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Failure of Reflection Positivity in the Quantum Heisenberg Ferromagnet

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Abstract. We show that reflection positivity does not hold in the finite-volume spin $\frac{1}{2}$ quantum Heisenberg ferromagnet in two cases: (i) for any dimension or degree of S^1-invariant anisotropy, above a volume independent temperature T_0, and (ii) for the isotropic model in one dimension, below a volume dependent temperature T_1.

0. Introduction

Reflection positivity (RP) has been a powerful tool for investigating the occurrence of phase transitions, but it is limited to very special models. Here we consider the spin $\frac{1}{2}$ quantum Heisenberg ferromagnet in dimension d, in finite volume with periodic boundary conditions. It was pointed out in [1, 2] that RP for the subalgebra of observables generated by the z components of the spin would suffice to establish the existence of a phase transition in $d \geqslant 2$ for the prolate anisotropic model (a result recently achieved by other methods [3]). Reflection positivity in the Heisenberg model does not follow from standard arguments, but the possibility of its existence was not ruled out.

In this Letter we present several examples which show that RP (with the standard reflection operator) in fact fails in several regimes; moreover, we know of no evidence for its validity in other regimes except for extremely small systems (see Section 2). Specifically: (i) for any dimension d and any S^1-symmetric anisotropy, RP fails above a volume independent temperature T_0, and fails for local observables above a volume dependent temperature $T_0(\Lambda)$; (ii) in dimension $d = 1$, RP fails for the isotropic model below a volume dependent temperature $T_1(\Lambda)$; and (iii) for the isotropic linear chain with six sites, numerical evidence indicates that reflection positivity fails at all temperatures.

1. The Model

Let Λ be the finite lattice $\Lambda = \{i \in \mathbb{Z}^d \mid -N_k + 1 \leqslant i_k \leqslant N_k\}$ and define $\theta\colon \Lambda \to \Lambda$ by $\theta(i_1, \ldots, i_d) = (1 - i_1, i_2, \ldots, i_d)$. Λ is partitioned as $\Lambda = \Lambda_+ \cup \Lambda_-$, with

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$\Lambda_+ = \{i \in \Lambda \mid i_1 \geqslant 1\}$ and $\Lambda_- = \theta(\Lambda_+)$. The Hilbert space of our theory is $\mathscr{H} = \otimes_{i \in \Lambda} \mathbb{C}^2$, and we define a reflection (also called θ) on operators in $\mathscr{H}$ by antilinear extension of $\theta(\otimes_\Lambda k_i) = \otimes_\Lambda \overline{K_{\theta i}}$. At each site i there is a spin $\frac{1}{2}$ operator $s^i = (s^i_x, s^i_y, s^i_z)$ which is represented by the standard 2×2 matrices. The Hamiltonian is

$$H = -2 \sum_{\langle i,j \rangle} [s^i_z s^j_z + \alpha(s^i_x s^j_x + s^i_y s^j_y)] + \tfrac{1}{2} d|\Lambda| ,$$

where $\alpha > 0$, the sum is over nearest neighbor pairs, defined with periodic boundary conditions, and the additive constant is chosen to give zero ground-state energy in the isotropic case.

Let $\mathscr{A}_+$ be the algebra of operators generated by $\{s^i_z \mid i \in \Lambda_+\}$. Reflection positivity is the property that, for all $F \in \mathscr{A}_+$,

$$\mathrm{Tr}(\mathrm{e}^{-\beta H} F\theta(F)) \geqslant 0 . \tag{1}$$

To rewrite (1) more explicitly, we introduce the orthonormal basis $\{\Psi_X \mid X \subset \Lambda\}$ for $\mathscr{H}$, defined by

$$\Psi_X = \bigotimes_{i \in \Lambda} \left\{[(-\chi_X(i)]\begin{pmatrix}1\\0\end{pmatrix} + \chi_X(i)\begin{pmatrix}0\\1\end{pmatrix}\right\}$$

with χ_X the characteristic function of X. For $A, B \subset \Lambda_+$ write $\Phi_{AB} = \Psi_{\theta(A) \cup B}$, and for $B \subset \Lambda_+$, let P_B be the projector

