Quantum Spins and Quasiperiodicity: A Real Space Renormalization Group Approach

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We study the antiferromagnetic spin-1/2 Heisenberg model on a two-dimensional bipartite quasiperiodic structure, the octagonal tiling, the aperiodic equivalent of the square lattice for periodic systems. An approximate block spin renormalization scheme is described for this problem. The ground state energy and local staggered magnetizations for this system are calculated and compared with the results of a recent quantum Monte Carlo calculation for the tiling. It is conjectured that the ground state energy is exactly equal to that of the quantum antiferromagnet on the square lattice.

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In this paper a renormalization group (RG) transformation is used to study the ground state of Heisenberg spins with antiferromagnetic couplings on a two-dimensional quasiperiodic tiling. This system poses a novel theoretical problem, namely, the nature of quantum fluctuations in a structure possessing a number of exact symmetries but no translational invariance. While periodic systems and disordered variants thereof have received much attention, little is known about aperiodic quantum models in two or more dimensions. In particular, the real space magnetic ordering of local moments in systems with quasiperiodic long range order remains to be elucidated and should present novel and complex features, different from properties of crystalline or disordered systems. The archetypal nonfrustrated two-dimensional antiferromagnetic system is that of spins on the square lattice, an old and until recently controversial problem, while the problem we consider now, with its fundamentally different symmetry properties, aims to understand a new class of unfrustrated systems.

Experimental work providing motivation for the study of such systems comes from neutron scattering studies of the magnetic phase in a Zn-Mg-Ho quasicrystal [1]. The magnetic diffuse scattering of the low temperature phase shows an icosahedral symmetry, reflecting the underlying quasiperiodicity of this compound. The nature of the ground state in such a quasicrystalline medium was recently discussed in [2] where quantum Monte Carlo (QMC) calculations were carried out for an antiferromagnetic Heisenberg model on one of the simplest two-dimensional quasiperiodic tilings available, the octagonal tiling. This tiling has been frequently used for numerical investigations of the effects of quasiperiodic modulations in two dimensions. More detailed, analytic and numerical results are available for one-dimensional quasiperiodic models, where quantum spins have been considered using real space renormalization transformation [3] and using density matrix renormalization or by using mappings to fermionic models (see [4] and references therein). However, the techniques used are particular to one dimension and not readily generalizable to the two-dimensional structure considered here.

The model considered in [2] has a Hamiltonian $H = J\sum_{\langle i,j\rangle}\vec{S}_i \cdot \vec{S}_j$ where the spins are located on vertices of the octagonal tiling, and J is coupling along each edge. Spin-spin correlations in the ground state were computed, and the staggered local moment at a given site was found to depend on the number of nearest neighbors z. We recall that the octagonal tiling has six z values ranging from 3 to 8 (see Ref. [2] for a picture). Figure 1 shows the six types of nearest neighbor configurations that occur, along with the nomenclature used in this paper (see below).

Within each of the six families the local order parameters have a fine structure reflecting the differences in the next-nearest neighbor shells, and there are further splittings due to even longer range spin-spin interactions. The observed z dependence of the local order parameters was qualitatively explained in [2] by an isolated cluster or Heisenberg star (HS) approximation. Doing better requires taking into account successive shells of next-nearest neighbors. The best way to do this is by a renormalization group calculation, using the self-similarity of the quasiperiodic structure. This is the aim of the present calculation.

The renormalization approach is a natural one for self-similar quasiperiodic tilings invariant under a scale transformation or inflation such as the one described by Gardner [5] for the Penrose tiling. For the octagonal (Ammann-Beenkker) tiling [6], one can start with tiles of some given edge length and reconnect a certain subset of vertices (inflation). The redrawn tiling is then similar to the original one, except for an overall scale factor, equal to the golden mean $\tau = (\sqrt{5} + 1)/2$ for the

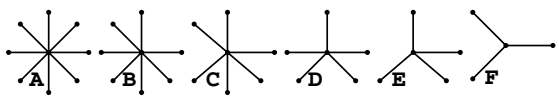

FIG. 1. The six nearest neighbor environments on the octagonal tiling

Fibonacci chain, 2D Penrose tiling, and its 3D generalization, or the silver mean $\lambda = (1 + \sqrt{2})$ in the case of the octagonal tiling. This structural property of tilings has been often exploited in order to establish recurrence relations for parameters occurring in discrete spin models, electron hopping models, etc., as mentioned before for the one-dimensional case, and for some two-dimensional models [7,8], where analytical methods remain hard to implement.

