotropy does not really matter [20]. For $n_0 \neq n_1$, the same analogy works now with the model of Ref. [4]. More rigorously, the above conjectured equivalence can be proven by showing that the models have the same low temperature thermodynamic properties.

In our model, we can, in fact, calculate exactly many thermodynamic quantities and find not only the low temperature but also the intermediate ($T \sim \phi_0$) temperature behavior. For instance, the uniform magnetic susceptibility is given by

$$\chi(T) = \beta \int_0^\infty dE \, \frac{\partial N}{\partial E} \, \frac{1}{2\cosh^2(\beta\sqrt{E}/2)},$$

and is plotted in Fig. 2 for the same values of ϕ_0, n_0, and n_1 as in Fig. 1.

From the asymptotic behavior of $N(E)$ for small E, we find that, at low T, $\chi(T) \sim T^{2\mu-1}$, for $\mu \neq 0$, and $\sim 1/(T \ln^2 T)$ for $\mu = 0$. The latter is exactly the result for the random XXZ Heisenberg model. Our model thus belongs, at low energy and for $\mu = 0$, to the same universality class. For all μ's smaller than $1/2$, the magnetic susceptibility still diverges at low temperature. Analogously, the specific heat vanishes as $C_v \sim T^{2\mu}$ ($C_v \sim 1/|\ln^3 T|$, for $\mu = 0$), which is compatible with the result of Ref. [4] with $2\mu = \alpha$, thus showing the equivalence with our model at $\mu \neq 0$. In addition, we obtain the full behavior of χ at intermediate temperatures, as shown in Fig. 2. We see that, at $T \sim \phi_0$, the susceptibility decreases as if a spin-Peierls gap were present, even though it finally diverges at low T. Moreover, for $E_* < T < \phi_0$, we predict a Curie-like behavior, with a Curie constant $\propto N_*$.

The behavior of the staggered part of the spin-spin correlation function $\chi_s(x)$ can be deduced by the analogies with the models analyzed in Refs. [1,4]. In particular, for $\phi \neq 0$, $\chi_s(x)$ decays exponentially with a correlation

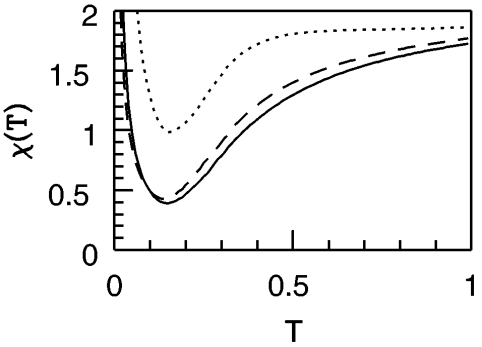

FIG. 2. Uniform magnetic susceptibility at zero staggered magnetic field, for the same cases as in Fig. 1.

length $\propto (1/\mu)^2$ [4]. On the contrary, for the case relevant to our model, which corresponds to $\phi = 0$, $\chi_s(x)$ decays as a power law $\sim 1/x^2$ [1]. At finite temperature and $\mu = 0$, $\ln \chi_s(x, T) \sim -x\sigma/\ln^2(T/\phi_0)$ [1], where $\sigma = 2\phi_0^2/(n_0 + n_1)$. This expression suggests a new energy scale E_c, which can be identified as the coherence energy for the antiferromagnetic fluctuations. In fact, when $T \geq E_c$, the correlation function should behave like $\exp(-2x\phi_0)$, which leads to $\ln(E_c/\phi_0^2) \sim -\sqrt{\sigma/\phi_0}$, that is, to a coherence energy exponentially small in the inverse square root of the disorder strength, but still much bigger than E_*. The appearance of an energy scale governing the spin-spin correlation function, which differs from that entering the average density of states, is not unexpected in the presence of disorder, which introduces basic differences between average and typical behaviors [21]. On the other hand, for $\mu \neq 0$, below another energy scale E_μ, we should recover the result of Ref. [4], which sets $\ln(E_\mu/\phi_0^2) \sim -1/\mu$.

We also exactly calculate the staggered susceptibility $\chi_s(T)$. By means of Eq. (2) we find that

$$\chi_s(T) = \int_0^\infty dE \, \frac{\partial N}{\partial E} \, \tanh\left(\frac{\beta\sqrt{E}}{2}\right) \frac{1}{\sqrt{E}} \, . \qquad (3)$$

For $\mu < 1/2$, this susceptibility diverges at low T like the uniform susceptibility. However, while the integral over E in the uniform susceptibility is cut off by T^2, the contribution to the singular behavior of the staggered susceptibility comes from all E up to approximately E_*. Moreover, all higher energies also contribute to the staggered susceptibility with a finite term as $T \to 0$. Therefore, while the singular behavior deriving from all $\epsilon = \sqrt{E} < T$ can be ascribed to local excitations, that deriving from $\epsilon > T$ is solely due to longer range antiferromagnetic fluctuations [1]. The rapid enhancement of antiferromagnetic fluctuations that we find is extremely suggestive in the light of that recently observed in $CuGeO_3$, as previously discussed (see also Ref. [10], for the Si-doping case). In fact, our model for a disordered spin-Peierls system clearly shows a coexistence of dimerization with long range antiferromagnetic fluctuations, the latter existing on energy scales lower than the pure spin-Peierls gap. These fluctuations may induce a magnetic ordering via the interchain coupling, below some Néel temperature T_N. The magnetic susceptibility would then still show the drop at the Peierls transition, but the low temperature divergence would finally be cut off by T_N, below which $\chi(T)$ would exponentially vanish, compatibly with the experimental evidences (see, e.g., Ref. [8]). Moreover, on the basis of the previous discussion, we expect that the Néel temperature is related to the energy scale governing the spin-spin correlation function, that is to E_c, which is exponentially small in $\sqrt{l/\lambda_{SP}}$, and therefore larger than the typical bandwidth of the low energy excitations E_*, which is exponentially small in l/λ_{SP}. This difference might be the explanation of the relatively large Néel temperatures found in the doped $CuGeO_3$.

It is a pleasure to acknowledge useful discussions with A. O. Gogolin, A. A. Nersesyan, and Yu Lu. A particular thanks goes to E. Tosatti, who has been the source of inspiration of this work. This work has been partly supported by EEC under Contract No. ERB CHR XCT 940438, and by the INFM, Project HTSC.

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