The hamiltonian of the tetrahedral spin-1/2 model

This text is part of section II of Ref.[1].

The hamiltonian of the tetrahedral spin-1/2 model (see Fig. 1 of Ref.[1]) is

$$\begin{aligned} H_t &= \sum_{i=1}^{N} \big\{ J_0(\sigma_i, \tau_i)_1 + J[(\sigma_i, \sigma_{i+1})_\Delta \\ &+ (\sigma_i, \tau_{i+1})_\Delta + (\tau_i, \sigma_{i+1})_\Delta + (\tau_i, \tau_{i+1})_\Delta] \\ &- h(\sigma_i^z \otimes \mathbf{1}_\tau + \mathbf{1}_\sigma \otimes \tau_i^z)\big\}. \end{aligned} \tag{1}$$

Along the ρ-line of the dumb-bell we have the spin-1/2 σ_i whereas along the r-line we have the distinct spin-1/2 τ_i. We use the notation: $(A_l, B_k)_\Delta \equiv A_l^x \otimes B_k^x + A_l^y \otimes B_k^y + \Delta A_l^z \otimes B_k^z$, with $A_l \equiv (A_l^x, A_l^y, A_l^z)$ and $B_k \equiv (B_k^x, B_k^y, B_k^z)$ to introduce the anisotropy in the z-direction. We impose periodic boundary conditions to the hamiltonian (1).

Hamiltonian (1) is a modified version of model B of Ref. [2] with $r_1 = \rho_1$ and $r_2 = \rho_2$. We introduce an anisotropy in the z-direction in the crossing interactions as well as in the interaction between first neighbours (see Fig. 1 of Ref.[1]). It is also a special case of the generalized spin ladder proposed by Kolezhuk and Mileska[3]to interpolate some quasi-one-dimensional gapped models. Hamiltonian (1) is the special case: $J_2 = J_3 = J_4$ of the hamiltonian in Ref.[4] that describes a frustrated spin ladder with diagonal couplings.

Defining the composite spin $\vec{S}_i$ at each site as

$$\vec{S}_i = \vec{\sigma}_i \otimes \mathbf{1}_\tau + \mathbf{1}_\sigma \otimes \vec{\tau}_i, \tag{2}$$

with $\mathbf{1}_\sigma$ being the identity in the σ-space and $\mathbf{1}_\tau$ being the identity in the τ-space, it is simple to realize that the tetrahedral spin-1/2 model (1) is mapped into the chain model

$$\begin{aligned} H_t &= \sum_{i=1}^{N} \big\{ -\frac{3}{4} J_0 \mathbf{1}_{4\times 4} + \frac{J_0}{2} S_i^2 \\ &+J[S_i^+ S_{i+1}^- + S_i^- S_{i+1}^+ + \Delta S_i^z S_{i+1}^z] - h S_i^z \big\}, \end{aligned} \tag{3a}$$

where $S_i^\pm \equiv \frac{1}{\sqrt{2}}(S_i^x \pm i S_i^y)$ and $S_i^2 \equiv \vec{S}_i \cdot \vec{S}_i$. The matrices in hamiltonian (3a), written in the basis of the eigenstates of S_i^z and S_i^2, are

$$S_i^2 = \begin{pmatrix} 2 & 0 & 0 & 0 \\ 0 & 2 & 0 & 0 \\ 0 & 0 & 2 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}_i, \quad S_i^z = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}_i, \tag{3b}$$

$$S_i^+ = \begin{pmatrix} 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}_i, \quad S_i^- = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}_i. \tag{3c}$$

The model described by hamiltonian (3a) is also subject to a periodic boundary condition. In matrices (3b) and (3c) we recognize the sectors $S = 0$ (singlet state) and $S = 1$ (triplet state) that come from the composite spin (2).

The method developed in Ref. [5] can be directly applied to the hamiltonian (3a) to obtain its thermodynamics in this region of temperature. The advantage of describing the tetrahedral spin-1/2 model in Fig. 1 of Ref.[1] by hamiltonian (3a) is that of recognizing a one-dimensional composite spin model that has already been studied in the literature[2, 6, 7].

References

[1] Onofre Rojas, E.V. Corra Silva, S.M. de Souza and M.T. Thomaz, "*The high temperature expansion of the tetrahedral spin-1/2 and spin-2 XXZ models*", Physical Review B vol. 69 (2004) 134405 (1-8). [link: http://dx.doi.org/10.1103/PhysRevB.69.134405].

[2] H. Niggemann, G. Uimin and J. Zittartz, J. Phys.: Condens. Matter **9**, 9031 (1997).

[3] A.K. Kolezhuk and H.-J. Mikeska, Phys. Rev. **B56**, R11 380 (1997).

[4] K. Totsuka and H.-J. Mikeska, Phys. Rev. **B66**, 054435 (2002).

[5] Onofre Rojas, S.M. de Souza and M.T. Thomaz), J. of Math. Phys. **43**, 1390 (2002).

[6] J. Sólyom and J. Timonen, Phys. Rev. **B34**, 487 (1986).

[7] J. Sólyom and J. Timonen, Phys. Rev. **B40**, 7150 (1989).