The effect of an external magnetic field on the MLRO in the global ground states of some antiferromagnetic models

1994 J. Phys. A: Math. Gen. 27 4043

(http://iopscience.iop.org/0305-4470/27/12/012)

J. Phys. A: Math. Gen. 27 (1994) 4043–4048. Printed in the UK

The effect of an external magnetic field on the MLRO in the global ground states of some antiferromagnetic models

Guang-Shan Tian

Department of Physics, Peking University, Beijing 100871, People's Republic of China and The Institute for Theoretical Physics, Academia Sinica, Beijing 100080, People's Republic of China

Received 14 January 1994

Abstract. In this paper, we shall study the effect of an external magnetic field on the magnetic long-range orders (MLRO) in the global ground states of the quantum XY model and the isotropic Heisenberg model on the simple cubic lattices. We shall rigorously prove that, while an external magnetic field (staggered in the antiferromagnetic case) which favours MLRO in a specific spin direction, say x-direction, is turned on, it completely suppresses the MLRO in the perpendicular spin directions in the global ground states of these models.

The discovery of magnetic long-range order (MLRO) in the superconducting layered perovskites [1–2] has motivated a surge of interest in the quantum antiferromagnetic Heisenberg model. As a model describing the magnetic properties of solids, the existence of MLRO in its ground states is of most concern to physicists. Over several decades, people have achieved many advances in understanding this model by either approximate or mathematically rigorous methods. As far as the rigorous results are concerned, Mermin and Wagner proved their famous theorem in 1966 [3] (it was also independently proved by Hohenberg [4]). Their theorem excludes the existence of MLRO in the one- and two-dimensional Heisenberg models when temperature $T \neq 0$. On the other hand, it was Dyson *et al* [5] who first established the existence of MLRO in the isotropic antiferromagnetic Heisenberg model on the three-dimensional simple cubic (SC) lattice when the localized spin angular momentum $s \geqslant 1$. This result was extended to the ground state of the Heisenberg model on the two-dimensional square lattice with $s \geqslant 3/2$ by Neves and Perez [6]. The best result was obtained by Kennedy *et al* [7]. They proved that, when $d \geqslant 3$ and $s \geqslant 1/2$, or, $d = 2$ and $s \geqslant 1$, the ground states of the antiferromagnetic Heisenberg models on SC lattices have antiferromagnetic long-range order. In a very recent article [8], we proved that, if the antiferromagnetic Heisenberg model is defined on a bipartite lattice Λ with macroscopic unequal numbers of sublattice points, then its ground states have both ferromagnetic and antiferromagnetic long-range order. Namely, the model represents a ferrimagnet proposed by Néel [9].

We notice that all these theorems were proved for Heisenberg models without external magnetic fields. A natural question which one would like to ask is what happens if a magnetic field is turned on. In general, one expects that an external magnetic field will introduce some kind of frustration into the system and hence, suppress the MLRO in the ground states. To study this problem on a rigorous basis, we shall consider a special case in which the ground state of the antiferromagnetic model has MLRO in several different spin directions. After turning on a magnetic field (staggered in the antiferromagnetic case) which favours MLRO in a specific spin direction, we show that the MLRO in other spin directions are completely suppressed, no matter how weak the magnetic field is.

For definiteness, we shall consider the quantum XY model on the two-dimensional square lattice in the following. As one will see, the final results of our analysis can be easily extended to some more complicated cases such as the isotropic antiferromagnetic Heisenberg model on SC lattices.

Take a finite square lattice Λ with $N_\Lambda = L^2$ lattice points. The Hamiltonian of the quantum XY model can be written as

$$H_\Lambda = -J \sum_{\langle ij \rangle} (s_{ix}s_{jx} + s_{iy}s_{jy}) \tag{1}$$

where s_{ix} and s_{iy} are spin-1/2 operators at lattice site i. $J > 0$ is a parameter and $\langle ij \rangle$ denotes a pair of nearest-neighbour lattice sites. With respect to this Hamiltonian, the square lattice is bipartite. Consequently, when the external magnetic field is absent, the sign of J does not play an important role in our analysis. In fact, one can show [10] that the positive- and negative-J quantum XY Hamiltonians on the square lattice are unitarily equivalent.

