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Magnetic order of the two-dimensional antiferromagnetic $\frac{1}{4}$-depleted square lattice

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Abstract
For a two-dimensional Heisenberg antiferromagnetic $\frac{1}{4}$-depleted square lattice, it has been analytically proved that its ground state possesses simultaneously ferromagnetic and antiferromagnetic long-range orders, and exhibits ferrimagnetism. Numerical simulations of finite lattices using exact diagonalization show that the $\frac{1}{4}$ depletion strengthens the short-range spin–spin correlations whereas it weakens the long-range ones. The $\frac{1}{4}$-depleted square lattice has a smaller susceptibility. This means that the geometric structure of the usual two-dimensional square lattice is more advantageous for establishing magnetic long-range order. By comparison of these two kinds of lattices, it is quite reliably inferred that Néel order exists in the ground state of the usual two-dimensional spin-$\frac{1}{2}$ Heisenberg antiferromagnetic square lattice.

1. Introduction

The subject of two-dimensional (2D) spin-$\frac{1}{2}$ quantum antiferromagnetism has witnessed a remarkable revival in recent years largely due to the experimental observation [1] that the parent compound of the high-T_c superconductor La_2CuO_4 is an antiferromagnetic (AF) insulator. Although the exact ground state (GS) of the 2D Heisenberg AF (HAF) model has not been obtained so far due to the mathematical complexity caused by quantum fluctuations, the Marshall–Peierls sign rule [2] indicates that the spin–spin correlation (SSC) is AF no matter how far two spins are away from each other (i.e. the correlation of two spins in the same sublattice is positive while that in the different sublattices is negative). However, this does not imply the existence of long-range order (LRO), which depends on the zero-point fluctuations. The decreasing of dimensionality will strengthen quantum fluctuations and be disadvantageous to the magnetic LRO. For a one-dimensional spin-$\frac{1}{2}$ HAF chain, the zero-point fluctuations

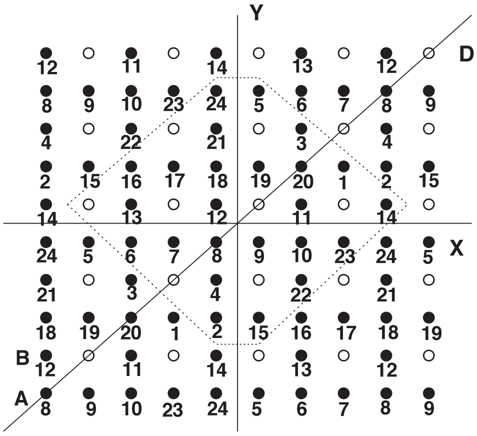

Figure 1. The geometries of two kinds of lattices. For the usual square lattice, all the sites have spins, while for the $\frac{1}{4}$-depleted square lattice, only sites denoted by full circles have spins. X, Y and D are the symmetric axes of reflections. A and B represent the two sublattices. The numbers below full circles are the index numbers of spins for the $\frac{1}{4}$-depleted square lattice of 24 spins under the tilted periodic boundary conditions.

destabilize the classic Néel order, and bring about a decay of SSCs in the power law. For a 2D spin-S isotropic HAF model, the Mermin–Wagner theorem [3] indicates that no magnetic LRO exists at any nonzero temperature. A question of fundamental importance is whether or not the zero temperature is a critical point. Many efforts have been devoted to this, and some significant results have been obtained. In the case of $S \geqslant 1$, it has been proved that AF LRO exists in the GS of a square or hexagonal lattice [4]. In order to investigate the stability of the AF LRO in the $S = \frac{1}{2}$ case, Kennedy *et al* [5] studied a cubic lattice with coupling γ in one lattice direction and 1 in the other two, and proved the existence of Néel order for $0.16 \leqslant \gamma \leqslant 1$. The 2D anisotropic HAF models have also been studied. For the spin-$\frac{1}{2}XXZ$ model ($J^x = J^y = 1$), LRO has been proved only for $0 \leqslant J^z < 0.13$ and $J^z > 1.78$ by Kubo *et al* [6]. Up to now, for a 2D spin-$\frac{1}{2}$ isotropic HAF bipartite lattice, a rigorous proof of the existence or nonexistence of the AF LRO has remained lacking. Many works based on analytical approximations or numerical simulations supported the notion that the zero-point fluctuations in the 2D spin-$\frac{1}{2}$ isotropic HAF square lattice do not suppress the classic Néel order but decrease the staggered magnetization (see Manousakis's review paper [7] and the related references therein). On the other hand, the RVB wavefunction without magnetic LRO can also give an energy very close to the exact GS energy [8]. The effect of quantum fluctuations on the GS is still somewhat plausible. It is meaningful to give an instance of the 2D spin-$\frac{1}{2}$ *isotropic* HAF model for which the magnetic LRO can be exactly examined.

