Applications of Yang-Baxter and Other Functional Equations in Periodic and Quasiperiodic Systems

Jacques H. H. Perk & Helen Au-Yang, Oklahoma State University

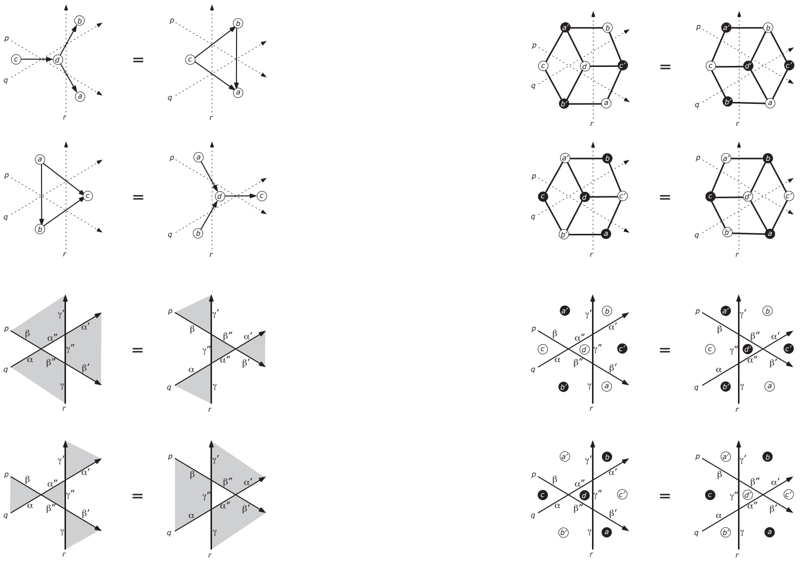
Outline:

- Z-invariant Ising lattices
  - ∗ Scaling limit results
  - ∗ Painlevé V and III
- Pentagrid Ising lattice
- Generalizations

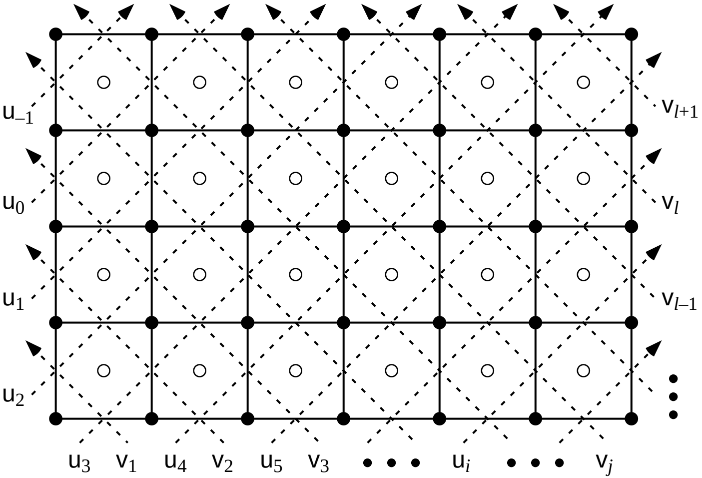
References:

- J. Stat. Phys. **127** (2007) 221–264, cond-mat/0409557.
- *Yang–Baxter Equation*, in *Encyclopedia of Mathematical Physics*, Vol. 5, (Elsevier Science, 2006), pp. 465–473. Extended version in math-ph/0606053.

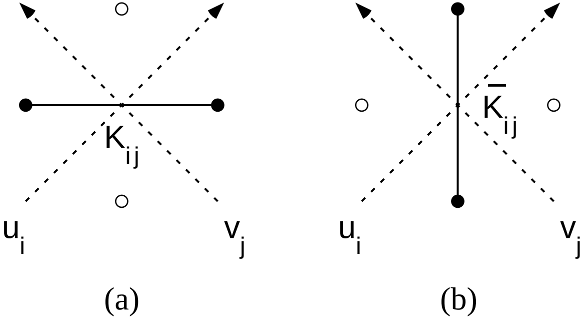
Yang-Baxter Equations



Baxter's z-invariant inhomogeneous Ising model



Parameterization in terms of elliptic functions of modulus k:



$$\sinh\big(2K(u_1,u_2)\big) = k\,\mathrm{sc}(u_1-u_2,k') = \mathrm{cs}\big(\mathrm{K}(k')+u_2-u_1,k'\big),$$
$$\sinh\big(2\bar{K}(u_1,u_2)\big) = \mathrm{cs}(u_1-u_2,k') = k\,\mathrm{sc}\big(\mathrm{K}(k')+u_2-u_1,k'\big),$$

$$k' = \sqrt{1-k^2}, \qquad \mathrm{sc}(v,k) = \mathrm{sn}(v,k)/\mathrm{cn}(v,k) = 1/\mathrm{cs}(v,k)$$

K and $\bar{K}$ are interchanged if we replace u_1 by $u_2 \pm \mathrm{K}(k')$ and u_2 by u_1: flipping the orientation of a rapidity line j is equivalent to changing its rapidity variable u_j to $u_j \pm \mathrm{K}(k')$.

Two-Point Correlation Functions

Only depends on elliptic modulus k and the values of the $2m$ rapidity variables $u_1, \ldots, u_{2m}$ that pass between the two spins, implying the existence of an infinite set of universal functions $g_2, g_4, \ldots, g_{2m}, \ldots$ such that for any permutation P and rapidity shift v

$$\langle \sigma\sigma' \rangle = g_{2m}(k; \bar{u}_1, \ldots, \bar{u}_{2m}) = g_{2m}(k; \bar{u}_{\mathrm{P}(1)} + v, \ldots, \bar{u}_{\mathrm{P}(2m)} + v).$$

$\bar{u}_j = u_j$ if the jth rapidity line passes between the two spins σ and σ' in a given direction and $\bar{u}_j = u_j + \mathrm{K}(k')$ if it passes in the opposite direction.

