

Lecture 21

Evaluating the partition function of the transverse-field Ising model by Trotter decomposition.

$$Z = \sum_{\{\sigma^z(\tau_n)\}} \cdots \sum_{\{\sigma^z(\tau_1)\}} \prod_{n=0}^{M-1} \langle \{\sigma^z(\tau_{n+1})\} | e^{-\epsilon H_0},$$

$$\cdot e^{-\epsilon H_0} | \{\sigma^z(\tau_n)\} \rangle, \quad \{\sigma^z(\tau_n)\} = \{\sigma^z(\tau_0)\}$$

Consider a single factor in the above product.

$$\begin{aligned} & \langle \{\sigma^z(\tau_{n+1})\} | e^{-\epsilon H_0} e^{-\epsilon H_0} | \{\sigma^z(\tau_n)\} \rangle = \\ & = \langle \{\sigma^z(\tau_{n+1})\} | e^{\epsilon h \sum_i \sigma_i^x} e^{\epsilon J \sum_{ij} \sigma_i^z \sigma_j^z} | \{\sigma^z(\tau_n)\} \rangle \\ & = \underbrace{\langle \{\sigma^z(\tau_{n+1})\} | e^{\epsilon h \sum_i \sigma_i^x} | \{\sigma^z(\tau_n)\} \rangle}_{\text{X}}. \end{aligned}$$

$$e^{\epsilon J \sum_{ij} \sigma_i^z (\tau_n) \sigma_j^z (\tau_n)}$$

$$e^{\epsilon h \sum_i \sigma_i^x} = \prod_i e^{\epsilon h \sigma_i^x}$$

$$e^{\epsilon h \sigma_i^x} = \cosh(\epsilon h) \sigma_i^0 + \sinh(\epsilon h) \sigma_i^x, \quad \sigma_i^0 = \left(\begin{smallmatrix} 0 & 1 \\ 1 & 0 \end{smallmatrix} \right)$$

This follows from $e^x = \cosh x + i \sinh x$ and $(\sigma^x)^2 = \sigma^0$

Now we obtain:

~~$$\langle \sigma^z(\tau_{n+1}) | \sigma^z(\tau_n) \rangle = \langle \sigma^z(\tau_n) | \sigma^z(\tau_{n+1}) \rangle$$~~

$$X = \langle \{ \sigma^z(\tau_{n+1}) \} | \prod_i [\cosh(\epsilon h) \sigma_i^x + \sinh(\epsilon h) \sigma_i^y] \rangle.$$

$$\langle \{ \sigma^z(\tau_n) \} \rangle = \prod_{i=1}^N \langle \sigma_i^z(\tau_{n+1}) | \cosh(\epsilon h) \sigma_i^x + \sinh(\epsilon h) \sigma_i^y | \sigma_i^z(\tau_n) \rangle = \prod_{i=1}^N C_{\sigma_i^z(\tau_{n+1}), \sigma_i^z(\tau_n)}$$

$$C = \begin{pmatrix} \cosh(\epsilon h) & \sinh(\epsilon h) \\ \sinh(\epsilon h) & \cosh(\epsilon h) \end{pmatrix}$$

C can be rewritten as:

$$C_{\sigma_1^z \sigma_2^z} = A e^{K_2 \sigma_1^z \sigma_2^z}$$

$$A e^{K_2} = \cosh(\epsilon h)$$

$$A e^{-K_2} = \sinh(\epsilon h)$$

$$A = \sqrt{\sinh(\varepsilon h) \cosh(\varepsilon h)} = \sqrt{\frac{1}{2} \sinh(2ch)}$$

$$K_2 = \frac{1}{2} \ln \coth(\varepsilon h)$$

Then we obtain:

$$X = A^N \prod_{i=1}^N e^{K_2 \sigma_i^z(t_{n+1}) \sigma_i^z(t_n)}$$

Z becomes:

$$Z = \sum_{\{\sigma^z(t_m)\}y} \cdots \sum_{\{\sigma^z(t_1)\}y} \prod_{n=0}^{M-1} \left\langle \sigma^z(t_{n+1})y \right|.$$

$$\cdot e^{-\varepsilon H_1} e^{-\varepsilon H_0} \left| \{\sigma^z(t_n)\}y \right\rangle =$$

$$= \sum_{\{\sigma^z(t_m)\}y} \cdots \sum_{\{\sigma^z(t_1)\}y} \prod_{n=0}^{M-1} e^{K_2 \sum_i \sigma_i^z(t_{n+1}) \sigma_i^z(t_n)}$$

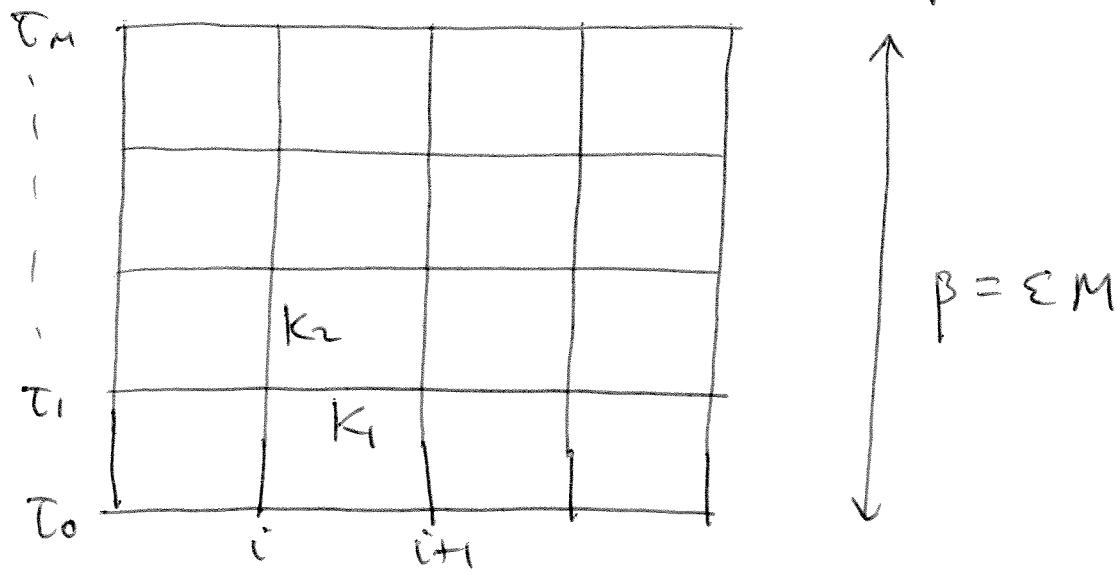
$$\cdot e^{K_1 \sum_{i,j} \sigma_i^z(t_n) \sigma_j^z(t_n)}$$

Here $K_1 = \varepsilon J$ and we neglected a constant prefactor A^N .

Thus we finally obtain :

$$Z = \sum_{\{\sigma^z(t_n)\}} \dots \sum_{\{\sigma^z(t_i)\}} e^{K_2 \sum_{n=0}^{m-1} \sum_i \sigma_i^z(t_{n+1}) \sigma_i^z(t_n)} \\ \cdot e^{K_1 \sum_{n=0}^{m-1} \sum_{\langle ij \rangle} \sigma_i^z(t_n) \sigma_j^z(t_n)}$$

This looks like a partition function of a classical Ising model on a $d+1$ -dimensional hypercubic lattice.



The extra dimension ~~is~~ corresponds to the temporal variable T . The extent of the system in the temporal direction is $\beta = \frac{1}{T}$
 \Rightarrow becomes infinite in the limit $T \rightarrow 0$.

