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Ground state properties of disordered and dimerized spin chains

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Abstract. Concerning the question of the (spin-)Peierls mechanism in the presence of disorder we present a detailed analysis of the ground state phase diagram of the dimerized anisotropic Heisenberg-XXZ chain containing one impurity. It is obtained by studying the destruction of the quantum coherence by the perturbations. The stability of the Peierls phase, i. e. the occurence of a stable dimerization, is determined by the energy gain and gap due to the coupling to the static phonons. The extension of the paramagnetic phase, found already in the clean dimerized chain, grows by adding the impurity, because the distortions weaken each other. The Peierls phase is reduced for two reasons: First, the energy gain of the spin-system decreases, which leads to a smaller stable dimerization and second, the energy gap itself is reduced.

Keywords: quantum spin systems, quantum coherence, disordered systems
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1 General remarks

Recent experiments on the doped one-dimensional Heisenberg system $Cu_{1-x}Zn_xGeO_3$ [1] have shown two subsequent magnetic transitions, the first to a nonmagnetic spin-Peierls state at $T_{\rm SP}$=10K, the second to antiferromagnetic order at $T_{\rm N}$=4K. This coexistence of antiferromagnetism and the spin-Peierls singlets lead to great interest in the question of the Peierls mechanism in the presence of disorder. Based on our experience with the randomly [2] or periodically [3] distorted Heisenberg chain, we investigate here the ground state properties of the randomly *and* periodically distorted chain. We clarify the interplay between interaction, periodic and random perturbation, which is not only relevant with regard to the afore mentioned experiments, but is also quite a general question in theoretical solid state physics. Fortunately, in one dimension, methods like the DMRG are available which allow quasi-exact quantitative statements. The antiferromagnetic correlations, on the other hand, cannot be explained by regarding only the ground state.

We consider in detail the anisotropic XXZ-Heisenberg model ($\hbar\vec{\sigma}/2 = \vec{S}$, $\hbar = 1$),

$$H = -\sum_{n=1}^{N} J_n(u)\left(\sigma_n^x\sigma_{n+1}^x + \sigma_n^y\sigma_{n+1}^y + \Delta\sigma_n^z\sigma_{n+1}^z\right) - h_1\sigma_1^z + \frac{NK_0}{2}u^2, \qquad (1)$$

where the alternating exchange coupling $J_n(u) = J[1 + (-)^n u]$ leads to dimerization

and the impurity is given by a local magnetic field. Thus, the impurities considered here are not the same as those realized in the doping experiments. Our choice, however, is usually investigated in theoretical treatments, see for example [4]. The clean model is integrable, showing three phases: a ferromagnetic phase for $\Delta \geq 1$, separated by a first order transition from a gapless phase for $-1 \leq \Delta < 1$, whose low lying excitations are given by those of a Luttinger liquid, and an antiferromagnetic phase for $\Delta < -1$. The transition to the antiferromagnet is of Kosterlitz-Thouless type and only found for zero total magnetization.

2 Ferromagnetic coupling: paramagnetic phase

In general, all perturbations of the clean XX-model (free fermions) lead to a phase with localized spins – either the spin glass phase of the disordered model or the spin singlets of the Peierls phase. Nevertheless, a paramagnetic phase, like the Luttinger phase of the clean model, is established for certain values of the anisotropic parameter Δ. Through a Jordan Wigner transformation, the model is related to spinless fermions and in terms of this description the localization of the spin moments is easy to understand. A periodic lattice distortion with a period of two lattice spacings, leads, for half filling (zero magnetization), to a $2k_F$ distortion which opens a gap at the Fermi level. Also the backscattering from the impurity tends to localize the ground state wave function. As shown in [2] (see also the references therein), the system enters the paramagnetic phase at $\Delta > 0$ in the case of a local impurity. The dimerized system shows the paramagnetic phase for $\sqrt{2} < \Delta < 1$, see [3]. We use the length dependence of the phase sensitivity, i.e. the reaction of the system to a change in the boundary conditions, $\sigma^-_{N+1} = \exp(i\Phi)\sigma^-_1$, to determine the transition from the phase with localized spin moments to the paramagnetic phase with free spins. In particular we determine below the energy difference for periodic ($\Phi = 0$) and antiperiodic ($\Phi = \pi$) boundary condi-

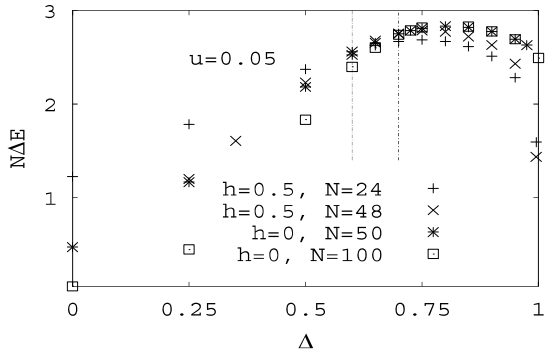

Fig. 1 Phase sensitivity versus interaction for a dimerized system without an impurity ($\diamond$, $\circ$) and with an impurity ($+$, $\times$). The above system sizes have been chosen for clear representation of the data. The vertical lines indicate the crossing points for the two lengths of each parameter pair (u, h), respectively.