Our renormalization group is a generalization of the calculation of Sierra and Martin-Delgado for the square lattice [9], where the authors considered blocks composed of five-spin star-shaped clusters. On the quasiperiodic tiling, the choice of block spins is suggested by site behavior under an inflation operation. Inflation results in the disappearance of low z sites. After inflation the sites that remain are those of high coordination numbers, A, B, C, and D_1 sites, having $z = 8, 7, 6, 5$, respectively. We refer to them collectively as α sites. Sites that disappear have $z = 5, 4$, and 3, respectively (the D_2, E, and F sites). Note that there are two types of fivefold sites that behave differently under inflation [10]. The relative number of sites of each kind, f_i, is preserved under inflation, whereas the density of sites is reduced by λ^{-2}. After inflation, sites have new coordination numbers z' as indicated in the following list of transformations: $A \rightarrow A$ or B or C or D_1; $B \rightarrow D_2$; $C \rightarrow E$; $D_1 \rightarrow F$.

A natural choice for block spins is to consider star clusters centered on sites of the α class. After inflation, the old z blocks will become the vertices of the inflated tiling, and new blocks defined at the high-z sites, and so on. The block spins and the couplings will renormalize to site-dependent values, grouped according to the local environments. Figure 2(a) shows a central D_1 site, which transforms after inflation to a $z' = 3$ site. The sites remaining after inflation are shown with large dots, and the dashed grey lines represent effective interactions between these sites. Intrablock couplings are shown by thick lines, while interblock couplings are shown by thin dotted lines. For an isolated block spin with z spins surrounding a central spin and antiferromagnetic interactions, the cluster has a spin of $S' = (z - 1)S$ in the ground state. The energy of the isolated block can be exactly found, while for the interblock couplings, we will follow the approach used in [9] for the square lattice (where all blocks carry the same value of $z = 4$), where one finds $S' = 3S$. The spin renormalization factors are taken to be equal to the classical value $\xi_z^{(0)} = 1/(z - 1)$ for simplicity. The new block spins S' are situated on the black circles representing the sites of the inflated lattice, while all of the nearest neighbors are decimated in the RG transformation.

However, on the octagonal tiling, blocks are not all isolated or disjoint as Figs. 2(b) and 2(c) show. Blocks as defined above can share pairs of sites, with a finite frequency of occurrence. This makes the tiling, a true two-dimensional structure, harder to solve than a fractal Sierpinski-type structure, which would have less connectivity. Figure 3 shows the tiling with grey dashes connecting such pairs of shared sites. To disconnect the clusters along the grey lines, the two spins are assigned to one or the other of the overlapping blocks. This is done by annulling one of the couplings for each of the spins. Thus we have a diluted version of the original tiling, with certain couplings annulled. The fraction of annulled couplings is finite and can be calculated exactly to be $\sqrt{2}/\lambda^3 \approx 0.10$ or 10%.

For example, Fig. 2(c) shows eight overlapping D_1 clusters surrounding an A site. They are decoupled by annulling one of the couplings on either side of each D site. The result is that the coordination numbers of all D_1 sites after dilution goes from $z = 5$ to $\tilde{z} = 3$. Similarly, C sites have their z reduced from 6 to 5.

For the seven local environments on the octagonal tiling, one has specific connectivity rules: an A site is always coupled to eight F sites, a B site is always coupled to five F sites and two E sites, etc. The new block spin variables take on environment dependent values, and after one inflation, one finds that $\mathbf{S}^{[1]} = (S_A^{(1)}, \ldots, S_F^{(1)}] = C\mathbf{S}^{(0)}$, with

$$C = \begin{pmatrix} -1 & 0 & 0 & 0 & 0 & 0 & 8 \\ -1 & 0 & 0 & 0 & 0 & 0 & 8 \\ -1 & 0 & 0 & 0 & 0 & 0 & 8 \\ -1 & 0 & 0 & 0 & 0 & 0 & 8 \\ 0 & -1 & 0 & 0 & 0 & 2 & 5 \\ 0 & 0 & -1 & 0 & 0 & 3 & 2 \\ 0 & 0 & 0 & -1 & 1 & 2 & 0 \end{pmatrix}, \qquad (1)$$

where $\mathbf{S}^{(0)} = (s_0, s_0, \ldots, s_0)$ and $s_0 = \frac{1}{2}$. One can follow the renormalizations as the tiling undergoes successive