Recently, the discovery of a spin gap of CaV_4O_9 [9] has stimulated the enthusiasm for studying the role of depletion in destabilizing the LRO. This compound can be described by the 2D spin-$\frac{1}{2}$ HAF model on the $\frac{1}{5}$-depleted square lattice (DSL), which has been investigated by many approximate methods [10–14]. It has been found that the depletion of $\frac{1}{5}$ strengthens the zero fluctuations and weakens the long-range SSC. For the 2D spin-$\frac{1}{2}$ HAF triangular lattice, which exhibits LRO, the depletion of $\frac{1}{4}$ leads to the Kagomé lattice. Numerical simulation [15] shows that the depletion not only weakens the SSC but also destabilizes the LRO.

In this paper, we study the 2D spin-S HAF $\frac{1}{4}$-DSL, in which there is one missing spin in each plaquette of four NN sites (figure 1). Without the solution of its exact GS, the existence of the magnetic LRO can be analytically proved. This lattice has the different geometric structure from the usual square lattice (USL). There are always four NN spins for each spin on the 2D USL. But for the 2D $\frac{1}{4}$-DSL, some of the spins have only two NN spins. In the case of $S = \frac{1}{2}$, the effect of depletion on SSCs is investigated by exact diagonalization. Also, we estimated its susceptibility and staggered magnetization. Comparing these two kinds of lattices, it is rather reliable to infer the existence of Néel order in the GS of the 2D spin-$\frac{1}{2}$ HAF USL.

2. Proof of the LRO of the $\frac{1}{4}$-depleted square lattice

The Hamiltonian of the spin-S HAF model reads

$$H = J \sum_{(i,j)} \vec{S}_i \cdot \vec{S}_j, \tag{1}$$

where the exchange integral $J > 0$, $\vec{S}_i$ ($\vec{S}_j$) is the spin operator on site i (j) and the sum runs over the pairs of NN spins. Only the bipartite lattice is considered in the present paper. It can be divided into two sublattices, A and B. When a spin belongs to sublattice A, its NN spins belong to sublattice B and vice versa. The maximum values of possible total spins of sublattices A and B are $S_A^{\max} = N_A S$ and $S_B^{\max} = N_B S$, respectively, where N_A and N_B represent the numbers of spins of two sublattices. For any HAF bipartite lattice, by the Lieb–Mattis theorem [16], the total spin (TS) of the GS

$$\Lambda = \left|S_A^{\max} - S_B^{\max}\right| = |N_A - N_B|\, S. \tag{2}$$

For the 2D $\frac{1}{4}$-DSL, $N_B = 2n$ when $N_A = n$, where n is an integer. The total number of spins is $N = N_A + N_B = 3n$. Unlike in the case of the USL, its GS does not take the lowest possible TS 0 (if the system has an odd number of spins, the lowest possible TS is equal to S) but a very large value. By the above equation, one can readily get

$$\Lambda = nS = \tfrac{1}{3} NS. \tag{3}$$

The GS of the $\frac{1}{4}$-DSL has a $(2\Lambda + 1)$-fold degeneracy due to the $SU(2)$ symmetry of Hamiltonian (1) in the spin space. Since there is no overlap between the different degenerate GSs, one can expand the GS of the M-subspace in the spin configuration complete set $\{\phi_\alpha\}$ in terms of the amplitudes f_α,

$$|\Lambda, M\rangle = \sum_\alpha f_\alpha \phi_\alpha, \tag{4}$$

where M is the magnetic quantum number. After a unitary transformation $\hat{U}_0 = \exp(\mathrm{i}\pi \sum_{k\in A} S_k^z)$, consisting of a rotation of sublattice A by π around the z-axis in the spin space, all the coefficients become positive [2, 16], i.e. $f_\alpha > 0$ for all the spin configurations α by the Perron–Fröbenius theorem [17]. The possibility of $f_\alpha = 0$ is excluded since for a HAF bipartite lattice, it is impossible that the GS takes the largest possible TS NS. Consequently, for any two spins,

$$\langle \Lambda, M| S_i^+ S_j^- + \mathrm{h.c.} |\Lambda, M\rangle > 0. \tag{5}$$

