The phase diagram of the Haldane chain mapped onto the surface roughening problem

S.V.Meshkov
Max-Planck Institut FKF, Hochfeld-Magnetlabor, Grenoble, France
Institute of Solid State Physics, Chernogolovka, Moscow distr., USSR

The world-line Monte Carlo approach is a very natural and powerful tool for the investigation of quantum spin systems. Here this method is applied to investigate dynamical properties (excitation spectrum) and, in general, to build consistently the phase diagram of 1D extended Heisenberg hamiltonian

$$\hat{H} = \sum_j [J_{xy}(S_j^x S_{j+1}^x + S_j^y S_{j+1}^y) + J_z S_j^z S_{j+1}^z + D(S_j^z)^2].$$

Here J_z and J_{xy} are exchange integrals, D is one-site anisotropy constant. The antiferromagnetic region $J_z > 0$ is considered, where intriguing properties have been conjectured by Haldane [1].

The full orthonormal basis required to develop the checkerboard Monte Carlo scheme [2] is taken as all possible products of eigen states of the S^z operator on each lattice site. An world line is a sequence of basic states, describing a discrete imaginary time τ evolution of the system. On a resulting two-dimensional Ising-like $S_z = 0, \pm 1$ lattice one can measure a general two-point correlator $Q^{zz}(j-j', \tau-\tau') \equiv < S^z(j,\tau) S^z(j',\tau') >$. In-plane correlators $Q^{xx}(j,\tau) = Q^{yy}(j,\tau)$ can also be obtained by a reorientation of the anisotropy axis.

Besides the correlators themselves, the the spectral density of excitations $\rho_k(\epsilon)$ can be extracted from the imaginary-time dependent spin correlator $\tilde{Q}(k,\tau) \equiv \sum_j Q^{zz}(j,\tau) e^{ikj}$. The corresponding integral equation $\tilde{Q}(k,\tau) = \int e^{-\epsilon\tau} \rho_k(\epsilon) d\epsilon$ (see e.g.[3]) is treated via a simplified version of the Maximum-Entropy method (least-mean-square regularized solution with the restriction $\rho_k(\epsilon) \geq 0$). An example presented in Fig.1 demonstrates a continuum of states in a low k region, but as a whole does not look like a superposition of one-magnon and two-magnon contributions [4].

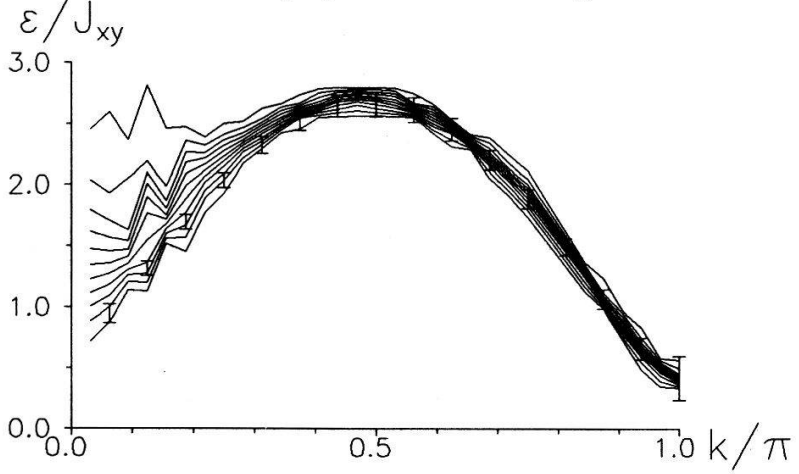

Fig.1
The spectral density $\rho_k(\epsilon)$ in a symmetric point $J_z = J_{xy}$, $D = 0$ for 64-site closed chain at $T = J_{xy}/32$. For each k the density of lines in a vertical direction is proportional to $\rho_k(\epsilon)$. Error bars show Takahashi result [5] for the lowest boundary of the spectrum.

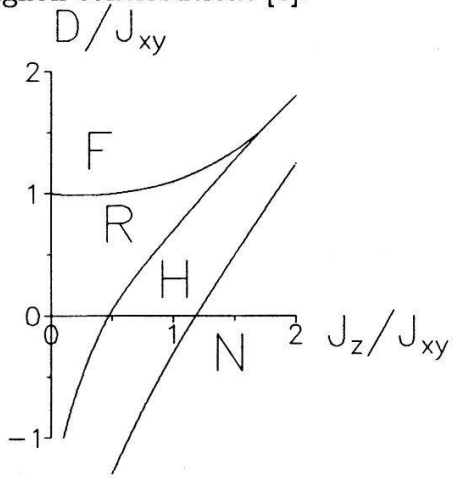

Fig.2
Antiferromagnetic region of the phase diagram $J_z > 0$. The phases are characterised in the text.

