

Density for harmonic oscillation:

$$\rho(x, x', \beta) = \left(\frac{m\omega_0}{\pi\hbar} \tanh \frac{\beta\hbar\omega_0}{2} \right)^{1/2} e^{-\frac{m\omega_0}{4\hbar} ((x+x') \tanh \frac{\beta\hbar}{2}\omega_0 + (x-x') \coth \frac{\beta\hbar}{2}\omega_0)}$$

Any potential:

$$\begin{aligned} \rho(x, x', \beta) &= \sum_m^{\prime} \psi_m^+(x) e^{-\beta H} \psi_m(x') \\ &= \sum_m^{\prime} \psi_m^+(x) e^{-\beta H/2} e^{-\beta H/2} \psi_m(x') \\ &= \sum_m^{\prime} \psi_m^+(x) e^{-\beta H/2} \int dx'' \delta(x' - x'') \\ &\quad e^{-\beta H/2} \psi_m(x'') \\ &= \sum_m^{\prime} \psi_m^+(x) e^{-\beta H/2} \int dx'' \\ &\quad \sum_m^{\prime} \psi_m(x') \psi_m^+(x'') e^{-\beta H/2} \psi_m(x'') \end{aligned}$$

$$\begin{aligned}
 &= \int dx'' \left(\sum_m^+ \psi_m(x) e^{-\beta H/2} \psi_m(x'') \right) \\
 &\quad \left(\sum_m^- \psi_m^+(x'') e^{-\beta H/2} \psi_m(x') \right) \\
 &= \int dx'' \rho(x, x''; \beta/2) \rho(x'', x'; \beta/2)
 \end{aligned}$$

Note the change in temperature:

$$\beta \rightarrow \beta/2 \quad \text{or} \quad T \rightarrow 2T.$$

This is of course true for the free particle Hamiltonian, but it is also true when

$$H = -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + U(x)$$

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Some potential.

The significance of the temperature change is that it reduces the relative importance of the potential $U =$ it goes down when T goes up.

We now divide the interval (x_0, x_p) into P equal parts:

$$\rho(x_0, x_p; \beta) = \int \dots \int dx_1 \dots dx_{p-1}$$

$$\rho(x_0, x_1; \beta/P) \cdots \rho(x_{p-1}, x_p; \beta/P)$$

P is called the Frobenius number.

If P is large enough:

$$\rho(x_p, x_{p+1}; \beta/P) \quad \text{Fermi energy.}$$

$$= \sum_m \psi_m^+(x_p) e^{-\frac{\beta}{P}(T + U(x))} \psi_m(x_{p+1})$$

$$\simeq \sum_m \psi_m^+(x_p) e^{-\frac{\beta}{P} T} \psi_m(x_{p+1})$$

$$e^{-\frac{\beta}{2P} (\mathcal{U}(x_p) + \mathcal{U}(x_{p+1}))}$$

$$= \rho_0(x_p, x_{p+1}; \beta/P) e^{-\frac{\beta}{2P} (\mathcal{U}(x_p) + \mathcal{U}(x_{p+1}))}$$

Diagonal element:

$$\rho(x_0, x_p = x_0; \beta)$$

$$= \left(\frac{mP}{2\pi\beta\hbar^2} \right)^{P/2} \int \dots \int dx_1 \dots dx_{p-1} e^{-\beta(\mathcal{H}_{\text{ext}} + \mathcal{H}_{\text{int}})}$$

where we have defined

$$\mathcal{H}_{\text{ext}} = \frac{1}{P} \sum_{p=0}^{P-1} \mathcal{H}(x_p)$$

$$\mathcal{H}_{\text{int}} = \frac{A\pi}{\beta} \sum_{p=0}^{P-1} (x_p - x_{p+1})^2$$

$$A = \frac{mP}{2\beta\pi\hbar^2}$$

Remember that

$$\rho_0(x, x'; \beta) = \left(\frac{m}{2\pi\beta\hbar^2} \right)^{1/2} e^{-\frac{m}{2\beta\hbar^2}(x-x')^2}$$

$U_{\text{ext}} + U_{\text{ring}}$ is the potential of a classical ring polymer! ($x_0 = x_p$).

