Absence of the Ferro-Quadrupole Ordering at Zero Temperature in One Dimension

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Abstract

By using the Shastry inequality and infrared bounds based on reflection positivity, we prove the absence of quadrupole ordering in the ground state of the spin-S isotropic Hamiltonian with bilinear $-J$ and biquadratic $-J^{'}$ exchange interactions in the one dimensional system in the region $J^{'} > 2S^2 J, J^{'} > 0$.

Key words: ferro-quadrupole moment; ground state; one dimension; Shastry inequality; infrared bounds; reflection positivity

At finite temperature the absence of spontaneous symmetry breaking (SSB) associated with dipole moment in one- and two-dimensional isotropic quantum spin systems with short range interactions has been established by the Mermin-Wagner theorem [1]. Its extension gives the proof of the absence of SSB associated with multipole moment in the isotropic multipole interaction systems [2,3].

On the other hand, at zero temperature the proof of the absence of dipole ordering (SSB or long range order (LRO)) for the one dimensional (1D) isotropic Heisenberg antiferromagnet has been given by the Shastry inequality [4] and the infrared bounds based on reflection positivity (RP) [5]. However, the absence of multipole ordering in the ground state (GS) of 1D systems have not been established yet.

In this paper we discuss the isotropic spin-S ($\boldsymbol{S} = (S_1, S_2, S_3)$) Hamiltonian with bilinear and biquadratic nearest-neighbor interactions:

$$\mathcal{H}_\Lambda = -\frac{J}{S^2}\sum_{\langle x,y\rangle} \boldsymbol{S}(x)\cdot\boldsymbol{S}(y) - \frac{J^{'}}{S^4}\sum_{\langle x,y\rangle}\left(\boldsymbol{S}(x)\cdot\boldsymbol{S}(y)\right)^2, \quad (1)$$

on a 1D chain Λ with an even number of sites $|\Lambda|$ and periodic boundary condition in the region $J^{'} > 2S^2 J, J^{'} \geq 0$, where the Hamiltonian satisfies RP [6]. In the case of $S = 1$, the GS of this model on a square or a simple cubic lattice is expected to be antiferromagnetic in the region $J < 0, J^{'} > 0$ and ferro-quadrupolar (FQ) in $J^{'} > J > 0$ [7]. In the case of $S > 1$, these phases are believed to be stable in the considered region. In the present paper we prove the absence of dipole and quadrupole ordering in the GS of the 1D system.

First, we prove the absence of quadrupole ordering. Now we use the quadrupole operators Q_q, $q = \{20, 22, xy, yz, zx\}$, then Hamiltonian (1) can be written as

$$\mathcal{H}_\Lambda = J_{\rm D}\sum_{\langle x,y\rangle}\boldsymbol{S}(x)\cdot\boldsymbol{S}(y) - J_{\rm Q}\sum_{\langle x,y\rangle}\sum_q Q_q(x)Q_q(y),$$

where $J_{\rm D} = -J/S^2 + J^{'}/(2S^4)$, $J_{\rm Q} = 2J^{'}/(3S^4)$ and $Q_{20} = [3S_3^2 - S(S+1)]/2$, $Q_{22} = (\sqrt{3}/2)(S_1^2 - S_2^2)$, $Q_{xy} = (\sqrt{3}/2)(S_1S_2 + S_2S_1)$, $Q_{yz} = (\sqrt{3}/2)(S_2S_3 + S_3S_2)$, $Q_{zx} = (\sqrt{3}/2)(S_3S_1 + S_1S_3)$.

In reference [4] Shastry derived the following inequality:

$$\left\langle\{B^\dagger, B\}\right\rangle \geq \frac{\left|\left\langle\left[A^\dagger, B\right]\right\rangle\right|^2}{\sqrt{\langle[[A^\dagger,\mathcal{H}],A]\rangle}\,\beta\,(A^\dagger, A)}$$

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$$\times \coth\left(\frac{\beta}{2}\sqrt{\frac{\langle[[A^\dagger,\mathcal{H}],A]\rangle}{\beta\,(A^\dagger,A)}}\right),$$

where the Duhamel-two point function $(A^\dagger, A)$ is defined by $Z^{-1}\int_0^1 \mathrm{Tr}(e^{-t\beta\mathcal{H}}A^\dagger e^{-(1-t)\beta\mathcal{H}}A)dt$ with partition function Z, and inverse temperature β. Setting the Fourier transformed operators $A = S_3(k)$, $B = Q_{xy}(k)$, and $\mathcal{H} = \mathcal{H}^{\mathrm{Q}}_\Lambda = \mathcal{H}_\Lambda - h\sqrt{|\Lambda|}Q_{22}(0)$, we have,

$$\left\langle\left\{Q^\dagger_{xy}(k), Q_{xy}(k)\right\}\right\rangle_{h\Lambda\beta} = 2\left\langle Q_{xy}(-k)Q_{xy}(k)\right\rangle_{h\Lambda\beta},$$

$$\left|\left\langle\left[S^\dagger_3(k), Q_{xy}(k)\right]\right\rangle_{h\Lambda\beta}\right|^2 = 4\left(m^{\mathrm{Q}}_{h\Lambda\beta}\right)^2,$$

$$\left\langle\left[\left[S^\dagger_3(k),\mathcal{H}^{\mathrm{Q}}_\Lambda\right],S_3(k)\right]\right\rangle_{h\Lambda\beta} = C_{h\Lambda\beta}E_k + 4hm^{\mathrm{Q}}_{h\Lambda\beta}$$

with

$$C_{h\Lambda\beta} = 2J_{\mathrm{D}}\sum_{i\neq 3}\langle S_i(x)S_i(y)\rangle_{h\Lambda\beta}$$

$$+2J_{\mathrm{Q}}\left(4\sum_{q=22,xy}\langle Q_q(x)Q_q(y)\rangle_{h\Lambda\beta} + \sum_{q=yz,zx}\langle Q_q(x)Q_q(y)\rangle_{h\Lambda\beta}\right),$$