Thus the techinique allows to capture 1) existence or absence of the long-range order, 2) power- or exponential-like decay of the space correlations, and 3) existence or absence of the gap in the spectrum of excitations. These qualitative criteria were used build the the phase diagram given in Fig.2.

Flat phase F comes form the limit $D \to +\infty$, where the nondegenerate ground state is the product of $S^z = 0$ states for all the sites. The energy per a site is $E_F \approx 0$, and the lowest excitation is formed by a nonzero S^z on one site $0000 + 0000$ with the energy $E_F^{\pm}(k) \approx D + 2J_{xy}cos(k)$. All the correlators decay exponentially.

Neel phase N, coming from the limit $D \to -\infty$ has a doubly degenerate Neel antiferromagnetic ground state $S_j^z = \pm(-1)^j$ with the energy $E_N \approx D - J_z$. The lowest excitation is a site with $S^z = 0$ between two half-spaces of opposite antiferromagnetic order $+-+-0+-+-$, the energy is $E_N^0 \approx D + 2J_{xy}cos(k)$. Correlators in xy-plane decay exponentially.

Rough phase R results from the quantum destruction of the phase F, when the negative energy of excitations $E_F^{\pm}$ near $k = \pi$ leads to spontaneous creation of defects with spin $+$ and $-$. The energy gap is zero at $k = \pi$ for excitations with $S^z = \pm 1$ and at $k = 0$ for ones with $S^z = 0$. All the correlators are power-like.

Haldane phase H can be treated as a result of the spontaneous creaction of $S^z = 0$ defects in a Neel state after vanishing of their gap at $k = \pi$ (the border NH). These defects destroy the long-range Neel order, but keep the order of nonzero S^z alternating [6].

One more way to treat the problem is provided by its equivalence [6] to the highly anysotropic limit of the restricted solid-on-solid model of the crystall surface. In the last reformulation each site with nonzero spin S^z is treated as a step up or down (for $S^z = +1$ or -1) when scanning along the space direction of the 2D lattice. The fluctuating level of the corresponding surface has the following possible variants of the distribution. In the F phase one atomic level is dominating with rare deviations up and down. The phase R corresponds to crystall surface with no dominating atomic levels. In the phases N ans H two levels are equally occupied and dominate on others, so the mean height is half-integer (phases). This fact helps to distinguish between the phases H and F, both of which are disordered and have a gap due to the finite energy of a step on the surface. The evolution of the crystall surface properties $H \to R \to F$ is illustrated in Fig.3.

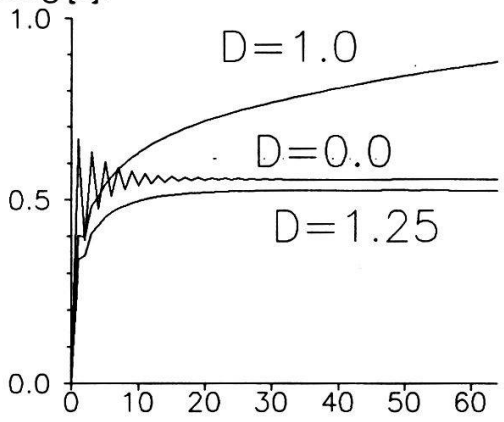

Fig.3

The correlator of the relative surface height $< [h(i) - h(0)]^2 >$ as a function of a distance along the chain for the symmetric exchange $J_z = J_{xy}$. Note the qualitative difference of the curve $D = 1.0$, corresponding to the *Rough* phase.

It should be noted that the existence of a wide region of the intermediate *Rough* phase between F and H cannot be strongly stated, because the measured correlations in xy-plane are decay with the distance l slightly faster than $l^{-1/4}$.

References:

[1] F.D.M.Haldane, Phys.Rev.Lett. **50**, 1153 (1983)
[2] J.E.Hirsch, D.J.Salapino, R.L.Sugar, R.Blankenbeckler, Phys.Rev.B **26**, 5033 (1982)
[3] J.Deiz, M.Jarrell, D.L.Cox, Phys.Rev.B **42**, 4869 (1990)
[4] G.Gomez-Santos, Phys.Rev.Lett. **63**, 790 (1989)
[5] M.Takahashi, Phys.Rev.Lett. **62**, 2313 (1989)
[6] M.den Nijs, K.Rommelse, Rhys.Rev.B **40**, 4709 (1989)