If two of the rapidity variables passing between the two spins differ by $\mathrm{K}(k')$, they can be viewed as belonging to a single rapidity line moving back and forth between these two spins:

$$g_{2m+2}\big(k; \bar{u}_1, \ldots, \bar{u}_{2m}, \bar{u}_{2m+1}, \bar{u}_{2m+1} + \mathrm{K}(k')\big) = g_{2m}(k; \bar{u}_1, \ldots, \bar{u}_{2m}).$$

Jin's Conjecture of Scaling Limit of Two-Point Function

In critical region, $k \to 1$, $\mathrm{K}(k') \to \mathrm{K}(0) = \frac{1}{2}\pi$, we have

$$\sinh\big(2K(u_1,u_2)\big) = \tan(u_1 - u_2) = \cot(\pm\tfrac{1}{2}\pi + u_2 - u_1),$$
$$\sinh\big(2\bar{K}(u_1,u_2)\big) = \cot(u_1 - u_2) = \tan(\pm\tfrac{1}{2}\pi + u_2 - u_1),$$

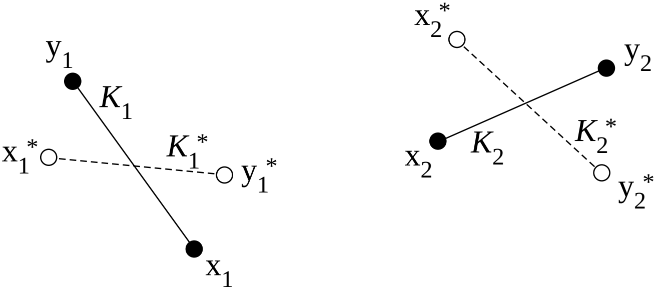
In terms of scaled distance $r = R/\xi_{\mathrm{d}}$, with $\xi_{\mathrm{d}}^{-1} = |\log k|$ and

$$R = \frac{1}{2}\bigg[\bigg\{\sum_{j=1}^{2m}\cos(2u_j)\bigg\}^2 + \bigg\{\sum_{j=1}^{2m}\sin(2u_j)\bigg\}^2\bigg]^{1/2}$$

with all u_j passing between the two spins. Then

$$\langle\sigma\sigma'\rangle \approx |1 - k^{-2}|^{1/4}F(r), \quad \langle\sigma\sigma'\rangle^* \approx |1 - k^{-2}|^{1/4}G(r).$$

Proof of Jin's Conjecture



$$\sinh(2K_1)\sinh(2K_2)\big\{\langle\sigma_{x_1}\sigma_{x_2}\rangle\langle\sigma_{y_1}\sigma_{y_2}\rangle - \langle\sigma_{x_1}\sigma_{y_2}\rangle\langle\sigma_{y_1}\sigma_{x_2}\rangle\big\}$$
$$+\big\{\langle\sigma_{x_1^*}\sigma_{x_2^*}\rangle^*\langle\sigma_{y_1^*}\sigma_{y_2^*}\rangle^* - \langle\sigma_{x_1^*}\sigma_{y_2^*}\rangle^*\langle\sigma_{y_1^*}\sigma_{x_2^*}\rangle^*\big\} = 0,$$

with two arbitrary nearest-neighbor pairs of spins at the sites $\{x_1, y_1\} \neq \{x_2, y_2\}$, and corresponding nearest-neighbor pairs of dual spins at $\{x_1^*, y_1^*\}$ and $\{x_2^*, y_2^*\}$, and $\sinh(2K_i)\sinh(2K_i^*) = 1$, $(i = 1, 2)$. (Orientations as in picture.)

Restricted to Z-invariant Ising model, quadratic identity reduces to

$$k^2\mathrm{sc}(u_2-u_1,k')\mathrm{sc}(u_4-u_3,k')$$
$$\times\big\{g(u_1,u_2,u_3,u_4,\cdots)\,g(\cdots)-g(u_1,u_2,\cdots)\,g(u_3,u_4,\cdots)\big\}$$
$$+\big\{g^*(u_1,u_3,\cdots)\,g^*(u_2,u_4,\cdots)-g^*(u_1,u_4,\cdots)\,g^*(u_2,u_3,\cdots)\big\}=0,$$

with "$\cdots$" short-hand for all other rapidity variables $u_5,u_6,\cdots$. In the scaling limit we have $k\longrightarrow 1$, $k'\longrightarrow 0$, this reduces to the leading nonvanishing term of

$$\tan(u_2-u_1)\tan(u_4-u_3)\big\{F(r_{1234})F(r)-F(r_{12})F(r_{34})\big\}$$
$$+\big\{G(r_{13})G(r_{24})-G(r_{14})G(r_{23})\big\}=0,$$

with subscripts to r indicating which u's are added to $u_5,u_6,\cdots$. Writing

$$r\cos\psi=\tfrac{1}{2}\xi_{\mathrm{d}}^{-1}\sum_{j\neq 1,2,3,4}\cos(2u_j),\qquad r\sin\psi=\tfrac{1}{2}\xi_{\mathrm{d}}^{-1}\sum_{j\neq 1,2,3,4}\sin(2u_j).$$

and expanding to second order in $1/\xi_{\mathrm{d}}$,

$$\cos(u_1+u_2-\psi)\cos(u_3+u_4-\psi)(FF''-F'^2+r^{-1}GG')$$
$$+\sin(u_1+u_2-\psi)\sin(u_3+u_4-\psi)(GG''-G'^2+r^{-1}FF')=0$$

