Penrose quantum antiferromagnet

A. Jagannathan and A. Szallas
Laboratoire de Physique des Solides, CNRS-UMR 8502, Université Paris-Sud, 91405 Orsay, France

Stefan Wessel
Institut für Theoretische Physik III, Universität Stuttgart, 70550 Stuttgart, Germany

Michel Duneau
Centre de Physique Théorique, CNRS-UMR 7644, Ecole Polytechnique, 91128 Palaiseau, France
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The Penrose tiling is a perfectly ordered two-dimensional structure with fivefold symmetry and scale invariance under site decimation. Quantum spin models on such a system can be expected to differ significantly from more conventional structures as a result of its special symmetries. In one dimension, for example, aperiodicity can result in distinctive quantum entanglement properties. In this work, we study ground-state properties of the spin-1/2 Heisenberg antiferromagnet on the Penrose tiling, a model that could also be pertinent for certain three-dimensional antiferromagnetic quasicrystals. We show, using spin-wave theory and quantum Monte Carlo simulation, that the local staggered magnetizations strongly depend on the local coordination number z and are minimized on some sites of fivefold symmetry. We present a simple explanation for this behavior in terms of Heisenberg stars. Finally, we show how best to represent this complex inhomogeneous ground state using the "perpendicular space" representation of the tiling.

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The Penrose tiling,[1] illustrated in Fig. 1, is one of the best known quasiperiodic tilings. Its counterpart in one dimension is the Fibonacci chain, while its three-dimensional counterpart is the three-dimensional Penrose or icosahedral tiling—the basic template for many quasicrystalline alloys. One of the most striking and experimentally observable features of the Penrose tiling is its fivefold symmetric structure factor with sharp peaks in reciprocal space. In real space, the tiling, built from two types of rhombuses, has a set of vertices of coordination number z ranging from 3 to 7, with an overall coordination number of exactly 4. The characteristics of the Penrose tiling, such as the tile shapes or the relative frequencies of vertices, can be expressed in terms of the golden mean $\tau=(\sqrt{5}+1)/2$. This irrational number also gives the length scale for the transformations called inflations (deflations) that leave the tiling invariant, in which the basic units of the tiling are redefined so as to give a Penrose tiling on a larger (smaller) scale. These and many other fascinating properties of the Penrose tiling have been extensively studied in the literature.[2] This type of ordered structure can lead to complex physics, as shown by a large number of studies on electronic properties in this and other quasiperiodic models.[3,4] Quasiperiodic quantum spin chains have also been the subject of many studies. The recent interest in quantum entanglement of spins has led, for example, to the investigation of one-dimensional critical aperiodic systems,[5] showing that the entanglement entropy depends on the strength of the aperiodicity. Quantum effects are biggest in low dimensions and small spin value, while 2 is the smallest dimension for which $T=0$ order can occur. It is therefore interesting to consider the Penrose $S=\frac{1}{2}$ antiferromagnet and compare its properties with those of simpler structures.

In an antiferromagnet, quantum fluctuations around the Néel state lead to a reduction of the order parameter with respect to its classical value, even at $T=0$. On bipartite Archimedean lattices, where all sites have the same value of z, the staggered magnetization is expected to increase with z toward the classical value of $\frac{1}{2}$. This effect is easily explained within linear spin-wave theory,[6] and it is confirmed in a number of numerical calculations. Thus, for example, the order parameter on the honeycomb lattice ($z=3$), $m_s \approx 0.235$,[7] is more strongly suppressed than on the square lattice ($z=4$), where $m_s \approx 0.307$.[8]

For inhomogeneous structures with more than one value of z, it was recently argued that, contrarily to naive belief based on the preceding remarks, quantum fluctuations in the ground state are typically *greater* on sites with greater z.[9] The Penrose tiling is the most complex of the structures so far studied, with more local environments and more complex transformation rules than the quasiperiodic octagonal tiling studied in Refs. 10 and 11. The ground state of the former has significantly stronger variations of the local-order parameters as compared to the latter. The results show a strong decrease of on-site magnetization with z for small z, followed by an upturn for larger z—a behavior we will explain by generalizing an argument presented in Ref. 9.

