Exactly solvable spin models in quasicrystals

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A general method is proposed for constructing fully-integrable dynamic models in quasicrystals. This method is illustrated using the example of a spin model for a quasiperiodic tiling of a plane by two rhombi. A second example constructed in this paper is a spin model for icosahedral filling of three-dimensional space. The free energy is calculated for these models.

1. INTRODUCTION

The quasiperiodic tiling of a plane by two rhombi which was proposed by Penrose^{1,2} is a canonical example of a twodimensional quasicrystal. The rhombi tile the entire plane and do not intersect one other, and no translation maps this covering into itself. However, any finite portion of this covering occurs within the covering an infinite number of times. In a number of cases the tiling can possess additional symmetries, for example a five-fold axis. De Bruijn³ succeeded in explaining the properties of this tiling with the help of duality transformations. It turns out that the lattice dual to this tiling is simply a set of straight lines on the plane. In Ref. 4 a three-dimensional generalization of the Penrose tiling was proposed, in which the rhombi are replaced by rhomboids. The rhomboid is a special case of the parallelepiped, in which all the sides are the same length while each face is a rhombus. The filling of three-dimensional space by two rhomboids has icosahedral symmetry.⁵ The experimental discovery of icosahedral symmetry⁶ (in the rapidly cooled alloy has played an important role: the crystal structure of this alloy was elucidated in Refs. 7-9. The Penrose tiling has attracted a great deal of interest (Refs. 10-14); in Refs. 3, 5 and 10-13 it was shown that the method of duality transformations provides a general method of constructing quasiperiodic tilings (in a space of arbitrary dimension). Specifically, this method will be used in the present paper to construct exactly solvable models in quasicrystals. The properties of dynamic systems in quasicrystals have been discussed in the literature (Refs. 15-18). On the other hand, fully integrable models have attracted the close attention of theorists; see, e.g., Refs. 19-30 and citations therein.

In the present paper, fully integrable models in quasicrystals (among them the two-dimensional Ising model) are constructed (and solved). A preliminary communication on this subject was published in Ref. 12. In the present paper a general method is presented for constructing exactly solvable dynamic models in quasicrystals. In Section 2 the basic properties of the quasiperiodic tiling of the plane by two rhombi are described; these properties allow us to construct the eight-vertex model of interacting spins for this tiling in Section 3. In Section 4 we described the icosahedral filling of three-dimensional space by two rhomboids. Section 5 is devoted to the Zamolodchikov model, which describes interacting spins in the three-dimensional case. The model is based on the solution of the tetrahedron equations. This solution is used in Section 6 to construct an exactly solvable spin model for icosahedral filling of three-dimensional space.

2. THE PENROSE COVERING

In this section the basic properties of quasiperiodic tilings of the plane by two rhombi are presented. This covering will be denoted by the letter Q. Each rhombus belonging to the tiling can be obtained by translations and rotations of one of a pair of rhombi. This pair consists of a wide rhombus (angles 72° and 108°) and a narrow rhombus (angles 36° and 144°). The length of each side equals one. So as to describe the orientation of the rhombi of the tiling, it is convenient to introduce five vectors:

$$\mathbf{d}_{j} = i \exp\left(\frac{1}{5}i\pi j\right), \quad j = 0, 1, 2, 3, 4.$$
 (2.1)

Here we use complex coordinates for the plane. All the vectors \mathbf{d}_i belong to the left half plane; with each pair of vectors \mathbf{d}_k , \mathbf{d}_i (k > j) we associate a rhombus r_{ki} . The vectors \mathbf{d}_k , \mathbf{d}_i are orthogonal to the sides of the rhombus r_{kj} , see Fig. 1; in this way the set of vectors (2.1) determine ten basic rhombi, five narrow and five wide (oriented in various ways). All rhombi belonging to the quasiperiodic tiling q can be obtained from the basic rhombi by translations alone. An important characteristic of the tiling ρ is the relative frequency ω_{ki} of occurrence of a basic rhombus within the entire covering. In the case where the tilin has the symmetry of a regular pentagon,^{1,2} the frequencies of all the narrow rhombi are the same, which is also the case for all the wide rhombi. Let us denote by ω_N the frequency of occurrence of a narrow rhombus, and that of a wide one by ω_{W} . These frequencies are given by the following expressions:

$$\omega_W = 1/5\tau, \quad \omega_N = 1/5\tau^2.$$
 (2.2)

Here, τ is the golden mean:

$$\tau = (1 + \sqrt{5})/2$$
 (2.3)

(we note that the plane can be tiled in a periodic fashion with the help of translations of one of the basic rhomboids).



