Random Bonds and Topological Stability in Gapped Quantum Spin Chains

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Using an asymptotically exact real space renormalization procedure, we find that the dimerized spin-1/2 chain is extremely stable against bond randomness. For weak dimerization or, equivalently, strong randomness, it is in a Griffiths phase with short-range spin-spin correlations and a divergent susceptibility. The string topological order persists. We conjecture that random integer spin chains in the Haldane phase exhibit similar thermodynamic and topological properties.

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Extensive theoretical work on random quantum magnetic systems has been carried out since the late 1970s [1–4]. Systems that behave critically in the absence of randomness are unstable against weak randomness and flow to the random singlet (RS) phase [1,3]. In the RS phase, spins far apart in space form weakly bound singlet pairs in a more or less random manner. The low temperature thermodynamic properties of these systems are dominated by the weakly bound pairs and are universal [1–3]. For instance, the susceptibility of the undimerized random antiferromagnetic Heisenberg or XXZ spin-1/2 chain diverges as $[T \log^2 T]^{-1}$ at low T, independent of the details of the randomness [3]. Universal power law behavior has also been found in disorder averaged spin-spin correlation functions [3]. Experiments, however, seem to find power law divergent susceptibilities with nonuniversal exponents [5]. It is of interest to study if there exist relevant perturbations at the RS fixed point that drive the system toward a state exhibiting the nonuniversal behavior found experimentally.

A related issue is the effect of randomness on spin chains that have an excitation gap in the absence of randomness [6]. The most prominent examples of such chains are integer spin chains in the Haldane phase [7]. Other examples include dimerized spin-1/2 chains [8] and spin chains with spontaneous dimerization [9]. All of these systems have topologically ordered [10] ground states. One might think that strong enough randomness will inevitably destroy the topological order of the ground state. However, Haldane has suggested [11] that there exists a class of random perturbations for which the the topological order in the ground state of integer spin chains is stable, regardless of the strength of the perturbations. We will show that the analog of this prediction for random bond dimerized spin-1/2 chains is correct.

An explicit example that provides strong support to Haldane's above conjecture can be found in the random version of the AKLT model [12]:

$$H = \sum_i J_i[\mathbf{S}_i \cdot \mathbf{S}_{i+1} + (1/3)(\mathbf{S}_i \cdot \mathbf{S}_{i+1})^2], \quad (1)$$

where $J_i > 0$. The exact ground state of this random model is identical to that of the pure model [12], i.e., a valence bond solid. Its excitation spectrum and thermodynamic properties will certainly depend on the distribution of J_i, yet the perfectly topologically ordered ground state is completely unaffected by randomness.

Without randomness, the spin-1 chain and dimerized spin-1/2 chains exhibit similar physical properties [13]. They both have a nondegenerate ground state with an excitation gap, and, more importantly, they both have string topological order [13]. Hida has shown that they can be continuously connected to each other without closing the gap or removing the topological order; i.e., they are in the same phase [13]. It is natural to expect that they also behave similarly in the presence of randomness.

In this paper we study the random bond dimerized spin-1/2 chain in detail. Using the asymptotically exact real space decimation renormalization group introduced by Dasgupta and Ma [1] and extended by Fisher [3], we find that enforced dimerization is a relevant operator at the RS fixed point that drives the system to a random dimer (RD) phase. The low temperature thermodynamic properties of the RD phase are *nonuniversal*. For weak dimerization, the spectrum of the RD phase is gapless and the susceptibility diverges as $\chi \sim T^{-1+\alpha}$ with $0 < \alpha \ll 1$ and dependent on the bond distribution (in agreement with the behavior found experimentally and qualitatively similar to the RS thermodynamics), but the averaged spin-spin correlation function remains short ranged. Thus for weak dimerization the RD phase is an example of a Griffiths phase. More importantly, we find that the string topological order is *not* destroyed by random bonds. We conjecture that these results also apply to random bond integer spin chains in the Haldane gapped phase. Comparison will also be made with spontaneously dimerized spin chains which behave very differently upon introducing disorder.