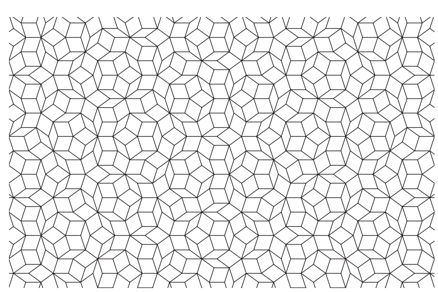

FIG. 1. Portion of the Penrose tiling.

The ground state of the Penrose antiferromagnet can be described in terms of the local staggered magnetizations. We calculate these by two different methods: linearized spin-wave (LSW) theory and quantum Monte Carlo (QMC). Although the real-space distribution of the local staggered magnetization thus found is complex, a compact visualization of it is possible in "perpendicular space," as will be explained below.

The model we consider is the nearest-neighbor Heisenberg antiferromagnet

$$\mathcal{H} = \sum_{\langle i,j \rangle} J\vec{S}_i \cdot \vec{S}_j, \tag{1}$$

where the sum is taken over pairs of linked sites and all bonds $J>0$ are of the same strength. The site index i takes values from 1 to N, for the finite-size systems considered. The first type of systems we consider are periodic approximants called Taylor approximants—after their use in the description of the Taylor phases of intermetallic compounds in the Al-Pd-Mn system[12]—which allow using periodic boundary conditions. These approximants can be constructed in such a way as to obtain sublattices of equal size, and we have considered four such systems, with $N=96$, 246, 644, and 1686 sites. These approximants have defects as compared to the infinite perfect tiling, but the relative number of defects becomes negligible as N increases. We also considered finite pieces of the perfect Penrose tiling and found that spin magnetizations in the interior of the finite sample are close to those obtained for the Taylor approximants, showing their relative insensitivity to boundary conditions.

The model of Eq. (1) is unfrustrated, and the ground state of this bipartite system breaks the SU(2) symmetry of H, with the order parameter being the staggered magnetization $M_s=\Sigma_i \epsilon_i \langle \vec{S}_i^z \rangle \equiv \Sigma_i m_{si}$, where $\epsilon_i = \pm 1$ depending on whether i lies in sublattice A or B and $m_{si}=|\langle S_i^z \rangle|$ are the local-order parameters.

Within the QMC simulations, we obtain $m_{si}^2 = \frac{3}{N}\Sigma_{j=1}^N \epsilon_i \epsilon_j \langle S_i^z S_j^z \rangle$ from the spin-spin correlation functions.[10] The QMC simulations were performed using the stochastic series expansion method[8] for the Taylor approximants at temperatures chosen low enough to obtain ground-state properties of these finite systems.[10]

To obtain the spin-wave Hamiltonian, one uses the Holstein-Primakoff boson representation of S^z on each sublattice in terms of the deviation from the classical values of $\pm S$, $S_i^z = S - a_i^\dagger a_i$ and $S_j^z = -S + b_j^\dagger b_j$, respectively.[13] The a_i, b_j $(i,j=1,\ldots,N/2)$ and their adjoints obey appropriate bosonic commutation relations and correspond to the sites of the A and B sublattices, respectively. The spin raising and lowering operators on the two sublattices are $S_i^+ = \sqrt{2S}\left(1-\frac{n_i}{2S}\right)^{1/2} a_i$ and $S_j^+ = \sqrt{2S} b_j^\dagger \left(1-\frac{n_j}{2S}\right)^{1/2}$, respectively. After expanding to order $1/S$, the (LSW) Hamiltonian can be diagonalized by a generalized Bogoliubov transformation.[14] The ground-state energy and m_{si} can then be calculated from the transformation matrix (cf., e.g., Ref. 11). The LSW result for the ground-state energy, extrapolated to the thermodynamic limit, is $E_0/N = -0.643J$, and compares well to the QMC result, $E_0/N = -0.6529(1)J$.

