Integrability in Statistical Mechanics Jacques H. H. Perk, Oklahoma State University Abstract:

There are two "integrability" criteria in statistical mechanics.

- * One is the star-triangle equation, also known as the Yang-Baxter equation;
- * the other is a generalization of Gaussian integration to fermionic or bosonic systems.

In this talk I plan to describe both criteria in a historical context and from different points of view, omitting the more technical details. Then I will discuss some of our recent results obtained using these techniques, showing some of our latest results for the pair correlation functions in the (planar) Z-invariant Ising model and the quantum Ising chain, ending with a few remarks on the chiral Potts model. This talk will be aimed at a non-specialist audience.

Integrability in Statistical Mechanics

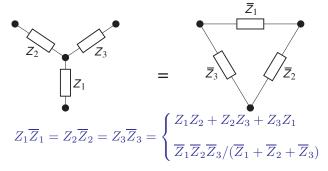
Canberra, September 4, 2008

Jacques H. H. Perk, Oklahoma State University

Outline:

- Integrability criteria
 - \ast Star-triangle equation
 - \ast Quadratic difference equations
- Square Ising lattice pair correlation
- Quantum Ising chain pair correlation
- Z-invariant Ising lattices
 - \ast Fibonacci Ising lattices
 - \ast Pentagrid Ising lattice
- Chiral Potts model

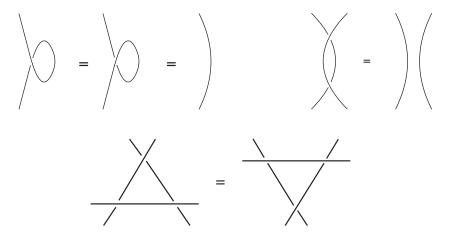
Star-Triangle Equation in Electric Networks In 1899 the Brooklyn engineer Kennelly published a short paper, entitled the equivalence of triangles and three-pointed stars in conducting networks.



The star-triangle transformation is also known under other names within the electric network theory literature as wye-delta $(Y - \Delta)$, upsilon-delta $(\Upsilon - \Delta)$, or tau-pi $(T - \Pi)$ transformation.

Knot Theory and Braid Group

Reidemeister moves of type I, II, and III to undo a knot (1926):

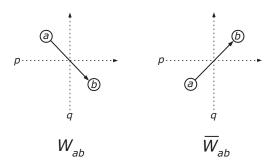


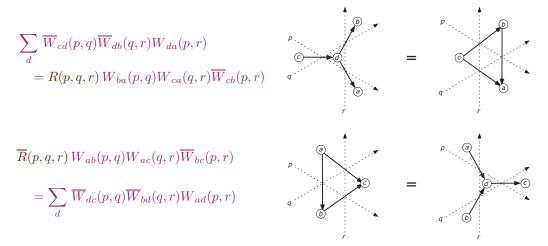
Star-Triangle Equation for Spin Models

Onsager—in his 1944 Ising model paper—made a brief remark on *an obvious* star-triangle transformation relating the model on the honeycomb lattice with the one on the triangular lattice.

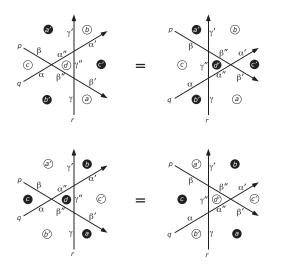
Generalizing, we introduce a lattice with spins $a, b, \dots = 1, \dots, N$ on the lattice sites and with interactions between spins a and b given in terms of Boltzmann weight factors W_{ab} and \overline{W}_{ab} .

The *integrability* of the model is expressed by the existence of spectral variables (rapidities p, q, r, ...) that live on oriented lines, drawn dashed here. One can distinguish two kinds of pair interactions depending on the orientations of the spins w.r.t. the *rapidity lines*. Integrability requires that the weights satisfy:





The two equations differ by the transposition of both spin variables in all six weight factors. In general there are scalar factors R(p, q, r) and $\overline{R}(p, q, r)$, which can often be eliminated by a suitable renormalization of the weights.



Generalizations:

The most general Yang–Baxter Equation has spin variables on the line segments of the rapidity lines and on the faces cut out by them, with faces alternatingly colored black and white.

If the spin variables only on all faces, one has an IRF model.

If the spin variables only live on rapidity lines, one has a vertex model.

JHHP & HAY, Yang-Baxter Equation, in Encyclopedia of Mathematical Physics, eds. J.-P. Françoise, G.L. Naber and Tsou S.T., Oxford: Elsevier, 2006, Vol. 5, pp. 465–473. See also arXiv:math-ph/0606053.

