# Some Recent Results on Pair Correlation Functions and Susceptibilities in Exactly Solvable Models 

Jacques H. H. Perk and Helen Au-Yang<br>Department of Physics, Oklahoma State University Stillwater, OK 74078-3072, USA

Detailed exact results on pair-correlation functions of $Z$-invariant models are still only available for Ising-type models. Using these we can write and run algorithms of polynomial complexity to obtain wavevector-dependent susceptibilities for a variety of Ising systems. We shall compare various periodic and quasiperiodic models, where the couplings and/or the lattice may be aperiodic, and where the Ising couplings may be either ferromagnetic, or antiferromagnetic, or of mixed sign, even fully-frustrated.

For the pentagrid Ising model we have developed a novel way of determining the pair probability of local environments on a Penrose tiling, which could also be used once more detailed results for pair correlations in e.g. the eight-vertex model or the chiral Potts model become available.

## Some Recent Results on Pair Correlation Functions

## and Susceptibilities in Exactly Solvable Models

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

## Outline:

- Z-invariant Ising lattices: Pair correlation and q-dependent susceptibility
- Generalized Fibonacci Ising lattices
- Pentagrid Ising lattice [cond-mat/0409557]
- Overlapping unit cells in 3d [cond-mat/0507117]

Baxter's Z-invariant inhomogeneous Ising model


Inhomogeneous Ising model Hamiltonian:

$$
-\beta \mathcal{H}=\sum_{m, n}\left(\bar{K}_{m, n} \sigma_{m, n} \sigma_{m, n+1}+K_{m, n} \sigma_{m, n} \sigma_{m+1, n}\right)
$$

Spin $\sigma_{m, n}= \pm 1, K=\beta J$ and $\bar{K}=\beta \bar{J}$ are "horizontal" and "vertical" couplings in the example lattice just shown.
(Rapidity lines can be moved at will, so do not have to take square lattice.)

$$
\begin{gathered}
\text { Wavevector-dependent susceptibility } \chi(\mathbf{q}): \\
k_{\mathrm{B}} T \chi(\mathbf{q}) \equiv \bar{\chi}(\mathbf{q})=\lim _{\mathcal{L} \rightarrow \infty} \frac{1}{\mathcal{L}} \sum_{\mathbf{r}} \sum_{\mathbf{r}^{\prime}} \mathrm{e}^{\mathrm{i} \mathbf{q} \cdot\left(\mathbf{r}^{\prime}-\mathbf{r}\right)}\left[\left\langle\sigma_{\mathbf{r}} \sigma_{\mathbf{r}^{\prime}}\right\rangle-\left\langle\sigma_{\mathbf{r}}\right\rangle\left\langle\sigma_{\mathbf{r}^{\prime}}\right\rangle\right]
\end{gathered}
$$

It is the Fourier transform of the connected pair correlation function.
$\mathcal{L}$ is the number of lattice sites, $\mathbf{r}$ and $\mathbf{r}^{\prime}$ run through all sites, $\mathbf{q}=\left(q_{x}, q_{y}\right)$.

Parameterization in terms of elliptic functions of modulus $k$ :

(a)

(b)

$$
\begin{aligned}
& \sinh \left(2 K\left(u_{1}, u_{2}\right)\right)=k \operatorname{sc}\left(u_{1}-u_{2}, k^{\prime}\right)=\operatorname{cs}\left(\mathrm{K}\left(k^{\prime}\right)+u_{2}-u_{1}, k^{\prime}\right), \\
& \sinh \left(2 \bar{K}\left(u_{1}, u_{2}\right)\right)=\operatorname{cs}\left(u_{1}-u_{2}, k^{\prime}\right)=k \operatorname{sc}\left(\mathrm{~K}\left(k^{\prime}\right)+u_{2}-u_{1}, k^{\prime}\right),
\end{aligned}
$$

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

$K$ and $\bar{K}$ are interchanged if we replace $u_{1}$ by $u_{2} \pm \mathrm{K}\left(k^{\prime}\right)$ and $u_{2}$ by $u_{1}$ : flipping the orientation of a rapidity line $j$ is equivalent to changing its rapidity variable $u_{j}$ to $u_{j} \pm \mathrm{K}\left(k^{\prime}\right)$.

