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<u>Wednesday 880.05</u>

· On left board (for reference): "anharmonic oscillator"

$$\boxed{\hat{H}(\hat{p},\hat{x}) = :\hat{H}(\hat{p},\hat{x}): = \frac{\hat{p}^2}{2m} + V(\hat{x}) \overset{\text{example}}{=} \frac{\hat{p}^2}{2m} + \frac{1}{2}a\hat{x}^2 + \frac{1}{4}\lambda\hat{x}^4}$$

(note: this will look like $\phi^4$ function field theory examples, but very different since long-distance confining forces)

$Z(\beta)$

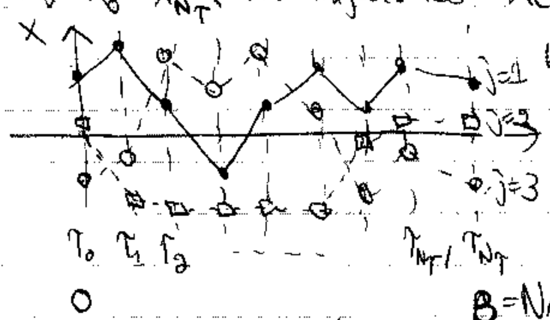
$$Z = \mathrm{Tr}\, e^{-\beta\hat{H}} = \int dx \langle x| e^{-\beta\hat{H}}|x\rangle$$

$$= \int dx \int_{x(0)=x}^{x(\beta)=x} \mathcal{D}(x(\tau))\, e^{-\frac{1}{\hbar}\int_0^\beta d\tau \left[\frac{m}{2}\left(\frac{dx(\tau)}{d\tau}\right)^2 + V(x(\tau))\right]}$$

$$= \int_{x(\beta)=x(0)} \mathcal{D}[x(\tau)]\, e^{-\frac{1}{\hbar}\int_0^\beta d\tau \left[\frac{m}{2}\left(\frac{dx(\tau)}{d\tau}\right)^2 + V(x(\tau))\right]} = \int_{x(\beta)=x(0)} \mathcal{D}[x(\tau)]\, e^{-S_E[x(\tau)]/\hbar}$$

$$\left[\int d^3x_1 \int d^3x_2 \int d^3x_3 \cdots \int d^3x_{N_\tau}\right] = \int_{-\infty}^{\infty} \prod_{k=1}^{N_\tau} dx_k \left(\frac{m}{2\pi\epsilon\hbar}\right)^{\frac{3N_\tau}{2}} e^{-\frac{\epsilon}{\hbar}\sum_{i=1}^{N_\tau}\left[\frac{m}{2}\left(\frac{x_i - x_{i-1}}{\epsilon}\right)^2 + V(x_{i-1})\right]}$$

where $\beta = N_\tau \epsilon$ (Monday $N_\tau$ was $M$ but notation is too confusing) and $x_0 = x_{N_\tau}$. The trajectories $x(\tau) \to \{x(\tau_i)\}_j$ begin and end at same $x$




· Recall that the $\frac{\hat{p}^2}{2m}$ went away after

$$\int \frac{d^3p_n}{(2\pi)^3} e^{-\epsilon\frac{p_n^2}{2m} + i p_n(x_n - x_{n-1})} = \left(\frac{m}{2\pi\epsilon}\right)^{3/2} e^{-\epsilon\frac{m}{2}\left(\frac{x_n - x_{n-1}}{\epsilon}\right)^2}$$

can be absorbed in defining $Z$ or hidden in $\mathcal{D}$.

Note: Using $\tau \in [-\beta/2, \beta/2]$ <u>instead of $\tau \in [0,\beta]$ is often simpler.</u>

· Plan for today:

1. Quick comments on MATLAB PS#1
2. Recap of intro to stochastic evaluation of path integrals
3. Brief follow-ups to one-particle path integral
   - spectral decomposition, perturbation theory, correlation functions
4. Generalization to many-particle states — (anti) symmetrization
   - issues for numerical evaluation

Monday → 5. Intro to alternative based on coherent states and field operators

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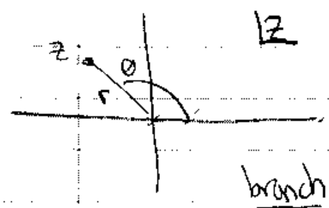
## MATLAB PS#2 Comments [any questions on diagrams?]

- Well executed solutions ~ we'll build on that when possible. (Eg. MATLAB code to illustrate SVM for PS#2.)