Partition Function, Free Energy and Correlation Function

The partition function is the sum of the Boltzmann weight over all state variables (spins) σ ; the Boltzmann weight is here a product of the weight factors for each vertex ℓ (intersection of a pair of rapidity lines) depending on the spin values $\{\sigma\}_{\ell}$ around that vertex:

$$Z = \sum_{\text{spins } \{\sigma\}} \prod_{\text{vertices } \ell} W_{\ell}(\{\sigma\}_{\ell}).$$

This provides the normalisation for the probability distribution.

The free energy is defined by $F = -k_{\rm B}T \ln Z$.

The correlation function of n spins $\sigma_1, \sigma_2, \ldots, \sigma_n$ at positions x_1, x_2, \ldots, x_n is

$$\langle \sigma_1 \sigma_2 \cdots \sigma_n \rangle = \frac{1}{Z} \sum_{\text{spins } \{\sigma\}} \prod_{\text{vertices } \ell} W_\ell(\{\sigma\}_\ell) \sigma_1 \sigma_2 \cdots \sigma_n.$$

Implications of Star-Triangle/Yang–Baxter Equation

- The partition function Z and the free energy are invariant under moving of rapidity lines. Baxter calls this Z-invariance.
- The order parameters (one-point correlation functions) cannot depend on the rapidity variables, as one can move all rapidity lines "to infinity" and move other ones with different values of the rapidity variables in. They can only depend on "moduli"—variables that are common to all rapidity lines.
- Pair correlation functions can only depend on rapidity variables of rapidity lines crossing between the two spins under consideration and the moduli.
- Integrable quantum chain hamiltonians can be found to be logarithmic derivatives of commuting transfer matrices of two-dimensional classical spin models.

Quadratic Difference/Differential Equations

The second integrability principle is a generalization of Gaussian integration. One can double the space and then employ rotational symmetry as in:

$$I \equiv \int_{-\infty}^{\infty} e^{-x^2} dx, \quad I_{2n} \equiv \int_{-\infty}^{\infty} x^{2n} e^{-x^2} dx \qquad \Longrightarrow \qquad$$

$$I^{2} = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} e^{-(x^{2} + y^{2})} dx dy = \int_{0}^{2\pi} \int_{0}^{\infty} e^{-r^{2}} r dr d\theta = \pi,$$

$$I I_{2n} = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} x^{2n} \mathrm{e}^{-(x^2 + y^2)} \mathrm{d}x \, \mathrm{d}y$$
$$= \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} (x \cos \theta + y \sin \theta)^{2n} \mathrm{e}^{-(x^2 + y^2)} \mathrm{d}x \, \mathrm{d}y.$$

Maclaurin at order θ^2 then gives

$$0 = -\frac{1}{2} 2n I I_{2n} + \frac{2n(2n-1)}{2} I_2 I_{2n-2} \implies I I_{2n} = (2n-1) I_2 I_{2n-2}.$$

Generalizations of the Wick Theorem

Applying this idea to bosonic or fermionic quantum systems, one can derive generalizations of the Wick theorem as Ward identities under rotations in the doubled space, e.g.

 $Tr(O_{1}O_{2}O_{3}O_{4}) Tr(\Gamma_{1}O_{1}\Gamma_{2}O_{2}\Gamma_{3}O_{3}\Gamma_{4}O_{4})$ $= Tr(\Gamma_{1}O_{1}\Gamma_{2}O_{2}O_{3}O_{4}) Tr(O_{1}O_{2}\Gamma_{3}O_{3}\Gamma_{4}O_{4})$ $\pm Tr(\Gamma_{1}O_{1}O_{2}\Gamma_{3}O_{3}O_{4}) Tr(O_{1}\Gamma_{2}O_{2}O_{3}\Gamma_{4}O_{4})$ $+ Tr(\Gamma_{1}O_{1}O_{2}O_{3}\Gamma_{4}O_{4}) Tr(O_{1}\Gamma_{2}O_{2}\Gamma_{3}O_{3}O_{4})$

with + for bosons and - for fermions. The Γ 's are linear combinations of creation and annihilation operators. The O's are products of factors that are either exponentials of quadratic forms or linear expressions.

More general, using traces with $2n \Gamma$'s, (n = 2, 3, ...), one gets recurrence relations determining Hafnians or Pfaffians.