$$P_B \Psi = \sum_{A \subset \Lambda_+} (\Phi_{AB}, \Psi)\Phi_{AB} .$$

Then any $F \in \mathscr{A}_+$ may be written $F = \Sigma_{B \subset \Lambda_+} f_B P_B$, $f_B \in \mathbb{C}$, and for any operator K,

$$\mathrm{Tr}(KF\theta(F)) = \sum_{A,B \subset \Lambda_+} \bar{f}_A \tilde{K}_{AB} f_B \equiv f^* \tilde{K} f, \tag{2}$$

with $\tilde{K}_{AB} \equiv (\Phi_{AB}, K\Phi_{AB})$. Thus, (1) becomes:

$$f^* \mathrm{e}^{-\beta H} f \geqslant 0 , \quad f \in \mathbb{C}^{2^{|\Lambda|}} . \tag{3}$$

2. Small Lattices

The quadratic form (2) may be computed explicitly for small systems; here we report results for the isotropic system in one dimension ($d = \alpha = 1$). For lattices with two or four sites, it can be shown that RP holds. For six sites, we have determined the eigenvalues of the quadratic form numerically, and conclude that RP fails at all temperatures.

3. High Temperature

Our main result in the high temperature regime is Theorem 3.2. We describe some additional conclusions in Remark 3.4. We first note

PROPOSITION 3.1. *The Heisenberg model is reflection positive at infinite temperature.*
Proof. Trivial ([2]).

THEOREM 3.2. *Suppose $N_1 \geqslant 5$. Then there is a β_0, depending on α and d but not on Λ, such that for some $F \in \mathscr{A}_+$ and any $\beta < \beta_0$, $\mathrm{Tr}(e^{-\beta H} F\theta(F)) < 0$; i.e., RP fails at temperatures $T > \beta_0^{-1}$.*

Proof. The theorem follows immediately on expanding $\mathrm{Tr}(e^{-\beta H} F\theta(F)) = f^* \widetilde{(e^{-\beta H})} f$ in powers of β and applying

LEMMA 3.3. *There exist Λ-independent constants c_1, c_2, and ρ such that for some $(f_A)_{A \subset \Lambda_+}$ we have (i) $f^*\widetilde{H^k}f = 0$, $k = 0, 1, 2, 3$; (ii) $f^*\widetilde{H^4}f \leqslant c_1 < 0$; (iii) $|f^*\widetilde{H^k}f| \leqslant c_2\rho^k k!$, $k \geqslant 0$.*

Proof. We must investigate $(\widetilde{H^k})_{AB} = (\Phi_{AB}, H^k\Phi_{AB})$. Now

$$
\begin{aligned}
H\Phi_{AB} &= m_{AB}\Phi_{AB} - \alpha \sum_{\langle i,j\rangle \in \Gamma_{AB}} \Phi_{A'B'} \\
&\equiv H^z\Phi_{AB} + \alpha H^{xy}\Phi_{AB},
\end{aligned}
\tag{4}
$$

where Γ_{AB} is the Peierls contour associated with $\theta(A) \cup B \subset \Lambda$, $m_{AB} = |\Gamma_{AB}|$, and $\Phi_{A'B'}$ is obtained from Φ_{AB} by flipping the i, j spins. For $k \leqslant 4$ write $H^k = X^{(k)} + \alpha^2 Y^{(k)} + \alpha^4 Z^{(k)}$ and consider these terms successively.

(a) From (4), $X_{AB}^{(k)} = m_{AB}^k$. Write

$$
m_{AB} = n_A + n_B - 2 \sum_{i \in \partial\Lambda_+} u_{Ai}u_{Bi},
$$

where

$$
\partial\Lambda_+ = \{i \in \Lambda \mid i_1 = 1 \text{ or } N\}, \qquad u_{Ai} = \chi_A(i) \quad \text{and} \quad n_A = \tfrac{1}{2}m_{AA} + u_A \cdot u_A .
$$

Then $f^*X^{(k)}f = 0$ for $0 \leqslant k \leqslant 4$ if for all ℓ, $m \geqslant 0$, $2\ell + m \leqslant 4$, and all $i_1, \ldots, i_m \in \partial\Lambda_+$,

$$
\sum_{A \subset \Lambda_+} f_A n_A^\ell u_{Ai_1} \ldots u_{Ai_m} = 0. \tag{5}
$$

From now on we consider only $F \in \mathscr{A}_+$ satisfying (5).

