The quest for solvability.

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CSIRO, Aspendale, March 17 2015

Outline of talk

- History and significance of the Ising model
- Crash course in Statistical Mechanics
- Three key quantites, free energy, magnetisation, susceptibility
- Solution in 1 dimension
- Solution in 2 dimensions (Onsager, free energy; Yang, magnetisation)
- Progress in finding the susceptibility
- Concept of a *differentiably finite* or *D-finite* function. A linear ODE with polynomial coefficients.
- Direct analysis, based on correlation functions
- An analysis based on *n*-particle contributions (Feynman-type integrals)

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- Proposed as a model of ferromagnetism.
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- Magnetism is due to the electron's spin.
- Short range interaction between electrons. How do local interactions have a global effect?
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- The gas-liquid transition.
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- **Neurology** Hopfield
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Statistical mechanics

- Write down the Hamiltonian $\mathcal{H}$. (Energy of a configuration).

$$\mathcal{H} = -J \sum_{<i,j>} \sigma_i \cdot \sigma_j + H \sum_i \sigma_i, \;\; \sigma_i = \pm 1.$$

- Then the partition function

$$Z(T, H) = \sum_{all\ configs.} \exp(-\mathcal{H}/kT).$$

(k is Boltzmann's const., T is temp., H is mag. field.)

- The (Helmholtz) free energy $F(T, H) = -kT \log Z(T, H)$.
- We need $\mathcal{F}(T, H) = \lim_{N \to \infty} F(T, H)/N$.
- All quantities follow by differentiation. These include:
- The specific heat $C_0 = -T \frac{d^2 \mathcal{F}(T,0)}{dT^2}$
- The (zero-field) magnetisation $m_0(T) = \frac{\partial \mathcal{F}(T,H)}{\partial H}|_{H=0}$
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ONE-DIMENSIONAL MODEL

- A one-dimensional array of “spins" $\{\mu_i, i = 1 \ldots N\}$, “up" or “down”, $\mu_i = \pm 1$. The Hamiltonian $\mathcal{H}$ of a configuration of spins, denoted $\{\mu\}$, is

$$\mathcal{H}\{\mu\} = -J \sum_{\langle i,j \rangle} \mu_i \mu_j + H \sum_{i=1}^{N} \mu_i = -J \sum_{i} \mu_i \mu_{i+1} + H \sum_{i=1}^{N} \mu_i.$$

$\sum_{\langle i,j \rangle}$ means a sum over nearest-neighbour pairs, J is the strength of the interaction between adjacent spins. The second sum gives the interaction of each spin with an external magnetic field H.

One-dimensional model

- The partition function is

$$Z_N = \sum_{\{\mu\}} \exp\left(-\beta\mathcal{H}\{\mu\}\right),$$

  where $\beta = 1/(k_B T)$.

- We want the Helmholtz free-energy, $\mathcal{F}/k_B T = -\lim_{N\to\infty} 1/N \log Z_N$.
- The zero-field free energy then follows (set H=0 in the above),
- the zero-field magnetisation, $\lim_{H\to 0} \partial(-\mathcal{F}/kT)/\partial H$,
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ONE-DIMENSIONAL MODEL

- In 1 dimension, impose cyclic boundary conditions, so that $\mu_{N+1} = \mu_1$. Then symmetrise the energy function

$$\begin{aligned}\mathcal{H}\{\mu\} &= -J\sum_{i=1}^{N}\mu_i\mu_{i+1} + H\sum_{i=1}^{N}\mu_i \\ &= -J\sum_{i=1}^{N}\mu_i\mu_{i+1} + H/2\sum_{i=1}^{N}(\mu_i + \mu_{i+1}).\end{aligned}$$

- The partition function sum $\sum_{\{\mu\}}$ can be written $\sum_{\mu_1=\pm1}\sum_{\mu_2=\pm1}\sum_{\mu_3=\pm1}\cdots\sum_{\mu_N=\pm1}$.

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- The summand is

$$e^{(-\beta\mathcal{H}\{\mu\})} = e^{[\beta J \sum_{i=1}^{N} \mu_i \mu_{i+1} + \beta H/2 \sum_{i=1}^{N} (\mu_i + \mu_{i+1})]}.$$

- Summing this over a particular value of μ_i is just taking a matrix product. Indeed, consider the matrix

$$T = \begin{pmatrix} e^{(\beta J + \beta H)} & e^{-\beta J} \\ e^{-\beta J} & e^{(\beta J - \beta H)} \end{pmatrix}$$

- Then

$$Z_N = \sum_{\mu_1 = \pm 1} T^N = \mathrm{Tr}(T^N) = \lambda_1^N + \lambda_2^N$$

- When $\beta J > 0$, $\lambda_1 > \lambda_2$, so in the TL we only consider λ_1.