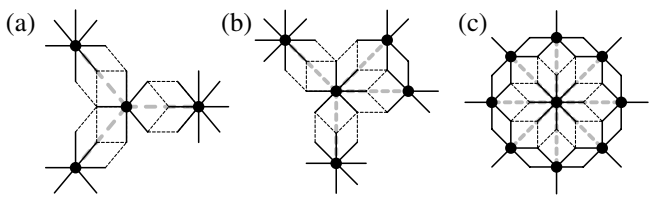

FIG. 2. Block spin centers (filled circles) showing the central and all peripheral blocks for three cases: (a) a $z = 5$, $z' = 3$ site; (b) a $z = 6$, $z' = 4$ site; (c) a $z = z' = 8$ site.

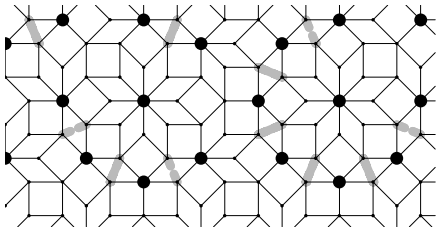

FIG. 3. Tiling showing block centers (black dots). The grey lines connect pairs of sites that are shared between two blocks.

inflations, with $\mathbf{S}^{(n)} = C\mathbf{S}^{(n-1)}$, and it is easy to show that for large n $\mathbf{S}^{(n)} \approx 3\mathbf{S}^{(n-1)}$, and spins tend to relative asymptotic values given by $(1, 1, 1, 1, 1, \frac{3}{4}, \frac{1}{2})$. In a star cluster where all spins have different lengths, with z spins of length $S_i = n_i s_0$ coupled by the same J to a central spin $S_0 = n_0 s_0$, the ground state energy is taken to be $(\sum_z n_i > n_0)$

$$\epsilon(J, z, \{n\}) = -n_0 J\left(\sum_{i=1}^{z} n_i + 2\right)/4. \tag{2}$$

If $\mathbf{n} = (n_A, n_B, n_C, n_{D1})$ are the number of blocks in a given region of each given type, the number of blocks of each type after one deflation is $N\mathbf{n}$, where

$$N = \begin{pmatrix} 1 & 0 & 0 & 8 \\ 1 & 0 & 2 & 5 \\ 1 & 0 & 4 & 2 \\ 1 & 1 & 4 & 0 \end{pmatrix}, \tag{3}$$

whose largest eigenvalue is equal to 7 so that the total number of blocks increases (decreases) with the number m of deflations (inflations) as 7^m for large m.

The effective interaction between block spins is determined by inspecting how links transform under inflation. A minimal model can be defined by considering just five types of links. The set of couplings retained in the model is represented in an array $\mathbf{j} = (j_{\alpha F}, j_{\alpha E}, j_{D_1 D_2}, j_{D_2 F}, j_{EF})$. Here, $j_{\alpha F}$ is used to denote the link between (A, F), (B, F), (C, F), and (D_1, F) pairs. Similarly, $j_{\alpha E}$ denotes the link connecting (B, E), (C, E), and (D_1, E) pairs. After inflation, the new couplings between sites are written in terms of the five old couplings, giving rise to a multiplicative renormalization scheme [11]. After one step of inflation the new couplings (the grey lines in Figs. 2) are found to be $\mathbf{j}^{(1)} = M^{(0)}\mathbf{j}^{(0)}$, where

