# Statistical and mathematical physics of discrete lattice models

Tony Guttmann

ARC Centre of Excellence for Mathematics and Statistics of Complex Systems
Department of Mathematics and Statistics
The University of Melbourne, Australia

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# Statistical mechanics

- Boltzmann (1844 – 1906) and Gibbs (1839 – 1903)

(a) The hotel where Boltzmann died

(b) Boltzmann's tombstone

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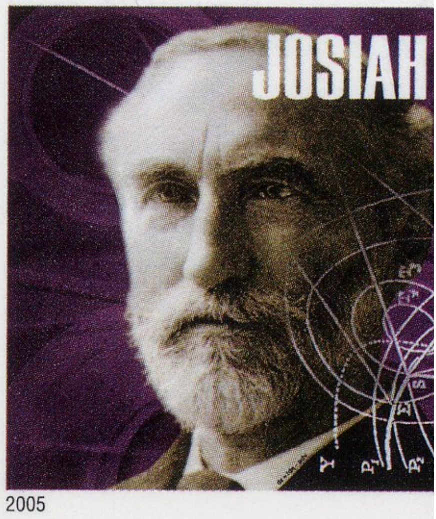


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# Ensembles

Canonical ensemble: $N$ particles of mass $m$, momentum $\mathbf{p}_i^2$, in a volume $V$ at temperature $T$, and $\beta = 1/k_B T$.

- Canonical partition function

$$Z(V, N, T) = \frac{1}{N!} \int d\Gamma \exp(-\beta H)$$

- Hamiltonian $H = \sum_{i=1}^{N} \frac{\mathbf{p}_i^2}{2m} + \sum_{1 \le i < j \le N} \phi(|\mathbf{r}_i - \mathbf{r}_j|)$
- Momentum integral gives $(2\pi m k_B T)^{3N/2}$, so

$$Z(V, N, T) = \lambda \int \cdots \int d\mathbf{r}_1 \cdots d\mathbf{r}_N \exp\left(-\beta \sum_{i<j} \phi(|\mathbf{r}_i - \mathbf{r}_j|)\right)$$

where $\lambda = \frac{(2\pi m k_B T)^{3N/2}}{N!}$.

- For lattices, integrals $\rightarrow$ sums, and $V$ disappears.

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# Thermodynamics

- Thermodynamics comes from

$$\Psi(V,N,T) = -k_B T \log Z(V,N,T).$$

- The *thermodynamic limit* exists for appropriate $\phi(r)$,

$$\lim_{N,V\to\infty,\ N/V\ \textit{fixed}} \frac{1}{N}\Psi(V,N,T) = \psi(\rho = N/V, T).$$

- The TL is essential for a phase transition
- For a variable number of particles, one has the Grand Canonical Partition Function – just the ogf of the CPF:

$$\mathcal{Z}(V,T,z) = \sum_{n=0}^{\infty} Z(V,n,T)z^n,$$

where $z$ is called the *fugacity*.
- Thermodynamics follow from, e.g. $PV = k_B T \log \mathcal{Z}(V,T,z)$, $\langle N\rangle = z\frac{\partial}{\partial z}\log \mathcal{Z}(V,T,z)$.

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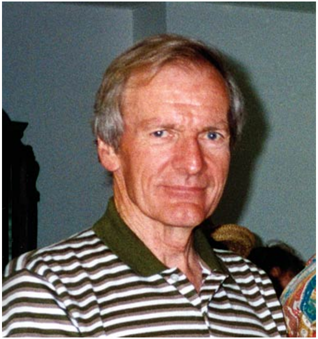
# Some well-known models

The Lenz-Ising (1900–1998) model and Potts (1925 – 2005) model

(e) E. Ising at 90



(f) Ren Potts

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# Lenz-Ising model

- $$H = -J \sum_{\langle i,j \rangle} \sigma_i \cdot \sigma_j, \quad \sigma_i = \pm 1.$$

- $$Z = \sum_{\sigma_1 = \pm 1} \cdots \sum_{\sigma_N = \pm 1} \exp(-\beta H).$$

- Generalise to the O($n$) model, where $\sigma_i$ is now an $n$-dimensional vector. (Stanley 1968).
- The Ising model is O(1). de Gennes pointed out that O(0) is the SAW model (1972).
- $n = \infty$ gives the spherical model. $n = 2$ the XY model, $n = 3$ the PCH model, $n = -2$ the Gaussian model.