- Most (if not all) of you encountered an error evaluating logm(A) when A had real negative eigenvalue.
  "Principal matrix logarithm not defined for A with nonpositive real eigenvalues. A non-principal matrix log is returned."
  - Let's remember what is going on in complex plane

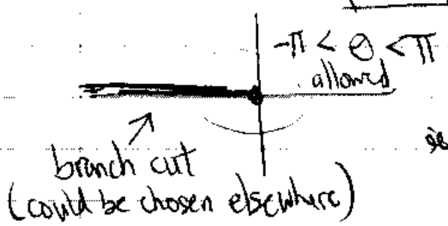



$\mathbb{Z}$ polar form $z = re^{i\theta}$

$$\Rightarrow \ln z = \ln r + \ln e^{i\theta} = \ln r + i\theta$$

branch point at $z=0$, multivalued as $\theta \to 0 \to 2\pi \to 4\pi \to$ ... keeps changing

So define principal logarithm by excluding negative real axis: $\Rightarrow$ single valued




- Not defined here for $\theta = \pi$ or $\theta = -\pi$ (although typically $-\pi < \theta \le \pi$ is used)
  ie is $\text{logm}(-1) = \ln^{0} 1 + i\pi$ or $-i\pi$ (chooses $+i\pi$)
  1x1 matrix

For a matrix, runs into this if eigenvalues lie on branch cut.

- MATLAB for loops

```
M = randn(5) + i*randn(5)
```

one way: `eye(5) + M + M*M/2 + M*M*M/6 + ...` (or `M^3/factorial(6)`)

another way:

```
sum = 0
for i = 0:10        ← or whatever
  sum = sum + M^i/factorial(i)      ← exclude ; to print each intermediate answer
end
disp(sum);          ← print ("display") final result
```

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- Recap & intro to stochastic evaluation of path integrals

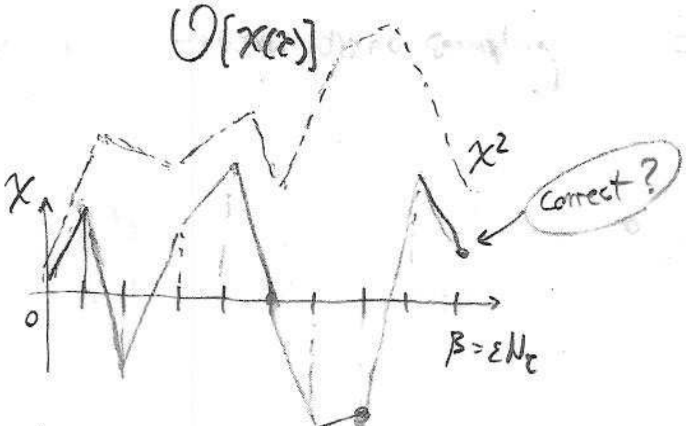
See Joaquin Drut notes.

Recap from Monday

(I) Numerical (in particular stochastic) methods are necessary to determine the properties of interacting many-body quantum systems, because pert. theory and saddle point approximations can fail (and they do in many interesting cases).

(II) Stochastic methods use the path integral formulation of QM. This means that expectation values are computed like so:

$$\langle \mathcal{O} \rangle = \frac{1}{Z} \int_{x(0)=x(\beta)} D[x(\tau)]\, e^{-S_E[x(\tau)]}\, \mathcal{O}[x(\tau)]$$




- Example: $\mathcal{O} = \frac{1}{\beta}\int_0^\beta x^2(\tau)\, d\tau$

(For each trajectory we compute $\frac{1}{\beta}\int_0^\beta x^2(\tau)\, d\tau$ and add it with weight $\frac{1}{Z}\exp\{-S_E[x(\tau)]\}$)

Get notation right!

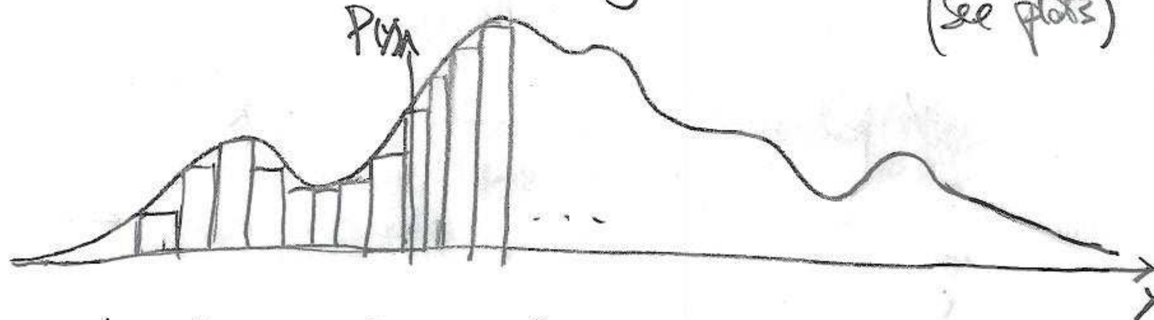
(III) Stochastic methods are based on the <u>central limit theorem</u>

Example: Consider $y$ distributed according to $\mathbb{P}(y)$

(see plots)

$\mathbb{P}(y) > 0$

$\int \mathbb{P}(y) dy = 1$




Drawing samples of $y$ according to $\mathbb{P}(y)$ and putting them in bins according to their value will eventually reproduce $\mathbb{P}(y)$ as a histogram.