Since this must hold for all values of ψ,

$$FF'' - F'^2 = -r^{-1}GG',$$
$$GG'' - G'^2 = -r^{-1}FF'.$$

Painlevé V Equation

Eliminating G' and G'',

$$G^2 = \frac{-2r^3(FF'' - F'^2)^2}{r^2(FF''' - F'F'') + r(FF'' - F'^2) - FF'},$$

$$(FF'' - F'^2)(r^4 F'''' - 2r^2 F'' + rF') + FF'^2 \\ + r^4(2F'F''F''' - FF'''^2 - F''^3) = 0.$$

Clearly, both $F(r)$ and $G(r)$ satisfy the same equation, which is an equation for the tau-function of a special Painlevé V equation. Set

$$\zeta = rF'/F, \qquad \text{or alternatively } \zeta = rG'/G,$$

$$r^3(\zeta'\zeta''' - \zeta''^2) - r^2(\zeta\zeta''' - \zeta'\zeta'') - r\zeta\zeta'' + \zeta\zeta' + 2r^2\zeta'^3 - 6r\zeta\zeta'^2 + 4\zeta^2\zeta' = 0.$$

This is the derivative of

$$\big(r^2\zeta''^2 + 4\zeta'^2(r\zeta' - \zeta) - \zeta'^2\big)/\big(4(r\zeta' - \zeta)^2\big) = \mu^2$$

where μ is a constant setting the "mass scale." Hence, we find

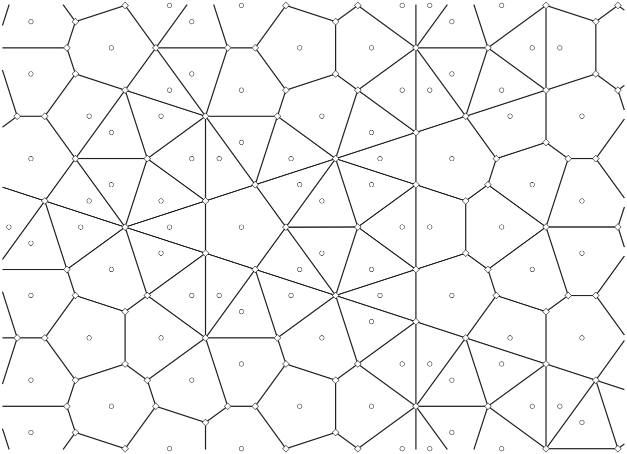
$$(r\zeta'')^2 = 4\mu^2(r\zeta' - \zeta)^2 - 4\zeta'^2(r\zeta' - \zeta) + \zeta'^2$$

and its derivative

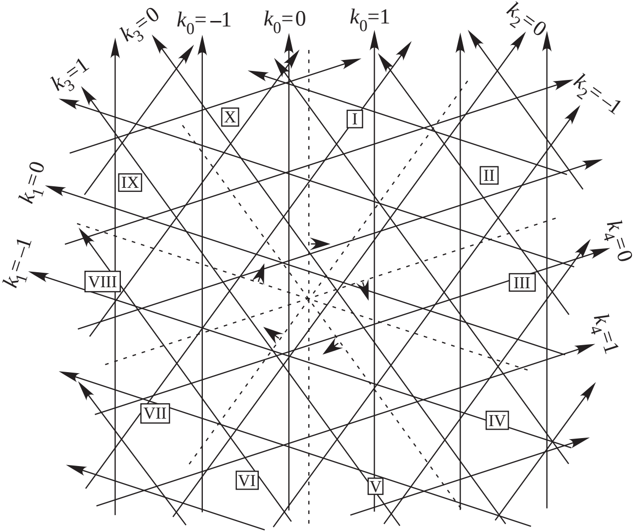
$$r^2\zeta''' + r\zeta'' = 4\mu^2 r(r\zeta' - \zeta) - 4\zeta'(r\zeta' - \zeta) - 2r\zeta'^2 + \zeta',$$

generalizing the Painlevé V Equation discovered by Jimbo and Miwa for the uniform rectangular Ising model to the scaled two-point functions of the general Z-invariant Ising model.

Pentagrid Ising lattice



De Bruijn's Pentagrid



Pentagrid in Mathematical Formulas

Regular pentagrid: no three lines have common intersection (vertex). Each vertex is surrounded by four meshes (faces). To label meshes, choose

$$\zeta = \mathrm{e}^{2\mathrm{i}\pi/5}, \qquad \zeta + \zeta^{-1} = 2\cos(2\pi/5) = p^{-1} = \tfrac{1}{2}(\sqrt{5} - 1),$$

$$\gamma_0 + \gamma_1 + \gamma_2 + \gamma_3 + \gamma_4 = 0, \quad \gamma_0, \gamma_1, \gamma_2, \gamma_3, \gamma_4 \in \mathbb{R}$$

Then the lines of the jth grid in the pentagrid are given by

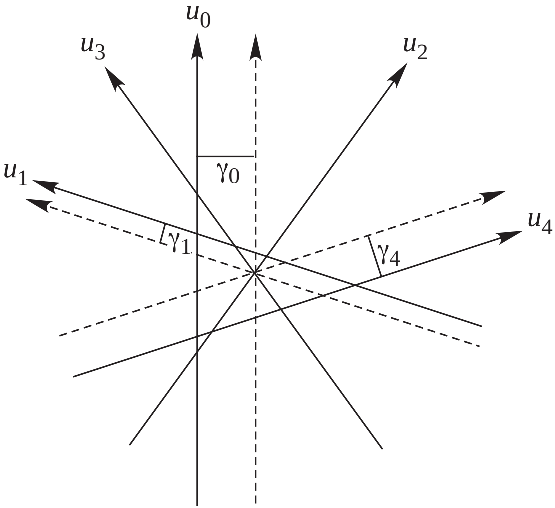
$$G_j = \{z \in \mathbb{C} | \mathrm{Re}(z\zeta^{-j}) + \gamma_j = k_j, k_j \in \mathbb{Z}\}, \qquad j = 0, \cdots, 4.$$