$$M^{(n)} = \begin{pmatrix} 0 & 0 & 0 & 0 & 2\xi_A^{(n)}\xi_D^{(n)} \\ 0 & 0 & 0 & 0 & 3\xi_A^{(n)}\xi_C^{(n)} \\ 0 & 0 & 0 & 0 & 4\xi_A^{(n)}\xi_B^{(n)} \\ 0 & \xi_B^{(n)}\xi_D^{(n)} & 0 & \xi_B^{(n)}\xi_D^{(n)} & \xi_B^{(n)}\xi_D^{(n)} \\ 0 & \xi_C^{(n)}\xi_D^{(n)} & 0 & \xi_C^{(n)}\xi_D^{(n)} & \xi_C^{(n)}\xi_D^{(n)} \end{pmatrix}, \tag{4}$$

with the initial condition (taking the zero order coupling $J = 1$) $\mathbf{j}^{(0)} = (1, 1, 1, 1, 1)$. After one inflation the new Hamiltonian is written using averaged values of the renormalization factors $\xi_i^{(1)}$ and couplings since the effective spins and couplings are no longer uniform. Block energies are obtained using Eq. (2) with a site-averaged value of the coupling, calculated appropriately for each of the seven families of sites (neglecting minor differences of the local environment in some cases). A sites, for example, have eight A–F links to their neighbors, so their average local coupling is $\overline{J}_A^{(n)} = j_{\alpha F}^{(n)}$. The matrix $M^{(n)}$ evolves under successive inflations to a fixed point whose maximum eigenvalue $\gamma_5 \approx 0.15$. Thus for large n, couplings decay as $\mathbf{j}^{(n)} = \gamma_5 \mathbf{j}^{(n-1)}$, while the corresponding eigenvector determines the fixed point relative couplings.

With these definitions, we now turn to the results obtained. The first quantity of interest is the ground state energy per site, e_0. The QMC data in [2] yield a value of $e_0 \approx -0.66$, while that of the square lattice was determined numerically [12] to be about -0.67. A plausible conjecture is that the octagonal tiling, with its two sublattice structure and its average coordination number of 4, has the same GS energy as the square lattice, however this remains to be proven. In the RG scheme, the ground state energy can be written as an infinite sum

$$e_0 = \sum_{i\in\alpha} f_i(\epsilon_i^{(0)} + \epsilon_i^{(1)}/\lambda^2 \cdots + \epsilon_i^{(n)}/\lambda^{2n} + \cdots), \tag{5}$$

using the fact that the frequency of blocks of type i is initially f_i[13] and is diminished by $1/\lambda^2$ at each step of RG. Here $\epsilon^{(n)}$ is a shorthand notation for the energy of an nth stage block having a spin $S_0^{(n)}$ at the center, an averaged coupling value $\overline{J}^{(n)}$, and surrounding spins of value $S_i^{(n)}$ as given by Eq. (2). The series for the energy gives $e_0 \approx -0.51$ (compared with the result of about -0.54 [9] for the square lattice). One reason for the discrepancy between renormalization and quantum Monte Carlo results for the quasiperiodic model is the appreciable bond dilution occurring at C and D sites, which leads to having fewer energy terms in the Hamiltonian. On the other hand, the loss of bonds is partly offset by the fact that the dilution tends also to suppress frustration and raise the local order parameter. A crude way to put back the "missing bond energies" is to add in half of the missing link energies at each of the C and D sites. This is easily done by adjusting the $\tilde{z}$ values ($\tilde{z}_C$ goes up from 5 to 5.5, while $\tilde{z}_{D1}$ is increased from 3 to 4). One then finds an adjusted ground state energy of about -0.59. This correction technique will be applied to the calculation of local order parameters discussed below, with good results.

The QMC data in [2] give values of local order parameters defined in terms of the local energies $E_i = J\sum\langle\vec{S}_i \cdot \vec{S}_{i+\delta}\rangle$, where the sum is over all nearest neighbors of a given site i and the spin correlations are evaluated in the ground state. The relation taken for the local order parameters is $m_{s,i} = \sqrt{E_i/z}$ [14]. We are therefore interested in the cluster energies, E_i, as a function of z. In the zeroth approximation the cluster energies are the HS energies obtained from Eq. (2), $\epsilon^{(0)} = -(z + 2)/4$. The RG allows us to calculate the cluster energy $E^{(n)}$ on increasingly bigger length scales, where z is the coordination number of the central spin at the end of n steps. For example, taking $n = 1$, consider an A site of the inflated tiling with eight F sites around it. The ancestor of the central A site is an A site with an associated block energy of $\epsilon_A^{(0)}$. The ancestors of the neighbors are D_1 sites, and each one contributes half its block energy to the cluster