tions, $\Delta E = E(\Phi = 0) - E(\Phi = \pi)$, numerically for systems with finite size. The result, in the Luttinger regime, can be evaluated exactly [5], and is given by $N\Delta E = \pi v g/2$, where v is the velocity of the spinon excitations and g parameterizes the anisotropy, $g = \pi/(4\eta)$, $\Delta = \cos(2\eta)$. Thus $N\Delta E$ is independent of system size in the paramagnetic phase, but expected to decrease in the localized phase. Concerning the given model, see Eq. (1), we show as an example in Fig. 1, the data obtained for the parameters $u = 0.05$ and $h_1 = 0.5J$. The behaviour of the phase sensitivity does not change by inverting the local field, since the effective $2k_F$-perturbation is given by $u_{\text{eff}} = \sqrt{u^2 + h^2/N^2}$. It is clearly seen that the system containing the impurity enters first the paramagnetic phase. The steep descent near $\Delta = 1$ is a finite size effect typical for the single impurity system, see [6]. Increasing the strength of the perturbations to very large values, an additional maximum of the phase sensitivity occurs in the localized regime at the point where the impurity becomes irrelevant and the system reacts to the true value of the dimerization. In summary, we have shown that the paramagnetic phase of the dimerized model grows, due to the weakening of the dimerization through the impurity.

3 Antiferromagnetic coupling: the Peierls state

The existence of a minimum in the total energy at finite u_0, $E(u) = \Delta E(u) + E_{\text{latt}}$, where $E_{\text{Latt}} = NK_0u^2/2$, is a criterion for the stability of the Peierls phase. Thus, we determine the exponent of the energy gain of the spins by coupling to the lattice, $\Delta E(u) = E(u,h) - E(u=0,h) = -NJc(\Delta)u^\alpha$. As commonly known, a stable dimerization, $u_0 = [\alpha c(\Delta)J/K_0]^{1/(2-\alpha)}$, can only develop in the antiferromagnetic chain. The numerical data, shown in Fig. 2, show that the energy gain decreases by adding a single impurity to the dimerized antiferromagnetic chain. In addition, the energy gain saturates for larger impurity strength. We see that α, in the clean system given by $\alpha = 2/(2-g)$, becomes more quadratic by increasing the impurity strength, in our example $\alpha = 1.7$. Therefore, the minimum of the total energy is found at smaller u_0.

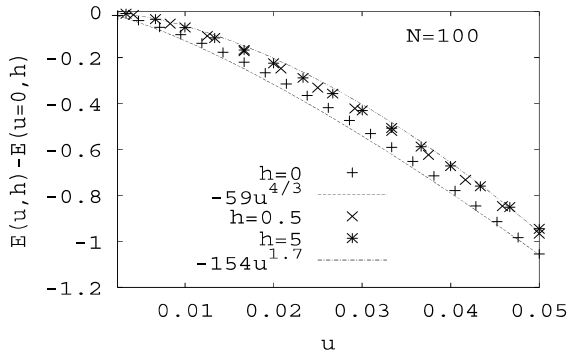

Fig. 2 Energy gain versus dimerization for $\Delta = -1$ and various impurity strengths.

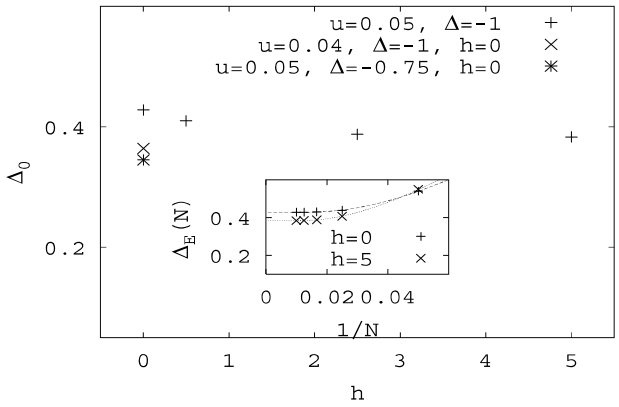

Fig. 3 Energy gap, obtained from finite size scaling, versus impurity strength at fixed dimerization $u = 0.05$ and fixed interaction, $\Delta = -1$. For comparison we include the data for $h = 0$, $\Delta = -1$, but smaller dimerization, $u = 0.04$ and for $h = 0$, $u = 0.05$, but $\Delta = -0.75$. The inset shows examples of the finite size scaling for $u = 0.05$, $\Delta = -1$.

Second, we consider the energy gap, Δ_0, due to the coupling to the lattice according $\Delta_E(N) = [E(S^z_{\rm tot} = 1) + E(S^z_{\rm tot} = -1) - 2E(S^z_{\rm tot} = 0)]/2$ and a subsequent finite size scaling with $\Delta_E(N) = \Delta_0 + A\exp(-N/N_0)/N$. As the numerical data presented in Fig. 3 show, the gap is only slightly reduced by such a local distortion. For comparison, we include the gap of a clean system, but smaller dimerization u or smaller anisotropy Δ to demonstrate the magnitude of the effect. A strong local impurity is equivalent to a (global) reduced dimerization (about 20%), or to a reduction of the anisotropy. Besides this observation, we note that the gap becomes independent of the impurity strength for strong enough impurities – as does the energy gain. Concerning the persistent gap, we can conclude that the Peierls state is stable even in the presence of a very strong impurity. Thus, the Peierls state can only become instable with the reduction of energy gain, whereas the energy gap is reduced but not closed.

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