Now consider $\langle \mathcal{O} \rangle = \int dy\, \mathcal{O}(y)\, \mathbb{P}(y)$ = "True mean"

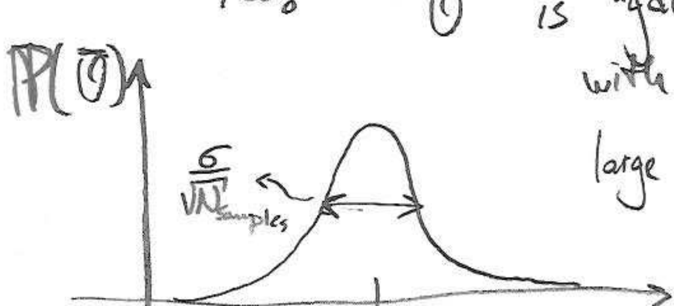
$\sigma^2 = \langle \mathcal{O}^2 \rangle - \langle \mathcal{O} \rangle^2$ = "True standard deviation" (squared)

Question: Can I approximate $\langle \mathcal{O} \rangle \simeq \frac{1}{N_{samples}} \sum_{n=1}^{N_{samples}} \mathcal{O}(y_n) \equiv \bar{\mathcal{O}}$

taking $y$ distributed according to $\mathbb{P}(y)$?

(see plots)

CLT: Yes! $\bar{\mathcal{O}}$ is "gaussianly distributed" around $\langle \mathcal{O} \rangle$ (True mean) with std deviation $\frac{\sigma}{\sqrt{N_{samples}}}$, in the limit of large $N_{samples}$.




$$\Rightarrow \langle \mathcal{O} \rangle \simeq \bar{\mathcal{O}} \pm \frac{\sigma}{\sqrt{N_{samples}}}$$

We don't know the true $\langle \mathcal{O} \rangle$, so this theorem tells us how to estimate it.

We also don't know the true $\sigma$, but we can estimate it as

$$\sigma \simeq \overline{\mathcal{O}^2} - \overline{\mathcal{O}}^2$$

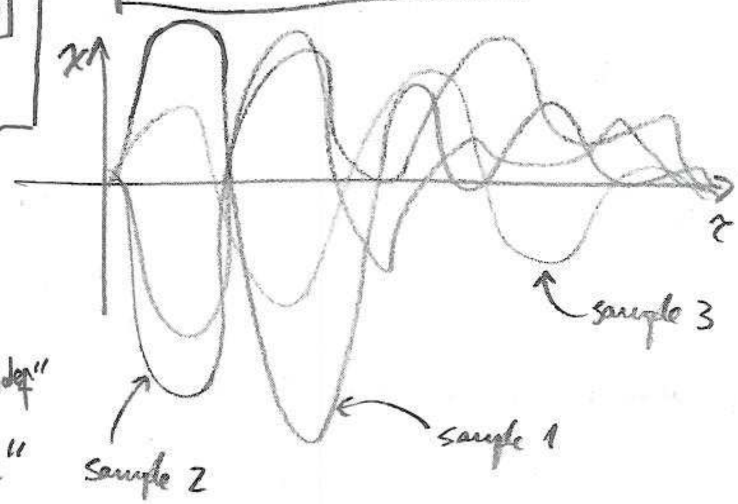
In QM, where $$\langle \mathcal{O} \rangle = \frac{1}{Z} \int \mathcal{D}[x(\tau)]\, e^{-S_E[x(\tau)]}\, \mathcal{O}[x(\tau)]$$

$$= \int \mathcal{D}[x(\tau)]\, \mathcal{O}[x(\tau)]\, \mathbb{P}[x(\tau)]$$

$$\boxed{\mathbb{P}[x(\tau)] = \frac{e^{-S_E[x(\tau)]}}{Z}}$$

We can estimate

$$\boxed{\langle \mathcal{O} \rangle \simeq \overline{\mathcal{O}} = \frac{1}{N_{\text{samples}}} \sum_{n=1}^{N_{\text{samples}}} \mathcal{O}[x_n(\tau)]}$$




Remember: This works only if $\mathbb{P}$ is well defined as a probability: $\mathbb{P}[x] \geq 0$ "positive semidef."