JHHP, Phys. Lett. A 79 (1980) 1–5, JHHP et al., Physica A 123 (1984) 1–49.

Ferromagnetic Symmetric Square-Lattice Ising Model

$$\mathcal{H} = -J \sum_{m,n} (\sigma_{m,n} \sigma_{m,n+1} + \sigma_{m,n} \sigma_{m+1,n}), \quad J > 0$$

[State $\{\sigma\}$ is map assigning to each site (m, n) spin $\sigma_{m,n} = \pm 1$.]

Elliptic modulus:
$$k = \sinh^2(2J/k_{\rm B}T) \equiv k_{>} \equiv 1/k_{<}$$

 $k < 1$ for $T > T_{\rm c}$ and $k > 1$ for $T < T_{\rm c}$
Kramers-Wannier duality: $k \leftrightarrow 1/k$

Spontaneous magnetization (Onsager & Yang)

$$\langle \sigma \rangle = \begin{cases} (1 - k^{-2})^{1/8}, & T < T_{\rm c}, \\ 0, & T \ge T_{\rm c}. \end{cases}$$

Usual and connected pair correlation functions

$$C(m,n) = \langle \sigma_{0,0}\sigma_{m,n} \rangle, \quad C^{(c)}(m,n) = \langle \sigma_{0,0}\sigma_{m,n} \rangle - \langle \sigma \rangle^2$$

Difference Equations for Pair Correlation Functions

$$\begin{bmatrix} C(m, n+1) C(m, n-1) - C(m, n)^2 \end{bmatrix} + k \begin{bmatrix} C^*(m+1, n) C^*(m-1, n) - C^*(m, n)^2 \end{bmatrix} = 0,$$

$$\begin{bmatrix} C(m+1,n) C(m-1,n) - C(m,n)^2 \end{bmatrix} + k \begin{bmatrix} C^*(m,n+1) C^*(m,n-1) - C^*(m,n)^2 \end{bmatrix} = 0,$$

$$\begin{bmatrix} C(m,n) C(m+1,n+1) - C(m+1,n) C(m,n+1) \end{bmatrix} = k \begin{bmatrix} C^*(m,n) C^*(m+1,n+1) - C^*(m+1,n) C(m,n+1) \end{bmatrix},$$

$$\sqrt{k} \left[C(m+1,n) C^*(m-1,n) + C(m-1,n) C^*(m+1,n) \right. \\ \left. + C(m,n+1) C^*(m,n-1) + C(m,n-1) C^*(m,n+1) \right] \\ \left. = (k+1) C(m,n) C^*(m,n), \right.$$

Susceptibility Series

$$\bar{\chi} \equiv k_{\rm B} T \chi = \sum_{m,n=-\infty}^{\infty} \left(\langle \sigma_{0,0} \sigma_{m,n} \rangle - \langle \sigma_{0,0} \rangle^2 \right).$$

High-temperature series, $s \equiv \sinh(2K)/2 = \sqrt{k}/2$, $(K = J/k_{\rm B}T)$:

$$\bar{\chi} = 1 + 4s + 12s^2 + 32s^3 + 76s^4 + 176s^5 + 400s^6 + \cdots$$

 $+ \begin{array}{c} 200733025882917299143116657228410703566232325184536 \backslash \\ 7545550226445723763406738301159160108585998318576 \hspace{0.1em} s^{323} \cdots \end{array}$

Low-temperature series,
$$s \equiv 1/(2\sinh(2K)) = 1/(2\sqrt{k})$$
:

$$\bar{\chi} = 4s^4 + 16s^6 + 104s^8 + 416s^{10} + 2224s^{12} + \cdots$$

 $+ 3051547724509044350855662072500389468463893273907 \\ 5732810211229434299420849612234517174982030845245 \\ 5331887458424846630637797467206682914215700492366 \\ 9271259707379855275224873707435550114462001144064 \\ s^{646} \cdots$

Spin $\frac{1}{2}$ Operator basis for Quantum Chain

$$\sigma_j^x := \cdots \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \otimes \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \otimes \overbrace{\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}}^{j-\text{th}} \otimes \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \otimes \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \otimes \cdots$$
$$\sigma_j^y := \cdots \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \otimes \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \otimes \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \otimes \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \otimes \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \otimes \cdots$$
$$\sigma_j^z := \cdots \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \otimes \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \otimes \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \otimes \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \otimes \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \otimes \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \otimes \cdots$$