(b) $Y^{(k)}$ is zero for $k < 2$; for $k \geqslant 2$ the two occurrences of H^{xy} must each flip the spins of the same pair $\langle i, j\rangle$. Using (5) we see that the contribution to $f^*Y^{(k)}f$ vanishes unless $i \in \Lambda_+$, $j = \theta(i) \in \Lambda_-$, unless $k = 4$, and unless the operators in H^4 act in the order $H^{xy}(H^z)^2H^{xy}$. Writing $A^{(i)} \equiv A\Delta\{i\}$ in this surviving case, we have a net contribution

$$
f^*Y^{(4)}f = 2 \sum_{i \in \partial\Lambda_+} \sum_{A, B \subset \Lambda_+} (\bar{x}_A n_{A^{(i)}})(x_B n_{B^{(i)}})(u_{Ai} - u_{Bi})^2 . \tag{6}
$$

(c) $Z^{(k)}$ vanishes unless $k = 4$, when $Z_{AB}^{(4)} = (\Phi_{AB}, (H^{xy})^4 \Phi_{AB})$. We can show that $f^*Z^{(4)}f = 0$ by repeated application of (5). Suppose, for example, that $(H^{xy})^4$ acts to flip four spin pairs on bonds which form a plaquette P, with corners $i_1, \ldots, i_4$ in cyclic order. A computation of various cases shows that the total contribution to $Z_{AB}^{(4)}$ from such, all such processes may be written as

$$
\sum_P \left[\left(\sum_{r=1}^{4} \gamma_{AB}(\langle i_r, i_{r+1}\rangle) \right) + 2 \sum_{r=1}^{2} \gamma_{AB}(\langle i_r, i_{r+2}\rangle)\gamma_{AB}(\langle i_{r+1}, i_{r+3}\rangle) \right], \tag{7}
$$

where γ_{AB} is the characteristic function of Γ_{AB}. Writing $\gamma_{AB}(\langle i, \theta(i)\rangle) = (u_{Ai} - u_{Bi})^2$ and applying (5) shows that the contribution to $f^*Z^{(4)}f$ from (7) vanishes. Other ways that $(H^{xy})^4$ may act are treated similarly.

We conclude that whenever f satisfies (5), $f^*\tilde{H}^k f$ vanishes for $0 \leqslant k \leqslant 3$ and for $k = 4$ is given (up to a factor α^2) by (6). We now choose f so that (6) is negative. Define Λ' by $\Lambda = [-N_1 + 1, N_1] \times \Lambda'$ and choose a fixed, nonempty $E \subset \Lambda'$. Let $A_r = \{1, \ldots, r\} \times E \subset \Lambda_+$ for $1 \leqslant r \leqslant 4$, $B_r = \{r+1\} \times E \subset \Lambda_+$ for $r = 1, 2$, and set $f_{A_1} = -f_{A_4} = y, f_{A_2} = -f_{A_3} = -3y, f_{B_1} = -f_{B_2} = z$, for y, z real, and $f_A = 0$ otherwise. Now u_{A_r}, u_{B_r}, and n_{B_r} are independent of r, while $n_{A_r} = |E| + r|\Gamma_E|$ with Γ_E the contour in Λ' defined by E (here we need $N_1 \geqslant 5$), so that (5) is satisfied. Evaluation of (6) is straightforward; using (5) repeatedly we have

$$f^*\tilde{H}^4 f = 4\alpha^2 \sum_{i \in E} \left(\sum_{r=1}^{4} n_{A(i)} f_{A_r}\right)\left(\sum_{s=1}^{2} n_{B(i)} f_{B_s}\right)$$
$$= 16\alpha^2 |E| yz .$$

Taking $y = 1$, $z = -1$ completes the proof of (i) and (ii) of Lemma 3.3 with $c_1 = -16\alpha^2|E|$.