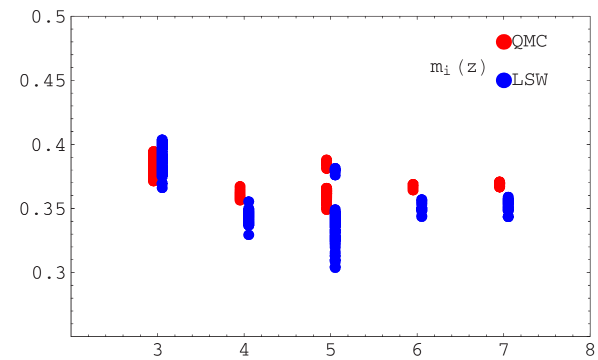

FIG. 2. (Color online) Local staggered magnetization plotted vs coordination number z as obtained by QMC (red) and by LSW theory (blue).

Figure 2 shows the values of m_{si} plotted against coordination number z for the largest approximant ($N=1686$) for both the LSW and QMC data. In comparison with the other known quasiperiodic structure, the octagonal tiling (see Ref. 11), the variations of the local-order parameters are larger, making it possible to identify some of the trends more clearly. The values initially decrease with z, but then tend to go upward. There appears, thus, to be a minimum in $m_s(z)$ at $z=5$—the median z value in this tiling. (On the infinite tiling as well as the approximants, the mean value of z is exactly 4.) The average value of the magnetizations is also higher on the Penrose tiling, compared to the octagonal tiling, showing a suppression of quantum fluctuations due to greater structural complexity.

Another noteworthy feature is the wide spread in the values for $z=5$. This is related to the complex structural properties of the lattice, as there are three sets of sites with $z=5$. The first set, which occurs most frequently, does not possess local fivefold symmetry and corresponds to the intermediate range of values of m_{si}. The two other sets of sites have a fivefold symmetry and are at the centers of football-shaped clusters (F) or star-shaped clusters (S). F sites correspond to the lowest m_{si} values, while the highest m_{si} values are obtained at the S sites.

This local hierarchy in the magnetic structure on the Penrose tiling becomes evident in the perpendicular space structural representation.[2] The vertices of the Penrose tiling can, in effect, be considered as the projection of vertices of a five-dimensional cubic lattice onto the x-y ("physical") plane. If those vertices are instead projected onto the three remaining dimensions or perpendicular space, one obtains dense packings of points lying on four distinct pentagon-shaped plane regions. In this perpendicular space projection, sites having the same environment map into the same subdomain of the selection windows (applied to a crystalline structure, the same operation would lead to as many points as there are distinct environments, of which there are a finite number, contrarily to the quasicrystal). The different domains are labeled in Fig. 3 by the value of z associated with each domain. In addition, the domains corresponding to the sets of F and S sites are shown, along with their appearance in real space.

