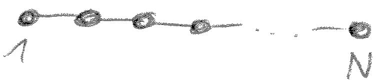
20/11/2014

Tutorial Statistical Physics

1D Ising Model:

- chain of N (classical) spins with nearest neighbour interactions



1) No external field:

can be >0 or <0

attractive interaction / repulsive interaction

can take values ± 1

Hamiltonian $\mathcal{H} = -J \sum_{i=1}^{N-1} \sigma_i \sigma_{i+1}$

Partition function

$$Z_N = \sum_{\sigma_1 = \pm 1} \cdots \sum_{\sigma_N = \pm 1} e^{\beta J \sum_{i=1}^{N-1} \sigma_i \sigma_{i+1}}$$

$$= Z_{N-1} \sum_{\sigma_N = \pm 1} e^{\beta J (\sigma_{N-1}) \sigma_N}$$

sloppy notation: the actual value of this does not matter for the outcome, leave it out if you want

$$= 2 Z_{N-1} \cosh(\beta J)$$

$$= (2\cosh(\beta J))^{N-2} Z_2$$

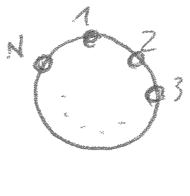
(with $Z_2 = \sum_{\sigma_1 = \pm 1} \sum_{\sigma_2 = \pm 1} e^{\beta J \sigma_1 \sigma_2} = 2(2\cosh(\beta J))$)

$$= 2(2\cosh(\beta J))^{N-1}$$

$\Rightarrow$ Free energy $F = -k_B T \ln Z_N = -k_B T \left[\ln 2 + (N-1)\ln(2\cosh \beta J)\right]$

$$\xrightarrow[\text{(therm. limit)}]{N \to \infty} -N k_B T \ln(2\cosh \beta J)$$

2) With an external magnetic field:



Now let $\mathcal{H} = -J \sum_{i=1}^{N} \sigma_i \sigma_{i+1} - h \sum_{i=1}^{N} \sigma_i$, where we consider a system with periodic boundary conditions such that $N+1 \Leftrightarrow 1$.

($\rightarrow$ the idea is that end effects will not matter for $N \to \infty$ and the calculations become much easier)

$\Rightarrow$ we can write

$$\mathcal{H} = -\sum_{i=1}^{N} \left[J \sigma_i \sigma_{i+1} + \frac{h}{2}(\sigma_i + \sigma_{i+1}) \right]$$

Then the partition function becomes

$$Z_N = \sum_{\sigma_1=\pm1} \cdots \sum_{\sigma_N=\pm1} e^{\beta \sum_{i=1}^{N} \left(J\sigma_i\sigma_{i+1} + \frac{h}{2}(\sigma_i+\sigma_{i+1})\right)}$$

$$= \sum_{\{\sigma_i\}} \prod_{i=1}^{N} e^{\beta(J\sigma_i\sigma_{i+1} + \frac{h}{2}(\sigma_i+\sigma_{i+1}))}$$

(Use the transfer matrix

$$P = \begin{bmatrix} P_{1,1} & P_{1,-1} \\ P_{-1,1} & P_{-1,-1} \end{bmatrix} = \begin{bmatrix} e^{\beta(J+h)} & e^{-\beta J} \\ e^{-\beta J} & e^{\beta(J-h)} \end{bmatrix}$$)

$$= \sum_{\{\sigma_i\}} P_{\sigma_1\sigma_2} P_{\sigma_2\sigma_3} P_{\sigma_3,\sigma_4} \cdots P_{\sigma_N,\sigma_1} = \mathrm{tr}\, P^N$$

always the same ⇒ like summing the diagonals of P^N

To calculate $\mathrm{tr}\, P^N$, the easiest way is to compute the eigenvalues of P, so that $\mathrm{tr}\, P^N = (\lambda_1^N + \lambda_2^N)$, with λ_1 & λ_2 the EV of P.