FIG. 1. Basic rhombus r_{ii} . The vectors \mathbf{d}_k , \mathbf{d}_i are orthogonal to its sides.

In Ref. 3, a lattice G was constructed which was dual to the tiling Q. This lattice was constructed in the following way; let us take one of the \mathbf{d}_j (2.1), and investigate the infinite set of equivalent straight lines parallel to this vector (the spacing between neighboring lines equals 1). Let us now investigate the five such sets which are created by each of the vectors \mathbf{d}_j in turn. The set of all these lines divides the plane into an infinite set of distinct polygons (the cells of the lattice); in this way we define the lattice G. The duality relation between G and Q is formulated as follows: each cell of the lattice corresponds to a vertex of the tiling Q. To each cell edge of G there corresponds an edge of Q. Each vertex of G corresponds to a cell of Q, where the cells of Q are rhombi.

We should point out that there exist many distinct quasiperiodic tilings. Duality transformations are a general method of constructing quasiperiodic tilings.^{5,10-13} The lattice always is an infinite set of straight lines on the plane. In the three-dimensional case the duality transformation is described in Section 4.

3. EXACTLY SOLVABLE SPIN MODELS IN A TWO-DIMENSIONAL QUASICRYSTAL

In this section we will construct an eight-vertex model for a quasiperiodic tiling of the plane by two rhombi. The spins σ are located at the vertices of the tiling (the vertices of the rhombi). Each spin takes on the two values ± 1 . The spins interact around the cells of Q. Each cell of Q is a rhombus.

The Hamiltonian H of the model is given by the expression:

$$-\frac{H}{T} = \sum_{i} \left(P_{kj}' \sigma_i \sigma_n + P_{kj} \sigma_p \sigma_m + P'' \sigma_i \sigma_m \sigma_n \sigma_p \right).$$
(3.1)

Here T is the temperature. The summation is taken over all the cells of Q (rhombi). The expression in square brackets is the contribution from a given rhombus r_{kj} . The positions of the spins at the vertices of the rhombus are shown in Fig. 1. The quantities P are dynamic coefficients. Let us investigate the pair of vectors \mathbf{d}_k , \mathbf{d}_i orthogonal to the sides of a given rhombus r_{kj} . We fill in the sector between the vectors (and also the opposite sectors) with hatching (see Fig. 1). One pair of vertices of the rhombus r_{ki} belongs to the dashed sectors (σ_n, σ_1) , while the other pair belongs to the unhatched sectors (σ_p , σ_m). The interaction of the spins in the dashed sectors are described by the dynamic coefficients P'_{kj} , while the interaction of spins in the unhatched sectors are described by the coefficients P_{kj} . The coefficients P_{kj} and P'_{ki} depend on the orientation of the rhombus; in all there are 21 dynamic coefficients. The partition function is defined in the usual way:

$$Z - \sum_{(\sigma)} \exp\left(-H/T\right). \tag{3.2}$$

In the thermodynamic limit, the free energy $F = -T \ln Z$ is proportional to the number of rhombi N. The free energy density has a finite limit

$$f = \lim \left(F/N \right). \tag{3.3}$$

The model (3.1) can be solved only in the case where the 21 dynamic coefficients P depend on only 6 independent parameters. This parametrization can be written in terms of

elliptic functions; the modulus k of the elliptic functions is one of the parameters. With each vector \mathbf{d}_j (2.1) we associate an independent parameter α_j ; they form an increasing sequence $\alpha_k > \alpha_j$ (if k > j). We will call α_j the spectral parameters. The final parameter is the coupling constant λ . With each basic rhombus r_{kj} we associate a value

$$\alpha_{kj}' \equiv \alpha_k - \alpha_j, \quad \alpha_{kj} \equiv \lambda + \alpha_j - \alpha_k, \quad k > j$$
(3.4)

and obtain the inequalities

$$0 < \alpha_{kj}, \quad \alpha_{kj}' < \lambda < 2K', \quad k > j.$$
(3.5)