Ising model is anisotropic - couplings in the spatial and temporal directions are different.

$$K_1 = \varepsilon \gamma \rightarrow 0 \quad \varepsilon \rightarrow 0$$

$$K_2 = \frac{1}{2} \ln \coth(\varepsilon h) \approx \frac{1}{2} \ln\left(\frac{1}{\varepsilon h}\right) \xrightarrow{\varepsilon \rightarrow 0} \infty$$

When $\varepsilon \rightarrow 0$ (or $\varepsilon \ll \frac{1}{h}, \frac{1}{\gamma}$):

$$K_1 = \varepsilon \gamma$$

$$K_2 \approx \frac{1}{2} \ln\left(\frac{1}{\varepsilon h}\right)$$

↓

$$\varepsilon h = e^{-2K_2}$$

$$\text{Now } K_1 = \frac{\gamma}{h} e^{-2K_2}$$

$$K_1 e^{2K_2} = \frac{\gamma}{h}$$

$$\text{Let } K_1 = \frac{\tilde{\gamma}_1}{\tilde{T}}, \quad K_2 = \frac{\tilde{\gamma}_2}{\tilde{T}}$$

\tilde{T} is the "temperature" in the $d+1$ -dimensional classical problem.

$$\text{Then } \frac{\tilde{\gamma}_1}{\tilde{T}} e^{2 \frac{\tilde{\gamma}_2}{\tilde{T}}} = \frac{\gamma}{h}$$

Thus $h \sim \tilde{T}$ - h behaves as temperature in the $d+1$ -dimensional model.

The variable t has dimensions of time. This is not an accident: turns out that quantum statistical mechanics may also be taught of as quantum dynamics in imaginary time.

To see this, recall path integral picture of quantum mechanics.

Time-dependent Schrödinger equation:

$$i \frac{\partial |\psi\rangle}{\partial t} = H |\psi\rangle$$

Solution can be written as:

$$|\psi(t_f)\rangle = e^{-iH(t_f-t_i)} |\psi(t_i)\rangle$$

Consider now wavefunction in the coordinate representation,

$$\psi(\vec{x}_f, t_f) = \langle \vec{x}_f | \psi(t_f) \rangle =$$

$$= \langle \vec{x}_f | e^{-iH(t_f-t_i)} | \psi(t_i) \rangle =$$

$$= \int d\vec{x}_i \langle \vec{x}_f | e^{-iH(t_f-t_i)} | \vec{x}_i \rangle \langle \vec{x}_i | \psi(t_i) \rangle =$$

$$= \int d\vec{x}_i U(\vec{x}_f, t_f; \vec{x}_i, t_i) \psi(x_i, t_i)$$

$$U(\vec{x}_f, t_f, \vec{x}_i, t_i) = \langle \vec{x}_f | e^{-iH(t_f-t_i)} | \vec{x}_i \rangle -$$

~~the~~ evolution operator in coordinate representation.

Let $t = t_f - t_i$.

Calculate $\langle \vec{x}_f | e^{-iHt} | \vec{x}_i \rangle$

Let $H = \frac{P^2}{2m} + V = T + V$, V -potential energy.

T and V don't commute: $[T, V] \neq 0$.

As before, deal with this problem using Trotter decomposition.

Divide t into M steps:

$\varepsilon = \frac{t}{M}$ - infinitesimal time interval.

~~$$e^{-iHt} = e^{-iH\varepsilon} \underbrace{\dots}_{M \text{ times}} e^{-iH\varepsilon}$$~~

$$e^{-i(T+V)\varepsilon} = e^{-i\varepsilon T} e^{-i\varepsilon V} \quad \text{up to terms } O(\varepsilon^2)$$

Then we obtain:

$$\langle \vec{x}_f | e^{-iHt} | \vec{x}_i \rangle = \int \prod_{n=1}^{M-1} d\vec{x}_n \langle \vec{x}_f | e^{-i\varepsilon H} | \vec{x}_{M-1} \rangle$$

$$\langle \vec{x}_{M-1} | e^{-i\varepsilon H} | \vec{x}_{M-2} \rangle \dots \langle \vec{x}_1 | e^{-i\varepsilon H} | \vec{x}_i \rangle$$