It remains to verify (iii) of the Lemma. But for $A, B \subset [1, 4] \times E$, an easy induction shows that

$$\tilde{H}^n \Phi_{AB} = \sum_{C, D \subset \Lambda_+} a_{CD}^{(n)} \Phi_{CD}$$

with

$$\sum_{C, D} |a_{CD}^{(n)}| \leqslant [16d\,|E|\,(1+\alpha)]^n\, n!$$

and with $m_{CD} \leqslant 2d(8|E| + n)$ whenever $a_{CD}^{(n)} \neq 0$. Thus, (iii) holds with $c_2 = 36$, $\rho = 16d|E|(1+\alpha)$. □

REMARK 3.4. (a) The observable constructed above has the form

$$F = \sum_{C} f_C P_C \tag{8}$$

with C running over $A_1, \ldots, A_4, B_1, B_2$. If in (8) we replace P_C by Q_C, where Q_C projects onto $\{\Psi \mid \Psi_i = (P_C\Psi)_i, i \in \Lambda_0\}$ with Λ_0 some fixed region amply containing $[1, 4] \times E$, we obtain an observable satisfying (i) and (ii), but not (iii), of Lemma 3.3. Thus, RP is violated by localized observables above some temperature $\beta_0(\Lambda)^{-1}$.

(b) Another modification of the example, involving $E = \Lambda'$ and, thus, global observables, and having Λ-dependent temperature $\beta_0(\Lambda)^{-1}$, disproves RP for all lattices with $N_1 \geqslant 3$. We omit details.

4. Low Temperature

In this section we consider only the isotropic ($\alpha = 1$) model. Our first observation is due to E. Lieb (private communication).

PROPOSITION 4.1. *The isotropic Heisenberg model is reflection positive at zero temperature.*

Proof. We must show that $\mathrm{Tr}(Q_0 F\theta(F)) \geqslant 0$ for any $F \in \mathscr{A}_+$, where Q_0 projects onto the subspace $\mathscr{H}_0$ of minimal (here zero) energy. $\mathscr{H}_0$ is the subspace of maximal total spin $N \equiv \frac{1}{2}|\Lambda|$ and is spanned by $\{\Theta_0^{(n)}\}_{n=0}^{2N}$, where $\Theta_0^{(n)} = \Sigma_{|X|=n}\Psi_X$. Using $(\Theta_0^{(n)}, \Theta_0^{(n)}) = \binom{2N}{n}$ and (2), and writing $u_\ell(F) = \Sigma_{|A|=\ell} f_A$, we have

$$\mathrm{Tr}(Q_0 F\theta(F)) = \sum_{n=0}^{2N} \binom{2N}{n}^{-1} \Big|\sum_{A,B\subset\Lambda_+} \bar{f}_A f_B\ (\Phi_{AB}, \Theta_0^{(n)})\Big|^2$$

$$= \sum_{\ell,m=0}^{N} \bar{u}_\ell u_m \binom{2N}{\ell+m}^{-1} \tag{9}$$

$$= [(2N)!]^{-1} \int_0^\infty \mathrm{d}t \int_0^\infty ds\, \mathrm{e}^{-(t+s)} s^{2N} \left(\sum_{\ell=0}^{N} u_\ell t^\ell s^{-\ell}\right)^2 .$$

Note that the quadratic form is positive definite in the u variables. □

The main result of this section is

THEOREM 4.2. *For the isotropic Heisenberg model in one dimension with at least six sites ($\alpha = d = 1$, $N \equiv N_1 \geqslant 3$) there exist $\beta_1(N) < \infty$ and $F \in \mathscr{A}_+$ so that if $\beta > \beta_1$,*

$$\mathrm{Tr}(\mathrm{e}^{-\beta H} F\theta(F)) < 0\,;$$

that is, RP fails at temperatures $T < \beta_1(N)^{-1}$.

