The hamiltonian of the S=1 spin ladder as a composite S =2 chain model

This text is part of Ref.[1].

The hamiltonian of the quasi-one-dimensional spin model is

$$
\begin{aligned}
H_{Q-1D} &= \sum_{i=1}^{N} \big\{ J_0[(\sigma_i,\tau_i)_{\Delta_0} + \frac{1}{2}(\Delta_0-1)((\sigma_i^z)^2\otimes \mathbf{1}_\tau + \mathbf{1}_\sigma \otimes (\tau_i^z)^2)] \\
&+ J[(\sigma_i,\sigma_{i+1})_\Delta \otimes \mathbf{1}_\tau + (\sigma_i,\tau_{i+1})_\Delta + (\tau_i,\sigma_{i+1})_\Delta + \mathbf{1}_\sigma \otimes (\tau_i,\tau_{i+1})_\Delta] \\
&- h(\sigma_i^z \otimes \mathbf{1}_\tau + \mathbf{1}_\sigma \otimes \tau_i^z)\big\}, \qquad (1)
\end{aligned}
$$

and it is subject to periodic boundary conditions. We use the same notation as in Ref.[2]: $(A_l,B_k)_\Delta \equiv A_l^x\otimes B_k^x + A_l^y\otimes B_k^y + \Delta A_l^z \otimes B_k^z$, with $A_l \equiv (A_l^x, A_l^y, A_l^z)$ and $B_k \equiv (B_k^x, B_k^y, B_k^z)$, introducing the anisotropy in the z-direction. For $\Delta_0 = 1$ and $\Delta = 1$, (1) equals to the sum of hamiltonians (2) and (3) of reference [3] for the $S=1$ ladder with second-neighbor exchanges ($J_3 = 0$), for the special case $J_1 = J_2$. The distinct $S=1$ variables σ_i and τ_i are related to the ρ- and r-lines of the dumb-bell, respectively (cf. Fig.1 of Ref.[2]).

We define the composite spin operators $\vec{S}_i$ at the i-th site as $\vec{S}_i = \vec{\sigma}_i \otimes \mathbf{1}_\tau + \mathbf{1}_\sigma \otimes \vec{\tau}_i$. Here, $\mathbf{1}_\sigma$ and $\mathbf{1}_\tau$ are the identity operators in σ- and τ-space, respectively. Using the composite spin $\vec{\mathbf{S}}_i$, the tetrahedral $S=1$ hamiltonian (1) is rewritten as a composite $S=2$ chain hamiltonian

$$
\begin{aligned}
\mathbf{H}_{Q-1D} &= \sum_{i=1}^{N} \left[-2J_0\mathbf{1} + g(\mathbf{S}_i,\mathbf{S}_i)_1 + J\left(\mathbf{S}_i^+\mathbf{S}_{i+1}^- + \mathbf{S}_i^-\mathbf{S}_{i+1}^+ + \Delta \mathbf{S}_i^z\mathbf{S}_{i+1}^z\right)\right. \\
&\qquad \left. -h\mathbf{S}_i^z + d(\mathbf{S}_i^z)^2 \right], \qquad (2)
\end{aligned}
$$

where $g \equiv \frac{J_0}{2}$, $d \equiv \frac{J_0}{2}(\Delta_0 - 1)$, $S_i^\pm \equiv \frac{1}{\sqrt{2}}(S_i^x \pm iS_i^y)$, and $\mathbf{1}$ is the identity operator, represented by a 9×9 identity matrix. The block matrix representations of the composite spin operators in (2), in the basis of eigenstates of $\mathbf{S}_i^z$ and $\vec{\mathbf{S}}_i^2$, are

$$
S_i^z = \begin{bmatrix} \Sigma^z_{(2)} & 0 & 0 \\ 0 & \Sigma^z_{(1)} & 0 \\ 0 & 0 & \Sigma^z_{(0)} \end{bmatrix} \quad \text{and} \quad S_i^+ = \begin{bmatrix} \Sigma^+_{(2)} & 0 & 0 \\ 0 & \Sigma^+_{(1)} & 0 \\ 0 & 0 & \Sigma^+_{(0)} \end{bmatrix}, \qquad (3)
$$

where the Σ square matrices refer to the different spin sectors,

$$\Sigma^z_{(2)} = \begin{bmatrix} -2 & 0 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 2 \end{bmatrix} \quad , \quad \Sigma^+_{(2)} = \begin{bmatrix} 0 & 0 & 0 & 0 & 0 \\ \sqrt{2} & 0 & 0 & 0 & 0 \\ 0 & \sqrt{3} & 0 & 0 & 0 \\ 0 & 0 & \sqrt{3} & 0 & 0 \\ 0 & 0 & 0 & \sqrt{2} & 0 \end{bmatrix},$$

$$\Sigma^z_{(1)} = \begin{bmatrix} -1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 1 \end{bmatrix} \quad , \quad \Sigma^+_{(1)} = \begin{bmatrix} 0 & 0 & 0 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{bmatrix},$$

$$\Sigma^z_{(0)} = \begin{bmatrix} 0 \end{bmatrix} \quad , \quad \Sigma^+_{(0)} = \begin{bmatrix} 0 \end{bmatrix}. \tag{4}$$

We point out that the operator $\vec{\mathbf{S}}_i^2$ is a constant of the motion, although the hamiltonian (2) can be interpreted as mixture of 3 kinds of spin ($S = 0, 1$ and 2), randomly distributed along the chain, with its probability depending on the constants of the hamiltonian and on the temperature.

An interesting limit of the hamiltonian (2) is $g = J_0/2 \to 0$, for finite values of $d \equiv \frac{J_0 \Delta_0}{2}$. In this limit it acquires a single-ion anisotropy term.

As in Ref.[2], the presence of a spin $S = 0$ in a site of the chain can be interpreted as nonmagnetic impurity at that site. The model thus encompasses the presence of randomly distributed impurities along the chain, without hindering the application of the method of Ref. [4], since the hamiltonian (2) has only nearest-neighbor interactions and is invariant under spatial translations.

References

[1] Onofre Rojas, E.V. Corra Silva, S.M. de Souza and M.T. Thomaz, "*Thermodynamics of the S=1 spin ladder as a composite S=2 chain model*", Physica A vol. 356 (2005) 575-588. [link: http://dx.doi.org/10.1016/j.physa.2005.02.091]

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[3] T. Sakai *et al.*, Phys. Stat. Sol.(b) **236**, 429 (2003).

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