After the inverse transformation $\hat{U}_0^{-1}$,

$$\Gamma_{ij} \langle \Lambda, M| S_i^+ S_j^- + \mathrm{h.c.} |\Lambda, M\rangle > 0, \tag{6}$$

where $\Gamma_{ij} = +1\,(-1)$ if spins i and j are in the same (different) sublattice(s). Performing the unitary transformation $\hat{U}_1 = \exp(\mathrm{i}\pi/2 \sum_k S_k^z)$, which rotates each spin around the z-axis by an angle $\pi/2$, one can obtain

$$\langle \Lambda, M| S_i^x S_j^x |\Lambda, M\rangle = \langle \Lambda, M| S_i^y S_j^y |\Lambda, M\rangle. \tag{7}$$

Since the $(2\Lambda + 1)$-fold degenerate GSs have the same statistical mechanics weight, the GS can be written as follows:

$$|G\rangle = \frac{1}{\sqrt{2\Lambda+1}} \sum_M |\Lambda, M\rangle .$$

Then,

$$\Gamma_{ij} \langle G|S_i^x S_j^x|G\rangle = \Gamma_{ij} \langle G|S_i^y S_j^y|G\rangle > 0. \tag{8}$$

In the above derivation, inequality (6) is used. Since $\hat{U}_2 = \exp(\mathrm{i}\pi/2 \sum_k S_k^y)$ commutes with Hamiltonian (1), the $2\Lambda+1$ degenerate GSs $|\Lambda, M\rangle$ will be transformed in terms of a $(2\Lambda + 1)$-dimensional irreducible unitary representation of the $SU(2)$ group [18]. We have

$$\begin{aligned}
\Gamma_{ij} \langle G|S_i^x S_j^x|G\rangle &= \frac{\Gamma_{ij}}{2\Lambda+1} \sum_{M=-\Lambda}^{\Lambda} \langle \Lambda, M|\hat{U}_2(\hat{U}_2^+ S_i^x \hat{U}_2)(\hat{U}_2^+ S_j^x \hat{U}_2)\hat{U}_2^+|\Lambda, M\rangle \\
&= \frac{\Gamma_{ij}}{2\Lambda+1} \sum_{M=-\Lambda}^{\Lambda} \langle \Lambda, M|\hat{U}_2 S_i^z S_j^z \hat{U}_2^+|\Lambda, M\rangle \\
&= \frac{\Gamma_{ij}}{2\Lambda+1} \sum_{M,M_1,M_2=-\Lambda}^{\Lambda} \bar{D}_{M_1 M} D_{M_2 M} \langle \Lambda, M_1|S_i^z S_j^z|\Lambda, M_2\rangle \\
&= \Gamma_{ij} \langle G|S_i^z S_j^z|G\rangle.
\end{aligned} \tag{9}$$

The fact that $\{D_{M_2 M}\}$ is a unitary matrix is used in the above derivation. Combining this with inequality (8), one can readily get

$$\Gamma_{ij} \langle G|\vec{S}_i \cdot \vec{S}_j|G\rangle > 0. \tag{10}$$

Inequality (10) shows that for the GS, the SSC is AF. However, it is not sufficient to establish the magnetic LRO since the rapidly decayed SSC cannot set up the magnetic LRO. To examine the magnetic LRO, it is necessary to calculate the magnetic susceptibility

$$\Omega(\mathbf{q}, N) \equiv \frac{1}{N} \langle G|\vec{S}(-\mathbf{q}) \cdot \vec{S}(\mathbf{q})|G\rangle, \tag{11}$$