The quantities K and K' are complete elliptic integrals of the first kind corresponding to the moduli k and $k' = (1 - k^2)^{1/2}$. The dynamic coefficients are expressed through the independent parameters via the following formulae:

$$2iP_{kj}' = \operatorname{am}[i(K' - \alpha_{kj}')], \quad 2iP_{kj} = \operatorname{am}[i(K' - \alpha_{kj})],$$
$$2iP'' = -\operatorname{am}[i(K' - \lambda)]. \quad (3.6)$$

In this way an exactly solvable spin model is constructed.

It is possible to solve this model in the following way. Let us reformulate the model on the lattice G dual to the tiling Q, see Section 2. The spins are found to be located in the cells of the lattice; they interact through a vertex of the lattice. With each straight line of the lattice there is associated a spectral parameter σ_j . Thus, the model is equivalent to a special case of the eight-vertex model on an irregular lattice.²⁰ This fact allows us to solve the model. The free energy density equals

$$f = \sum \omega_{kj} f_0(P_{kj}, P_{kj'}, P'').$$
 (3.7)

The summation extends over ten basic rhombi, while $r \ge k > j \ge 0$; ω_{kj} is the relative frequency (2.2); f_0 is the free energy density for the periodic case. In the case of a periodic tiling of the plane by shifts of one of the basic rhombi, the spin model is determined analogously, and is equivalent to the standard eight-vertex model.¹⁹ The solution to this model in the periodic case was solved within the context of quantum-mechanical methods for the inverse problem in Ref. 21. The periodic model depends only on three dynamic coefficients P, P', P''. The dependence of the free energy on the dynamic coefficients possesses a certain symmetry (the duality property),^{19,20} This allows us to investigate the dynamic coefficients only in the region

$$e^{(P+P'+P'')} \ge e^{(P-P'-P'')} + e^{(-P+P'-P'')} + e^{(-P-P'+P'')}.$$
 (3.8)

In this region the free energy density f_0 (for the periodic case) equals

$$-\frac{1}{T}f_{0}(P, P', P'')$$

$$= P + P' + P'' + \sum_{n=1}^{\infty} \frac{x^{-n}(x^{2n} - q^{n})^{2}(x^{n} + x^{-n} - z^{n} - z^{-n})}{n(1 - q^{2n})(1 + x^{2n})}.$$
(3.9)

Here

$$q = \exp\left(-2\pi \frac{K'}{K}\right), \quad x = \exp\left(\frac{-\pi\lambda}{2K}\right),$$
$$z = \exp\left[\frac{\pi(\alpha - \alpha')}{2K}\right]. \quad (3.10)$$

The local magnetization and polarization for the quasiperiodic tiling equal

$$\langle \sigma_i \rangle = \prod_{n=1}^{\infty} \frac{1 - x^{4n-2}}{1 + x^{4n-2}},$$
 (3.11)

$$\langle \sigma_i \sigma_m \rangle = \prod_{n=1}^{\infty} \left(\frac{1+q^n}{1-q^n} \right)^2 \left(\frac{1-x^{2n}}{1+x^{2n}} \right)^2. \tag{3.12}$$

Thus, the spin model for the two-dimensional quasicrystal has been solved. In the case P'' = 0 it is equivalent to two noninteracting Ising models.

In conclusion, it must be emphasized that we have presented a general method of constructing exactly solvable models in quasicrystals. The quasicrystal can be obtained with the help of a duality transformation from the lattice.^{3,5,10-13} The eight-vertex model can be solved for an arbitrary lattice.²⁰ It is clear that not only the eight-vertex model but an arbitrary R matrix satisfying the Yang-Baxter model relations^{19,21,22} can be used to construct an exactly solvable model in some quasicrystal. However, the models we can construct are not limited to fundamental²² (spin) models; any *L*-operator satisfying the bilinear relations²³ with some R matrix generates a fully integrable model in the quasicrystal.