## Two-Point Correlation Functions

Only depends on elliptic modulus $k$ and the values of the $2 m$ rapidity variables $u_{1}, \ldots, u_{2 m}$ that pass between the two spins, implying the existence of an infinite set of universal functions $g_{2}, g_{4}, \ldots, g_{2 m}, \ldots$ such that for any permutation P and rapidity shift $v$

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

$\bar{u}_{j}=u_{j}$ if the $j$ th rapidity line passes between the two spins $\sigma$ and $\sigma^{\prime}$ in a given direction and $\bar{u}_{j}=u_{j}+\mathrm{K}\left(k^{\prime}\right)$ if it passes in the opposite direction.

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

$$
g_{2 m+2}\left(k ; \bar{u}_{1}, \ldots, \bar{u}_{2 m}, \bar{u}_{2 m+1}, \bar{u}_{2 m+1}+\mathrm{K}\left(k^{\prime}\right)\right)=g_{2 m}\left(k ; \bar{u}_{1}, \ldots, \bar{u}_{2 m}\right) .
$$

## Quadratic Identity for Pair Correlation



$$
\begin{aligned}
& \sinh \left(2 K_{1}\right) \sinh \left(2 K_{2}\right)\left\{\left\langle\sigma_{\mathrm{x}_{1}} \sigma_{\mathrm{x}_{2}}\right\rangle\left\langle\sigma_{\mathrm{y}_{1}} \sigma_{\mathrm{y}_{2}}\right\rangle-\left\langle\sigma_{\mathrm{x}_{1}} \sigma_{\mathrm{y}_{2}}\right\rangle\left\langle\sigma_{\mathrm{y}_{1}} \sigma_{\mathrm{x}_{2}}\right\rangle\right\} \\
&+\left\{\left\langle\sigma_{\mathrm{x}_{1}^{*}} \sigma_{\mathrm{x}_{2}^{*}}\right\rangle^{*}\left\langle\sigma_{\mathrm{y}_{1}^{*}} \sigma_{\mathrm{y}_{2}^{*}}\right\rangle^{*}-\left\langle\sigma_{\mathrm{x}_{1}^{*}} \sigma_{\mathrm{y}_{2}^{*}}\right\rangle^{*}\left\langle\sigma_{\mathrm{y}_{1}^{*}} \sigma_{\mathrm{x}_{2}^{*}}\right\rangle^{*}\right\}=0
\end{aligned}
$$

with two arbitrary nearest-neighbor pairs of spins at the sites $\left\{\mathrm{x}_{1}, \mathrm{y}_{1}\right\} \neq\left\{\mathrm{x}_{2}, \mathrm{y}_{2}\right\}$, and corresponding nearest-neighbor pairs of dual spins at $\left\{\mathrm{x}_{1}^{*}, \mathrm{y}_{1}^{*}\right\}$ and $\left\{\mathrm{x}_{2}^{*}, \mathrm{y}_{2}^{*}\right\}$, and $\sinh \left(2 K_{i}\right) \sinh \left(2 K_{i}^{*}\right)=1,(i=1,2)$. (Orientations as in picture.)

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

$$
\begin{aligned}
& k^{2} \operatorname{sc}\left(u_{2}-u_{1}, k^{\prime}\right) \operatorname{sc}\left(u_{4}-u_{3}, k^{\prime}\right) \\
& \quad \times\left\{g\left(u_{1}, u_{2}, u_{3}, u_{4}, \cdots\right) g(\cdots)-g\left(u_{1}, u_{2}, \cdots\right) g\left(u_{3}, u_{4}, \cdots\right)\right\} \\
& +\left\{g^{*}\left(u_{1}, u_{3}, \cdots\right) g^{*}\left(u_{2}, u_{4}, \cdots\right)-g^{*}\left(u_{1}, u_{4}, \cdots\right) g^{*}\left(u_{2}, u_{3}, \cdots\right)\right\}=0,
\end{aligned}
$$

with " $\ldots$ " short-hand for all other rapidity variables $u_{5}, u_{6}, \cdots$, common to all $g$ 's and $g^{*}$ 's (passing between all eight sites).