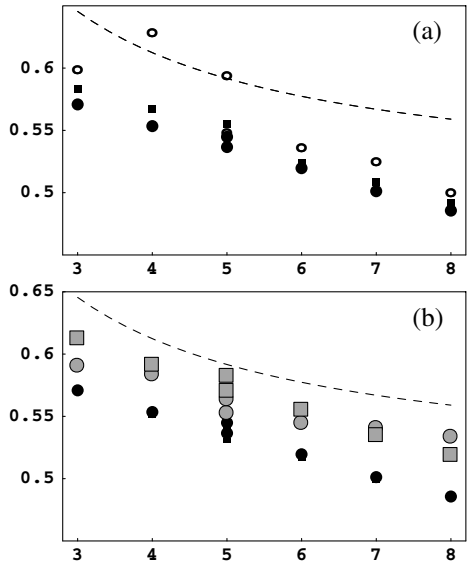

FIG. 4. m_s values plotted versus z for increasing orders of RG. (a) zero (dashed line), first (open circles), second (rectangles), and third (filled circles) order RG. (b) QMC data (grey circles), third (black circles), and fourth (black rectangles) order RG, and corrected fourth order data (grey rectangles).

energy. The total energy $E_A^{(1)}$ is therefore the sum of the cluster energy for A sites having a first-order coupling $\overline{J}_A^{(1)}$, plus a zeroth order A block energy term, plus half the zeroth order block energies of its neighbors as follows:

$$E_A^{(1)} = \epsilon_A^{(1)} + \epsilon_A^{(0)} + 4\epsilon_{D1}^{(0)}, \tag{6}$$

and similar expressions are written for the other six types of site. At each stage of RG, the cluster energies $E^{(n)}$ are used to find the corresponding values of the local order parameters. For $n = 2$, cluster energies for the twice-inflated tiling can be written out in terms of the energies $\epsilon_i^{(k)}$ ($k = 0, 1, 2$). The number of terms contributing to the cluster energy is governed by the largest eigenvalue of N, so that $E^{(n)}/7^n$ tends to a limit as $n \to \infty$. In that limit, the quantities $m_s = \sqrt{z^{-1}E^{(n)}/7^n}$ therefore have asymptotic values which are compared to the available numerical data. In Fig. 4(a) we have compared the m_s obtained after zero (dashed line), one and two and three RG steps (open circles, squares, and filled circles, respectively). After two steps, the values of m_s converge quickly. In Fig. 4(b) are shown the third (circles) and fourth order (squares) results which overlap on the scale of the figure. The limiting values of m_s are clearly below the QMC data, shown as grey circles, and this is expected due to the bond dilution. If the bond reduction is compensated by putting back half the bonds as we did earlier to estimate e_0, we get estimates for m_s values on the original octagonal tiling. The grey squares of Fig. 4(b) were obtained by correcting the $n = 4$ data in this way, in fairly good agreement with the QMC data.

In conclusion, we have presented an RG scheme for a two-dimensional quasiperiodic tiling that can be completely solved, under certain approximations. The problem is of importance as being the simplest 2D aperiodic quantum antiferromagnetic spin model possible, like the square lattice antiferromagnet for periodic systems. The results of the approximate RG in regards to the local order parameters are close to those calculated for the full undiluted model, and we believe the model takes into account important aspects of the quasiperiodic geometry of the tiling. The method is less good at obtaining the ground state energy. We note that the ground states of the octagonal tiling and the square lattice appear to share the same value of the ground state energy—a conjecture awaiting proof. One notes finally that the RG calculation after appropriate modifications can be extended to electronic, vibrational, and other discrete problems (work in progress).

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[11] Intercluster bonds are not considered to be affected by bond dilution. Thus a central A site linked to eight D_1 clusters around it by 16 links retains all those links to the eight clusters, i.e., retains two links per D_1 cluster (in a sort of bond-moving step).
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[14] Note a slight change of definition of m_s from that of Ref. [3].