4. ICOSAHEDRAL FILLING OF THREE-DIMENSIONAL SPACE

The three-dimensional case is investigated in a way analogous to the two-dimensional case. The quasicrystal Q here is a quasiperiodic filling of three-dimensional space by shifts of a finite number of rhomboids. (The rhomboid is a special case of a parallelepiped, all of whose faces are identical rhombi.) The rhomboids are constructed as follows: we take an icosahedron, which has six fivefold axes. Let us investigate the six unit vectors

$$\mathbf{e}_{j}, j=1, 2, 3, 4, 5, 6,$$
 (4.1)

directed along these axes. Each triad of these vectors generates a rhomboid F_{iki} :

$$F_{ikj} = \mu_i \mathbf{e}_i + \mu_k \mathbf{e}_k + \mu_j \mathbf{e}_j, \quad 0 \leq \mu_{i, k, j} < 1.$$

The quantity μ is a real number. In all there are twenty $\binom{6}{3}$ of

these rhomboids, which form the basic rhomboids. By shifting these rhomboids we can fill the entire space. Ten of these rhomboids can be obtained by rotation from a narrow rhomboid which is generated (see (4.2)) by the vectors

$$\mathbf{e}_{i} = \gamma(0, 1, \tau), \quad \mathbf{e}_{2} = \gamma(-\tau, 0, -1), \quad \mathbf{e}_{3} = \gamma(\tau, 0, -1),$$

$$\gamma = (1 + \tau^{2})^{1/2} \tau = (1 + \sqrt{5})/2.$$
(4.3)

The other ten basic rhomboids are obtained by rotation from the wide rhomboid, which is generated (see (4.2)) by the vectors

$$\mathbf{e}_{4} = \gamma(0, -1, \tau), \quad \mathbf{e}_{5} = \gamma(\tau, 0, 1), \quad \mathbf{e}_{6} = \gamma(0, 1, \tau).$$
 (4.4)

The relative frequency ω_{ikj} of appearance of a given basic rhomboid F_{ikj} throughout the quasicrystal Q is also of interest. In the case of icosahedral symmetry¹⁴ the individual frequency for each narrow rhomboid equals

$$\omega_N = 1/10\tau^2. \tag{4.5}$$

The individual frequency of each wide rhomboid equals

$$\omega_W = 1/10\tau. \tag{4.6}$$

The lattice G is dual to the quasicrystal Q, and will play an important role in constructing exactly solvable models. The lattice is constructed in the following way: we investigate an infinite equivalent set of planes orthogonal to a given vector \mathbf{e}_i (4.1) (the spacing between neighboring planes equals 1). In all there are six of these sets of planes (4.1): we investigate them all. This system of planes divides the threedimensional space into an infinite set of polyhedrons (each of which is a cell of the lattice); this is how the lattice is constructed. The duality relation between G and Q can be expressed in the following way (see Refs. 5, 10–13): to each cell of the lattice there corresponds a vertex of Q, while to each face of G there corresponds an edge of Q and to each edge of G corresponds a face of Q. Cells of Q (rhomboids) correspond to vertices of G.

In conclusion we should point out that there exist many distinct quasiperiodic fillings (quasicrystals) of this sort. Icosahedral symmetry is not necessarily one of their properties. The dual transformation is a general method of constructing quasicrystals,^{3,5,10–13} for which the lattice is always a system of planes. In Section 6 we will construct an exactly solvable spin model for an arbitrary quasicrystal, using a solution to the tetrahedron equations described in the next section.

5. THE ZAMOLODCHIKOV MODEL

Zamolodchikov constructed a fully integrable model of interacting spins in the three-dimensional case.^{24,25} The Boltzmann weights of this model satisfy the tetrahedron equations. In order to prove that they satisfy all the tetrahedron equations, it is convenient to reformulate the model on the dual lattice²⁶; this formulation will be used below. Let us investigate a standard cubic lattice \mathscr{L} (with an edge of 1) in the three-dimensional space. The spin σ are located at the vertices of this lattice. Each spin σ can take on two values ± 1 . They interact around the cube, and there is a Boltzmann weight W associated with each unit cube. The locations of spins a, \ldots, h at the vertices of a unit cube are shown in Fig. 2. The Boltzmann weight connected with this cube we will write as

$$W(a|e, f, g|b, c, d|h; \theta_{23}, \theta_{13}, \theta_{12}).$$
(5.1)