$\int \mathbb{P}[x]\, dx = 1$ "normalizable"

Main problem: How to generate configurations distributed according to $\mathbb{P}[x(\tau)]$. → Sampling strategies.

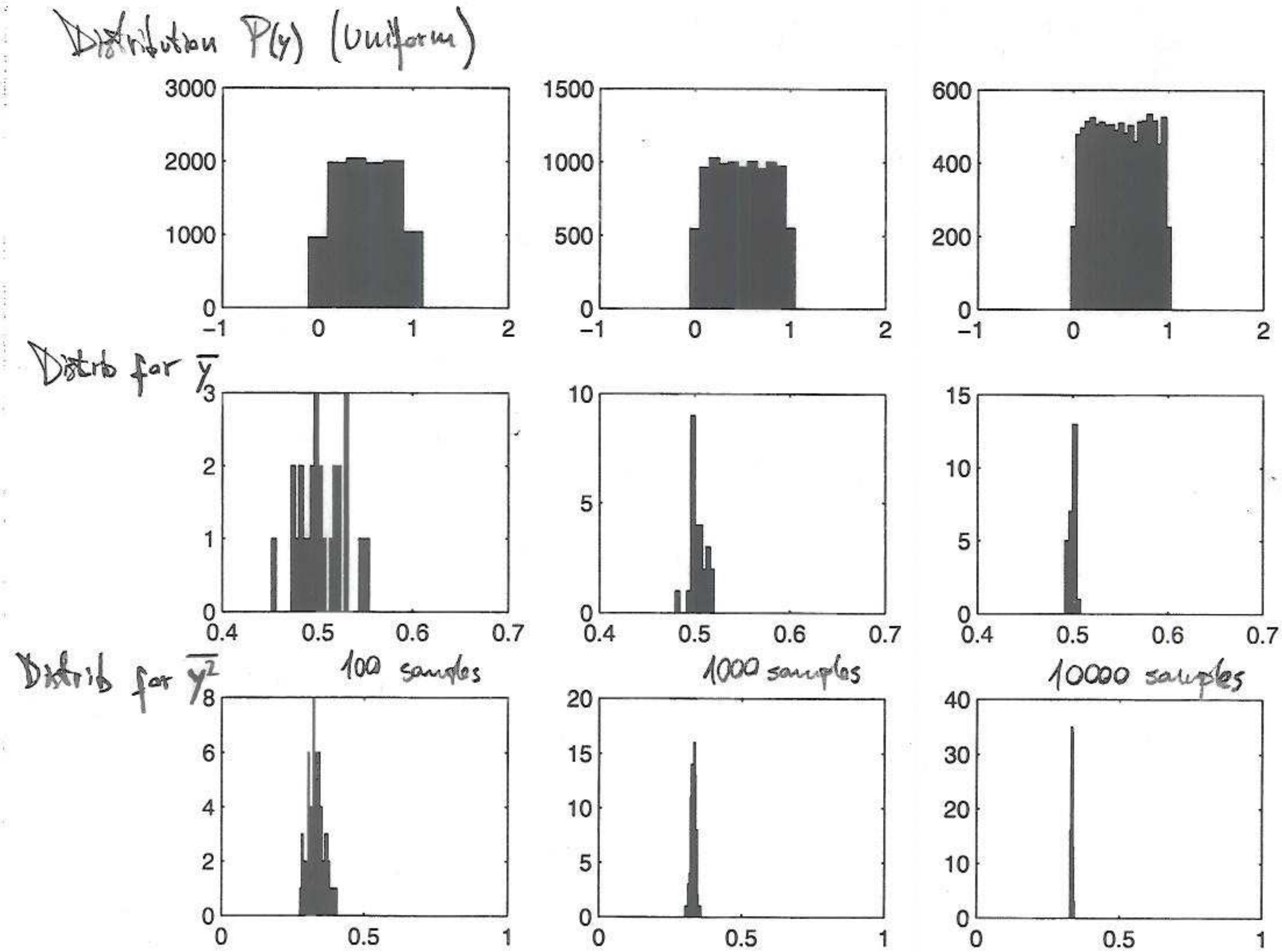
# IV) Sampling strategies

- Heat-bath
- Metropolis ⟵ typical for Ising model
- Molec. dynamics
- Hybrid

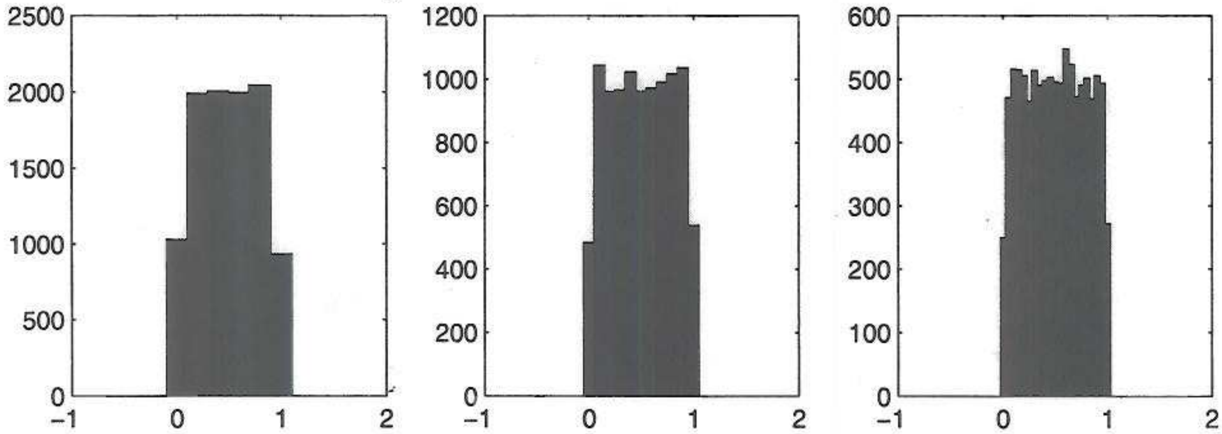
— Markov chain-based

All of them can generate good samples if used properly.

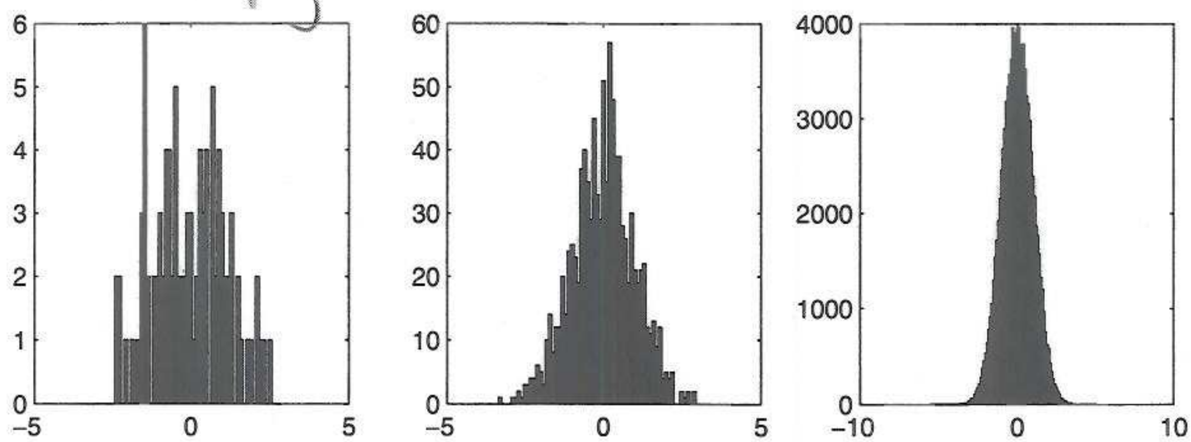
- Equilibrated
- Uncorrelated


Distribution P(y) (Uniform)
Distrib for $\overline{y}$
Distrib for $\overline{y^2}$
100 samples
1000 samples
10000 samples

Uniform distribution sampling (10000 samples, variable bin size).




Gaussian distrib. sampling




100 samples 1000 samples 10000 samples

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Followup comments on $Z$ for one particle...

- The "real time" version comes from $\tau \to it$ (or $t \to -i\tau$) so that

$$\boxed{U_E(x_f\tau_f;x_i\tau_i) = \langle x_f|e^{-\frac{\hat{H}}{\hbar}(\tau_f-\tau_i)}|x_i\rangle \longrightarrow U(x_f t_f;x_i t_i) = \langle x_f|e^{-i\frac{\hat{H}}{\hbar}(t_f-t_i)}|x_i\rangle}$$

[recall that $i\hbar\frac{\partial}{\partial t}\Psi(x,t) = \hat{H}\Psi(x,t) \Rightarrow \Psi(x,t_f) = e^{-i\hat{H}(t_f-t_i)/\hbar}\Psi(x,t_i)$ for any $x$]

What about the physics content? Do we lose anything going from $U$ to $U_E$?