Schrödinger time dependence in Heisenberg picture with Hamiltonian \mathcal{H} :

$$\sigma_j^{\alpha}(t) := \mathrm{e}^{\mathrm{i}\mathcal{H}t}\sigma_j^{\alpha}\,\mathrm{e}^{-\mathrm{i}\mathcal{H}t}, \qquad \mathrm{in \ units \ for \ which \ } \hbar \equiv 1, \quad (\alpha = x, y, z).$$

Quantum Ising Chain

$$\mathcal{H} = -\frac{1}{2} \sum_{j=-\infty}^{\infty} (J\sigma_j^x \sigma_{j+1}^x + B\sigma_j^z), \qquad \mathcal{H}^* = -\frac{1}{2} \sum_{j=-\infty}^{\infty} (B\sigma_j^x \sigma_{j+1}^x + J\sigma_j^z)$$

The dual chain corresponds to the interchange of J and B. The pair correlation function

$$X_n(t) \equiv \langle \sigma_j^x(t) \sigma_{j+n}^x \rangle \equiv \frac{\operatorname{Tr}\left(\mathrm{e}^{\mathrm{i}t\mathcal{H}} \sigma_j^x \, \mathrm{e}^{-\mathrm{i}t\mathcal{H}} \sigma_{j+n}^x \, \mathrm{e}^{-\beta\mathcal{H}}\right)}{\operatorname{Tr}\left(\mathrm{e}^{-\beta\mathcal{H}}\right)}$$

satisfies

$$\begin{cases} X_n(t)\ddot{X}_n(t) - \dot{X}_n(t)^2 = B^2 \left(X_{n-1}^*(t) X_{n+1}^*(t) - X_n^*(t)^2 \right) \\ X_n^*(t)\ddot{X}_n^*(t) - \dot{X}_n^*(t)^2 = J^2 \left(X_{n-1}(t) X_{n+1}(t) - X_n(t)^2 \right) \end{cases}$$

At the critical field B = J this reduces to

$$X_n(t)\ddot{X}_n(t) - \dot{X}_n(t)^2 = J^2 \left(X_{n-1}(t)X_{n+1}(t) - X_n(t)^2 \right)$$

JHHP, Phys. Lett. A **79** (1980) 1–2.

These equations can be shown to satisfy a discrete generalization of a hyperbolic partial differential equation. Therefore, we expect the initial-value problem to be stable. At zero temperature, the initial values relate to the diagonal correlation in the 2d Ising model with k = B/J or J/B:

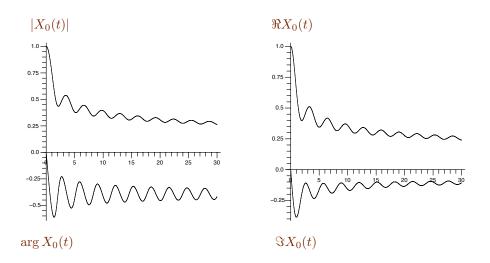
$$X_n(0) = \langle \sigma_{00} \sigma_{nn} \rangle, \quad \dot{X}_n(0) = \dot{X}_0(0) \,\delta_{n0}$$

For J = B, we have the simple result

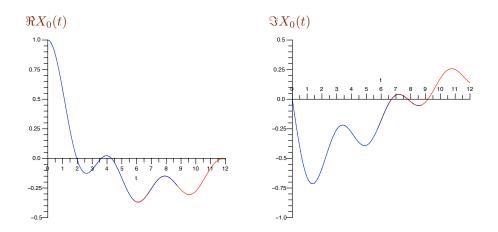
$$X_n(0) = \left(\frac{2}{\pi}\right)^n \prod_{\ell=1}^{n-1} \left(1 - \frac{1}{4\ell^2}\right)^{l-n}, \quad \dot{X}_n(0) = \frac{2}{\pi} \,\delta_{n0}$$

Also for $B \neq J$ these are known to high precision from our earlier work and a newly derived asymptotic expansion for large n. Next we can find as many time-derivatives at t = 0 as we want from the differential equations. We can then calculate $X_n(\delta t)$ and $\dot{X}_n(\delta t)$ to high precision using Taylor expansion to, say, five orders for sufficiently small δt .