Knowing $g(u, u, \cdots, u)$ and $g(v, u, \cdots, u)$, with all or all but one of the rapidities equal, all other $g$ 's can be calculated by recurrence. Therefore, the knowledge of the diagonal and next-to-diagonal pair correlations in the uniform asymmetric $(K \neq \bar{K})$ square-lattice Ising model suffices.
[H. Au-Yang and J.H.H. Perk, MathPhys Odyssey 2001: Integrable Models and Beyond, M. Kashiwara and T. Miwa, eds., (Birkhäuser, Boston, 2002), pp. 1-48.]

## Summary of Findings

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

- Periodic lattice with periodic couplings: Periodic $\chi(\mathbf{q})$, with peaks at sites commensurate with reciprocal lattice, becoming sharper and sharper as $T \rightarrow T_{\mathrm{c}}$. This includes fully-frustrated cases.
- Periodic lattice with ferromagnetic couplings varying quasiperiodically: Periodic $\chi(\mathbf{q})$, with peaks at reciprocal lattice sites, sharper and sharper as $T \rightarrow T_{\mathrm{c}}$
- Periodic lattice with mixed FM and AFM couplings quasiperiodically arranged: Periodic $\chi(\mathbf{q})$, with more and more incommensurate peaks within unit cell as $T \rightarrow T_{\mathrm{c}}$
- Quasiperiodic lattice: Quasiperiodic $\chi(\mathbf{q})$, more and more peaks visible closer to $T_{\mathrm{c}}$

For $Z$-invariant lattices, we can evaluate $\chi(\mathbf{q})$ numerically to high accuracy from the recurrence relations for the pair correlations. However, the structure is clearer in density plots.

## Generalized Fibonacci Ising lattices

We arrange couplings according to quasiperiodic sequences in horizontal, vertical, and/or diagonal directions. We used de Bruijn's generalized Fibonacci sequences, assigning different couplings according to the sequence of zeros and ones

$$
p_{j}(n) \equiv\left\lfloor\gamma+(n+1) / \alpha_{j}\right\rfloor-\left\lfloor\gamma+n / \alpha_{j}\right\rfloor
$$

with

$$
\alpha_{j} \equiv \frac{1}{2}\left[(j+1)+\sqrt{(j+1)^{2}+4}\right]
$$

Ferromagnetic cases differ very little from periodic cases.
For the mixed ferro/antiferro case, the simplest examples follow adding signs to the couplings of the Onsager square lattice model by gauge transform. We show four examples with $j=0, \cdots, 3$, with $j=0$ the golden ratio (Fibonacci) case and $j=1$ the silver mean case:

## Generalized Fibonacci Ising lattices



$$
j=1
$$



$$
j=3
$$

## 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

$$
\begin{gathered}
\zeta=\mathrm{e}^{2 \mathrm{i} \pi / 5}, \quad \zeta+\zeta^{-1}=2 \cos (2 \pi / 5)=p^{-1}=\frac{1}{2}(\sqrt{5}-1), \\
\gamma_{0}+\gamma_{1}+\gamma_{2}+\gamma_{3}+\gamma_{4}=0, \quad \gamma_{0}, \gamma_{1}, \gamma_{2}, \gamma_{3}, \gamma_{4} \in \mathbb{R}
\end{gathered}
$$

Then the lines of the $j$ th grid in the pentagrid are given by

$$
G_{j}=\left\{z \in \mathbb{C} \mid \operatorname{Re}\left(z \zeta^{-j}\right)+\gamma_{j}=k_{j}, k_{j} \in \mathbb{Z}\right\}, \quad j=0, \cdots, 4
$$