The weight depends not only on the spins but also on three real parameters θ_{23} , θ_{13} , θ_{12} (angles). So as to define these parameters, we will introduce three unit vectors \mathbf{n}_1 , \mathbf{n}_2 , \mathbf{n}_3 (they need not necessarily coincide with vectors belonging to the lattice \mathcal{L}). The vectors n_1 , n_2 , n_3 are analogous to the spectral parameters, and define the angles θ :

 $(\mathbf{n}_1\mathbf{n}_2) = \cos \theta_{12}, \quad (\mathbf{n}_1\mathbf{n}_3) = \cos \theta_{13}, \quad (\mathbf{n}_2\mathbf{n}_3) = \cos \theta_{23}.$ (5.2)

So as to write out an explicit expression for W, it is convenient to introduce the spherical excesses

$$2\boldsymbol{\vartheta}_{0} = \boldsymbol{\theta}_{12} + \boldsymbol{\theta}_{13} + \boldsymbol{\theta}_{23} - \boldsymbol{\pi}, \qquad \boldsymbol{\vartheta}_{i} = \boldsymbol{\theta}_{jk} - \boldsymbol{\vartheta}_{0}. \tag{5.3}$$

Here i, j, k is a permutation of 1, 2, 3. We further define



FIG. 2. Positions of spins a, \ldots, h on the vertices of a cube.

$$t_{l} = [tg(\vartheta_{l}/2)]^{\frac{1}{2}}, \quad s_{l} = [sin(\vartheta_{l}/2)]^{\frac{1}{2}}, \\ c_{l} = [cos(\vartheta_{l}/2)]^{\frac{1}{2}}, \quad l = 0, 1, 2, 3,$$
(5.4)

and also

$$P_{0}=1, \quad Q_{0}=t_{0}t_{1}t_{2}t_{3}, \quad R_{0}=s_{0}/c_{1}c_{2}c_{3}, \\ P_{i}=t_{j}t_{k}, \quad Q_{i}=t_{0}t_{i}, \quad R_{i}=s_{i}/c_{0}c_{j}c_{k}.$$
(5.5)

In terms of these quantities, the Boltzmann weight W are presented in the table. The partition function Z is standard:

$$Z = \sum_{(\sigma)} \prod W(a | e, f, g | b, c, d | h),$$
 (5.6)

where the product is carried out over all cubes. The free energy density f_0 is calculated in Ref. 27:

$$-f_{0}(\theta_{23},\theta_{13},\theta_{12})/k_{B}T = -\ln(c_{0}c_{1}c_{2}c_{3})$$

$$+\Phi(\pi-s) + \Phi(s-a_{1}) + \Psi(s-a_{2})$$

$$+\Phi(s-a_{3}) + \frac{1}{2\pi}\sum_{i=1}^{3} \left\{a_{i}\ln\sin\left(\frac{\theta_{ik}}{2}\right)\right\}$$

$$+(\pi-a_{i})\ln\cos\left(\frac{\theta_{ik}}{2}\right)\right\}.$$
(5.7)

Here k_B is the Boltzmann constant, T the temperature. The quantities a_1, a_2, a_3 are the three sides of the spherical triangle opposite the angles $\theta_{23}, \theta_{13}, \theta_{12}$. The perimeter of this triangle we denote by 2s:

$$2s = a_1 + a_2 + a_3. \tag{5.8}$$

The polylogarithm function $\Phi(x)$ is defined thus:

$$\Phi(x) = \sum_{m=1}^{\infty} \frac{\sin(2mx)}{2\pi m^2}.$$
 (5.9)

In this way we reformulate and solve the model.

If we turn from the model with lattice \mathcal{L} to its dual lattice \mathcal{L}_D (which also is a standard cubic lattice), we can obtain the original formulation of Zamolodchikov. Here the Boltzmann weights are related to the vertices of the lattice \mathcal{L}_D . In analogy with the two-dimensional case, the Zamo-

TABLE I.

lodchikov model can be formulated on an arbitrary set of planes; the partition function will be Z-invariant. It should be noted that Bazhanov and Stroganov proposed still another three-dimensional exactly solvable model,²⁸ which also can be used to construct fully integrable models in quasicrystals.