Define $S_z = \sum_{i\in\Lambda} s_{iz}$ to be the total spin z-component operator. It is easy to see that $[H_\Lambda, S_z] = 0$. Therefore, S_z is a good quantum number of the quantum XY model and the Hilbert space of H_Λ can be divided into numerous subspaces. Each of these is characterized by a quantum number $S_z = M$. Affleck and Lieb [11] showed that, in each subspace $V(M)$, H_Λ has a unique ground state and the global ground state $\Psi_0(\Lambda)$ of H_Λ coincides with its ground state in the subspace $V(M = 0)$.

Furthermore, for the positive-J quantum XY model on the square lattice, Kennedy *et al* [12] proved the existence of the momentum-0 transverse MLRO in its non-degenerate global ground state $\Psi_0(\Lambda)$. More precisely, they proved that if one defines

$$S_x(q) \equiv \frac{1}{\sqrt{N_\Lambda}} \sum_{j\in\Lambda} s_{jx} \exp(-\mathrm{i}q \cdot j) \qquad S_y(q) \equiv \frac{1}{\sqrt{N_\Lambda}} \sum_{j\in\Lambda} s_{jy} \exp(-\mathrm{i}q \cdot j) \tag{2}$$

where q is a reciprocal vector of the square lattice, then one can find a positive constant $\alpha > 0$, independent of N_Λ, such that

$$\langle \Psi_0(\Lambda) \mid S_x^\dagger(0) S_x(0) \mid \Psi_0(\Lambda) \rangle = \langle \Psi_0(\Lambda) \mid S_y^\dagger(0) S_y(0) \mid \Psi_0(\Lambda) \rangle \geqslant \alpha N_\Lambda \tag{3}$$

holds. The equals sign in (3) is due to the fact that the quantum XY Hamiltonian is invariant under rotations about the S_z axis. In other words, the global ground state $\Psi_0(\Lambda)$ of H_Λ has both spin x- and y-direction MLRO.

Now, we turn on an external magnetic field which favours the spin x-direction MLRO. The new Hamiltonian reads

$$H'_\Lambda = H_\Lambda + V = -J \sum_{\langle ij \rangle} (s_{ix}s_{jx} + s_{iy}s_{jy}) - h \sum_{i\in\Lambda} s_{ix} \tag{4}$$

where $h > 0$ is a constant. We choose a negative magnetic field only for technical convenience. As a matter of fact, by applying the unitary operator $U_1 = \exp(\mathrm{i}\pi S_z)$ to H'_Λ, we can easily show that it is equivalent to the negative-h Hamiltonian of the same form.

Introduce operators $s_{i+} \equiv s_{ix} + \mathrm{i}s_{iy}$ and $s_{i-} \equiv s_{ix} - \mathrm{i}s_{iy}$. The Hamiltonian H'_Λ can be rewritten as

$$H'_\Lambda = -\tfrac{1}{2} J \sum_{\langle ij \rangle} (s_{i+}s_{j-} + s_{i-}s_{j+}) - \tfrac{1}{2} h \sum_{i\in\Lambda} (s_{i+} + s_{i-}). \tag{5}$$

For such a Hamiltonian, we have the following theorem.

Theorem 1. The global ground state $\Psi_0(\Lambda)$ of H'_Λ is non-degenerate. Furthermore, for a pair of distinct lattice points $\boldsymbol{k}$ and $\boldsymbol{h}$, we have

$$\langle\Psi_0(\Lambda)|s_{k-}s_{h+}|\Psi_0(\Lambda)\rangle \geqslant 0 \qquad \langle\Psi_0(\Lambda)|s_{k+}s_{h-}|\Psi_0(\Lambda)\rangle \geqslant 0. \tag{6}$$