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

$$
\vec{K}(z)=\left(K_{0}(z), \cdots, K_{4}(z)\right), \quad K_{j}(z)=\left\lceil\operatorname{Re}\left(z \zeta^{-j}\right)+\gamma_{j}\right\rceil
$$

Map each mesh to vertex of Penrose tiling:

$$
z \rightarrow f(z)=\sum_{j=0}^{4} K_{j}(z) \zeta^{j}
$$



Five different kinds of rapidity lines and shifts $\gamma_{j}$ 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

$$
\sinh 2 K_{j}=s_{j}=k \operatorname{sc}\left(j \lambda / 5, k^{\prime}\right), \quad \lambda=\mathrm{K}\left(k^{\prime}\right), \quad k^{\prime}=\sqrt{1-k^{2}}
$$

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

$$
\begin{aligned}
\left\langle\sigma_{\vec{K}^{\prime}} \sigma_{\vec{K}^{\prime}}\right\rangle & =\left\langle\sigma \sigma^{\prime}\right\rangle_{\left[\ell_{0}, \cdots, \ell_{4}\right]} \\
& =g(\overbrace{u_{0}^{\prime}, \ldots, u_{0}^{\prime}}^{\left|\ell_{0}\right|}, \overbrace{u_{1}^{\prime}, \ldots, u_{1}^{\prime}}^{\left|\ell_{1}\right|}, \overbrace{u_{2}^{\prime}, \ldots, u_{2}^{\prime}}^{\left|\ell_{2}\right|}, \overbrace{u_{3}^{\prime}, \ldots, u_{3}^{\prime}}^{\left|\ell_{3}\right|}, \overbrace{u_{4}^{\prime}, \ldots, u_{4}^{\prime}}^{\left|\ell_{4}\right|}),
\end{aligned}
$$

where $u_{j}^{\prime}=u_{j}$ for rapidity lines of type $j$ with arrows pointing to the same side of the line joining the two spins, and $u_{j}^{\prime}=u_{j} \pm \lambda$ 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 $u_{0}^{\prime}, \ldots, u_{4}^{\prime}$ by the same amount, depending on the region, such that $\min _{j} u_{j}^{\prime}=0$, and using the permutation property, we reduce the calculation to

$$
g\left[m_{4}, m_{3}, m_{2}, m_{1}, m_{0}\right] \equiv
$$

$$
g(\overbrace{\frac{4 \lambda}{5}, \ldots, \frac{4 \lambda}{5}}^{m_{4}}, \overbrace{\frac{3 \lambda}{5}, \ldots, \frac{3 \lambda}{5}}^{m_{3}}, \overbrace{\frac{2 \lambda}{5}, \ldots, \frac{2 \lambda}{5}}^{m_{2}}, \overbrace{\frac{\lambda}{5}, \ldots, \frac{\lambda}{5}, 0, \ldots, 0}^{m_{1}} \overbrace{0}^{m_{0}}),
$$



