Tutorial 10, Statistical Mechanics: Concepts and applications
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Tutorial exercises

I. THE ROUGHENING TRANSITION

1. **The Chui–Weeks model** *Source: S. T. Chui and J. D. Weeks, Phys. Rev. B* **23***, 2438 (1981)*
J. M. Yeomans, Statistical Mechanics of Phase Transitions (Oxford, 1992), chapter 5

The model: Here we consider a version of the Chui-Weeks model, which describes solid-on-solid surface growth. The surface is parametrized by the height h_i above site i of the lattice, which we are going to assume to be discrete and non-negative $h_i \in \mathbb{N}$ (there is an impenetrable substrate). The Hamiltonian is given by

$$H = J \sum_{i=1}^{N} |h_i - h_{i+1}| - K \sum_{i=1}^{N} \delta_{h_i 0} \, , \tag{1}$$

where the first term represents the contribution of surface tension to the total energy, and K parametrizes an energy binding the surface to the substrate. Assume a one dimensional model with periodic boundary conditions.

(a) Write down the transfer matrix of this model in terms of $\omega = e^{-\beta J}$ and $\kappa = e^{\beta K}$.

:

$$T_{ss'} = \omega^{|s-s'|}(\delta_{s0}\kappa + 1 - \delta_{s0}) \tag{2}$$

for $s, s' \geq 0$

(b) Consider a family of eigenvectors of the form

$$\vec{v}^t = \begin{pmatrix} \Psi_0 & \cos(q+\theta) & \cos(2q+\theta) & \dots \end{pmatrix} . \tag{3}$$

Find the corresponding eigenvalues.

: *We have*

$$[T\vec{v}]_0 = \kappa(\Psi_0 + \sum_{s=1}^{\infty} \omega^s \cos(sq+\theta)) = \kappa(\Psi_0 + \mathrm{Re} \sum_{s=1}^{\infty} \omega^s e^{isq+i\theta}) = \kappa(\Psi_0 + \mathrm{Re} \frac{e^{i\theta}}{e^{\beta J - iq} - 1}) = \kappa\Big[\Psi_0 + \frac{\omega\cos(q+\theta) - \omega^2\cos\theta}{1 - 2\omega\cos q + \omega^2}\Big] \tag{4}$$

$$[T\vec{v}]_{s\geq 0} = e^{-\beta J s}\Psi_0 + \sum_{s'=1}^{\infty} e^{-\beta J|s-s'|}\cos(qs'+\theta) = e^{-\beta J s}\Psi_0 + \sum_{s'=1}^{s-1} e^{-\beta J(s-s')}\cos(qs'+\theta) + \sum_{s'=0}^{\infty} e^{-\beta J s'}\cos(qs'+qs+\theta)$$
$$= e^{-\beta J s}\Psi_0 + \frac{e^{\beta J(1-s)}\cos(\theta+q) - e^{(2-s)\beta J}\cos\theta + (e^{2\beta j} - 1)\cos(qs+\theta)}{1 + e^{2\beta J} - 2e^{\beta J}\cos q} \, . \tag{5}$$

Thus we must impose

$$\begin{aligned} e^{\beta K}\left[\Psi_0 + \frac{e^{\beta J}\cos(q+\theta)-\cos\theta}{e^{2\beta J}-2e^{\beta J}\cos q+1}\right] &= \lambda\Psi_0 \\ \omega^s\Psi_0 + \frac{e^{\beta J(1-s)}\cos(\theta+q)-e^{(2-s)\beta J}\cos\theta+(e^{2\beta j}-1)\cos(qs+\theta)}{1+e^{2\beta J}-2e^{\beta J}\cos q} &= \lambda\cos(qs+\theta)\,. \end{aligned} \tag{6}$$

From the second equation we find

$$\Psi_0 = \frac{e^{2\beta J}\cos\theta - e^{\beta J}\cos(q+\theta)}{1+e^{2\beta J}-2e^{\beta J}\cos q} \tag{7}$$

which, plugged into the first equation gives

$$\lambda = e^{\beta K}\cos\theta\frac{e^{2\beta J}-1}{e^{2\beta J}\cos\theta - e^{\beta J}\cos(q+\theta)} \tag{8}$$