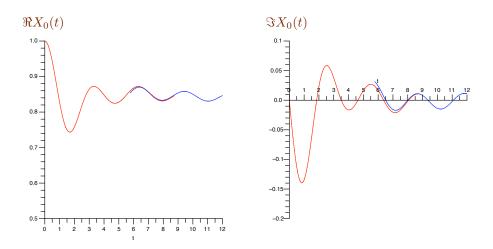
Repeating this process N times we can calculate $X_n(N\delta t)$ and $X_n(N\delta t)$ using initial conditions in the "past light-cone." This is a discrete version of the method of characteristics. $X_0(t)$ for B = J = 1



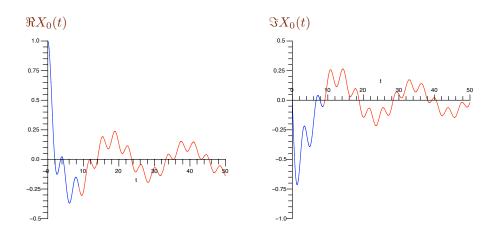
 $X_0(t)$ for B/J = 0.7



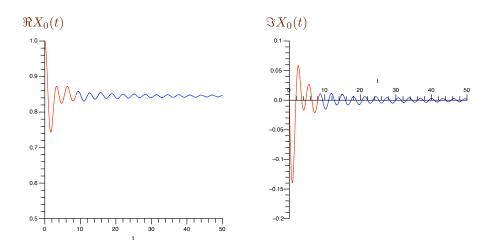
 $X_0(t)$ for J/B = 0.7



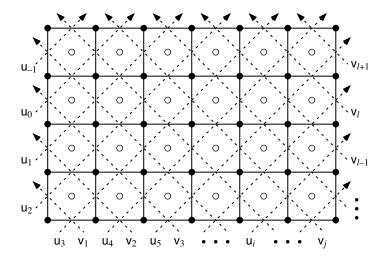
 $X_0(t)$ for B/J = 0.7



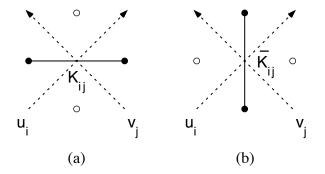
 $X_0(t)$ for J/B = 0.7



Baxter's Z-invariant inhomogeneous Ising model



Parameterization in terms of elliptic functions of modulus k:



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

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

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

Two-Point Correlation Functions

Pair correlations only depend 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

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

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

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

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

[See also: R.J. Baxter, Phil. Trans. Roy. Soc. A 289 (1978) 315.]

Jin's Conjecture of Scaling Limit of Two-Point Function In critical region, $k \to 1$, $K(k') \to K(0) = \frac{1}{2}\pi$, we have

$$\sinh\left(2K(u_1, u_2)\right) = \tan(u_1 - u_2) = \cot(\pm \frac{1}{2}\pi + u_2 - u_1),$$

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

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

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

with all u_j passing between the two spins. Then

$$\begin{split} \langle \sigma \sigma' \rangle &\approx |1 - k^{-2}|^{1/4} F(r), \quad \langle \sigma \sigma' \rangle^* \approx |1 - k^{-2}|^{1/4} G(r), \\ FF'' - F'^2 &= -r^{-1} GG', \qquad GG'' - G'^2 = -r^{-1} FF'. \end{split}$$

Wavevector-Dependent Susceptibility

$$\bar{\chi}(q_x, q_y) \equiv k_{\rm B}T \,\chi(q_x, q_y)$$
$$= \lim_{\mathcal{N} \to \infty} \frac{1}{\mathcal{N}} \sum_{m_1, n_1} \sum_{m_2, n_2} \left(\langle \sigma_{m_1, n_1} \sigma_{m_2, n_2} \rangle - \langle \sigma_{0, 0} \rangle^2 \right) \mathrm{e}^{\mathrm{i}(q_x x + q_y y)}.$$

where (x, y) is the physical distance vector between positions (m_1, n_1) and (m_2, n_2) , and \mathcal{N} is number of sites. Note, $\chi(0, 0)$ is the usual susceptibility. In the scaling limit, we can write

$$\langle \sigma_{m_1,n_1} \sigma_{m_2,n_2} \rangle - \langle \sigma_{0,0} \rangle^2 = |1 - k^{-2}|^{1/4} F_{\pm}(\kappa R)$$

where

$$\begin{cases} F_+(\kappa R) = F(R/\xi_{\rm d}), & T > T_{\rm c}, \\ F_-(\kappa R) = G(R/\xi_{\rm d}) - 1, & T < T_{\rm c}, \end{cases}$$

and $\kappa = 1/\xi_d = |\log k|$. F(r) and G(r) satisfy a Painlevé V differential equation.