Integer vector: $z \in \mathbb{C} \to \vec{K}(z) \in \mathbb{Z}^5$:

$$\vec{K}(z) = (K_0(z), \cdots, K_4(z)), \quad K_j(z) = \lceil \mathrm{Re}(z\zeta^{-j}) + \gamma_j \rceil,$$

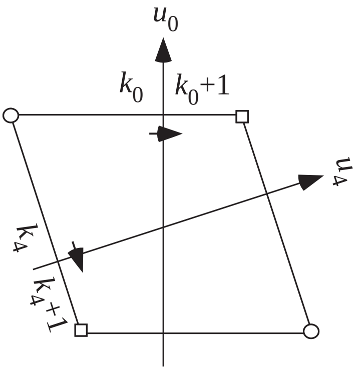
Map each mesh to vertex of Penrose tiling:

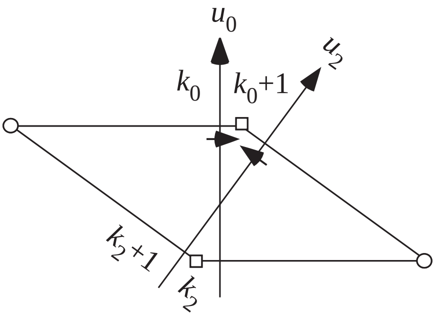
$$z \to f(z) = \sum_{j=0}^{4} K_j(z)\zeta^j$$



Five different kinds of rapidity lines and shifts γ_j to make pentagrid regular.

Pentagrid Ising Model





Following Korepin, each fat or skinny rhombus of Penrose tiling has two rapidity lines associated, with rapidity u_j for the$j$th grid. On the vertices we put alternatingly Ising spins and dual Ising spins. The rapidity lines become "Conway worms" (no longer straight) in the Penrose tiling.

The lengths of the four diagonals of the two rhombuses are all different. The interactions between the spins are chosen to depend on the interparticle spacings only, but not on the orientations. Hence,

$$u_0 - u_1 = u_2 - u_3 = u_4 - u_0 = \lambda + u_1 - u_2 = \lambda + u_3 - u_4.$$

From this, we find

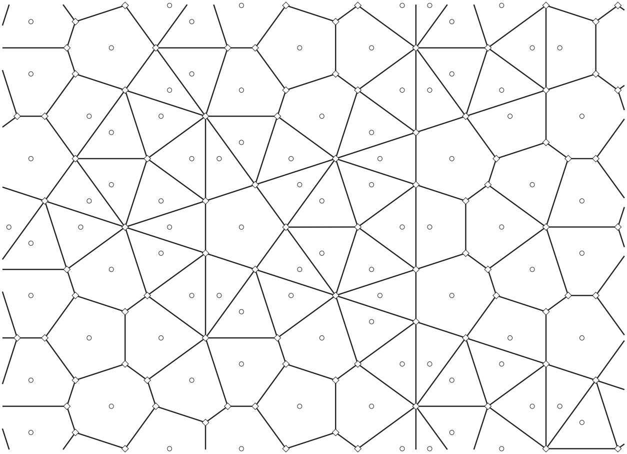
$$u_4 - u_1 = \frac{4\lambda}{5}, \quad u_2 - u_1 = \frac{3\lambda}{5}, \quad u_0 - u_1 = \frac{2\lambda}{5}, \quad u_3 - u_1 = \frac{\lambda}{5}.$$

If we let

$$\sinh 2K_j = s_j = k \, \mathrm{sc}(j\lambda/5, k'), \quad \lambda = \mathrm{K}(k'), \quad k' = \sqrt{1-k^2}$$

then for the thick rhombus, we assign s_2 to the longer diagonal and s_3 to the shorter diagonal, while for the thin rhombus s_4 to the shorter diagonal and s_1 to the longer one.

Pentagrid Ising lattice



The Pair Correlation Function

$$\langle \sigma_{\vec{K}} \sigma_{\vec{K}'} \rangle = \langle \sigma \sigma' \rangle_{[\ell_0, \cdots, \ell_4]}$$

$$= g(\overbrace{u'_0, \ldots, u'_0}^{|\ell_0|}, \overbrace{u'_1, \ldots, u'_1}^{|\ell_1|}, \overbrace{u'_2, \ldots, u'_2}^{|\ell_2|}, \overbrace{u'_3, \ldots, u'_3}^{|\ell_3|}, \overbrace{u'_4, \ldots, u'_4}^{|\ell_4|}),$$

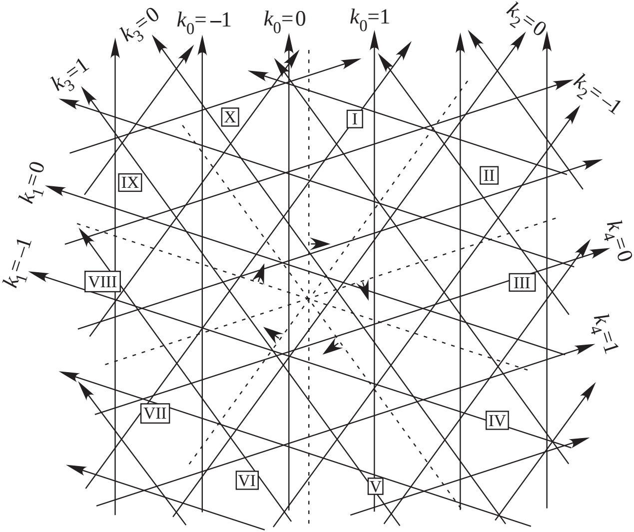
where $u'_j = u_j$ for rapidity lines of type j with arrows pointing to the same side of the line joining the two spins, and $u'_j = u_j \pm \lambda$ for rapidities with arrows pointing to opposite sides of the line. The position of each spin is labeled by its integer vector $\vec{K}$.