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# Ising and Onsager

- It is simple to solve the 1d Ising model. The free-energy in the TL is:

$$\frac{-\psi}{k_B T} = \log(2\cosh(\beta J)).$$

- No phase transition. Boring!
- Rescued by metallurgists interested in binary alloys.
- Onsager, in 1944, solved the 2d model:

$$\frac{-\psi}{k_B T} = \frac{\log 2}{2} + \frac{1}{2\pi}\int_0^\pi \log\left(c^2 + \sqrt{s^2 + 1 - 2s\cos\theta}\right) d\theta.$$

  Here $c = \cosh(2K)$, $s = \sinh(2K)$.
- A phase transition when $s = 1$. Statistical mechanics is a “complete” theory. Hallelujah!

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# de Gennes and Onsager

(g) Pierre-Gilles de Gennes 1932–2007, Nobel Physics 1991

(h) Lars Onsager 1903–1976, Nobel Chem. 1968

# From Stat. Mech. to Combinatorics

- $$Z = \sum_{\{\sigma\}} \prod_{\langle i,j \rangle} \exp(K\sigma_i\sigma_j); \;\; K = J/k_B T.$$
- As $\sigma_i\sigma_j = \pm 1$, $\exp(K\sigma_i\sigma_j) = \cosh K(1 + \sigma_i\sigma_j \tanh K)$.
- On a lattice, $\sigma_i\sigma_j$ can be represented by a bond from $\sigma_i$ to neighbouring bond $\sigma_j$.
- Summing over all configurations, only those in which any $\sigma$ occurs an even number of times survives.
- Thus $Z$ is a sum over all graphs on the lattice with every vertex of even degree. We now have a combinatorial counting problem!

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# The Potts model

- At each lattice site place one of $q$ colours, $\{1, 2, \ldots, q\}$. The Hamiltonian is

$$H = -J \sum_{\langle i,j \rangle} \delta(\sigma_i, \sigma_j),$$

so the interaction is 1 if adjacent spins have the same colour, and 0 otherwise. Then with $K = J/k_B T$,

- $$Z(q, K) = \sum_{\{\sigma_i\}} \exp\left( K \sum_{\langle i,j \rangle} \delta(\sigma_i, \sigma_j) \right)$$

- When $q = 2$ it is just the Ising model. But as $q \to 1$ we get a percolation problem. As $q \to 0$ one obtains the number of spanning forests. Other interesting limits exist.

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- One connection with combinatorics is through the Tutte polynomial. Set $x = 1 + \frac{qe^{-K}}{1-e^{-K}}, \; y = e^k$, then $T(x, y) = \sum_{i,j \geq 0} t_{i,j} x^i y^j$.
- The Tutte polynomial coincides with the Potts model along the hyperbola $(x-1)(y-1) = q$.
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# Some mathematical connections

- Near a (second-order) phase transition, as exhibited, e.g. by the Ising model, thermodynamic quantities behave as

$$f(z) = \sum a_n z^n \sim A(1 - z/z_c)^\gamma.$$

Then $a_n \sim \frac{A \cdot n^{-\gamma-1}}{\Gamma(\gamma) \cdot z_c^n}$.

- In combinatorics, we ideally seek closed form expressions for the generating functions, or rigorous asymptotics.
- In statistical mechanics, one is often content to identify $\gamma$, $z_c$ and $A$, the critical exponent, critical point and critical amplitude respectively.
- Universality: The exponent is common across many different problems.

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# Scaling

- If $f(\xi) \sim A\xi^{\gamma}$ where $\xi = 1 - z/z_c$, this can be considered a solution of
$$f(\lambda\xi) = \kappa f(\xi),$$
with $\kappa = A\lambda^{\gamma}$. That is, a scaling of $\xi$ corresponds to a rescaling of $f$. (Equivalently, $f(\lambda^{1/\gamma}\xi) = \lambda f(\xi)$.)
- This rescaling can be applied to functions of more than one variable, so for a magnetic system (Hamiltonian has a second, field variable, say $H$), we have
$$f_s(\lambda^{y_t}\xi, \lambda^{y_h}H) = \lambda^{d} f_s(\xi, H),$$
where $d$ is the spatial dimension, and $y_t$ and $y_h$ are exponents in terms of which all other related exponents may be derived.
- This then implies
$$f_s(\xi, H) \sim |\xi|^{-d/y_t} F(H|\xi|^{y_t/y_h})$$