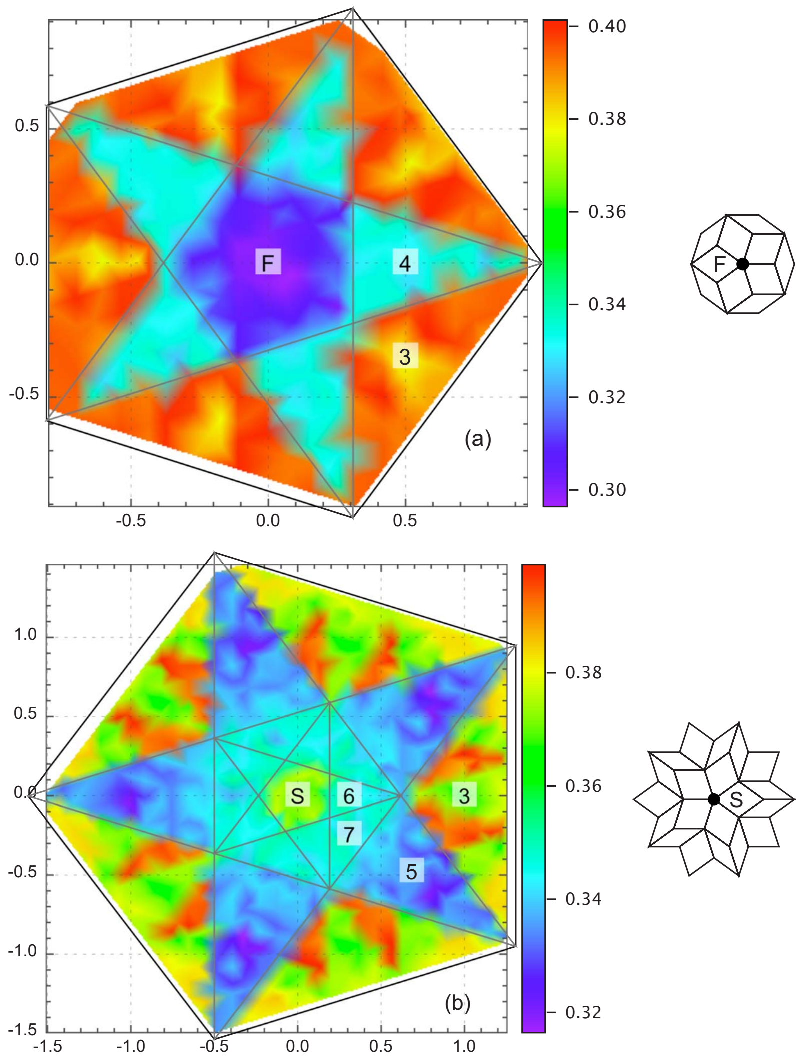

FIG. 3. (Color online) Two out of the four perpendicular space projected domains of the Penrose tiling, with a color coding of the sites according to the value of the local staggered magnetization determined by linear spin-wave theory.

Using a color map to represent the local-order-parameter strengths, we obtain compact representations of the ground state as in Fig. 3, which thus shows the LSW magnetizations of sites corresponding to two of the perpendicular space planes (the two others being identical up to rotations). The points in the central star-shaped region of Fig. 3(a) correspond to the F sites and have the smallest staggered magnetizations. In Fig. 3(b), the central pentagon corresponds to the S sites, which have the highest staggered magnetizations at $z=5$.

A simple model for the local staggered magnetization is based on a Heisenberg star cluster consisting of a central spin coupled to z neighboring spins.[9] One considers the external spins to be embedded in an infinite medium, so that there is a finite net staggered magnetization. By carrying out the standard expansion in boson operators, one then finds that the center magnetization is smaller than that of the outer spins.[9] This model, which takes into account only the nearest neighbors, is clearly inadequate to describe the nonmonotonic dependence of magnetizations observed. We consider, therefore, a generalization to a two-level Heisenberg star in order to investigate the effects of next-nearest neighbors on the central spin magnetization. The cluster we consider is shown in Fig. 4, where the central site has z nearest neighbors and zz' next-nearest neighbors. All the couplings (represented by the links in the figure) are taken equal, with $J>0$.

The Hamiltonian of this cluster of $1+z(1+z')$ spins can be diagonalized in linear spin-wave theory, with the following result for the central spin's staggered magnetization:

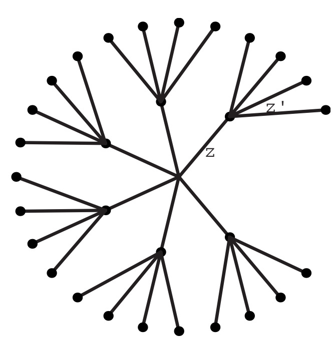

FIG. 4. A two-level Heisenberg star showing the central spin and its z nearest neighbors and zz' next-nearest neighbors. In the example shown, $z=6$ and $z'=4$.