6. EXACTLY SOLUBLE SPIN MODEL IN A THREE-DIMENSIONAL QUASICRYSTAL

The three-dimensional case is investigated in a way analogous to the two-dimensional case, see Section 3. Let us investigate the icosahedral filling of R^3 , see Section 4. Below we will construct an exactly soluble spin model for this quasicrystal Q. The spins σ are located on the vertices of Q; each spin takes on the two values ± 1 . They interact around the rhomboid. The Boltzmann weight associated with a given rhomboid F_{ikj} (4.2) is denoted by

$$W(a|e, f, g|b, c, d|h; \theta_{jk}, \theta_{ik}, \theta_{ij}).$$

$$(6.1)$$

The spins a, \ldots, h are located on the vertices of the rhomboid just as they were on the vertices of the cube in Fig. 2. The weight W depends on the angles θ ; so as to introduce these angles, we associate a unit vector \mathbf{n}_j with each of the six vectors \mathbf{e}_j (4.1) which belong to the crystal. (The vectors \mathbf{n}_j do not necessarily coincide with \mathbf{e}_j .) The Boltzmann weight W associated with the rhomboid F_{ikj} (4.2) depends on three angles θ which are defined by

$$(\mathbf{n}_{i}\mathbf{n}_{k}) = \cos \theta_{ik}, \quad (\mathbf{n}_{i}\mathbf{n}_{k}) = \cos \theta_{ik}, \quad (\mathbf{n}_{i}\mathbf{n}_{j}) = \cos \theta_{ij}.$$
 (6.2)

The explicit expression for W is given in the table (after replacing $\theta_{23} \rightarrow \theta_{kj}$, $\theta_{13} \rightarrow \theta_{ik}$, $\theta_{12} \rightarrow \theta_{ij}$). The partition function is standard:

$$Z = \sum_{\langle \sigma \rangle} \prod W(a \mid e, f, g \mid b, c, d \mid h), \qquad (6.3)$$

the product extends over all rhomboids. It depends on 9 angles (the scalar products of the six unit vectors \mathbf{n}_j). The partition function is Z-invariant, so that the weights W satisfy the tetrahedron equation. This implies that the model can be solved in a way analogous to the two-dimensional case. It is sufficient to reformulate the model on a lattice dual to the quasicrystal. This will be a special case of the Zamolodchi-kov model on an arbitrary set of planes. Using the unitarity hypothesis,^{29,30} we obtain the following expression for the free energy density f for the spin model in a quasicrystal (6.3):

$$f = \sum \omega_{ikj} f_0(\theta_{jk}, \theta_{ik}, \theta_{ij}).$$
 (6.4)

The summation is limited by the condition $6 \ge j > k > i \ge 1$. The sum consists of twenty terms, each of which corresponds to one of the basic rhomboids (4.2). The quantities ω_{ikj} are the relative frequencies of occurrence of the rhom-

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abeh	$ac \hbar$	adgh	$ \begin{array}{c} W(a \mid e, f, g \mid b, \\ c, d \mid h; \theta_{23}, \\ \theta_{13}, \theta_{12}) \end{array} $	ab eh	ac/h	adgh	$ \begin{array}{c} W(a \mid e, f, \\ g \mid b, c, d \mid h; \\ \theta_{23}, \theta_{13}, \theta_{12}) \end{array} $
+	+	+	$P_0 - abcdQ_0$	+	-	_	$abP_1 + cdQ_1$
	+	+	R_1	_	+	-	acP_2+bdQ_2
+	-	+	R_2	-	-	+	acP_2+bdQ_2
+	+	-	R_3^-		-		R_0

boid F_{ikj} (4.5), (4.6); f_0 is the free energy density for the periodic case (5.7).

An exactly soluble model can be constructed in an analogous way for any quasicrystal.

It should be emphasized that the properties of the dynamic models in quasicrystals constructed in this paper are closer to the properties of analogous models in the periodic case than properties of dynamic quasicrystal models discussed previously in the literature.

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