| Regions | $u_{4}^{\prime}$ | $u_{2}^{\prime}$ | $u_{0}^{\prime}$ | $u_{3}^{\prime}$ | $u_{1}^{\prime}$ |
| :--- | :--- | :--- | :--- | :--- | :---: |
| 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 $\left(\ell_{0}, \ell_{1}, \ell_{2}, \ell_{3}, \ell_{4}\right)$ | $\left\langle\sigma \sigma^{\prime}\right\rangle_{\left[\ell_{0}, \cdots, \ell_{4}\right]}=$ |
| :--- | :--- | :---: |
| I \& VI | $(+,+,+,-,-) \&(-,-,-,+,+)$ | $g\left[\left\|\ell_{0}\right\|,\left\|\ell_{3}\right\|,\left\|\ell_{1}\right\|,\left\|\ell_{4}\right\|,\left\|\ell_{2}\right\|\right]$ |
| II \& VII | $(+,+,-,-,-) \&(-,-,+,+,+)$ | $g\left[\left\|\ell_{2}\right\|,\left\|\ell_{0}\right\|,\left\|\ell_{3}\right\|,\left\|\ell_{1}\right\|,\left\|\ell_{4}\right\|\right]$ |
| III \& VIII | $(+,+,-,-,+) \&(-,-,+,+,-)$ | $g\left[\left\|\ell_{4}\right\|,\left\|\ell_{2}\right\|,\left\|\ell_{0}\right\|,\left\|\ell_{3}\right\|,\left\|\ell_{1}\right\|\right]$ |
| IV \& IX | $(+,-,-,-,+) \&(-,+,+,+,-)$ | $g\left[\left\|\ell_{1}\right\| \cdot\left\|\ell_{4}\right\|,\left\|\ell_{2}\right\|,\left\|\ell_{0}\right\|,\left\|\ell_{3}\right\|\right]$ |
| V \& X | $(+,-,-,+,+) \&(-,+,+,-,-)$ | $g\left[\left\|\ell_{3}\right\|,\left\|\ell_{1}\right\| \cdot\left\|\ell_{4}\right\|,\left\|\ell_{2}\right\|,\left\|\ell_{0}\right\|\right]$ |

## Enumeration/Statistics of Sites via Pentagrid

Let $P\left(k_{j}, k_{j+1}\right)$ 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 $P\left(k_{j}, k_{j+1}\right)$ ?
- What values of $k_{j+2}, k_{j+3}, k_{j+4}$ occur for these spins?

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

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

At the corner $\epsilon_{j}=\epsilon_{j+1}=0$, can derive $\quad(\{x\}=x-\lfloor x\rfloor=$ fractional part $)$
$k_{j+2}=k_{j+2}^{\mathrm{ref}} \equiv\lceil\alpha\rceil-k_{j}, \quad \alpha \equiv \hat{\alpha}\left(k_{j+1}\right) \equiv p^{-1}\left(k_{j+1}-\gamma_{j+1}\right)+\gamma_{j}+\gamma_{j+2}$,
$k_{j+4}=k_{j+4}^{\text {ref }} \equiv\lceil\beta\rceil-k_{j+1}, \quad \beta \equiv \hat{\beta}\left(k_{j}\right) \equiv p^{-1}\left(k_{j}-\gamma_{j}\right)+\gamma_{j+1}+\gamma_{j+4}$,
$k_{j+3}=\left\{\begin{array}{ll}k_{j+3}^{\mathrm{ref}}-1 & \text { for } \quad\{\alpha\}+\{\beta\} \geq 1, \\ k_{j+3}^{\mathrm{ref}} & \text { for } \quad\{\alpha\}+\{\beta\}<1,\end{array} \quad k_{j+3}^{\mathrm{ref}} \equiv 2-\lceil\alpha\rceil-\lceil\beta\rceil=-\lfloor\alpha\rfloor-\lfloor\beta\rfloor\right.$.

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: $\sum_{j} k_{j}^{\text {ref }}=2$. There are 24 configurations of $P\left(k_{j}, k_{j+1}\right)$, 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:

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

Writing $q=q_{x}+\mathrm{i} q_{y}, q^{*}=q_{x}-\mathrm{i} q_{y}$, the $\mathbf{q}$-dependent susceptibility is

$$
\begin{aligned}
& k_{\mathrm{B}} T \chi(\mathbf{q})=\lim _{\mathcal{M} \rightarrow \infty} \frac{1}{\mathcal{N} \mathcal{M}^{2}} \sum_{\vec{K}(z \in \mathbb{C})} \sum_{\vec{K}\left(z^{\prime} \in \mathbb{C}\right)} \cos \operatorname{Re}\left\{q^{*} \sum_{j=0}^{4}\left[K_{j}\left(z^{\prime}\right)-K_{j}(z)\right] \zeta^{j}\right\} \\
& \quad \times\left[\left\langle\sigma_{\vec{K}(z)} \sigma_{\vec{K}\left(z^{\prime}\right)}\right\rangle-\left\langle\sigma_{\vec{K}(z)}\right\rangle\left\langle\sigma_{\vec{K}\left(z^{\prime}\right)}\right\rangle\right]=\left\{\begin{array}{cc}
2 \hat{\chi}^{\mathrm{o}}(\mathbf{q}), & \text { (model 1), } \\
2 \hat{\chi}^{\mathrm{e}}(\mathbf{q}), & \text { (model 2), } \\
\hat{\chi}^{\mathrm{o}}(\mathbf{q})+\hat{\chi}^{\mathrm{e}}(\mathbf{q}), & \text { (model 3) }
\end{array}\right.
\end{aligned}
$$