$m^{\mathrm{Q}}_{h\Lambda\beta} = |\Lambda|^{-1}\sum_{x\in\Lambda}\langle Q_{22}(x)\rangle_{h\Lambda\beta}$, and $E_k = 1 - \cos k$. Expectation values of X in the following cases are denoted by $\lim_{h\to 0}\lim_{\Lambda\to\infty}\lim_{\beta\to\infty}\langle X\rangle_{h\Lambda\beta} = \lim_{h\to 0}\lim_{\Lambda\to\infty}\langle X\rangle_{h\Lambda} = \lim_{h\to 0}\langle X\rangle_h = \langle X\rangle$. An upper bound on the Duhamel two-point function is given by

$$\beta\left(S^\dagger_3(k), S_3(k)\right) \leq 1/(2E_{k-\pi}) \qquad (2)$$

in the region $J^{'} > 2S^2J, J^{'} \geq 0$, where $\mathcal{H}_\Lambda$ satisfies RP [5,6]. Since the uniform field term $-h\sqrt{|\Lambda|}Q_{22}(0)$ does not invalidate RP and the derivation of inequality (2) is independent of this field term, this upper bound remains intact for $\mathcal{H}^{\mathrm{Q}}_\Lambda$.

By using inequality (2), we have, in the limit $\beta\to\infty$,

$$\langle Q_{xy}(-k)Q_{xy}(k)\rangle_{h\Lambda} \geq \left(m^{\mathrm{Q}}_{h\Lambda}\right)^2\sqrt{\frac{8}{C_{h\Lambda}}}\sqrt{\frac{E_{k-\pi}}{E_k + \gamma^{\mathrm{Q}}_{h\Lambda}h}}$$

with $\gamma^{\mathrm{Q}}_{h\Lambda} = 4m^{\mathrm{Q}}_{h\Lambda}/C_{h\Lambda}$. Summing both sides of this inequality over k and dividing by $|\Lambda|$, we obtain,

$$\left\langle(Q_{xy}(x))^2\right\rangle_{h\Lambda} \geq \frac{\left(m^{\mathrm{Q}}_{h\Lambda}\right)^2}{|\Lambda|}\sqrt{\frac{8}{C_{h\Lambda}}}\sum_k\sqrt{\frac{E_{k-\pi}}{E_k + \gamma^{\mathrm{Q}}_{h\Lambda}h}}.$$

Finally, taking $\Lambda\to\infty$, we have,

$$\left\langle(Q_{xy}(x))^2\right\rangle_h \geq \left(m^{\mathrm{Q}}_h\right)^2\sqrt{\frac{8}{C_h}}\frac{1}{2\pi}\int_{-\pi}^{\pi}\sqrt{\frac{E_{k-\pi}}{E_k + \gamma^{\mathrm{Q}}_h h}}dk$$

$$= \frac{2\left(m^{\mathrm{Q}}_h\right)^2}{\pi}\sqrt{\frac{8}{C_h}}\tanh^{-1}\left(\sqrt{\frac{2}{2+\gamma^{\mathrm{Q}}_h h}}\right).$$

Taking $h\to 0$, we see that the right hand side diverges, but the left hand side takes a finite value. Therefore, m^{Q} must vanish. Following the argument in reference [9], we see that the absence of SSB associated with FQ moment assures the absence of FQ-LRO in the GS.

On the other hand, in the region $J^{'} \geq 2S^2J, J^{'} > 0$, an upper bound on the Fourier transformed two-point quadrupole correlation function for $k \neq 0$ (i.e., infrared bound) in finite volume GS can be constructed [5,6]. Thus, quadrupole-LRO which would be realized in the infinite volume GS is a ferro-type.

We have proven the absence of quadrupole-LRO in the region $J^{'} > 2S^2J, J^{'} > 0$ (strictly speaking, the absence of SSB associated with FQ-moment and quadrupole-LRO for $k \neq 0$).

Next, we prove the absence of dipole ordering. In this case, we choose $A = S_3(k), B = S_2(k+\pi), \mathcal{H} = \mathcal{H}_\Lambda - h\sqrt{|\Lambda|}S_1(\pi)$. Then we have, in the infinite volume GS,

$$\left\langle(S_2(x))^2\right\rangle_h \geq \frac{\left(m^{\mathrm{D}}_h\right)^2}{\pi}\sqrt{\frac{2}{C_h}}\tanh^{-1}\left(\sqrt{\frac{2}{2+\gamma^{\mathrm{D}}_h h}}\right)$$

with $m^{\mathrm{D}}_h = \lim_{\Lambda\to\infty}\lim_{\beta\to\infty}|\Lambda|^{-1}\sum_{x\in\Lambda}(-1)^x\langle S_1(x)\rangle_{h\Lambda\beta}$ and $\gamma^{\mathrm{D}}_h = m^{\mathrm{D}}_h/C^{\mathrm{D}}_h$ (here we should note that the staggered field term also does not invalidate RP). Following the same arguments as for the quadrupole case, this inequality leads to $m^{\mathrm{D}} = 0$. From the infrared bound on the Fourier transformed dipole correlation function for $k \neq \pi$ in the region $J^{'} > 2S^2J, J^{'} \geq 0$ [5,6], dipole-LRO for $k \neq \pi$ is absent in infinite volume GS. Thus we reach similar conclusion to the one for the quadrupole case in $J^{'} > 2S^2J, J^{'} \geq 0$ [9].

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