$$\Rightarrow |P - \lambda \mathbb{1}| = 0 \quad \Rightarrow \lambda_{1,2} = e^{\beta J}\cosh(\beta h) \pm \left(e^{2\beta J}\sinh^2\beta h + e^{-2\beta J}\right)^{\frac{1}{2}}$$

$$\Rightarrow \lambda_1 > \lambda_2$$

This means, in the therm. limit ($N \to \infty$) we can approximate

$Z_N = \mathrm{tr}\, P^N = \lambda_1^N + \lambda_2^N \longrightarrow \lambda_1^N$ is the dominant contribution to

$$F = -\frac{1}{\beta}\ln(\lambda_1^N + \lambda_2^N) = -\frac{1}{\beta}\Bigg(N\ln\lambda_1 + \underbrace{\ln\left(1+\left(\frac{\lambda_2}{\lambda_1}\right)^N\right)}_{\to 0}\Bigg) \to -Nk_BT\ln\lambda_1$$

$$= -Nk_BT\ln\left[e^{\beta J}\cosh(\beta h) + \left(e^{2\beta J}\sinh^2\beta h + e^{-2\beta J}\right)^{\frac{1}{2}}\right]$$

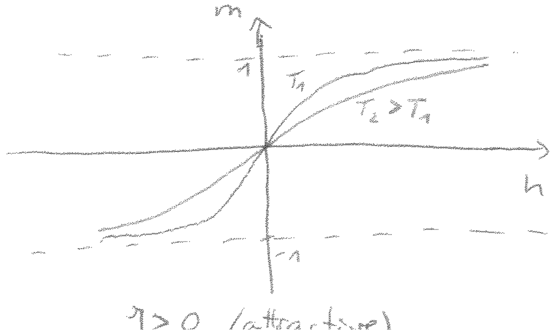
(for $h=0$ previous result of $-Nk_BT\ln(2\cosh\beta J)$)

Now, for the magnetization we find

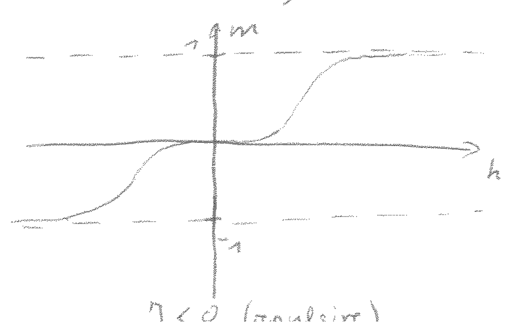
needs a bit of tedious calculation & rearrangement (or mathematica or so)

$$m = \langle\sigma_0\rangle = -\frac{1}{N}\frac{\partial F}{\partial h} = \frac{1}{\beta\lambda_1}\frac{\partial\lambda_1}{\partial h} = \frac{\sinh(\beta h)}{(\sinh^2(\beta h) + e^{-4\beta J})^{1/2}}$$

per particle



$J > 0$ (attractive)



$J < 0$ (repulsive)

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A few comments:

- basically the same model as the interacting lattice gas treated in the lectures
- for $h=0$, no long-range order for $T>0$ (magnetization vanishes)
- For $J>0$, as $T\to 0$ $\sinh^2(\beta h) \gg e^{-4\beta J}$ and so for small h, $m\to 1$ still very quickly. Also, the mean free energy per particle goes to $F(T\to 0) = -NJ$ (here take $h=0$), corresponding to completely aligned spins $\to$ we say we "have a phase transition at $T=0$"
- Phase transitions for $T>0$ will only occur in higher dimensions!

Spin correlation function:

$\Gamma_\ell = \langle \sigma_i \sigma_{i+\ell}\rangle - \langle\sigma_i\rangle\langle\sigma_{i+\ell}\rangle$. As there is no spin ordering for $h=0$, in this case we have $\langle\sigma_i\rangle = 0$ and so

$$\Gamma_\ell = \langle \sigma_i\sigma_{i+\ell}\rangle = \frac{1}{Z_N}\sum_{\{\sigma_j\}} \sigma_i\sigma_{i+\ell}\, e^{\beta\sum_{k=1}^{N-1} J_k\sigma_k\sigma_{k+1}}$$

in our case, $J_k = J$, but we could have looked at more general systems and also this is convenient!