- 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 $P=P\left(k_{j}, k_{j+1}\right)$ also $P^{\prime}=P^{\prime}\left(k_{j}+\ell, k_{j+1}+\ell^{\prime}\right)$, then

$$
\begin{aligned}
& \left\{\alpha^{\prime}\right\}=\left\{\begin{array}{ccc}
\{\alpha\}+a & \text { for } & \{\alpha\}+a<1 \\
\{\alpha\}+a-1 & \text { for } & \{\alpha\}+a \geq 1
\end{array}\right\},
\end{aligned} \begin{array}{lll}
\{\alpha\} & a=\left\{p^{-1} \ell^{\prime}\right\}, \\
\left\{\beta^{\prime}\right\} & =\left\{\begin{array}{ccc}
\{\beta\}+b & \text { for } & \{\beta\}+b<1 \\
\{\beta\}+b-1 & \text { for } & \{\beta\}+b \geq 1
\end{array}\right\}, & b=\left\{p^{-1} \ell\right\} .
\end{array}
$$



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


Left: The sixteen even spin configurations of $P\left(k_{j}, k_{j+1}\right)$.
Right: The eight odd spin configurations of $P\left(k_{j}+1, k_{j+1}+1\right)$.
Note the bijection given by inversion, used to prove equality of $\chi\left(q_{x}, q_{y}\right)$ 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 $k=.4912758, \xi \approx 2$.

$$
\text { Same for } \xi \approx 4 \text { and } \xi \approx 8
$$



## Overlapping Unit Cells in 3 Dimensions

Petra Gummelt, motivated by physical considerations, proposed a description of quasicrystals in terms of overlappings of decagons. Here we use a multigrid method to produce a new example of 3-dimensional overlapping unit cells.
N.G. de Bruijn has shown that a Penrose tiling can be obtained by the projection of the 5 -d euclidean lattice $\mathbb{Z}^{5}$ onto a particular 2-d cut-plane $\mathcal{D}$, by allowing only those lattice points $\boldsymbol{k}$ in $\mathbb{Z}^{5}$ whose projections into the 3-d orthogonal space $\mathcal{W}$ are inside the window of acceptance. This window is the projection of the 5 -d unit cell $\mathrm{Cu}(5)$ with $2^{5}$ vertices into this 3 -d space $\mathcal{W}$. Each facet shared by two neighboring 5 -d unit cell cubes is 4 -d and when projected into 3 -d space it produces a polyhedron $\mathcal{K}$ with 12 faces. Thus the idea of overlapping decagons must have its extension to three dimension, by projecting the 5 -d lattice into the space $\mathcal{W}$.

Choose projection operators $\boldsymbol{D}^{\mathrm{T}}=\left(\boldsymbol{d}_{0}, \cdots, \boldsymbol{d}_{4}\right)$ and $\boldsymbol{W}^{\mathrm{T}}=\left(\boldsymbol{w}_{0}, \cdots, \boldsymbol{w}_{4}\right)$ on $\mathcal{D}$ and $\mathcal{W}$, where

$$
\boldsymbol{d}_{j}^{\mathrm{T}}=(\cos j \theta, \sin j \theta), \quad \boldsymbol{w}_{j}^{\mathrm{T}}=(\cos 2 j \theta, \sin 2 j \theta, 1)=\left(\boldsymbol{d}_{2 j}^{\mathrm{T}}, 1\right), \quad \theta=2 \pi / 5
$$