- Consider eigenstates of $\hat{H}$: $\boxed{\hat{H}|\varphi_n\rangle = E_n|\varphi_n\rangle \text{ and } \langle x|\varphi_n\rangle = \varphi_n(x)}$

$$\Rightarrow U(x_f t_f;x_i t_i) = \sum_n \langle x_f|\varphi_n\rangle\langle\varphi_n|e^{-\frac{i\hat{H}}{\hbar}(t_f-t_i)}|x_i\rangle = \sum_n \varphi_n(x_f)\varphi_n^*(x_i)\,e^{-iE_n(t_f-t_i)/\hbar}$$

$$\Rightarrow U_E(x_f\tau_f;x_i\tau_i) = \sum_n \langle x_f|\varphi_n\rangle\langle\varphi_n|e^{-\frac{\hat{H}}{\hbar}(\tau_f-\tau_i)}|x_i\rangle = \sum_n \varphi_n(x_f)\varphi_n^*(x_i)\,e^{-E_n(\tau_f-\tau_i)/\hbar}$$

"Spectral representation" shows same content. [that doesn't mean there can't be subtle complications in relating real and imaginary path integrals!]

Note: $\tau_i = 0$, $\tau_f = \beta$ and $\beta \to \infty$ limit! ← if $E_1 - E_0 > 0$

$$\boxed{U_E(x_f\beta;x_i 0) \xrightarrow[\beta\to\infty]{} \varphi_0(x_f)\varphi_0^*(x_i)\,e^{-\beta E_0/\hbar}}$$ so $$\boxed{-\frac{1}{\beta}\ln U_E \xrightarrow{\beta\to\infty} E_0 - \cancel{\frac{1}{\beta}\ln(\varphi_0(x_f)\varphi_0^*(x_i))}^{\,0}}$$

independent of $x_f, x_i$ so true for $Z$

in particular ⇒ $\boxed{-\frac{1}{\beta}\ln Z \xrightarrow[\beta\to\infty]{} E_0}$ project ground state by $\beta\to\infty$ limit

- Note that $\tau \to it$ means $$\boxed{S_E[x(\tau)] \to -S[x(t)] = -\int_{t_i}^{t_f} dt\left[\frac{1}{2}m\left(\frac{dx}{dt}\right)^2 - V(x(t))\right]}$$

usual action functional

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- How does perturbation theory work in this case? [Note: See Zinn-Justin ch. 2 for more general $U_E$ instead of $Z$]

- In the model partition function $\boxed{Z \Rightarrow Z[j] = \int d\xi\, e^{-(a\xi^2 + \frac{\lambda}{4}\xi^4) + j\xi}}$ and used $\partial_j$: $e^{\frac{\lambda}{4}\xi^4} \Rightarrow e^{-\frac{\lambda}{4}(\frac{\partial}{\partial j})^4}[\quad]$

- Here: analog is to add $f(\tau)$ to $H$ in path integral:

$$\boxed{H(p,x) \to H(p,x;t) = \frac{1}{2m}p^2 + V(x) - x f(\tau)}$$

- This is a time dependent driving (external) force $\Rightarrow$ like a $j$ at each time
  - Also $f(0) = f(\beta)$.

- For concreteness, take $V(x) = \frac{1}{2}ax^2 + \frac{\lambda}{4}x^4$ and think about perturbation $\frac{\lambda}{4}x^4$ about harmonic oscillator $\frac{p^2}{2m} + \frac{1}{2}ax^2$.

In discrete version of $Z[f]$, $f(\tau) \to \{f(\tau_i)\} \equiv \{f_i\}$, $i = 1, \dots, N_\tau$

$\hbar = 1$

$$\Rightarrow \boxed{Z[f] = C\int_{-\infty}^{\infty}\prod_k dx_k\; e^{-\epsilon\sum_{i=1}^{N_\tau}\left[\frac{m}{2}\left(\frac{x_i - x_{i-1}}{\epsilon}\right)^2 + \frac{1}{2}ax_i^2 + \frac{\lambda}{4}x_i^4 - x_i f_i\right]}}$$ (like having a different $j$ at each time step)

So $\frac{1}{\epsilon}\frac{\partial Z[f]}{\partial f_j} = C\int\prod_k dx_k\; x_j\, e^{-\epsilon\sum_i[\qquad]}$ ← one of these has $i = j$

$f(\tau_k) \to$ a particular $j$

so $\boxed{\langle x_{j_1} x_{j_2}\rangle = \frac{1}{Z}\left(\frac{1}{\epsilon}\frac{\partial}{\partial f_{j_1}}\frac{1}{\epsilon}\frac{\partial}{\partial f_{j_2}}\right)Z[f]\Big|_{f_j = 0}}$ "correlation function"

continuum limit $N_\tau \to \infty$ $\boxed{\langle x(\tau_1)x(\tau_2)\rangle = \frac{1}{Z}\left(\frac{\delta}{\delta f(\tau_1)}\frac{\delta}{\delta f(\tau_2)}\right)Z[f]\Big|_{f(\tau)=0}}$ generalizes $\langle\xi^2\rangle$ from model partition function