Proof. Let $\mathscr{H}^{(n)} \subset \mathscr{H}$ be the space of 'n-magnon' states, i.e., the subspace of $\mathscr{H}$ spanned by $\{\Psi_X \ |X| = n\}$. $\mathscr{H}^{(n)}$ is an invariant space for H; let $H|_{\mathscr{H}^{(n)}}$ have eigenvalues $E_0^{(n)} < E_1^{(n)} < \ldots$ and corresponding eigenspaces $\{\mathscr{H}_k^{(n)}\}$ with orthogonal projections $\{Q_k^{(n)}\}$. (We know as above that $E_0^{(n)} = 0$ with $\mathscr{H}_0^{(n)}$ spanned by $\Theta_0^{(n)}$.) Now let $\mathscr{A}_+^{(m)} \subset \mathscr{A}_+$ consist of observables of the form

$$F = \sum_{|A|=m} f_A P_A\,; \quad \text{for } F \in \mathscr{A}_+^{(m)},$$

$$\mathrm{Tr}(\mathrm{e}^{-\beta H} F\theta(F)) = \sum_k \mathrm{e}^{-\beta E_k^{(2m)}} \mathrm{Tr}(Q_k^{(2m)} F\theta(F)) .$$

Hence, Theorem 4.2 (with $F \in \mathscr{A}_+^{(1)}$) will follow from

LEMMA 4.3. *There exists an $F \in \mathscr{A}_+^{(1)}$ such that $\mathrm{Tr}(Q_0^{(2)} F\theta(F)) = 0$ and $\mathrm{Tr}(Q_1^{(2)} F\theta(F)) < 0$.*

We need a lemma, whose proof will be delayed until the Appendix, describing $Q_1^{(2)}$:

LEMMA 4.4. *$E_1^{(2)} = 4\sin^2(\pi/2N)$, and $\mathscr{H}_1^{(2)}$ is a two-dimensional space spanned by the (spin wave) states*

$$\Theta_{\pm 1}^{(2)} \equiv \sum_{\substack{j,k\in\Lambda \\ j\neq k}} \mathrm{e}^{\pm i\pi j/N}\, \Psi_{\{j,k\}} \,.$$

Proof of Lemma 3.3. Introduce the basis $\{F^{(\ell)}\}_{\ell=1}^{N}$ for $\mathscr{A}_{+}^{(1)}$ given by

$$F^{(\ell)} = \sum_{j \in \Lambda_+} e^{i2\pi\ell j/N} P_{\{j\}},$$

and for $F \in \mathscr{A}_{+}^{(1)}$ write $F = \Sigma \hat{f}_j F^{(j)}$. The condition

$$\hat{f}_N \equiv u_1(F) = 0 \tag{10}$$

implies by (9) that $\mathrm{Tr}(Q_0 F\theta(F)) = 0$; we consider only $F \in \mathscr{A}_{+}^{(1)}$ satisfying (10). Set $C = (\Theta_{\pm 1}^{(2)}, \Theta_{\pm 1}^{(2)}) = 4N(N-1)$; then by Lemma 4.4 and a direct calculation

$$\begin{aligned}\mathrm{Tr}(Q_1^{(2)} F\theta(F)) &= C^{-1} \sum_{\sigma = \pm 1} \sum_{\ell, m = 1}^{N-1} \hat{f}_\ell \hat{f}_m (\Theta_\sigma^{(2)}, F^{(m)}\theta(F^{(\ell)})\Theta_\sigma^{(2)}) \\ &= 16 C^{-1}\, \mathrm{Re}[(\hat{f}^* g)(h^* \hat{f})],\end{aligned} \tag{11}$$

with

$$g_\ell = e^{i\pi/2N}[1 - e^{i\pi(2\ell+1)/N}]^{-1},$$

$$h_m = e^{-i\pi/2N}[1 - e^{i\pi(2m-1)/N}]^{-1}.$$

But (11) cannot define a positive form, since g and h are linearly independent. For, consider $\hat{f} = \|g\|^{-1} g + \zeta \|h\|^{-1} h$ with $|\zeta| = 1$. Then

$$(\hat{f}^* g)(h^* \hat{f}) = \|g\|\, \|h\|\, (\zeta + \zeta^{-1}\eta)^2,$$

with $\eta = h^* g / \|g\|\, \|h\|$ and, hence, $|\eta| < 1$; since the map $w(z) = (z^{-1} = \eta z)^2$ vanishes at $z = \pm(-\eta)^{-1/2}$ inside the unit disc, we must have $w(\zeta) < 0$ for some ζ with $|\zeta| = 1$.