Call $\vec{x}_i = \vec{x}_0$, $\vec{x}_f = \vec{x}_M$

Consider a general factor in the above product:

$$\langle \vec{x}_{n+1} | e^{-i\varepsilon H} | \vec{x}_n \rangle = \langle \vec{x}_{n+1} | e^{-i\varepsilon T} e^{-i\varepsilon V} | \vec{x}_n \rangle =$$

$$= \langle \vec{x}_{n+1} | e^{-i\varepsilon T} | \vec{x}_n \rangle e^{-i\varepsilon V(\vec{x}_n)}$$

$$\langle \vec{x}_{n+1} | e^{-i\varepsilon T} | \vec{x}_n \rangle = \langle \vec{x}_{n+1} | e^{-i\varepsilon \frac{p^2}{2m}} | \vec{x}_n \rangle =$$

$$= \int d\vec{p} \langle \vec{x}_{n+1} | \vec{p} \rangle e^{-i\varepsilon \frac{p^2}{2m}} \langle \vec{p} | \vec{x}_n \rangle = *$$

$$\langle \vec{x} | \vec{p} \rangle = \frac{1}{(2\pi)^{3/2}} e^{i\vec{p} \cdot \vec{x}}$$

$$* = \int \frac{d\vec{p}}{(2\pi)^3} e^{-i\varepsilon \frac{p^2}{2m}} e^{i\vec{p} \cdot (\vec{x}_{n+1} - \vec{x}_n)} =$$

$$= \left(\frac{m}{m\varepsilon} \right)^{3/2} e^{i\frac{m}{2\varepsilon} (\vec{x}_{n+1} - \vec{x}_n)^2}$$

From we obtain:

$$\langle \vec{x}_f | e^{-iHt} | \vec{x}_i \rangle = \prod_{n=1}^N \langle \vec{x}_n | e^{-i\varepsilon_n t} | \vec{x}_n \rangle$$

We obtain:

$$\langle \vec{x}_f | e^{-iHt} | \vec{x}_i \rangle = \left(\frac{m}{m\epsilon} \right)^{\frac{3M}{2}} \int_{\vec{x}_i}^{\vec{x}_f} d\vec{x}_n \cdot e^{-i\epsilon \sum_{n=1}^{M-1} \left[\frac{m}{2} \left(\frac{\vec{x}_{n+1} - \vec{x}_n}{\epsilon} \right)^2 - V(\vec{x}_n) \right]}$$

Taking the limit $\epsilon \rightarrow 0$ we obtain:

$$\langle \vec{x}_f | e^{-iHt} | \vec{x}_i \rangle = \int_{\vec{x}(0)=\vec{x}_i}^{\vec{x}(t)=\vec{x}_f} D\vec{x} e^{i \int_0^t L[\vec{x}(t')] dt'}$$

$$L[\vec{x}] = \frac{m\dot{\vec{x}}^2}{2} - V(\vec{x}) \quad \text{-classical lagrangian.}$$

$$S[\vec{x}] = \int_0^t (L[\vec{x}(t')]) dt' \quad \text{-action.}$$

$$\langle \vec{x}_f | e^{-iHt} | \vec{x}_i \rangle = \int D\vec{x} e^{i S[\vec{x}]}$$

Evaluating this path integral in the saddle-point approximation gives classical mechanics.