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# Scaling

- If $f(\xi) \sim A\xi^{\gamma}$ where $\xi = 1 - z/z_c$, this can be considered a solution of
$$f(\lambda\xi) = \kappa f(\xi),$$
with $\kappa = A\lambda^{\gamma}$. That is, a scaling of $\xi$ corresponds to a rescaling of $f$. (Equivalently, $f(\lambda^{1/\gamma}\xi) = \lambda f(\xi)$.)
- This rescaling can be applied to functions of more than one variable, so for a magnetic system (Hamiltonian has a second, field variable, say $H$), we have
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# Polygons – Richard, Jensen, Guttmann

- For square lattice polygons,

$$P(x,q) \sim P^{(reg)}(x,q) + (1-q) \cdot F\left(\frac{x_c - x}{(1-q)^{2/3}}\right) + C(q)$$

- Here,

$$F(s) = const.\log Ai(const.s),$$

and $C(q) = \frac{1}{12\pi}(1-q)\log(1-q)$.

- These scaling ideas, due to Kadanoff, Widom, Fisher and others in the '60s are a mathematical manifestation of the physical idea that at the critical point, all length scales are important.

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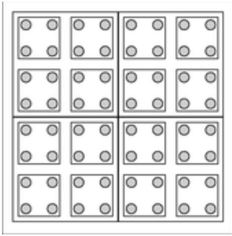
# Block renormalization - L Kadanoff

- Precedes K Wilson, Kadanoff 1966



- Assume physics stays the same as we reblock. Then $H(T, J) \to H(T', J') \to H(T'', J'')$ etc. Iterates to a fixed point.
- For the 1d Ising model, the RG flow goes from order ($T = 0$) to disorder ($T = \infty$.)
- For the 2d Ising model, the critical fixed point $K_c$ lies in between, and flow is away in both directions.

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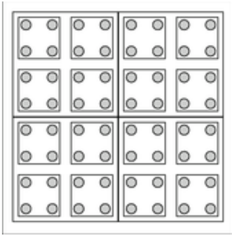

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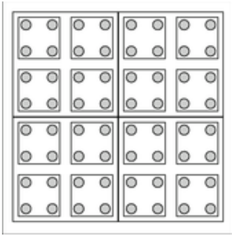

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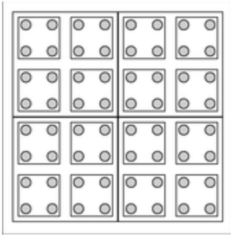

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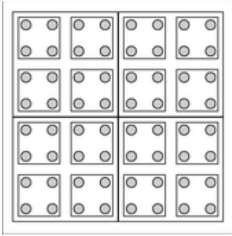

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# The renormalization group - K Wilson

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- Not a group. No renormalization. "The" is inappropriate. (Cardy).
- More generally, if $\{\sigma_i\} \to \{\sigma_i'\}$, and $\{J_k\} \to \{J_k'\}$ such that

$$Z(\{\sigma_i\}, \{J_k\}) = Z(\{\sigma_i'\}, \{J_k'\}),$$

  the system is *renormalizable.*
- Then $\{J_k'\} = \beta\{J_k\}$. The $\beta$-function is said to induce a renormalization flow on the $J$ space.
- In momentum space, one applies a Fourier transform, and the renormalization idea corresponds to integrating out the highest momentum components. Reminiscent of QED, which is renormalizable.
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# Scale invariance

- Scaling and RG theory explained global scale invariance.
- This gave *scaling laws* between exponents.
- In 1984 Belavin, Polyakov, Zamolodchikov investigated local scale invariance: conformal invariance
- In 2d, the conformal group is infinite.
- This implies that many systems can be labelled by a single parameter $c$ (central charge/conformal anomaly).
- Blöte, Cardy and Nightingale (1986) showed how to calculate $c$, via the transformation

$$z \to \frac{W}{2\pi} \log z$$

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# Conformal invariance

- Hence the free-energy of a critical model on an infinite cylinder of circumference $W$ has the scaling form

$$F = Wf_{\infty} - \frac{\pi c}{6W} + o(1/W).$$

- Precise numerical work can be done on finite-sized systems, and $c$ thus determined from the leading order correction to the bulk value $f_{\infty}$.
- Knowing $c$ is not sufficient to determine the universality class or ther exponents.
- Rather, for many systems, with $c < 1$, the possible exponents are restricted by the Kac formula, which gives possible exponents in terms of $c$.
- Systems can be in different universality classes with the same value of central charge.