Consider the model Hamiltonian

$$H = \sum_i J_i[S_i^x S_{i+1}^x + S_i^y S_{i+1}^y + \Delta S_i^z S_{i+1}^z], \quad (2)$$

where S_i^α are spin-1/2 operators, J_i are (random) positive coupling constants, and $0 \le \Delta \le 1$. Here we will concentrate on the cases $\Delta = 0$ (XX) and $\Delta = 1$ (Heisenberg

chain), since it has been shown that, for the case of random bonds, the Ising coupling is irrelevant when $\Delta < 1$ [3]. We assume that the distribution functions of the couplings J_i depend on whether i is even or odd, which are $P_e(J, J_0)$ and $P_o(J, J_0)$, respectively. Here J_0 is the cutoff in the distribution function corresponding to the strongest bond in the system. As Fisher [3] has shown, in the absence of dimerization, i.e., when $P_e(J, J_0) = P_o(J, J_0)$, the low energy, long-distance behavior of Eq. (2) is universal, and the XX and Heisenberg chains behave in essentially the same way.

Following Fisher [3], we introduce a decimation renormalization group procedure in which we pick the bond in the system with the largest J, say J_2 between spins 2 and 3. Since this is such a strong bond, spins 2 and 3 are likely to form a singlet pair and become unimportant at low energies (on scales much smaller than J_2). The major physical effect of the existence of spins 2 and 3 is to generate an induced coupling between their neighboring spins 1 and 4. For the XX chain, $\tilde{H}_{1-4} = \tilde{J}_{14}(S_1^x S_4^x + S_1^y S_4^y)$ where $\tilde{J}_{14} = J_1 J_3/J_2 + O(1/J_2^2)$ and for the Heisenberg chain, $\tilde{H}_{1-4} = \tilde{J}_{14}\mathbf{S}_1 \cdot \mathbf{S}_4$ where $\tilde{J}_{14} = J_1 J_3/2J_2 + O(1/J_2^2)$. The effect of this decimation procedure is to get rid of the strongest bond (and also its two neighbors) in the system, generate a weaker bond between the spins neighboring the decimated ones, and lower the overall energy scale. This procedure becomes asymptotically exact in the low energy limit [3]. The new energy cutoff is then lowered to $\Omega = \max\{\tilde{J}\}$ [14]. Following Fisher and anticipating that the bond distribution will become broad on logarithmic scales at low energy [3], we transform to logarithmic variables and define $\Gamma = -\log(\Omega/J_0)$ and $\zeta = \log(\Omega/\tilde{J})$, so that both Γ and ζ are positive and a larger Γ and a larger ζ correspond to a lower energy scale and a weaker bond, respectively. The recursion relations now become

$$\tilde{\zeta}_{1-4} = \zeta_1 + \zeta_3 - \zeta_2 + \kappa = \zeta_1 + \zeta_3 + \kappa, \quad (3)$$

where we used the fact that $\zeta_2 = 0$ since $J_2 = \Omega$. The constant $\kappa = 0$ for the XX chain and $\log(2)$ for the Heisenberg chain. The flow equations for the bond strength distribution functions $\rho_e(\zeta, \Omega)$ and $\rho_o(\zeta, \Omega)$ in terms of ζ are then

$$\partial\rho_{e,o}(\zeta,\Gamma)/\partial\Gamma = \partial\rho_{e,o}/\partial\zeta + [\rho_{e,o}(0,\Gamma) - \rho_{o,e}(0,\Gamma)]\rho_{e,o} + \rho_{o,e}(0,\Gamma)\int\int d\zeta_1\, d\zeta_2\, \rho_{e,o}(\zeta_1,\Gamma)\rho_{e,o}(\zeta_2,\Gamma)\delta(\zeta - \zeta_1 - \zeta_2 - \kappa). \quad (4)$$