where $\vec{S}(\mathbf{q}) = \frac{1}{\sqrt{N}} \sum_k \vec{S}_k \exp(\mathrm{i}\mathbf{q}\cdot\mathbf{R}_k)$, $\mathbf{q}$ is the reciprocal vector and $\mathbf{R}_k$ is the coordinate vector of site k. The criterion for the AF LRO is that $\Omega(\mathbf{q}, \infty)$ is finite at $\mathbf{q} = \mathbf{\Pi} \equiv (\pi, \pi)$. Using equation (10), we have

$$\begin{aligned}
\Omega(\mathbf{\Pi}, N) &= \frac{1}{N^2} \sum_{ij} \Gamma_{ij} \langle G|\vec{S}_i \cdot \vec{S}_j|G\rangle \\
&> \frac{1}{N^2} \sum_{ij} \langle G|\vec{S}_i \cdot \vec{S}_j|G\rangle \\
&= \frac{1}{N^2} \langle G|(\vec{S}^T)^2|G\rangle \\
&= \frac{(\Lambda+1)\Lambda}{N^2},
\end{aligned} \tag{12}$$

where $\vec{S}^T \equiv \sum_k \vec{S}_k$ is the TS operator. In the thermodynamic limit, it is obtained that

$$\Omega(\mathbf{\Pi}) = \lim_{N\to\infty} \Omega(\mathbf{\Pi}, N) > \tfrac{1}{9} S^2. \tag{13}$$

Equation (3) is used in the above derivation. The finite $\Omega(\mathbf{\Pi})$ means the existence of the AF LRO.

Table 1. The spin–spin correlations of the usual square lattice of 32 spins and the $\frac{1}{4}$-depleted square lattice of 24 spins. $\vec{R}_i$ is the coordinate vector of spin i. Subscripts s and d are for the usual square lattice and the $\frac{1}{4}$-depleted square lattice, respectively.

$R = \left\|\vec{R}_i - \vec{R}_j\right\|$	1	$\sqrt{2}$	2	$\sqrt{5}$
$\langle G\|\vec{S}_i \cdot \vec{S}_j\|G\rangle_{\rm s}$	−0.3401	0.2090	0.1874	−0.1830
$\langle G\|\vec{S}_i \cdot \vec{S}_j\|G\rangle_{\rm d}$	−0.3572	0.2172	0.1880	−0.1625

The GS TS is proportional to the total number of spins by equation (3). This means that the GS has unsaturated ferromagnetism, which is measured by the quantity

$$\Omega(\mathbf{0}) = \lim_{N\to\infty} \Omega(\mathbf{0}, N) = \lim_{N\to\infty} \frac{(\Lambda+1)\Lambda}{N^2} = \frac{1}{9}S^2, \tag{14}$$

where $\mathbf{0} \equiv (0, 0)$. Equation (11) is used in the above derivation. The finite $\Omega(\mathbf{0})$ means the existence of ferromagnetic (F) LRO. This kind of F LRO, which comes from the AF spin–spin interactions and depends on the difference $|N_A - N_B|$, is different from that produced by the F spin–spin interactions. It is only a by-product of the AF LRO. The F and AF LROs exhibit the same spin status, i.e. the Néel order. In conclusion, the AF and F LROs coexist in the GS of the 2D spin-S HAF $\frac{1}{4}$-DSL. Its GS displays ferrimagnetism since $\Omega(\mathbf{\Pi})$ is larger than $\Omega(\mathbf{0})$.

The model with $S = \frac{1}{2}$ is more attractive due to the strong zero-point fluctuations. It is noticed that inequality (13) and equation (14) are true for any spin S. In the case of $S = \frac{1}{2}$,

$$\Omega(\mathbf{\Pi}) > \Omega(\mathbf{0}) = \tfrac{1}{36}. \tag{15}$$

This means that the zero-point fluctuations cannot suppress the Néel order. Although the lattice investigated is not the USL, the conclusion is meaningful since at least it gives an example of a 2D spin-$\frac{1}{2}$ *isotropic* ($J^x = J^y = J^z$) HAF bipartite lattice for which one can exactly prove the existence of magnetic LRO in the GS.