[Note $\langle x(\tau_1)x(\tau_2)\rangle = \langle T[\hat{x}(\tau_1)\hat{x}(\tau_2)]\rangle$ where $\hat{x}(\tau) = e^{\tau H}\hat{x}e^{-\tau H}$ ]

↖ "functional derivatives"

Check $\boxed{\frac{\delta}{\delta f(\tau)}\int d\tau'\, f(\tau')g(\tau') \underset{\text{discrete}}{=} \frac{1}{\epsilon}\frac{\delta}{\delta f_i}\sum_k \epsilon f_k g_k = g_i \overset{\text{continue}}{=} g(\tau)}$ ✓

↖ $\tau_i$ — so makes an integral go away!

* What if just $\boxed{\frac{\delta}{\delta f(\tau)}f(\tau')? \to \frac{1}{\epsilon}\frac{\delta}{\delta f_i}f_k = \frac{1}{\epsilon}\delta_{ik} \to \delta(\tau - \tau')}$

(Check that $\int\delta(\tau-\tau')d\tau' = 1$ translates $\to \sum_{k=1}^{N_\tau}\epsilon\left(\frac{1}{\epsilon}\delta_{ik}\right) = \sum_k \delta_{ik} = 1$ ✓ )

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Now we can also play the same game as before where we replace $\boxed{x_i^4 \longrightarrow \left(\frac{1}{\epsilon}\frac{\partial}{\partial f_i}\right)^4}$

so

$$\boxed{\begin{aligned} Z[f] &= e^{-\epsilon\sum_{i=1}^{N_\tau}\frac{\lambda}{4}\left(\frac{1}{\epsilon}\frac{\partial}{\partial f_i}\right)^4} C\int_{x_0=x_{N_\tau}} \prod_k dx_k\, e^{-\epsilon\sum_{i=1}\left[\frac{m}{2}\left(\frac{x_i-x_{i-1}}{\epsilon}\right)^2+\frac{1}{2}ax_i^2-x_if_i\right]} \\ \xrightarrow{\text{continuum}} &\ e^{-\int_0^\beta d\tau\frac{\lambda}{4}\left(\frac{\delta}{\delta f(\tau)}\right)^4} C\int_{x(\beta)=x(0)}\mathcal{D}x(t)\, e^{\underbrace{-\int_0^\beta d\tau\left[\frac{m}{2}\left(\frac{dx}{d\tau}\right)^2+\frac{1}{2}ax^2-xf(t)\right]}_{S_E}} \end{aligned}}$$

- The discrete form of the integral is a Gaussian form with matrices. If we look up the general result (see Zinn-Justin chap. 1 handout):

$$\boxed{I[J]\equiv\int_{-\infty}^{\infty}dy_1\cdots dy_n\, e^{-\frac{1}{2}y_iA_{ij}y_j+y_iJ_i} = (2\pi)^{n/2}[\det A]^{-1/2}e^{\frac{1}{2}J_iA^{-1}_{ik}J_k}}$$

If $J=0$, then $\boxed{I[0]=(2\pi)^{n/2}(\det A)^{-1/2}} \Rightarrow \boxed{I[J]=I[0]\,e^{\frac{1}{2}\underline{J}^T\underline{\underline{A}}^{-1}\underline{J}}}$

- If we know $I[0]$ from elsewhere, we are done. (We'll assume that here.)

- So what is $J_i$ and $y_i$ here? $y_i\to x_i$, $J_i\to f_i$
What is $A_{ij}$? It is the quadratic part: so match $x_iA_{ij}x_j$ to terms in the exponent with two $x_i$'s.

$$-\frac{1}{2}x_iA_{ij}x_j = -\frac{1}{2}\times(x_1\ x_2\ \cdots\ x_{N_\tau})\begin{pmatrix}A_{11} & A_{12} & A_{13} \\ A_{21} & A_{22} & A_{23} \\ & \vdots & \end{pmatrix}\begin{pmatrix}x_1\\x_2\\ \vdots \\ x_{N_\tau}\end{pmatrix} = -\frac{1}{2}\left(A_{11}x_1^2+A_{12}x_1x_2+A_{21}x_2x_1+A_{22}x_2^2+\ldots\right)$$

$$-\epsilon\sum_{i=1}^{N_\tau}\frac{1}{2}ax_i^2 = -\frac{1}{2}\epsilon a\left[x_1^2+x_2^2+x_3^2+\ldots\right] \Rightarrow (A_{ij})_{\text{this term}} = \epsilon a\delta_{ij} = \begin{pmatrix}\epsilon a & & 0\\ & \epsilon a & \\ 0 & & \epsilon a \\ & & & \ddots\end{pmatrix}$$