When $\kappa = 0$ (XX chain), these flow equations are identical to those encountered in the transverse field Ising model if we identify the even bonds as the bonds between Ising spins and odd bonds as the transverse fields [4]. In order to find fixed point solutions of the renormalization group (RG) flow, it is necessary to rescale variables. Following Fisher [3,4], we introduce the rescaled variable $\eta = \zeta/\Gamma$ and the new distribution function $Q_{e,o}(\eta, \Gamma) = \Gamma P_{e,o}(J, \Omega)$. The flow equations for Q are

$$\Gamma\,\partial Q_{e,o}/\partial\Gamma = Q_{e,o} + (1+\eta)\partial Q_{e,o}/\partial\eta + [Q_{e,o}(0,\Gamma) - Q_{o,e}(0,\Gamma)]Q_{e,o} + Q_{o,e}(0,\Gamma)\int d\eta_1 d\eta_2 Q_{e,o}(\eta_1)Q_{e,o}(\eta_2)\delta(\eta - \eta_1 - \eta_2 - \kappa/\Gamma). \quad (5)$$

As Fisher has shown [3,4], the flow equations (5) have only one generic fixed point [15]

$$Q_e = Q_o = Q^*(\eta) = e^{-\eta}\Theta(\eta). \quad (6)$$

This fixed point distribution corresponds to the random spin-1/2 chain without dimerization, a model studied extensively before [3]. Going back to the original variable ζ, we find the fixed point distribution corresponds to

$$\rho(\zeta) = (1/\Gamma)e^{-\zeta/\Gamma}; \quad (7)$$

i.e., the width of the distribution on the logarithmic scale grows linearly with the logarithim of the energy scale Γ. For small deviation away from the fixed point $Q_e = Q^* + q_e$ and $Q_o = Q^* + q_o$, there is only one *relevant* eigenperturbation [4] behaving as $q_{e,o}(\eta, \Gamma) = q_{e,o}(\eta)\Gamma^\lambda$ with eigenvalue $\lambda = 1$, and the eigenvector is $q_e = (\eta - 1)e^{-\eta}$ and $q_o = -(\eta - 1)e^{-\eta}$. The relevant perturbation, like the fixed point distribution, is independent of κ; hence, the XX and Heisenberg chains will behave similarly.

The relevant perturbation corresponds to the *difference* in the distributions for even and odd bonds. Therefore, we find that dimerization is a *relevant* perturbation near the RS fixed point, with eigenvalue $+1$.

For weak dimerization, the system barely knows that there is a small difference between even and odd bonds in the early stages of the RG flow. Both distributions initially flow toward the RS fixed point solution with a small relevant perturbation reflecting the dimerization:

$$Q_o(\Gamma) = Q^* + \delta\Gamma(\eta - 1)e^{-\eta}, \qquad Q_e(\Gamma) = Q^* - \delta\Gamma(\eta - 1)e^{-\eta}, \quad (8)$$

where δ characterizes the strength of the dimerization (distance from criticality). In general, δ depends in a complicated way on the shape of the original distributions

and at what energy scale it is defined. As the flow away from the RS point continues, the even (odd) bonds get much weaker than the odd (even) bonds if originally the even (odd) bonds were only slightly weaker than the odd (even) bonds. The relevant perturbation grows linearly with Γ and becomes of $O(1)$ as $\Gamma = \Gamma_0 \sim 1/|\delta|$. The flow equation for the density of spins not yet decimated at energy scale Γ is [3]

$$\partial n(\Gamma)/\partial\Gamma = -2Q(\eta = 0, \Gamma). \tag{9}$$

Using the RS fixed point distribution Eq. (6) in Eq. (9), we find that $n \sim 1/\Gamma^2$ [3,4] so when the relevant perturbation becomes large, the density of active spins is $n \sim \delta^2$. The corresponding length scale L, which is the typical distance between the remaining spins, is $L_0 \sim \Gamma_0^2 \sim 1/\delta^2$. At this stage the existence of dimerization becomes dominant and under RG most of the bonds decimated are odd bonds.