3. Spin–spin correlations

The effects of missing spins, which distribute periodically on the 2D $\frac{1}{4}$-DSL, are not independent but coherent. This may result in a significant change of the long-range SSC. It is meaningful to investigate the effect of depletion since the global magnetic properties such as the magnetic LRO depend on the long-range SSC. By means of exact diagonalization based on the Lanczös technique, we calculated the SSC of the finite USL and $\frac{1}{4}$-DSL which have 32 and 24 spins, respectively. In our numerical simulations, $S = \frac{1}{2}$ and tilted periodic boundary conditions are taken. The distance of two sites which have the same index number is $R \equiv |\vec{R}_i - \vec{R}_j| = 4\sqrt{2}$ (figure 1), where $\vec{R}_i$ is the coordinate vector of site i and the distance of two NN sites is taken as the unit. Only the data for the SSCs with $R < 2\sqrt{2}$ are meaningful. For the $\frac{1}{4}$-DSL, the SSCs with the same distance R may have different magnitudes because of the different distributions of spins on the lattice directions. For example, for a spin in sublattice B, the SSCs of the third neighbours ($R = 2$) are different in X and Y directions (figure 1). In this case, their average value is taken. The numerical results are listed in table 1. When $R = 1$ and $\sqrt{2}$, the SSCs of the $\frac{1}{4}$-DSL are stronger than those of the USL. The values of SSCs of two kinds of lattices are close when $R = 2$. But the SSC of the $\frac{1}{4}$-DSL becomes weaker when $R > 2$. Our calculations support the conclusion that the depletion of $\frac{1}{4}$ strengthens the short-range SSC but weakens the long-range ones.

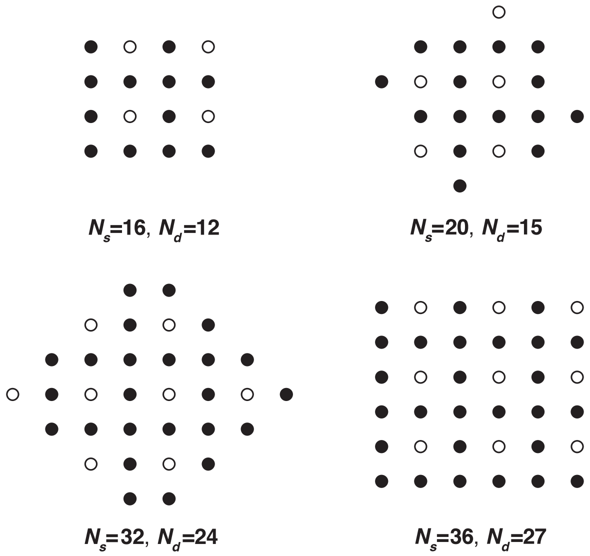

Figure 2. The geometries of several finite systems on the usual square lattice and the $\frac{1}{4}$-depleted square lattice. The full and empty circles have the same meanings as those in figure 1. N_s and N_d are their numbers of spins.

In order to further study the effect of depletion, the susceptibilities of these two kinds of lattices are investigated by calculating a series of the spin-$\frac{1}{2}$ finite lattices (see figure 2). The sizes of the finite USLs are $N = 16, 20, 32$ and 36 while the corresponding finite $\frac{1}{4}$-DSLs have 12, 15, 24 and 27 spins, respectively. The finite USLs of 18 and 26 spins are not involved since their numbers of spins are not integer multiples of 4, so there is no counterpart of the finite $\frac{1}{4}$-DSL. In our calculations, all or part of the symmetries of translation, reflections on X and Y axes and on the diagonal, and up–down (i.e. spin inversion) are used. The symmetric axes of reflections are drawn in figure 1. The usual (or tilted) periodic boundary conditions are taken. The data for the GS energies of the finite USLs are consistent with those obtained by Schultz *et al* [19]. We calculated the GS TS and obtained $\Lambda = 2, \frac{5}{2}, 4$ and $\frac{9}{2}$ for the $\frac{1}{4}$-DSLs of 12, 15, 24 and 27 spins, respectively. They accord with the Lieb–Mattis theorem (i.e. equation (3)). For finite systems, according to the suggestion of Bernu *et al* [20], the susceptibility is normalized by the factor $\frac{1}{N(N+2)}$. The numerical results are plotted in figure 3. They show that the susceptibility of the $\frac{1}{4}$-DSL is smaller than that of the USL. This is consistent with the conclusion that the depletion weakens the long-range SSC since the long-range SSC is responsible for the susceptibility.