Introduce the five grids in $\mathbb{R}^{3}$ consisting of bundles of equidistant planes defined by

$$
x \cos 2 j \theta+y \sin 2 j \theta+z+\gamma_{j}=\boldsymbol{w}_{j}^{\mathrm{T}} \boldsymbol{r}+\gamma_{j}=k_{j},
$$

for $\quad j=0, \cdots, 4, k_{j} \in \mathbb{Z}$, with $\boldsymbol{r}^{\mathrm{T}}=(x, y, z)$. The $\gamma_{j}$ are real numbers which shift the grids from the origin with sum

$$
\gamma_{0}+\gamma_{1}+\gamma_{2}+\gamma_{3}+\gamma_{4}=c, \quad c \leq 0<1
$$

Let the integer $k_{j}$ be assigned to all points sandwiched between the grid planes defined by $k_{j}-1$ and $k_{j}$. Then, five integers

$$
K_{j}(\boldsymbol{r})=\left\lceil\boldsymbol{w}_{j}^{\mathrm{T}} \boldsymbol{r}+\gamma_{j}\right\rceil, \quad j=0, \cdots, 4,
$$

are uniquely assigned to every point $r$ in $\mathbb{R}^{3}$. A mesh in $\mathbb{R}^{3}$ is now an interior volume, enclosed by grid planes, containing points with the same five integers.

One next maps each mesh to a vertex in $\mathcal{W}$ by

$$
\boldsymbol{f}(\boldsymbol{r})=\sum_{j=0}^{4} K_{j}(\boldsymbol{r}) \boldsymbol{w}_{j}=\boldsymbol{W}^{\mathrm{T}} \boldsymbol{K}(\boldsymbol{r}), \quad \boldsymbol{K}^{\mathrm{T}}(\boldsymbol{r})=\left(K_{0}(\boldsymbol{r}), \cdots, K_{4}(\boldsymbol{r})\right) .
$$

This results in a 3 -dimensional aperiodic lattice $\mathcal{L}=\left\{\boldsymbol{f}(\boldsymbol{r}) \mid \boldsymbol{r} \in \mathbb{R}^{3}\right\}$, which is aperiodic in two directions, but periodic after five steps in the third.

A point $\boldsymbol{k}$ in $\mathbb{Z}^{5}$ satisfies the so-called mesh condition and therefore can be mapped into $\mathcal{L}$ if and only if $\boldsymbol{D}^{\mathrm{T}}(\boldsymbol{k}-\boldsymbol{\gamma})=\boldsymbol{D}^{\mathrm{T}} \boldsymbol{\lambda}$, where $\boldsymbol{\gamma}^{\mathrm{T}}=\left(\gamma_{0}, \cdots, \gamma_{4}\right)$ and $\boldsymbol{\lambda}^{\mathrm{T}}=\left(\lambda_{0}, \cdots, \lambda_{4}\right)$ with $0<\lambda_{j}<1$ so that $\boldsymbol{\lambda}$ is point inside 5 -d unit cube $\mathrm{Cu}(5)$.

Thus, the window of acceptance is the interior of the convex hull of the points $\boldsymbol{D}^{\mathrm{T}} \boldsymbol{n}_{i}$, where $\boldsymbol{n}_{i}$ are the $2^{5}$ vertices of the 5 -d unit cube $\mathrm{Cu}(5)$.

- The projection of $\mathrm{Cu}(5)$ with these 32 points into $\mathcal{W}$ is a polytope $\mathcal{P}$ with 40 edges connecting the 22 vertices, and with 20 faces.
- The orthogonal projection of $\operatorname{Cu}(5)$ into $\mathcal{D}$ is a decagon $\mathcal{Q}$ with 10 edges connecting the 10 vertices.

Using ideas of de Bruijn, we may find out the condition for both $\boldsymbol{k}$ and $\boldsymbol{k}+\boldsymbol{n}_{i}$ to satisfy the mesh condition-to lie both in the window of acceptance.