REMARK 4.5. Similar arguments might be used to disprove RP in dimensions $d > 1$. For example if $N_1 > \max\{N_2, \ldots, N_d\}$, we would again expect the lowest energy excitations to be two-spin-wave states of momenta 0 and $(\pm(\pi/N), 0, 0 \ldots 0)$; if so, the same mechanism as above gives a counter example.

Appendix

The spectrum of the Heisenberg ferromagnet in the two-magnon sector has been intensively investigated (see [4] and references therein) and Lemma 4.4 is hardly a surprising result: we sketch a proof from the development in [4]. Write $E_1 = 4\sin^2(\pi/2N)$. It is immediate that $H\Theta_{\pm 1}^{(2)} = E_1 \Theta_{\pm 1}^{(2)}$; we verify that the only eigenvalue of H less than E_1 (in $\mathscr{H}^{(2)}$)) is 0, and that 0 and E_1 have degeneracies 1 and 2, respectively. For the case $\sigma = 0, 1$ let Λ_σ^* be the dual lattice $\Lambda_\sigma^* = \{q = (2j - \sigma)\pi/2N \mid -(N-1) \leqslant j \leqslant N\}$, and for $q \in \Lambda_0^*$ define $\sigma(q)$ by $\frac{1}{2}q \in \Lambda_{\sigma(q)}^*$. Then by a slight extension of [4] it suffices to show: for any $K \in \Lambda_0^*$ and any $E \leqslant E_1$,

$$S_{K,K}(E) \neq 1, \tag{A1}$$

where

$$S_{Q,K}(E) = \frac{4}{N} \sum_{q \in \Lambda_{\sigma(K)}^*}{}' \frac{(\cos Q/2 - \cos q)\cos q}{E - 4(1 - \cos Q/2 \cos q)} \tag{A2}$$

and in Σ' we omit $q = \pm(K/2)$ for $K = 0, \pm\pi/N$. Clearly we may restrict consideration to $0 \leqslant K \leqslant \pi$.

To check (A1), we observe that

$$\frac{\mathrm{d}}{\mathrm{d}(\cos Q/2)} S_{Q,K}(E) = \frac{4}{N} \sum_{q \in \Lambda^*_{\sigma(K)}} \frac{(E - 4\sin^2 q)\cos q}{[E - 4(1 - \cos Q/2 \cos q)]^2}. \tag{A3}$$

Pair the q and $\pi - q$ terms in (A3); for $E \leqslant E_1$ each pair except $(0, \pi)$ (occurring only for $\sigma(K) = 0$), and each unpaired term (occurring only for $K = 0, \pm\pi/N$), gives a zero or negative contribution. Thus, for $\sigma(K) = 1$ or $K = 0$, (A3) is nonpositive, and integrating this inequality from $Q = \pi$ to $Q = K$ shows that

$$S_{K,K}(E) \leqslant S_{\pi,K}(E) = \frac{2}{4 - E} < 1$$

for $\sigma(K) = 1$ or $K = 0$. If $K \neq 0$ but $\sigma(K) = 0$, we compute the $q = 0$ term in $S_{K,K}(E)$ directly and treat the others as above, finding

$$S_{K,K}(E) \leqslant \left[\frac{2}{4 - E} - \frac{4}{N(4 - E)} + \frac{4}{N}\left[\frac{\cos K/2 - 1}{E - 4(1 - \cos K/2)}\right]\right] < 1 \tag{A4}$$

(the last term in (A4) is maximized at $\frac{1}{3}$ by $E = E_1$, $K = 2\pi/N$, $N = 3$).

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