The above conclusion can also be achieved by means of the expansion parameter $\delta = (zS)^{-1}$ of spin wave theory [21, 22], where z is the coordinate number. In the case of high dimensionality and large spin, the zero-point fluctuations are weakened so that the quantum spin system the behaviours similar to the classical spin one. But for the case of low dimensionality or small S, the zero-point fluctuations may heavily affect the GS and cause a significant change of spin status. For instance, for the spin-$\frac{1}{2}$ HAF chain, the zero-point fluctuations suppress the Néel order and result in a disordered GS. This means that the zero-point fluctuations can be qualitatively measured by δ. For a 2D USL, z is always equal to 4 for all the sites. But for the $\frac{1}{4}$-DSL, $z = 4$ and 2 for the sites of sublattices A and B, respectively. The effective coordinate number of the 2D $\frac{1}{4}$-DSL must be smaller than 4. The zero-point fluctuation in the USL should

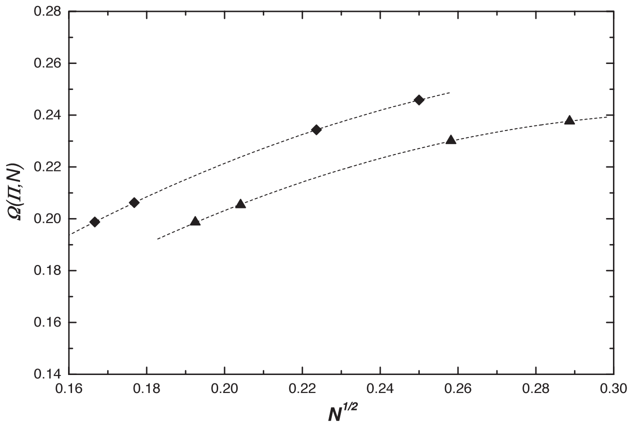

Figure 3. The susceptibilities of the finite $\frac{1}{4}$-depleted square lattice (triangle points) and the usual square lattice (diamond points). $\Omega(\mathbf{\Pi}, N)$ is normalized by the factor $\frac{1}{N(N+2)}$.

be weaker than that in the $\frac{1}{4}$-DSL. The mean field spin wave theory describes not the local but the average property. The weakening of zero-point fluctuations does not mean that all the SSCs are strengthened. In fact, the global magnetic property depends on the long-range SSC. In other words, for the $\frac{1}{4}$-DSL, the strengthening of zero-point fluctuations indicates the weakening of the long-range SSC. The analysis based on the expansion of the spin wave is consistent with our calculations of SSCs.

Our numerical simulation shows that the depletion of $\frac{1}{4}$ weakens the long-range SSC and the susceptibility. For the $\frac{1}{5}$-DSL [10, 14] and the $\frac{1}{4}$-depleted triangular lattice [15], similar results have been obtained. This means that the periodic distribution of missing spins is disadvantageous to the magnetic LRO. In other words, the geometric structure of the USL is more favourable for the establishment of the magnetic LRO. One can infer the existence of the AF LRO in the GS of the USL based on the exact result that the GS of the $\frac{1}{4}$-DSL has the AF LRO.

4. The AF LRO of the 2D spin-$\frac{1}{2}$ square lattice

For the 2D spin-$\frac{1}{2}$ USL, whether or not the AF LRO exists is an important subject. Unfortunately, the above scheme, which is used to prove the existence of the magnetic LRO in the GS of the 2D $\frac{1}{4}$-DSL, becomes useless for the 2D USL since its two sublattices have the same numbers of spins, i.e. $N_A = N_B$. But it is possible to examine the AF LRO in the GS of the 2D spin-$\frac{1}{2}$ HAF USL by comparison of these two kinds of lattices. We introduce the quantity

$$Q(N) \equiv N^2\Omega(\mathbf{\Pi}, N). \tag{16}$$

The Q quantities of the clusters shown in figure 2 have been calculated by means of exact diagonalization. When the number of spins of a USL lattice is N, that of the corresponding $\frac{1}{4}$-DSL is $\frac{3}{4}N$. The numerical results of Q quantities are listed in table 2 and plotted in figure 4. Our calculations show that for all the finite systems investigated, the Q quantity of the USL is always larger than that of the corresponding $\frac{1}{4}$-DSL, i.e.