Shifting $u'_0, \ldots, u'_4$ by the same amount, depending on the region, such that $\min_j u'_j = 0$, and using the permutation property, we reduce the calculation to

$$g[m_4, m_3, m_2, m_1, m_0] \equiv$$

$$g\Bigg(\overbrace{\frac{4\lambda}{5}, \ldots, \frac{4\lambda}{5}}^{m_4}, \overbrace{\frac{3\lambda}{5}, \ldots, \frac{3\lambda}{5}}^{m_3}, \overbrace{\frac{2\lambda}{5}, \ldots, \frac{2\lambda}{5}}^{m_2}, \overbrace{\frac{\lambda}{5}, \ldots, \frac{\lambda}{5}}^{m_1}, \overbrace{0, \ldots, 0}^{m_0}\Bigg),$$

The Ten Regions



Regions	u'_4	u'_2	u'_0	u'_3	u'_1
I and VI	$u_4 - \lambda$	$u_2 - \lambda$	u_0	u_3	u_1
II and VII	$u_4 - \lambda$	u_2	u_0	u_3	u_1
III and VIII	u_4	u_2	u_0	u_3	u_1
IV and IX	u_4	u_2	u_0	u_3	$u_1 + \lambda$
V and X	u_4	u_2	u_0	$u_3 + \lambda$	$u_1 + \lambda$

Regions	Signs of $(\ell_0, \ell_1, \ell_2, \ell_3, \ell_4)$	$\langle \sigma\sigma' \rangle_{[\ell_0,\cdots,\ell_4]} =$
I & VI	$(+,+,+,-,-)$ & $(-,-,-,+,+)$	$g[\|\ell_0\|, \|\ell_3\|, \|\ell_1\|, \|\ell_4\|, \|\ell_2\|]$
II & VII	$(+,+,-,-,-)$ & $(-,-,+,+,+)$	$g[\|\ell_2\|, \|\ell_0\|, \|\ell_3\|, \|\ell_1\|, \|\ell_4\|]$
III & VIII	$(+,+,-,-,+)$ & $(-,-,+,+,-)$	$g[\|\ell_4\|, \|\ell_2\|, \|\ell_0\|, \|\ell_3\|, \|\ell_1\|]$
IV & IX	$(+,-,-,-,+)$ & $(-,+,+,+,-)$	$g[\|\ell_1\|.\|\ell_4\|, \|\ell_2\|, \|\ell_0\|, \|\ell_3\|]$
V & X	$(+,-,-,+,+)$ & $(-,+,+,-,-)$	$g[\|\ell_3\|, \|\ell_1\|.\|\ell_4\|, \|\ell_2\|, \|\ell_0\|]$

Enumeration/Statistics of Sites via Pentagrid

Let $P(k_j, k_{j+1})$ denote the parallelogram sandwiched between four grid lines $k_j - 1$, k_j, $k_{j+1} - 1$ and k_{j+1} for any j. Inside, $K_j(z) = k_j$ and $K_{j+1}(z) = k_{j+1}$.

- How many spin sites in $P(k_j, k_{j+1})$?
- What values of k_{j+2}, k_{j+3}, k_{j+4} occur for these spins?

Parametrize the internal points of $P(k_j, k_{j+1})$ as

$$z = \frac{\mathrm{i}\,[\zeta^j(k_{j+1} - \gamma_{j+1} - \epsilon_{j+1}) - \zeta^{j+1}(k_j - \gamma_j - \epsilon_j)]}{\sin(2\pi/5)}, \quad 0 < \epsilon_j, \epsilon_{j+1} < 1$$

At the corner $\epsilon_j = \epsilon_{j+1} = 0$, can derive $\quad (\{x\} = x - \lfloor x \rfloor = \text{fractional part})$

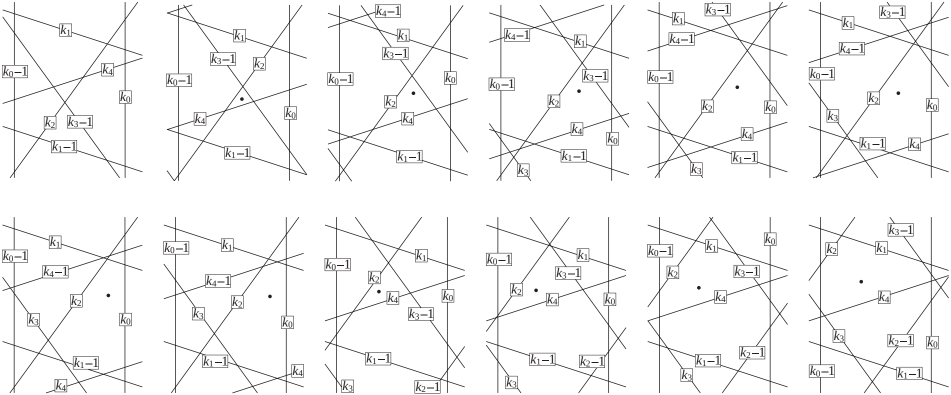
$$k_{j+2} = k_{j+2}^{\mathrm{ref}} \equiv \lceil \alpha \rceil - k_j, \quad \alpha \equiv \hat{\alpha}(k_{j+1}) \equiv p^{-1}(k_{j+1} - \gamma_{j+1}) + \gamma_j + \gamma_{j+2},$$