$$m_s(z,z') = \frac{1}{2} - \frac{z f_1^2(z,z')}{f_2^2(z,z') - z f_1^2(z,z') - 4z'}, \tag{2}$$

where $f_{1(2)} = -z' \pm [2 - z + \sqrt{4 - 4z + (z+z')^2}]$. This yields a staggered magnetization that approaches the classical limit of 0.5 in the limit of large z and/or z'. In addition, for fixed z, this function $m_s(z,z')$ has a minimum for a value of z' between $z-1$ and z. In other words, the quantum fluctuations on the central site are largest when this site and its neighbors have similar coordinations.

Turning now to the Penrose tiling, effective values of z' can be assigned for each site by counting the number of its next-nearest neighbors. One finds that sites of small z have higher values of z' (next-nearest-neighbor number), with the opposite being true for sites of high z. This means that the density of sites, in other words, does not have large local fluctuations on the Penrose tiling. A single effective z' is found for all the sites except for the values $z=3$ and $z=5$. For the $z=3$ sites, we find $z'=4$, 4.3, and 4.7, where the nonintegral values result from the fact that the clusters on the tiling do not have the regular tree structure of the model shown in Fig. 4. This leads to a spread in the values of the local staggered magnetizations. The generic $z=5$ sites correspond to $z'=2.8$, while F and S sites have $z'=2.4$ and 4, respectively. The resulting values for the $m_s(z,z')$ obtained using Eq. (2) along with the values of z and z' for each class of site are shown in Fig. 5.

The predictions of the simple analytical model, which is based on the number of nearest and next-nearest neighbors only, agree qualitatively quite well with the numerical results shown in Fig. 2 for most z. The complete description must, of course, include longer ranged structural differences, seen clearly in Fig. 3: the domains of sites of a given coordination number are not colored uniformly but are instead further separated into subdomains. The hierarchical invariance of the original structure, which has not been exploited in these calculations (as was done in Ref. 15 using a renormalization-group approach for the octagonal tiling), is expected to lead to self-similarities in the order-parameter distribution function. This analysis, which requires considering much bigger sample sizes, is left for further investigations.

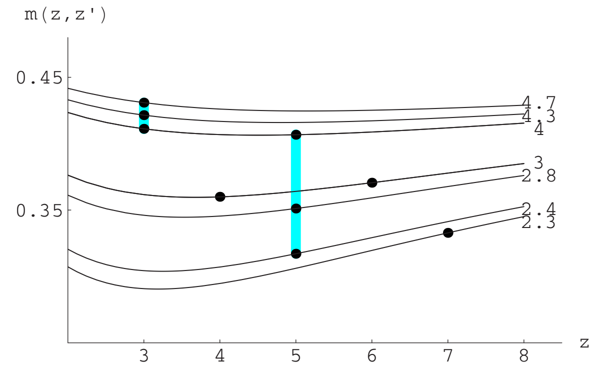

FIG. 5. (Color online) Staggered magnetization as predicted by Eq. (2) as a function of z for different z' values. The points indicate the value of z' computed (see text) for sites of the Penrose tiling.

In conclusion, we have considered quantum fluctuations in the Penrose tiling, a two-dimensional structure that has perfect long-range structural order but with an infinite number of spin environments. The overall value of the staggered magnetization is higher than on the octagonal tiling, which is, in turn, higher than on the square lattice. This indicates a progressive suppression of quantum fluctuations in going from the periodic to the simple quasiperiodic, and finally, to the more complex quasiperiodic structure. The geometry of the Penrose tiling leads to an antiferromagnetic ground state with extremely large variations of the local staggered magnetization compared to other systems studied recently in this context. The heirarchical symmetry present in the ground state is best seen in perpendicular space projections such as the ones shown in this Brief Report. Finally, to explain our results, we present a two-level Heisenberg star argument showing that quantum fluctuations tend to be maximized when the site coordination number and the next-nearest-neighbor coordination numbers are closely matched in value.

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