$$Q_{\mathrm{s}}(N) > Q_{\mathrm{d}}(\tfrac{3}{4}N), \tag{17}$$

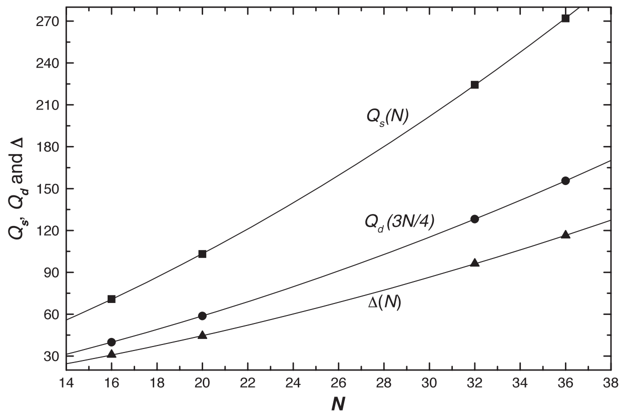

Figure 4. $Q_{\mathrm{s}}(N)$, $Q_{\mathrm{d}}(\frac{3}{4}N)$ and $\Delta(N)$ versus N. The square, circle and triangle point data were calculated using exact diagonalization. The solid curves are the polynomial fits up to the second order.

Table 2. The Q quantities for the usual square lattice and the $\frac{1}{4}$-depleted square lattice, and their difference Δ.

N	16	20	32	36
$Q_{\mathrm{s}}(N)$	70.79	103.09	224.36	271.94
$Q_{\mathrm{d}}(\frac{3}{4}N)$	39.92	58.67	128.13	155.54
$\Delta(N)$	30.87	44.42	96.23	116.40

where $Q_{\mathrm{s}}(N)$ and $Q_{\mathrm{d}}(\frac{3}{4}N)$ denote the Q quantities of the USL and the $\frac{1}{4}$-DSL, respectively. For convenience of discussion, we calculated their difference

$$\Delta(N) = Q_{\mathrm{s}}(N) - Q_{\mathrm{d}}(\tfrac{3}{4}N), \tag{18}$$

and found that it increases obviously as N increases (figure 4). Inequality (17) seems to be valid for the systems with larger scales. In other words, one can rather reasonably assume that this inequality holds true in the thermodynamic limit. So,

$$\lim_{N\to\infty} \frac{1}{N^2}\Delta(N) \geqslant 0. \tag{19}$$

Then,

$$\lim_{N\to\infty} \frac{1}{N^2}\left[Q_{\mathrm{s}}(N) - Q_{\mathrm{d}}\left(\frac{3}{4}N\right)\right] = \lim_{N\to\infty}\left[\frac{1}{N^2}Q_{\mathrm{s}}(N)\right] - \frac{9}{16}\lim_{N\to\infty}\left[\frac{1}{(3N/4)^2}Q_{\mathrm{d}}\left(\frac{3}{4}N\right)\right]$$
$$= \Omega_{\mathrm{s}}(\mathbf{\Pi}) - \tfrac{9}{16}\Omega_{\mathrm{d}}(\mathbf{\Pi}) \geqslant 0.$$

where $\Omega_{\mathrm{s}}(\mathbf{\Pi})$ and $\Omega_{\mathrm{d}}(\mathbf{\Pi})$ are the susceptibilities of the USL and the corresponding $\frac{1}{4}$-DSL, respectively. From equation (15),

$$\Omega_{\mathrm{s}}(\mathbf{\Pi}) > \tfrac{1}{64}. \tag{20}$$

Finite $\Omega_{\mathrm{s}}(\mathbf{\Pi})$ means that the AF LRO exists in the GS of the 2D spin-$\frac{1}{2}$ HAF USL. Its staggered magnetization satisfies

$$\mathcal{F}_{\mathrm{s}} = 2\sqrt{\Omega_{\mathrm{s}}(\mathbf{\Pi})} > \tfrac{1}{4}.$$

This result is compatible with the previous ones (for example, $\mathcal{F}_{\mathrm{s}} = 0.614$ from series expansions [23] and $\mathcal{F}_{\mathrm{s}} = 0.615$ from quantum Monte Carlo simulation [24]).