$$= \frac{1}{Z_N}\sum_{\{\sigma_j\}} (\sigma_i\sigma_{i+1})(\sigma_{i+1}\sigma_{i+2})\cdots(\sigma_{i+\ell-1}\sigma_{i+\ell})\, e^{\beta\sum_{k=1}^{N-1} J_k\sigma_k\sigma_{k+1}}$$

$(\sigma_j)^2 = 1$

$$= \frac{1}{Z_N\beta^\ell}\left.\frac{\partial^\ell Z_N(J_0\ldots J_N)}{\partial J_i\,\partial J_{i+1}\,\partial\ldots\partial J_{i+\ell-1}}\right|_{J_i=J}$$

$$= (\tanh\beta J)^\ell = e^{-\ell/\xi}$$

with $\boxed{\xi = -\left(\ln(\tanh\beta J)\right)^{-1}}$ (so $\xi>0$)

correlation length!

$\Rightarrow$ exponential decay with increasing ℓ (for $T>0$)

$\Rightarrow$ for small T, ξ can get quite large though!

$$\ln(\tanh\beta J) \approx -2e^{-2\beta J} \Rightarrow \xi = \frac{1}{2}e^{2\beta J}$$

$\Rightarrow$ however, this is not long-range order (for that we require $\langle\sigma_i\sigma_{i+\ell}\rangle \underset{\ell\to\infty}{\not\to} 0$).

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Extra: Susceptibility! (compare with 5.1.3 in skript)

We calculate

$$\chi_{zz} = \frac{1}{N k_B T}\left(\langle M^2\rangle - \langle M\rangle^2\right), \text{ with } M = \sum_{i=1}^{N} \sigma_i .$$

$$\rightarrow \chi_{zz} = \frac{1}{N k_B T}\left(\left\langle \sum_{ij} \sigma_i \sigma_j \right\rangle - \left(\left\langle \sum_i \sigma_i \right\rangle\right)^2\right)$$ vanishes for $h=0$

$$= \frac{1}{N k_B T} \sum_{i=1}^{N}\sum_{j=1}^{N} \Gamma_{|i-j|}$$

$$= \frac{1}{N k_B T} \sum_{i=1}^{N}\sum_{j=1}^{N} (\tanh \beta J)^{|i-j|}$$

limit of large N

$$\approx \frac{1}{N k_B T} \sum_{i=1}^{N}\left(1 + 2\sum_{j=1}^{\infty} (\tanh\beta J)^j\right)$$

$$= \frac{1}{k_B T}\left(1 + 2\sum_{j=1}^{\infty} (\tanh\beta J)^j\right)$$

$$= \frac{1}{k_B T}\left(1 + \frac{2\tanh\beta J}{1-\tanh\beta J}\right) = \frac{1}{k_B T}\left(\frac{1+\tanh\beta J}{1-\tanh\beta J}\right)$$

For high temperatures this becomes

$$\chi_{zz} \approx \frac{1}{k_B T}\left(1 + 2\tanh\beta J\right)\left[= \frac{1}{k_B T}\left(1 + 2\frac{e^{\beta J} - e^{-\beta J}}{e^{\beta J} + e^{-\beta J}}\right)\right]$$

$$\rightarrow \frac{1}{k_B T}.$$

For small temperatures, χ_{zz} diverges in the ferromagnetic case ($J>0$) as

$$\chi_{zz} \approx \frac{1}{k_B T}\left(\frac{1 + (e^{\beta J} - e^{-\beta J})/(e^{\beta J} + e^{-\beta J})}{1 - (e^{\beta J} - e^{-\beta J})/(e^{\beta J} + e^{-\beta J})}\right)$$

$$\approx \frac{1}{k_B T}\left(\frac{2 - e^{-2\beta J} - e^{-2\beta J}}{1 - (1 - e^{-2\beta J} - e^{-2\beta J})}\right) \approx \frac{1}{k_B T} e^{2\beta J}$$ ($\rightarrow$ diverges very fast)