The fact that a small difference in the bond distributions grows as one lowers the energy is physically easy to see. Assume the odd bonds are slightly stronger than the even bonds in general. Then, in the decimation procedure, it is slightly more likely that an odd bond gets decimated. When that happens, typically two intermediate strength neighboring even bonds also disappear, and a *much weaker even bond* is generated. Hence, the width of the even bond distribution grows faster than the odd bond distribution, and its overall strength also decreases faster. Thus, in the low energy limit, the system can be viewed as a trivially soluble collection of uncoupled spin pairs (isolated odd bonds). We refer to this phase as the RD phase.

After renormalization the distribution of odd bonds takes the form $\rho_o(\zeta) \sim (1/\Gamma_0)e^{-\zeta/\Gamma_0}\Theta(\zeta)$. In terms of the original variables the odd bond distribution is

$$P_o(J) = (\alpha/\Omega_0)(J/\Omega_0)^{-1+\alpha}\Theta(1 - J/\Omega_0), \tag{10}$$

where $\Omega_0 = J_0 \exp(-\Gamma_0)$ and $\alpha \propto \delta$.

This effective independent pair Hamiltonian with a power law bond distribution is identical to that introduced by Clark and Tippie [16] to explain the low-temperature thermodynamics of the random spin chains. Here we have *derived* it using RG from the realistic model. [We note in passing that dimerization does exist in some members of the $R^+(\mathrm{TCNQ})_2^-$ compound family [5] studied experimentally, in the absence of disorder [17]; thus the random dimer model studied here may be relevant to some of these systems in the presence of randomness.] The leading temperature dependence of thermodynamic properties can be determined by assuming that all spins connected by bonds with energy greater than the temperature have paired up into singlets, and all spins connected by bonds with energy less than the temperature are essentially free. This is a good approximation for broad bond distributions. In this way, the specific heat and susceptibility in the low temperature limit can be easily calculated. As the temperature goes to zero, the the spin susceptibility (in any direction, with possible direction dependent prefactors) diverges like $\chi \sim T^{\alpha-1}$, and the specific heat goes to zero like $C_v \sim T^{\alpha}$. The averaged spin-spin correlation function is short ranged, with the correlation length (distance between spins) $\xi \sim |\delta|^{-\nu} \sim |\delta|^{-2}$. The existence of a divergent magnetic susceptibility away from the critical point is characteristic of a Griffiths phase. The divergent susceptibility arises from magnetically active gapless excitations. For the RS phase discussed by Fisher [3], the averaged spin-spin correlation function decays as $1/R^2$ at long distance so the system is critical and one expects a divergent susceptibility. The Griffiths phase in the random dimerized spin-1/2 chain is exactly analogous to the Griffiths phase that appears in the random transverse field Ising chain [4]. If the initial dimerization is large, the flow begins far from the RS phase, the bond distribution of the stronger bonds does not flow to a power law, and the gap does not close up. When this happens, thermodynamic properties depend strongly on the initial distribution and the susceptibility remains finite.

The dimer phase has a novel kind of topological order that measures the dimerization of the chain. The "string-topological correlation function" is [13]

$$T_{ij} = \langle\Psi_0|S_i^z \exp\left[i\pi \sum_{i<k<j} S_k^z\right] S_j^z|\Psi_0\rangle, \tag{11}$$

where $|\Psi_0\rangle$ is the ground state. T_{ij} is similar to the topological correlation function for the spin-1 chain [10]. For a completely dimerized ground state, $T_{ij} = -1/4$ if i is a left spin of a dimer and j is the right spin of a (possibly different) dimer. This is because every spin between i and j in the completely dimerized model is paired up with another spin between i and j. $T_{ij} = 0$ otherwise. Therefore, this special topological correlation function is long ranged although there is only short-range spin-spin correlation, a situation similar to the special kind of off-diagonal long-range order (ODLRO) in the fractional quantum Hall effect (FQHE) [18].