Proof. First, we notice that the Hilbert space of H'_Λ is no longer reducible. In other words, all the subspaces $V(M)$ are connected by the external field Hamiltonian. Choose a basis of vectors of the Hilbert space by

$$\phi_\alpha = (s_{1+})^{m_1}(s_{2+})^{m_2}\dots(s_{N_\Lambda+})^{m_{N_\Lambda}}|\chi\rangle \tag{7}$$

where $|\chi\rangle$ is the state with all spins down and m_i takes on values of either 0 or 1. In terms of this basis, H'_Λ can be written as a matrix. Since both s_{i+} and s_{i-} are non-negative operators $(s_+|\uparrow\rangle = 0, s_+|\downarrow\rangle = |\uparrow\rangle, s_-|\uparrow\rangle = |\downarrow\rangle, s_-|\downarrow\rangle = 0)$ with respect to $\{\phi_\alpha\}$, we find that all the non-zero matrix elements of H'_Λ are negative. For such a matrix, we have the famous Perron–Fröbenius theorem [13]. It tells us that the lowest eigenvalue of H'_Λ is non-degenerate. Furthermore, the ground state $\Psi_0(\Lambda)$ is a linear combination of $\{\phi_\alpha\}$ with positive coefficients. Consequently, inequality (6) holds since s_+ and s_- are non-negative operators. □

A direct corollary of theorem 1 is as follows.

Corollary 1. Let

$$S_+(\boldsymbol{q}) \equiv \frac{1}{\sqrt{N_\Lambda}}\sum_{j\in\Lambda} s_{j+}\exp(\mathrm{i}\boldsymbol{q}\cdot\boldsymbol{j}) \tag{8}$$

and $S_-(\boldsymbol{q}) \equiv S_+^\dagger(\boldsymbol{q})$, where $\boldsymbol{q}$ is a reciprocal vector of the square lattice. Define

$$g(\boldsymbol{q}) \equiv \langle\Psi_0(\Lambda)|S_+(\boldsymbol{q})S_-(\boldsymbol{q}) + S_-(\boldsymbol{q})S_+(\boldsymbol{q})|\Psi_0(\Lambda)\rangle. \tag{9}$$

Then, the following inequality

$$g(0) \geqslant g(\boldsymbol{q}) \tag{10}$$

holds for any reciprocal vector $\boldsymbol{q}$.

Proof. By the definition of $g(\boldsymbol{q})$ and inequality (6), we immediately obtain inequality (10). □

By corollary 1, if $\Psi_0(\Lambda)$ has a momentum-$\boldsymbol{q}$ MLRO, i.e. if $g(\boldsymbol{q}) \geqslant \alpha N_\Lambda$ for some reciprocal vector $\boldsymbol{q}$, then $\Psi_0(\Lambda)$ must also have a momentum-0 MLRO. Considering the magnetic field strengthens the momentum-0 MLRO in the spin x-direction, corollary 1 can be easily understood.

We now show that, while the spin x-direction MLRO may be strengthened by the external magnetic field, the spin y-direction MLRO is completely suppressed. Our result can be summarized in the following theorem.

Theorem 2. Let $\Psi_0(\Lambda)$ be the global ground state of H'_Λ on the square lattice. Then, for any reciprocal vector q, we have

$$\langle\Psi_0(\Lambda)|S_y^\dagger(q)S_y(q)|\Psi_0(\Lambda)\rangle = O(1). \tag{11}$$

Consequently, the MLRO in the spin y-direction is absent in $\Psi_0(\Lambda)$.

Proof. To prove theorem 2, we shall apply a technique which we developed in a previous paper [14] for showing the absence of some type of long-range orderings in a strongly-correlated many-body system.

First, we notice that the Hamiltonian H'_Λ on the square lattice enjoys the so-called reflection positivity [5, 7]. Consequently, by following the proof of the main theorem in [6] step by step, we can show that there is a positive function $f(q)$ which is of order O(1) for any $q \neq 0$ as $N_\Lambda \to \infty$, such that

$$0 \leqslant g(q) \leqslant f(q). \tag{12}$$

Therefore, $\Psi_0(\Lambda)$ can have, at most, a momentum-0 MLRO. On the other hand, by the definitions of s_{i+} and s_{i-}, $g(q)$ can be written as

$$g(q) = 2\{\langle\Psi_0(\Lambda)|S_x^\dagger(q)S_x(q)|\Psi_0(\Lambda)\rangle + \langle\Psi_0(\Lambda)|S_y^\dagger(q)S_y(q)|\Psi_0(\Lambda)\rangle\}. \tag{13}$$