(See Chandler et al., J. Chem. Phys. 74, 4078 (1981)).

Hence, we have transformed a quantum particle into a classical ring polymer.

Path integral Monte Carlo for
one particle

Quantum particle in external
potential $U(x) \rightarrow$ Ring potential

$$U_{\text{ext}} = \frac{1}{p} \sum_{p=0}^{p-1} U(x_p)$$

Internal potential of rigid polymer:

$$M_{int} = \frac{mP}{2\beta h^2} \sum_{p=0}^{P-1} (x_p - x_{p+1})^2$$

(A)

$$U = M_{int} + U_{ext}$$

(1)

Move $x \rightarrow x + \Delta x$

$\underbrace{\hspace{1cm}}$
↑

Same quantity added
to all x_p ; $x_p \rightarrow x_p + \Delta x$.

(2) move every x_p an extent Δx_p .

This is the new configuration. x'

(B)

$$\text{Calculate } U(x') - U(x) = \Delta U$$

(C) Metropolis step:

Draw random # ξ from flat distribution on unit interval.

If $\Delta u \leq 0$, $x \rightarrow x'$

If $\Delta u > 0$ and $\xi \leq e^{-\Delta u / \beta}$, $x \rightarrow x'$

If $\Delta u > 0$ and $\xi > e^{-\Delta u / \beta}$, $x \rightarrow x$

(unchanged).

① Return to ④.

$$\text{Mint}(x_p, x_{p+1}) = \underbrace{\frac{4\pi}{\beta}}_{\text{Spring constant.}} (x_p - x_{p+1})^2$$

Spring constant.

The spring constant is proportional to the Trotter number P .

The importance of the external potential:

$$\frac{1}{P} U(x_p)$$

decreases with increasing P.

Stiffer springs demand smaller mouth parts, while weaker external potential allows for larger mouth parts.

We combine the opposite tendencies by using a large S_x and smaller S_{xp} .

A way to do this:

Construct a new ring for each little step by using a narrow

Multivariate Gaussian distribution

$$p(x_0, \dots, x_{p-1}) \propto e^{-\frac{m_p}{2\beta_{\text{eff}}} \sum_{p=0}^{p-1} (x_p - \bar{x}_{p,\text{eff}})^2}$$

Move centre of mass of chain by
a large random step.

N particles that interact through
pair potential $U(|x_i - x_j|)$

Each particle is represented by a
 P -element ring.

Position of each element p in ring i is:

$$x_{i,p}$$

Diagonal elements of density matrix:

$$\rho(x_0, x_0, \beta) = A^{\frac{NP}{2}}$$

$$\int \dots \int dx_{1,1} \dots dx_{N,p-1}$$

$$e^{-A\pi \sum_{i=1}^N \sum_{p=0}^{P-1} (x_{i,p} - x_{i,p+1})^2}$$

$$e^{-\frac{\beta}{P} \sum_{i=1}^N \sum_{i>j} \sum_{p=0}^{P-1} M(|x_{i,p} - x_{j,p}|)}$$

Statistical mechanics

Critical slowing down.

"Most important source of difficulties
in the study of phase transitions."

New second order (continuous) phase
transitions, (critical points) time
"slows down".

Defining correlation time.

$$f_E(t-t') = \frac{\langle E(t)E(t') \rangle - \langle E \rangle^2}{\langle E^2 \rangle - \langle E \rangle^2}$$

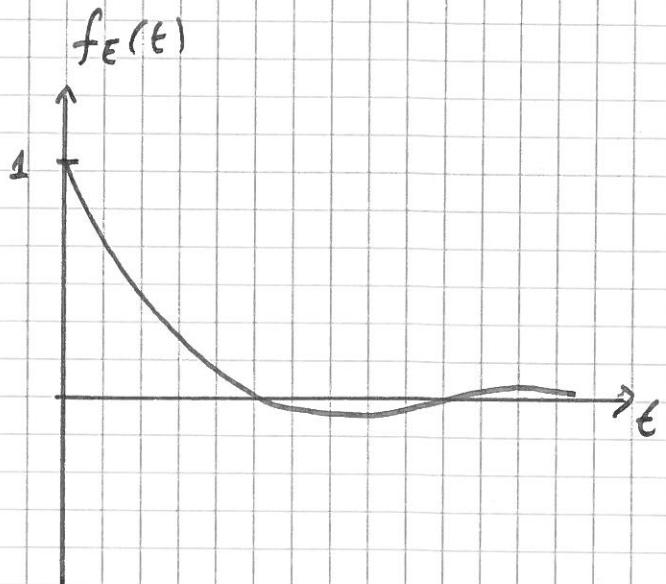


(Stationary ensemble)