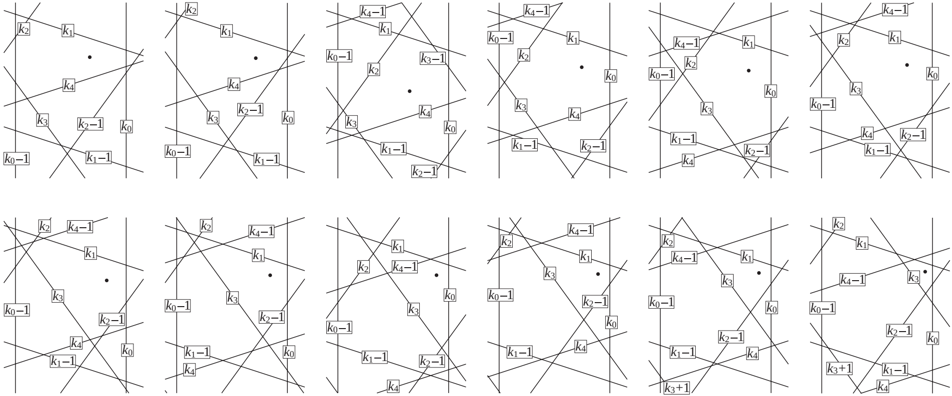
$$k_{j+4} = k_{j+4}^{\mathrm{ref}} \equiv \lceil \beta \rceil - k_{j+1}, \quad \beta \equiv \hat{\beta}(k_j) \equiv p^{-1}(k_j - \gamma_j) + \gamma_{j+1} + \gamma_{j+4},$$

$$k_{j+3} = \begin{cases} k_{j+3}^{\mathrm{ref}} - 1 & \text{for} \quad \{\alpha\} + \{\beta\} \ge 1, \\ k_{j+3}^{\mathrm{ref}} & \text{for} \quad \{\alpha\} + \{\beta\} < 1, \end{cases} \qquad k_{j+3}^{\mathrm{ref}} \equiv 2 - \lceil \alpha \rceil - \lceil \beta \rceil = -\lfloor \alpha \rfloor - \lfloor \beta \rfloor.$$

The *index of a mesh* is defined as $\sum_j K_j(z)$. For *odd* spins it has values 1 or 3, and for *even* spins 2 or 4. For the reference integer vector: $\sum_j k_j^{\rm ref} = 2$.

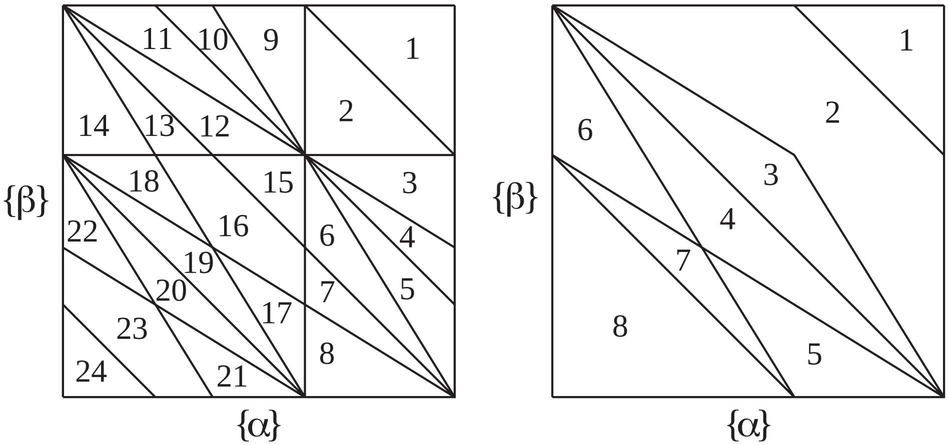
There are 24 configurations of $P(k_j, k_{j+1})$, depending on $\{\alpha\}$ and $\{\beta\}$. (The even mesh with the reference integer vector is indicated with a dot. Only for first one it does not occur.)





The number of spin sites/meshes per parallelogram varies between 6 and 12, whereas the number of odd (or even) sites varies between 3 and 7.

Which configuration occurs only depends on $\{\alpha\}$ and $\{\beta\}$, and is determined by simple inequalities (linear programming):



On the left: The 24 regions for the 24 different configurations.

On the right: The 8 regions for the 8 different odd configurations.

The golden ratio is irrational, the probabilities are proportional to the areas:

$$\begin{aligned} A(1) &= A(2) = \tfrac{5}{2} - \tfrac{3}{2}p = \tfrac{1}{2}p^{-4}, \\ A(3) &= A(5) = A(6) = A(8) = A(9) = A(11) = A(12) \\ &\quad = A(14) = A(19) = A(20) = \tfrac{5}{2}p - 4 = \tfrac{1}{2}p^{-5}, \\ A(4) &= A(7) = A(10) = A(13) = A(15) = A(17) = A(18) \\ &\quad = A(21) = A(22) = A(24) = \tfrac{13}{2} - 4p = \tfrac{1}{2}p^{-6}, \\ A(16) &= A(23) = 9p - \tfrac{29}{2} = \tfrac{1}{2}p^{-3} - p^{-6}. \end{aligned}$$

Writing $q = q_x + \mathrm{i}q_y$, $q^* = q_x - \mathrm{i}q_y$, the $\mathbf{q}$-dependent susceptibility is

$$k_{\mathrm{B}}T\chi(\mathbf{q}) = \lim_{\mathcal{M}\to\infty} \frac{1}{\mathcal{N}\mathcal{M}^2} \sum_{\vec{K}(z\in\mathbb{C})} \sum_{\vec{K}(z'\in\mathbb{C})} \cos \mathrm{Re}\Big\{q^* \sum_{j=0}^{4} [K_j(z') - K_j(z)]\zeta^j\Big\}$$

$$\times\big[\langle\sigma_{\vec{K}(z)}\sigma_{\vec{K}(z')}\rangle - \langle\sigma_{\vec{K}(z)}\rangle\langle\sigma_{\vec{K}(z')}\rangle\big] = \begin{cases} 2\hat{\chi}^{\mathrm{o}}(\mathbf{q}), & \text{(model 1)}, \\ 2\hat{\chi}^{\mathrm{e}}(\mathbf{q}), & \text{(model 2)}, \\ \hat{\chi}^{\mathrm{o}}(\mathbf{q}) + \hat{\chi}^{\mathrm{e}}(\mathbf{q}), & \text{(model 3)}. \end{cases}$$