Therefore, $\langle\Psi_0(\Lambda)|S_y^\dagger(q)S_y(q)|\Psi_0(\Lambda)\rangle \geqslant \beta N_\Lambda$ (β is a positive constant independent of N_Λ) may only hold at $q = 0$ since $\langle\Psi_0(\Lambda)|S_x^\dagger(q)S_x(q)|\Psi_0(\Lambda)\rangle$ is a positive quantity. Consequently, if $\langle\Psi_0(\Lambda)|S_y^\dagger(0)S_y(0)|\Psi_0(\Lambda)\rangle$ is of order O(1) as $N_\Lambda \to \infty$, then the spin y-direction MLRO is completely suppressed. We now prove this fact by the method developed in [14].

Consider the commutator of H'_Λ and $S_z = \sum_{i\in\Lambda} s_{iz}$.

$$[H'_\Lambda, S_z] = [H_\Lambda, S_z] + [V, S_z] = -h\left[\sum_{i\in\Lambda} s_{ix}, \sum_{i\in\Lambda} s_{iz}\right] = \mathrm{i}h\sum_{i\in\Lambda} s_{iy}. \tag{14}$$

A direct consequence of this commutator is

$$\langle\Psi_0(\Lambda)|S_y(0)|\Psi_0(\Lambda)\rangle = \langle\Psi_0(\Lambda)|S_y^\dagger(0)|\Psi_0(\Lambda)\rangle = 0. \tag{15}$$

Let $\{\Psi_n(\Lambda)\}$ be the complete set of the eigenvectors of H'_Λ. Then, the commutator (14) can be written in the following equivalent form

$$|\langle\Psi_n(\Lambda)|S_z|\Psi_0(\Lambda)\rangle|^2(E_n - E_0)^2 = h^2|\langle\Psi_n(\Lambda)|S_y|\Psi_0(\Lambda)\rangle|^2 \tag{16}$$

where $E_n(\Lambda)$ is the eigenvalue of $\Psi_n(\Lambda)$. By identities (15) and (16), we obtain the following inequality

$$\begin{aligned}
0 &\leqslant \langle\Psi_0(\Lambda)|S_y^\dagger(0)S_y(0)|\Psi_0(\Lambda)\rangle \\
&= \tfrac{1}{2}\sum_n [|\langle\Psi_n(\Lambda)|S_y^\dagger(0)|\Psi_0(\Lambda)\rangle|^2 + |\langle\Psi_n(\Lambda)|S_y(0)|\Psi_0(\Lambda)\rangle|^2] \\
&= \tfrac{1}{2}\sum_n \left\{\left[|\langle\Psi_n(\Lambda)|S_y^\dagger(0)|\Psi_0(\Lambda)\rangle|\sqrt{E_n - E_0}\right]\frac{|\langle\Psi_n(\Lambda)|S_y^\dagger(0)|\Psi_0(\Lambda)\rangle|}{\sqrt{E_n - E_0}}\right.
\end{aligned}$$

$$+\left[|\langle\Psi_n(\Lambda)|S_y(0)|\Psi_0(\Lambda)\rangle|\sqrt{E_n-E_0}\right]\frac{|\langle\Psi_n(\Lambda)|S_y(0)|\Psi_0(\Lambda)\rangle|}{\sqrt{E_n-E_0}}\Bigg\}$$

$$\leqslant \tfrac{1}{2}\sum_n\Bigg\{(E_n-E_0)[|\langle\Psi_n(\Lambda)|S_y^\dagger(0)|\Psi_0(\Lambda)\rangle|^2+|\langle\Psi_n(\Lambda)|S_y(0)|\Psi_0(\Lambda)\rangle|^2]$$

$$\times\sum_n\frac{|\langle\Psi_n(\Lambda)|S_y^\dagger(0)|\Psi_0(\Lambda)\rangle|^2+|\langle\Psi_n(\Lambda)|S_y(0)|\Psi_0(\Lambda)\rangle|^2}{E_n-E_0}\Bigg\}$$