5. Summary and discussion

For the 2D spin-S HAF $\frac{1}{4}$-DSL, although the existence of the AF LRO is proved by means of the existence of the F LRO, the F LRO is not the basis for the existence of the AF LRO. The F LRO comes from the alignment of spins in the AF Néel ordered way and the different numbers of spins in two sublattices. This kind of F LRO will disappear when the difference of the numbers of spins of two sublattices vanishes (by the Lieb–Mattis theorem, the GS is a singlet, i.e. $\Lambda = 0$). In general, from equations (2) and (14), one can conclude that for a spin-S HAF bipartite lattice which has $|N_A - N_B| < \mathrm{O}(N)$, its GS has no F LRO in the thermodynamic limit.

Missing spins, which distribute periodically on the $\frac{1}{4}$-DSL, make the SSC different from that of the 2D USL. The simulation of finite systems shows that compared to the 2D USL, the short-range SSC of the $\frac{1}{4}$-DSL is stronger, whereas the long-range SSC is weaker. Since the magnetic LRO depends on the long-range SSC, this numerical result means that the geometric structure of the USL is more favourable for the magnetic LRO.

By comparison of the Q quantities of the two kinds of lattices, it is concluded that the GS of the 2D spin-$\frac{1}{2}$ HAF USL has the AF LRO. In the procedure, all the approaches except for inequality (19) are analytically rigorous. From equations (11) and (16),

$$Q(N) = \sum_{ij} \Gamma_{ij} \langle G|\vec{S}_i \cdot \vec{S}_j|G\rangle. \tag{21}$$

Q is the summation of SSCs with the (π, π) phase factor. By inequality (10), each term in the sum remains positive. So, $Q(N)$ is equal to the sum of the magnitudes of all the SSCs. One notices that for the USL of N sites, there are N^2 terms in the summation of equation (21), while for the corresponding $\frac{1}{4}$-DSL, the sum runs only over $\frac{9}{16}N^2$ terms. The difference in number of terms for these two kinds of lattices is $\frac{7}{16}N^2$. It increases with N as N^2. This is responsible for $\Delta(N)$ remaining positive and increasing rapidly with N. In other words, the extrapolation of $\Delta(N) > 0$ is rather reliable. We fitted the data for $\Delta(N)$ to a second-order polynomial, and obtained

$$\Delta(N) = 0.051\,66N^2 + 1.601\,05N - 8.078\,13. \tag{22}$$

For the GS of the 2D spin-$\frac{1}{2}$ HAF USL [24], the staggered magnetization $\digamma_s = 0.615$. Thus its susceptibility $\Omega_s(\mathbf{\Pi}) = \frac{1}{4}\digamma_s^2 = 0.094\,56$. From equations (18) and (22), the susceptibility of the 2D spin-$\frac{1}{2}$ HAF $\frac{1}{4}$-DSL is

$$\Omega_d(\mathbf{\Pi}) = 0.076\,27$$

and its staggered magnetization is

$$\digamma_d = 2\sqrt{\Omega_d(\mathbf{\Pi})} = 0.552\,34.$$

In the above derivations, $\lim_{N\to\infty} \Delta(N)/N^2 = 0.051\,66$ is used. The depletion of $\frac{1}{4}$ leads to about 19% loss of susceptibility.

The reliability of the conclusion that the GS of the spin-$\frac{1}{2}$ HAF USL has the AF LRO depends on inequality (19). This inequality holds true as long as $\Omega_s(\mathbf{\Pi}) \geqslant \frac{9}{16}\Omega_d(\mathbf{\Pi})$. It is a quite weak condition since it does not require that $\Omega_s(\mathbf{\Pi})$ must be larger than $\Omega_d(\mathbf{\Pi})$. Thus, the conclusion of the existence of the AF LRO in the GS of the 2D spin-$\frac{1}{2}$ HAF USL, which is derived from inequality (19), is rather reliable.

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