From the second equation instead we have

$$\lambda = \frac{e^{2\beta J}-1}{1+e^{2\beta J}-2e^{\beta J}\cos q} \tag{9}$$

which results in the consistency condition

$$e^{\beta K}(1+e^{2\beta J}-2e^{\beta J}\cos q) = e^{2\beta J} - e^{\beta J}\frac{\cos(q+\theta)}{\cos\theta}\,. \tag{10}$$

For any given q, the quantity $\frac{\cos(q+\theta)}{\cos\theta}$ can assume any value, therefore there is always a value of θ for which this condition is satisfied. Consequently, the family of eigenvalues associated with eigenvectors of the form (**??**) *is parametrized as in* (**??**) *for arbitrary q. We can therefore conclude*

$$\lambda \in \left[\frac{1-\omega}{1+\omega}, \frac{1+\omega}{1-\omega}\right]. \tag{11}$$

(c) Now consider a different eigenvector:

$$\vec{w}^t = \begin{pmatrix}\Phi_0 & e^{-\mu} & e^{-2\mu} & \dots\end{pmatrix}. \tag{12}$$

Find the corresponding eigenvalue and, if necessary, specify in what temperature regime it exists.

: *We find*

$$[T\vec{w}]_0 = \kappa\Big(\Phi_0 + \sum_{s=1}^{\infty}\omega^s e^{-\mu s}\Big) = \kappa\Big(\Phi_0 + \frac{1}{e^{\beta J+\mu}-1}\Big) \equiv \lambda\Phi_0 \tag{13}$$

$$[T\vec{v}]_{s\geq 0} = \omega^s\Phi_0 + \sum_{s'=1}^{\infty}\omega^{|s-s'|}e^{-\mu s'} \overset{\beta J<\mu}{=} e^{-\beta J s}\Phi_0 + \frac{e^{-\beta J(s-1)-\mu}-e^{-\mu s}}{1-e^{\beta J-\mu}} + \frac{e^{-\mu s}}{1-e^{-\beta J-\mu}} \equiv \lambda e^{-\mu s} \tag{14}$$

From the second equation we deduce

$$\Phi_0 = \frac{1}{1 - e^{-\beta J + \mu}} \tag{15}$$

which plugged into the first equation gives

$$e^{\beta K}\left(\frac{e^{\beta J} - e^{-\beta J}}{e^{\beta J} - e^{-\mu}}\right) = \lambda \tag{16}$$

while the second equation results in the constraint

$$e^{-\mu} = \frac{\omega}{1 - \kappa^{-1}}. \tag{17}$$

Since $\mu > 0$ (otherwise the eigenvector would not be normalizable), this places a condition on the temperature:

$$\omega < 1 - \kappa^{-1}. \tag{18}$$

The discrete eigenvalue that exists in the temperature range satisfying the condition above is given by

$$\lambda_0 = \frac{\kappa(1 - \omega^2)(\kappa - 1)}{\kappa(1 - \omega^2) - 1}. \tag{19}$$

(d) Find the eigenvalue that dominates the thermodynamics below the critical temperature (temperature at which the *roughening transition* occurs), and discuss what this means for the two phases.

: *Lets check whether this inequality holds:*

$$\frac{\kappa(1 - \omega^2)(\kappa - 1)}{\kappa(1 - \omega^2) - 1} > \frac{1 + \omega}{1 - \omega},$$

$$\kappa\omega^2 - 2(\kappa - 1)\omega - 2 + \kappa + 1/\kappa > 0,$$

The quadratic equation has one root $\omega = \frac{K-1}{K}$, so no part of the parabola lies below the x-axis and the inequality holds. Therefore, where λ_0 exists (i.e., below T_c), it is the largest eigenvalue. Roughly speaking, the right eigenvector $\vec{w}^t$, and the corresponding left eigenvector of T give the probabilities of various heights: the product of the two vectors' kth components is proportional to the probability of $h = k$ on a given site.
You can then see that below T_c the width of the substrate is bound, whereas above the roughening transition it is not.