$$=\tfrac{1}{2}\langle\Psi_0|[S_y^\dagger(0),[H'_\Lambda,S_y(0)]]|\Psi_0\rangle\left(\frac{1}{h^2}\langle\Psi_0|[S_z^\dagger(0),[H'_\Lambda,S_z(0)]]|\Psi_0\rangle\right)$$

$$=\frac{1}{2N_\Lambda^2h^2}\langle\Psi_0|h\sum_{i\in\Lambda}s_{ix}-2\sum_{\langle ij\rangle}(s_{ix}s_{jx}-s_{iz}s_{jz})|\Psi_0\rangle\langle\Psi_0|h\sum_{i\in\Lambda}s_{ix}|\Psi_0\rangle. \tag{17}$$

In the above derivation, we used the Cauchy inequality. Obviously, each of the expectation values in the last line of inequality (17) is, at most, a quantity of order $O(N_\Lambda)$. Therefore, $\langle\Psi_0(\Lambda)|S_y(0)S_y(0)|\Psi_0(\Lambda)\rangle$ is bounded above by a quantity of order O(1). It implies that the global ground state $\Psi_0(\Lambda)$ of H'_Λ has no spin y-direction MLRO. □

Although we have only proved our theorem for the quantum XY model on the square lattice, it is not difficult to see that the proof can be easily extended to the isotopic antiferromagnetic Heisenberg model on SC lattices. In this case, we should replace $V=h\sum_{j\in\Lambda}s_{jx}$ with $V'=h\sum_{j\in\Lambda}(-1)^{iQ\cdot j}s_{jz}$, $(Q\equiv(\pi,\pi,\ldots,\pi))$ which favours the longitudinal MLRO of the isotropic antiferromagnetic Heisenberg model [5]. By repeating the proof of theorem 2, we find that the transverse MLRO in the global ground state $\Psi_0(\Lambda)$ of the Heisenberg Hamiltonian is completely suppressed.

In summary, we have studied in this paper the effect of an external magnetic field on the existence of the MLRO in the antiferromagnetic XY and Heisenberg model on SC lattices. We find that, turning on a magnetic field, which may favour MLRO in a specific spin direction, totally destroys the MLRO of the system in the perpendicular spin directions.

Acknowledgments

We would like to thank Professor E Lieb for critically reading the manuscript of this paper. We would also like to thank our referee for his valuable and constructive suggestions. This work is partially supported by the Chinese National Science Foundation under grant no 19274003.

References

[1] Vaknin D, Sinha S K, Moncton D E, Johnston D C, Newsam J M, Safinya C R and King H E Jr 1987 *Phys. Rev. Lett.* **58** 2801
[2] Sato M, Shamoto S, Tranquada J M, Shirane G and Kleiner B 1988 *Phys. Rev. Lett.* **61** 1317
[3] Mermin N D and Wagner H 1966 *Phys. Rev. Lett.* **17** 1133
[4] Hohenberg P 1967 *Phys. Rev.* **158** 383
[5] Dyson F J, Lieb E H and Simon B 1978 *J. Stat. Phys.* **18** 335
[6] Jordão Neves E and Fernando Perez J 1968 *Phys. Lett.* **144A** 331
[7] Kennedy T, Lieb E H and Shastry B S 1988 *J. Stat. Phys.* **53** 1019
[8] Tian Guang-Shan to be published

[9] Néel L 1948 *Ann. Phys., Paris* **3** 137
[10] Lieb E H and Mattis D C 1962 *J. Math. Phys.* **3** 749
[11] Affleck I and Lieb E H 1986 *Lett. Math. Phys.* **12** 57
[12] Kennedy T, Lieb E H and Shastry B S 1988 *Phys. Rev. Lett.* **61** 2582
[13] Horn R A and Johnson C R 1985 *Matrix Analysis* (Cambridge: Cambridge University Press)
[14] Tian Guang-Shan 1993 *J. Phys. A: Math. Gen.* **26** 2325