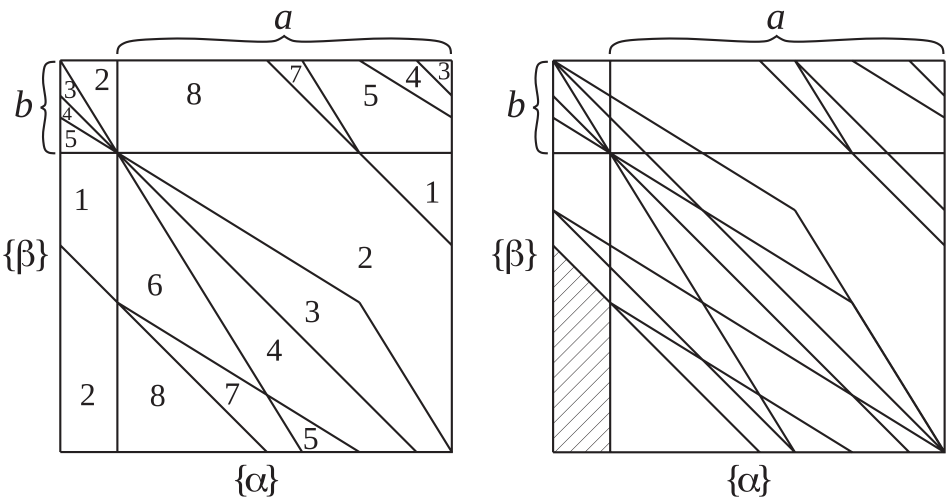
- Model 1: spins on odd sites only.
- Model 2: spins only on even (dual) sites.
- Model 3: spins on all sites, factors into two independent Ising models.

Can show $\hat{\chi}^{\mathrm{o}}(\mathbf{q}) = \hat{\chi}^{\mathrm{e}}(\mathbf{q})$, so that all three models have the same $\chi(\mathbf{q})$.

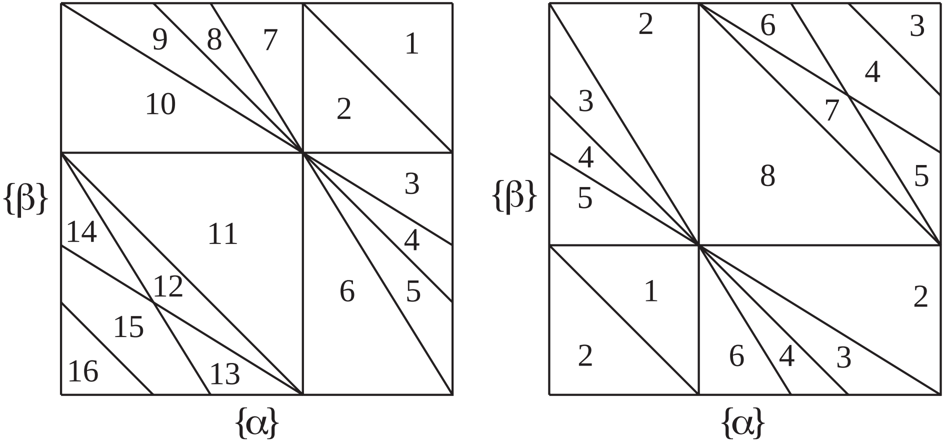
Consider next to $P = P(k_j, k_{j+1})$ also $P' = P'(k_j + \ell, k_{j+1} + \ell')$, then

$$\{\alpha'\} = \left\{ \begin{matrix} \{\alpha\} + a & \text{for} & \{\alpha\} + a < 1 \\ \{\alpha\} + a - 1 & \text{for} & \{\alpha\} + a \geq 1 \end{matrix} \right\}, \quad a = \{p^{-1}\ell'\},$$

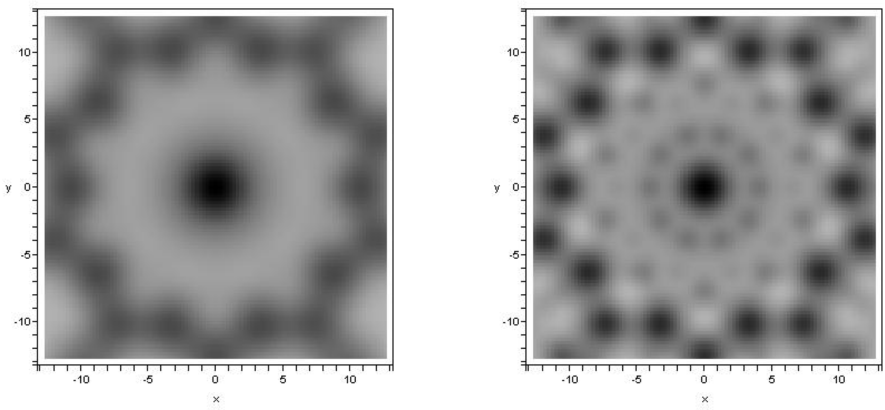
$$\{\beta'\} = \left\{ \begin{matrix} \{\beta\} + b & \text{for} & \{\beta\} + b < 1 \\ \{\beta\} + b - 1 & \text{for} & \{\beta\} + b \geq 1 \end{matrix} \right\}, \quad b = \{p^{-1}\ell\}.$$