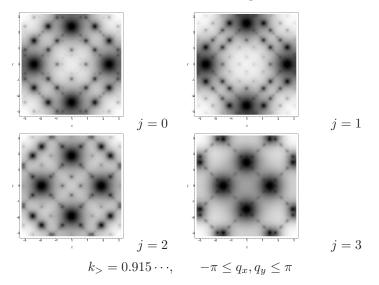
Fibonacci Ising lattices

We can make the couplings J and/or the lattice aperiodic. Findings:

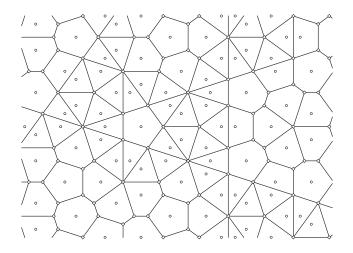
- Periodic lattice ferromagnetic couplings: Periodic $\chi(\mathbf{q})$, with peaks at reciprocal lattice sites, sharper and sharper as $T \to T_c$
- Periodic lattice mixed couplings: Periodic $\chi(\mathbf{q})$, with more and more incommensurate peaks as $T \to T_c$
- Aperiodic lattice: Quasiperiodic $\chi(\mathbf{q})$, more and more peaks visible closer to $T_{\rm c}$

For Z-invariant lattices, we can evaluate $\chi(\mathbf{q})$ numerically to high accuracy. However, the structure is clearer in density plots. For the mixed ferro/antiferro case, the simplest examples follow adding signs to the couplings of the square lattice by gauge transform. Next, we show four examples based on de Bruijn's generalized Fibonacci sequences, with j = 0 based on the golden ratio and j = 1 on the silver mean, flipping signs depending the sequence of zeros and ones $p_j(n) \equiv \lfloor \gamma + (n+1)/\alpha_j \rfloor - \lfloor \gamma + n/\alpha_j \rfloor$, with $\alpha_j \equiv \frac{1}{2} [(j+1) + \sqrt{(j+1)^2 + 4}]$.

Generalized Fibonacci Ising lattices



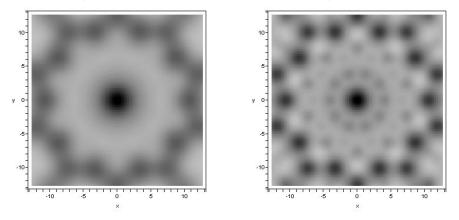
Pentagrid Ising lattice



Far from Criticality

 $k_{<}=0.048\cdots$

 $k_{<}=0.236\cdots$

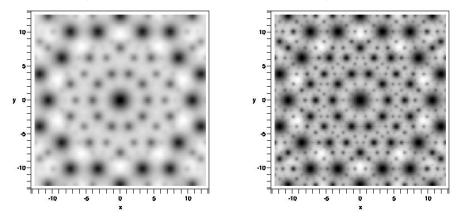


 $-4\pi \le q_x, q_y \le 4\pi$

Close to Criticality

 $k_{<} = 0.701 \cdots$

 $k_{>} = 0.701 \cdots$

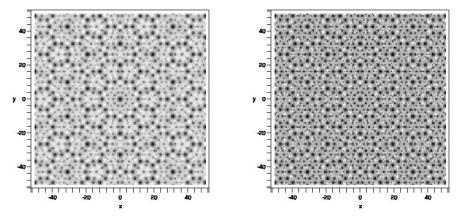


 $-4\pi \le q_x, q_y \le 4\pi$

Close to Criticality

 $k_{<} = 0.701 \cdots$

$$k_{>} = 0.701\cdots$$



 $-16\pi \le q_x, q_y \le 16\pi$

Some Remarks about the Integrable Chiral Potts Model

- The Boltzmann weights W and \overline{W} break parity invariance in general, as $W_{pq}(a-b) \neq W_{pq}(b-a)$ for nearest-neighbour spins a and b. They solve the Yang–Baxter equations, but are parametrized by higher-genus functions.
- Due to the parity breaking, the classical 2d model and the related quantum chain model behave differently in their respective physical domains.
- There is a deep relationship with cyclic (basic) hypergeometric functions $(q^N = 1)$, with N the number of states per spin. For $N \to \infty$ these relations become known and new identities for ordinary hypergeometric functions.
- Detailed results for free energies, interfacial tensions and critical exponents are known, giving information on the multicritical point in the more general non-integrable model.
- The 1988 conjecture on order parameters was finally proved by Baxter.
- For pair correlation functions one needs eigenvectors of the transfer matrix. This is where we plan to spend much effort during our stay.

Some Selected References of Ours

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