Correlation function.

$$f_E(0) = 1$$

$$f_E(\infty) = 0$$



Correlation time:

$$\tau^2 = \frac{\int_0^\infty dt t^2 f_E(t)}{\int_0^\infty dt f_E(t)}$$

Correlation length:

$$g_0(r) = \frac{\langle \sigma(\vec{r} + \vec{r}) \sigma(\vec{r}) \rangle - \langle \sigma \rangle^2}{\langle \sigma^2 \rangle - \langle \sigma \rangle^2}$$

$r = 1\bar{r}1$, assuming isotropy.

Spins in a spin system.

Spatial correlation function.

Correlation length:

$$\xi^2 = \frac{\int_0^\infty dr r^2 g_0(r)}{\int_0^\infty dr g_0(r)}$$

Second order phase transition:

$$T \rightarrow T_c$$



Critical temperature.

$\xi \rightarrow \infty$ as $T \rightarrow T_c$:

$$\xi \propto |T - T_c|^{-\nu}$$

Correlation length exponent.

Likewise

335

$$\tau \rightarrow \infty \text{ as } T \rightarrow T_c$$

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Correlation time.

We have

$$\boxed{\tau \propto \xi^z}$$

dynamical critical exponent.

In a finite system of size L at $T=T_c$:

$$\boxed{\xi = L}$$

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This is the fundamental assumption behind finite size scaling analysis.

Hence, at $T = T_c$:

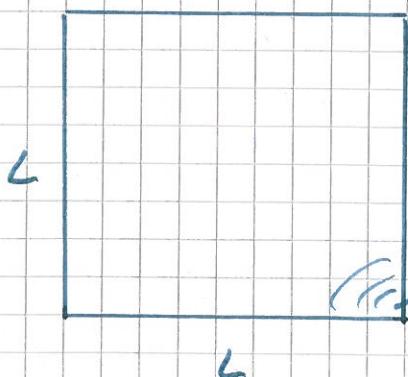
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$$\boxed{\tau(L) \propto L^z}$$

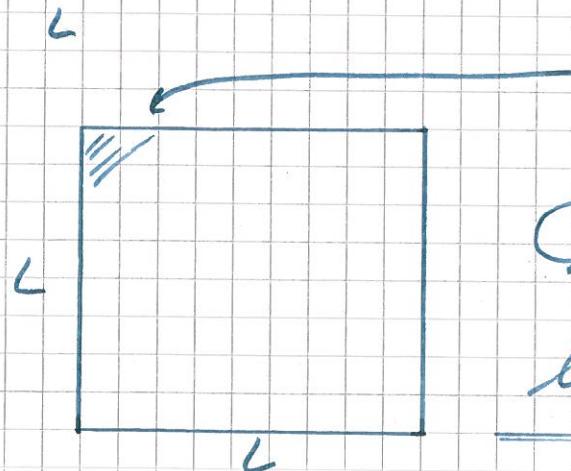
Away from criticality, correlation time typically behaves as

$$\tau \propto L^2$$

This is based on an assumption of information spreading in a diffusive way.



at $t=0$,
perturb. region here.



at $t = L^2$, full
effect here.

Diffusion:
length $\propto \sqrt{\text{time}}$

At criticality, $T = T_c$:

$$\tau \propto L^{\frac{z}{\beta}}$$

$z > 2$

This is critical slowing down.

The number of Monte Carlo sweeps needed to reach steady state grows very fast with system size.

Methods to fight critical slowing down:

* Jordan acceleration

* multigrid methods (based on renormalization group ideas)

* Cluster algorithms

(e.g. Swendsen - Wang).