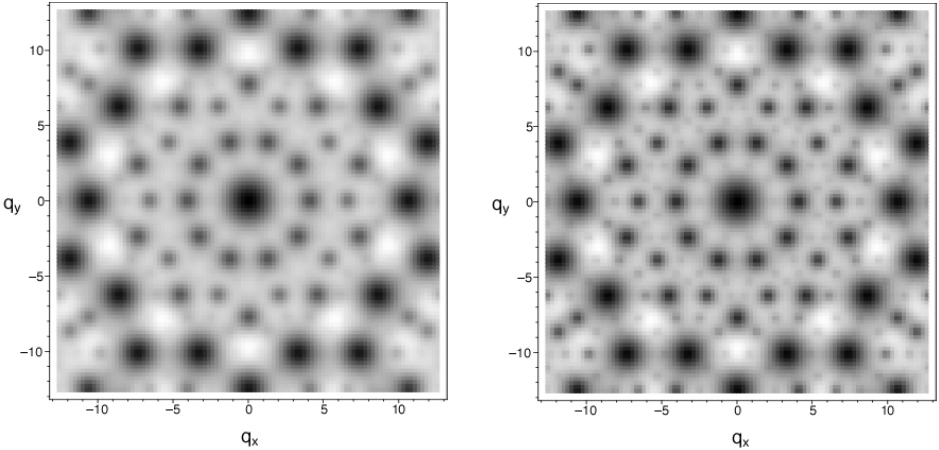
Left: The eight odd spin configurations for $P' = P(k_j + 2, k_{j+1} + 3)$.
Right: Overlapping with configurations for $P = P(k_j, k_{j+1})$. The shaded area represents the probability that P is in state $m = 8$ and P' in $m' = 2$.



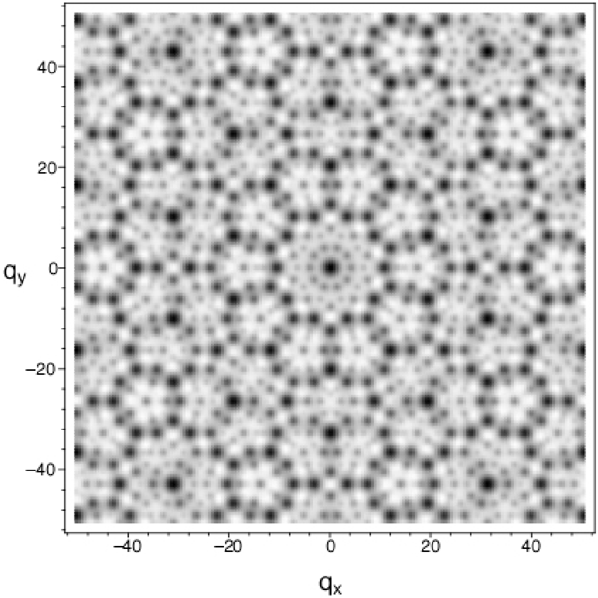
Left: The sixteen even spin configurations of $P(k_j, k_{j+1})$.
Right: The eight odd spin configurations of $P(k_j+1, k_{j+1}+1)$.
Note the bijection given by inversion, used to prove equality of $\chi(q_x, q_y)$ for odd and even (dual) sublattices.



Density plots for (a) $\xi \approx 0.5$, $k = .04847302$ and (b) $\xi \approx 1$, $k = .2363562$.

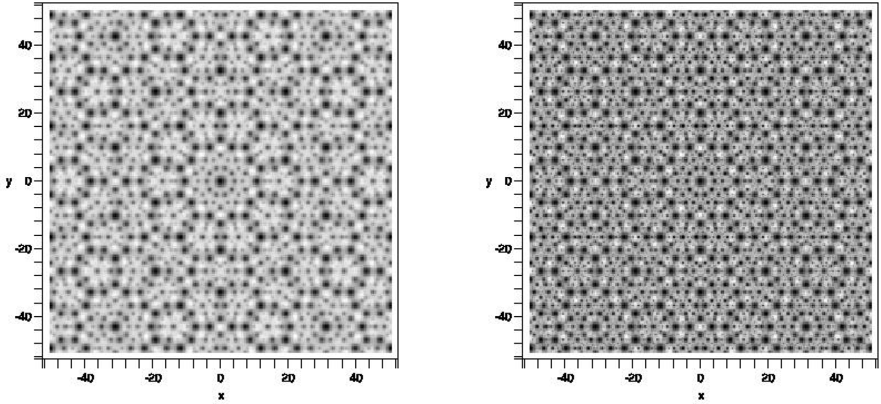


Density plots for (a) $k = .7018662$, $\xi \approx 4$ and (b) $k = .8379187$, $\xi \approx 8$.



Density plot for $k = .4912758$, $\xi \approx 2$.

Same for $\xi \approx 4$ and $\xi \approx 8$



Generalizations

The method can be extended to any multigrid such that no three lines meet in a point. Each vertex corresponds to a rhombus of a tiling. The multigrid lines are the rapidity lines of the Yang-Baxter equation.

The method can be extended to higher dimensions. For example, given a multigrid of parallel planes in three dimensions (3d), such that no more than three meet in a point, one can assign to each vertex a 3d rhombus. The grid planes are the planes where the spectral parameters of the 3d Yang–Baxter equations live.

Obtaining the multigrid from a projection from a higher dimensional lattice, one can also use the orthogonal complement to construct new aperiodic lattices. [See, e.g., *Overlapping Unit Cells in 3d Quasicrystal Structure*, J. Phys. A: Math. Gen. **39** (2006) 9035-9044, cond-mat/0507117.]