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# Vertex models

- Put arrows on the square lattice bonds, 2 pointing in/out.
- There are only 6 possible configurations.
- Give a Boltzmann weight $w_i$ to configuration $i \in [1, \cdots, 6]$.
- The partition function is

$$Z = \sum_{\{configs\}} \prod_{i=1}^{6} w_i^{m_i}$$

  where there are $m_i$ vertices of type $i$.
- Different choices of weights lead to different models. Solved by Lieb/Sutherland in 1967, for $w_{1,2} = a$, $w_{3,4} = b$, $w_{5,6} = c$.
- Adding two extra vertices (4 arrows in/out with $w_{7,8} = d$) leads to the 8-vertex model. Solved by Baxter in 1973.

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# Transfer matrices

- The vertex models can be set up as a transfer matrix problem. (Introduced into stat. mech, by Kramers and Wannier in 1942).
- The partition function is then given by eigenvalues of the TM.
- For the 6-v problem, the arrow conservation rules leads to a block diagonal structure of the TM.
- For small lattices, Lieb produced an Ansatz for the eigenvectors (the Bethe Ansatz. Bethe 1931 1d a-f H model)
- In fact the TM commutes, $T(a,b,c)T'(a',b',c') = T'(a',b',c')T(a,b,c)$, and Baxter realized that invoking this bypasses the Bethe Ansatz.

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# 8-vertex model

- In this case the TM doesn't commute.
- Baxter investigated the conditions under which $T(a, b, c, d)$ and $T'(a', b', c', d')$ commute.
- He introduced a model with a third set of weights $(a'', b'', c'', d'')$, and found that if a condition relating the three models holds, then the TMs commute.
- This equation is called the *star-triangle* or *Yang-Baxter* equation.
- To solve the 6-v model, the weights are parameterised in terms of trig. functions. For the 8-v model a parameterisation in terms of Jacobi $\vartheta$ functions is needed.
- Invoking symmetries, one finds, in the TL, a functional equation for the eigenvalues of the TM, from which the free energy follows.

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- The Bethe Ansatz gives TM eigenvectors, but the CTM method does not.
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- One merely restricts the heights to the set $\{1, \cdots, L\}$.
- In 1987 Pasquier rewrote the weights in terms of elements of an adjacency matrix, and realised that it could be replaced by *any* symmetric $L \times L$ matrix with elements 0 and 1, and all solvability properties still held.
- Now such adjacency matrices can of course be represented as graphs! Hence any graph gives rise to an associated solvable RSOS model. *Graph state models*.
- These models with ABF Boltzmann weights satisfy a T-L algebra with a simple set of generators.
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# Nienhuis's calculation for honeycomb SAW

- Nienhuis and colleagues showed that the p.f of an O($n$) model can be written as a loop model
- Take a honeycomb lattice of $2N$ sites. Place arrows on edges such that at each vertex there are 0 or 2 arrows (1 in, 1 out). Gives oriented loops.
- Let $L = \#$ of arrows, $l, r = \#$ of vertices with a left/right turn.
- For each loop there are 6 more/less turns to left than right.
- So

$$Z_{loop} = \sum_{\{configs\}} t^{2N-L}(2\cos 6\alpha)^P,$$

where $P = \#$ of loops, and $\alpha$ is a fugacity.

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- Next consider a $q$-state Potts model on the triangular lattice, with $N$ sites $\sigma_i$, with $i \in 1, \cdots, q$.
- Then $Z_{Potts} = \sum_{\{\sigma\}} \exp\left(K \sum_{\langle ij \rangle} \delta(\sigma_i, \sigma_j)\right)$,
- Both the loop model and the Potts model are equivalent to a 6-v model on a kagomé lattice of $3n$ sites
- They are equivalent to the *same* model, and to one another, iff

$$n = 2\cos(6\alpha) = 2 - (2 - t^2)^2, \;\; q = 4 - t^2 = 2 - 2\sin(3\alpha), \;\; e^{(}-K) =$$

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- The proof is based on establishing a parafermionic operator, using discrete holomorphicity.
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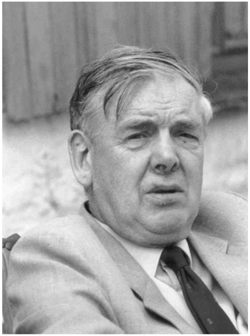
# John Hammersley 1920–2004



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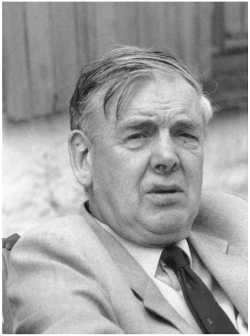

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