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One-dimensional model

- So to solve the 1d Ising model we need only the eigenvalues of a 2×2 matrix
- Thus

$$\frac{\mathcal{F}(T,H)}{-kT} = \left[\beta J + \log\left(\cosh \beta H + \sqrt{\sinh^2 \beta H + \exp(-4\beta J)}\right)\right].$$

- Thus

$$\mathcal{F}(T,0) = -kT \log(2\cosh \beta J),$$

- $m_0(T) = 0$ for $T > 0$, and $m_0(T) = \pm 1$ for $T = 0$.
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$$\mathcal{F}(T,0) = -kT\log(2\cosh\beta J),$$

- $m_0(T) = 0$ for $T > 0$, and $m_0(T) = \pm 1$ for $T = 0$.
- $\chi_0(T) = \exp(2\beta J)/kT$.

TWO-DIMENSIONAL MODEL

- In 1942 Onsager solved the two-dimensional model for the zero-field free energy (published 1944), noting that the transfer matrices generated a finite Lie algebra.
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Two-dimensional model

- Onsager's solution was refined by Kaufmann, who pointed out that a Clifford algebra could be used. Kac and Ward sought a simpler solution. Sherman pointed out a flaw. Feynman conjectured a fix. Sherman proved Feynman's conjecture.
- Later, Schutzenberger informed Sherman that his proof extended an identity of W. Witt on *"the dimension of the linear space of Lie elements of degree r in a free Lie algebra with k generators over a field of characteristic zero,"* and made some remarks on further extensions that might be of use in proving results in three dimensions.

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- Let $\mu_{i,j}$ be the spin at lattice site (i,j) of a lattice of m rows and n columns, wrapped as a cylinder. The Hamiltonian is

$$\mathcal{H}\{\mu\} = -J\sum_{i,j}\mu_{i,j}\mu_{i+1,j} - J\sum_{i,j}\mu_{i,j}\mu_{i,j+1} - H\sum_{i,j}\mu_{i,j}$$

  The partition function

$$Z = \sum_{\{\mu\}}\exp(-\mathcal{H}\{\mu\}/kT)$$

  can be calculated by diagonalising a $2^m \times 2^m$ matrix in the limit as $m \to \infty$.

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- The final result for the internal energy is relatively simple:

$$U = -J \coth 2K \left[1 + (2 \tanh^2 2K - 1) \frac{2}{\pi} K(k_1) \right]$$

$k_1 = 2 \sinh 2K / \cosh^2 2K$, $K = J/kT$ and $K(k_1)$ is the complete elliptic integral of the first kind.

- Denote by $\mathcal{M}$ the magnetisation. It is zero for $T > T_c$ and, $\mathcal{M} = (1 - s^{-4})^{1/8}$ for $T < T_c$, where $s = \sinh(2J/kT)$.
- The two-point correlation function is

$$C(m, n) = \langle \mu_{0,0} \mu_{m,n} \rangle.$$

- In terms of this two-point correlation function, the susceptibility χ is given by

$$kT \cdot \chi = \sum_m \sum_n \left(C(m, n) - \mathcal{M}^2 \right),$$

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THE SUSCEPTIBILITY

- No one has managed to find a closed form expression for the susceptibility, despite strenuous efforts by many of the world's greatest mathematical physicists.
- However, considerable progress has been made.
- In 1976, Wu, McCoy, Tracy and Barouch showed that the susceptibility can be expressed as an infinite sum of *n-particle contributions.* The susceptibility is given by

$$kT\chi_H(w) = \frac{1}{s} \cdot (1 - s^4)^{\frac{1}{4}} \sum_n \tilde{\chi}^{(2n+1)}(w)$$

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$$\tilde{\chi}^{(n)}(w) \;=\; \frac{1}{n!} \cdot \Big(\prod_{j=1}^{n-1} \int_0^{2\pi} \frac{d\phi_j}{2\pi}\Big) \Big(\prod_{j=1}^{n} y_j\Big) \cdot R^{(n)} \cdot \; \Big(G^{(n)}\Big)^2,$$

$$G^{(n)} \;=\; \prod_{1 \,\le\, i \,<\, j \,\le\, n} h_{ij}, \quad h_{ij} \;=\; \frac{2 \sin\left((\phi_i - \phi_j)/2\right) \cdot \sqrt{x_i\, x_j}}{1 - x_i x_j},$$

$$R^{(n)} \;=\; \frac{1 \,+\, \prod_{i=1}^{n} \, x_i}{1 \,-\, \prod_{i=1}^{n} \, x_i},$$

$$x_i \;=\; \frac{2w}{1 - 2w\cos(\phi_i) \,+\, \sqrt{(1 - 2w\cos(\phi_i))^2 - 4w^2}},$$

$$y_i \;=\; \frac{2w}{\sqrt{(1 \,-\, 2w\cos(\phi_i))^2 \,-\, 4w^2}}, \qquad \sum_{j=1}^{n} \phi_j = \; 0$$