For a general spin-1/2 chain with randomness, we introduce a topological order parameter

$$T = \lim_{j-i\to\infty} (\overline{T_{2i,2j-1}} - \overline{T_{2i+1,2j}}), \tag{12}$$

where the overbar stands for average over randomness. In the absence of dimerization, T vanishes. For a random system, T measures the probability that the two end spins survive decimation until the dimerization becomes large, and the low energy physics becomes that of the completely dimerized chain. This probability is just the square of the density of spins at the dimerization crossover scale. Therefore, for small δ, T scales like

$$T \sim -|\delta|^{2\beta}\mathrm{sgn}(\delta), \tag{13}$$

with $\beta = \nu = 2$, and $\mathrm{sgn}(\delta)$ is $+$ if even bonds are stronger and $-$ if odd bonds are stronger. In the absence of randomness, β is found to be $1/12$ [13].

The topological order described here is not a spontaneous order like the spontaneous magnetization of a ferromagnetic Ising chain in the absence of magnetic field; it is

dynamically *enforced* by the Hamiltonian. Its sign is determined by the sign of the dimerization, unlike the spontaneous magnetization which can take any direction allowed by the symmetry. In this sense it is more like the magnetization of an Ising chain in the *presence* of a magnetic field. The existence of the topological order simply reflects the fact that the Hamiltonian favors singlet pairs to be formed over even bonds, if the even bonds are stronger in general. In the absence of odd bond couplings, the ground state is a trivial collection of singlet pairs over even bonds and the dimer or topological order is perfect. In the presence of odd bond couplings (but weaker than even bonds in general), quantum and statistical fluctuations generate regions where singlet pairs are formed over odd bonds. Between regions of different topological structures there has to be a spin unpaired to its neighbors (a soliton). In the presence of dimerization, the energy cost of the "wrong region" (the area having singlets formed over the odd bonds in this case) is proportional to its length (at least at long enough length scales); hence the unpaired spins are confined by a linear confining potential [19]. This is similar to the confinement of domain walls of the Ising chain in the *presence* of a magnetic field. The confinement length in the weak dimerization limit is the length scale at which dimerization becomes significant under RG, which is also the spin-spin correlation length. We hence find that although the gap vanishes in the presence of strong randomness, the dimer phase is stable and the topological order persists due to the confinement of unpaired spins [20]. This should be contrasted with the case of spontaneous dimerization. In that case the two degenerate ground states also have finite topological order, but it is a *spontaneous* order associated with the spontaneously broken translation symmetry. The spinons carried by the domain walls separating the two different ground state configurations are *unconfined*, just as the unconfined domain walls in the Ising chain without a magnetic field. In this case, the state is unstable against *weak* randomness, and both the gap and topological order immediately disappear upon introducing randomness [21].

We have shown that the dimerized spin-$1/2$ chain is stable against disorder. This can be seen as due to the confinement of unpaired spins. When the dimerization is weak or the randomness is strong, the system is in a Griffiths phase, in which the spin-spin correlation function is short ranged yet the susceptibility diverges. The susceptibility and specific heat follow simple power laws with nonuniversal exponents at low temperatures. The string-topological order is not destroyed by randomness. We conjecture that these results apply to other systems with dynamically generated topological order, such as the spin-1 chain in the Haldane phase. A detailed analysis using a real space RG procedure that is proper for the random spin-1 chain will be presented elsewhere [21]. We also conjecture that spontaneously generated topological order is unstable against randomness [21]. The relevance of the random dimer model studied here to the experiments [5] deserves further investigation. Experimentally there has been some work on effects of hole doping in the spin-1 chains [22]. The effect of hole doping is probably different from random bonds because it introduces unconfined topological defects into the system [21].

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