Now imagine we want to evaluate the partition function for the same problem - particle in an external potential.

$$Z = \text{Tr } e^{-\beta H} = \int d\vec{x} \langle \vec{x} | e^{-\beta H} | \vec{x} \rangle$$

Go back to the evolution operator and set:

$$it = \beta, \quad it' = T - \text{imaginary time}.$$

$$\text{Set } \bar{X}_f = \bar{x}_c = \bar{x}$$

$$\frac{dx}{dt'} = i \cdot \frac{dx}{dt}$$

Then we obtain:

$$Z = \int D\bar{x} e^{-S[\bar{x}]}$$

$$S[\bar{x}] = \int_0^\beta dt \left[\frac{m}{2} \left(\frac{d\bar{x}}{dt} \right)^2 + V(\bar{x}) \right]$$

$S[\bar{x}]$ is called imaginary time action.

$$\bar{x}(0) = \bar{x}(\beta)$$

~~partition function~~

This evaluation of the partition function in a quantum statistical mechanics problem is equivalent to evaluation of a ~~backward~~ probability amplitude for a particle to come back to the same point after time $\beta = \frac{1}{T}$.

This statistical mechanics is related to real-time quantum dynamics by the $it = T$ transformation (Wick rotation).

Quantum statistical mechanics = dynamics in imaginary time.

Go back to the transverse field Ising model:

$$Z = \sum_{\{\sigma^z(t_m)\}} \dots \sum_{\{\sigma^z(t_{m'})\}} e^{-S[\sigma^z]}$$

$$S[\sigma^z] = -K_2 \sum_{n=0}^{M-1} \sum_i \sigma_i^z(t_{n+1}) \sigma_i^z(t_n) -$$

$$-K_1 \sum_{n=0}^{M-1} \sum_{i < j} \sigma_i^z(t_n) \sigma_j^z(t_n) \quad -\text{imaginary-time}$$

action for the transverse-field Ising model.

To obtain continuum φ^n theory use Hubbard-Stratonovich transformation:

$$S[\varphi] = \sum_{ij} \varphi_i K_{ij}^{-1} \varphi_j + \frac{1}{2} \sum_i \varphi_i^2 + \frac{n}{4!} \sum_i \varphi_i^4 \dots$$

Tacoy continuum limit ~~and~~ we obtain:

$$S[\varphi] = \int_0^\beta dt \int d^d x \left[\frac{1}{2} (\partial_t \varphi)^2 + \frac{1}{2} (\vec{\nabla} \varphi)^2 + \right. \\ \left. + \frac{1}{2} \varphi^2 + \frac{n}{4!} \varphi^4 \right]$$

Thus we get φ^n theory in $D=d+1$ space-time dimension.

RG developed for classical φ^n theory carries over without any change.

Upper critical dimension is $d+1=4 \Rightarrow d=3$.

Can set up 3- ε expansion.

Spatial fluctuations are characterized by average correlation length ξ . In this problem we also need to introduce correlation time T . At a quantum phase transition both diverge, however in general they may diverge differently:

$$T = \xi^z, \quad z \text{ is dynamical critical exponent.}$$

In the case of the transverse field Ising model $z=1$ space-time and space enter on equal footing (action has relativistic form). In general $z \neq 1$.

A somewhat nontrivial problem here is how to translate correlation function ~~of~~ of the classical Ising model in $d+1$ -dimensional space-time into time-dependent correlation function of the d -dimensional transverse field Ising model.

Consider imaginary time correlation function,

$$G_{ij}(\tau) = T \langle \sigma_i^z(\tau) \sigma_j^z(0) \rangle$$

$$\sigma_i^z(\tau) = e^{H\tau} \sigma_i^z e^{-H\tau}$$

—imaginary time Heisenberg representation.

T_τ is the time-ordering operator, puts operators with later times to the left.

Since we have periodic b.e. in imaginary time:

$$G_{ij}(\tau + \beta) = G_{ij}(\tau)$$

Then we have $G_{ij}(\tau) = \frac{1}{\beta} \sum_{w_n} G_{ij}(iw_n) e^{-iw_n \tau}$

Here $w_n = \frac{\pi n}{\beta}$ - Matsubara frequencies.