The projection of the 5 -d unit cube $\mathrm{Cu}(5)$ into the orthogonal 2 d space $\mathcal{D}$.

There are only five different possibilities:
(1) The points inside a quadrilateral of type (a1) correspond to a polytope intersecting with four other polytopes sharing with each a polyhedron of type $\mathcal{J}$ with six faces.
(2) Points inside triangles of type (a2) or (a3) correspond to a polytope intersecting with five other polytopes, sharing with one of them a polyhedron $\mathcal{K}$ with 12 faces and with the other four polyhedra of type $\mathcal{J}$.
(3) If the point is inside triangles of type (a4) or (a6), the polytope intersects with four other polytopes sharing with one of them a polyhedron $\mathcal{K}$ and with the other three polyhedra of type $\mathcal{J}$.
(4) If the point is in a triangle (a5) or (a7), the polytope intersects with five other polytopes sharing with two of them polyhedra of type $\mathcal{K}$ and with the other three polyhedra $\mathcal{J}$.
(5) Finally, if the point is inside a pentagon (a8), the polytope intersects with six other polytopes sharing with two of them a $\mathcal{K}$ and with the other four a $\mathcal{J}$.

Their relative frequencies are related to the ratios of their areas:

$$
\begin{aligned}
& P_{\mathrm{a} 1}=2 p^{-3}, \quad P_{\mathrm{a} 2}=P_{\mathrm{a} 3}=p^{-6}, \quad P_{\mathrm{a} 4}=P_{\mathrm{a} 6}=p^{-5}, \\
& P_{\mathrm{a} 5}=P_{\mathrm{a} 7}=p^{-6}, \quad P_{\mathrm{a} 8}=p^{-5}+p^{-7} .
\end{aligned}
$$



Cases (a1) or (a2): Polytope sharing interior point with four or five neighbors.

To simplify the mesh condition, we introduce parallelepiped $P\left(k_{4}, k_{0}, k_{1}\right)$ sandwiched between the six grid planes $k_{4}-1, k_{4}, k_{0}-1, k_{0}, k_{1}-1$, and $k_{1}$. We find for every point $\boldsymbol{r}$ in $P\left(k_{4}, k_{0}, k_{1}\right)$ :

$$
\begin{aligned}
& K_{0}(\boldsymbol{r})=k_{0}, \quad K_{1}(\boldsymbol{r})=k_{1}, \quad K_{2}(\boldsymbol{r})=\lfloor\alpha\rfloor+k_{4}+m, \\
& K_{3}(\boldsymbol{r})=\lfloor\beta\rfloor+k_{1}+n, \quad K_{4}(\boldsymbol{r})=k_{4},
\end{aligned}
$$

with some integers $m$ and $n$ satisfying $-1 \leq m, n \leq 2$, and

$$
\begin{aligned}
\alpha & =p^{-1}\left(k_{0}-k_{1}-\gamma_{0}+\gamma_{1}\right)+\gamma_{2}-\gamma_{4} \\
\beta & =p^{-1}\left(k_{0}-k_{4}-\gamma_{0}+\gamma_{4}\right)+\gamma_{3}-\gamma_{1} .
\end{aligned}
$$

Next, we now project $\boldsymbol{K}(\boldsymbol{r})$ to $\mathcal{D}$ and find

$$
\boldsymbol{D}^{\mathrm{T}}(\boldsymbol{K}(\boldsymbol{r})-\gamma)=\sum_{j=0}^{4}\left(K_{j}(\boldsymbol{r})-\gamma_{j}\right) \boldsymbol{d}_{j}=(m-a) \boldsymbol{d}_{2}+(n-b) \boldsymbol{d}_{3}
$$

in which $a \equiv\{\alpha\} \equiv \alpha-\lfloor\alpha\rfloor$ and $b \equiv\{\beta\} \equiv \beta-\lfloor\beta\rfloor$. Thus each window of acceptance is a decagon.


The projection of $\mathcal{L}$ in the $x y$-plane.