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- To evaluate $\tilde{\chi}^{(n)}$ convert to an n-fold integration with the explicit phase constraint $\sum \phi_i = 0$ now in the integrand. A Fourier transform decouples all ϕ_i integrations at the expense of a sum over the Fourier integer k. Next expand all denominator factors in the integrand, thereby converting it into a sum of n-fold products $\prod y_i x_i^{n_i}$. Each i integration picks out the k^{th} Fourier coefficient of $y_i x_i^{n_i}$. This coefficient is proportional to a ${}_4F_3$ hypergeometric function. The integrand becomes a nested sum of products of hypergeometric functions.

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- In particular, both the Ising free-energy and magnetisation are holonomic functions (i.e. *differentiably finite* or *D-finite* functions), while the susceptibility, they argued, was not.
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- Many 2d lattice models are solvable for some properties and/or some lattices.
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The two-dimensional Ising model

- Take $t_1 = \tanh(J_x/kT)$ and $t_2 = \tanh(J_y/kT)$ in directions x, y.
- The log of the reduced p.f. is

$$\log \Lambda(t_1, t_2) = \sum_{n,m} a_{n,m} t_1^{2m} t_2^{2n} = \sum_n R_n(t_1^2) t_2^{2n}.$$

- Baxter showed that $R_n(t_1^2) = P_{2n-1}(t_1^2)/(1 - t_1^2)^{2n-1}$.
- R_n rational, with num. and den. pols of degree $2n - 1$,
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- Remarkably, these two relations, plus the structure of R_n suffices to determine, order by order, the numerator polynomials.
- Alternatively, the two functional relations, and the structure of R_n implicitly gives the Onsager solution.
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- $\chi(t_1, t_2) = \sum_{n,m} c_{n,m} t_1^m t_2^n = \sum_n H_n(t_1) t_2^n.$
- The corresponding inversion and symm. relations are

$$\chi(t_1, t_2) + \chi(1/t_1, -t_2) = 0, \quad \chi(t_1, t_2) = \chi(t_2, t_1).$$

- The first few denominators of $H_n(t_1)$ are:

$$\begin{aligned}
D_0(x) &= (1 - t_1) \\
D_1(x) &= (1 - t_1)^2 \\
D_2(x) &= (1 - t_1)^3 (1 + t_1) \\
D_3(x) &= (1 - t_1)^4 \\
D_4(x) &= (1 - t_1)^4 (1 + t_1)^3 (1 - t_1^3) \\
D_5(x) &= (1 - t_1)^6 (1 + t_1)^2 \\
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2D ISING SUSCEPTIBILITY

- The numerators are the same degree as denoms, and symmetric, unimodal with positive coefficients.
- But the degree of the polynomials increases non-linearly.
- The functional relations are insufficient to determine the numerator.
- In the famous paper by Wu, McCoy, Tracy and Barouch, $\chi(t) = \sum \chi^{(2n+1)}(t)$, where $\chi^{(2n+1)}(t) = O(t^{(2n+1)^2-1})$.
- $H_4(t)$ sees the first occurrence of $(1 - t^3)$ in the denominator, and reflects the $O(t^8)$ term that enters with $\chi^{(3)}$.
- Similarly, $H_{12}(t)$ sees the first occurrence of $(1 - t^5)$ in the denominator, and reflects the $O(t^{24})$ term that enters with $\chi^{(5)}$.

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2D ISING SUSCEPTIBILITY STRUCTURE

- $H_n(t)$ is rational, with poles on the unit circle in the t-plane.
- These become dense as $n \to \infty$.
- Then (barring miraculous cancellation) $\chi(t_1, t_2)$ as a function of t_1 for t_2 fixed (a) has a natural boundary, and (b) is neither algebraic nor D-finite, despite the fact that $H_n(t_1)$ is rational.
- Some models can be refined into a proof (absence of cancellations).
- If we could prove positivity and unimodality, that would do. (No cancellations then possible).
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CONCLUSION FROM THIS METHOD

- A frequently exact method for models that can be exactly solved.
- Fails for non-D-finite models.
- Provides a powerful tool for predicting solvability.
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- Glossed over Ian's other seminal contribution, developing the techniques to produce the enumerative data. Nathan will speak more on this.

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