$$-\epsilon\sum_{i=1}^{N_\tau}\frac{m}{2}\left(\frac{x_i-x_{i-1}}{\epsilon}\right)^2 = -\frac{1}{2}\frac{\epsilon m}{\epsilon^2}\left[(x_1-x_0)^2+(x_2-x_1)^2+(x_3-x_2)^2\right] = -\frac{1}{2}\frac{m}{\epsilon}\left[x_1^2-x_1x_0-x_0x_1+x_0^2+x_2^2-x_1x_2 -x_2x_1+x_1^2+x_3^2-x_3x_2-x_2x_3+x_2^2+\ldots\right]$$

$$\Rightarrow A_{11}=\frac{m}{\epsilon}\cdot 2+\epsilon a,\ A_{12}=-\frac{m}{\epsilon},\ A_{21}=-\frac{m}{\epsilon},\ A_{22}=\frac{m}{\epsilon}\cdot 2+\epsilon a,\ \ldots$$

$A_{10}=A_{1N_\tau}=-1=A_{N_\tau 1}$

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note the boundary conditions

or

$$\underline{A} = \frac{m}{\epsilon}\begin{pmatrix} 2 & -1 & 0 & 0 & -1 \\ -1 & 2 & -1 & \cdots & \\ 0 & -1 & 2 & \cdots & \\ 0 & & & \ddots & \\ -1 & & & & 2 \end{pmatrix} + \epsilon a \begin{pmatrix} 1 & & 0 \\ & 1 & \\ & \ddots & \\ 0 & & 1 \end{pmatrix}$$

so we can construct $\underline{A}$ explicitly in the discrete representation.
Then we have

$$\boxed{Z[f] = e^{-\epsilon \sum_i \frac{\lambda}{4}\left(\frac{1}{\epsilon}\frac{\partial}{\partial f_i}\right)^4} Z_0\, e^{\frac{1}{2} f_i A^{-1}_{ik} f_k}}$$

How do we understand the continuum version?

$$\int_{x(\beta)=x(0)} \mathcal{D}x(\tau)\, e^{-\int_0^\beta d\tau \left[\frac{m}{2}\left(\frac{dx}{d\tau}\right)^2 + \frac{1}{2}a x^2 - x f(\tau)\right]}$$

$$= \int \mathcal{D}x(\tau)\, e^{-\int_0^\beta d\tau \left\{ x\left[-\frac{m}{2}\frac{\partial^2}{\partial \tau^2} + \frac{1}{2}a\right] x - x f(\tau)\right\}}$$ (What about surface term? Remember boundary condition! $\Rightarrow$ surface term $= 0$)

$$= \int \mathcal{D}x(\tau)\, e^{-\int_0^\beta d\tau \int_0^\beta d\tau' \left\{ x(\tau)\underbrace{\left[-\frac{m}{2}\frac{\partial^2}{\partial\tau^2} + \frac{1}{2}a\right]\delta(\tau-\tau')}_{\frac{1}{2}A(\tau,\tau')} x(\tau') - x(\tau)\delta(\tau-\tau')f(\tau)\right\}}$$

$$= \underbrace{\int \mathcal{D}x(\tau)\, e^{-\int d\tau\, d\tau' \frac{1}{2}(x + fA^{-1})A(x + A^{-1}f)}}_{Z_0 \text{ (after shift of } x(\tau))}\; e^{+\frac{1}{2}\int_0^\beta d\tau \int_0^\beta d\tau' f(\tau) A^{-1}(\tau,\tau') f(\tau')}$$

$$\Rightarrow \boxed{Z[f] = e^{-\int_0^\beta d\tau \frac{\lambda}{4}\left[\frac{\delta}{\delta f(\tau)}\right]^4} Z_0\, e^{\frac{1}{2}\int_0^\beta d\tau \int_0^\beta d\tau' f(\tau) A^{-1}(\tau,\tau') f(\tau')}}$$

$\Rightarrow$ $A^{-1}(\tau,\tau')$ is the inverse of the differential operator $\left(-\frac{m}{2}\frac{\partial^2}{\partial\tau^2} + \frac{1}{2}a\right)\delta(\tau-\tau')$ or the Green's function, with the periodic boundary condition.

$\Rightarrow$ solution to $\left(-\frac{m}{2}\frac{\partial^2}{\partial\tau^2} + \frac{1}{2}a\right)A^{-1}(\tau) = \delta(\tau)$ with $A^{-1}(0) = A^{-1}(\beta)$

(we've used $A^{-1}(\tau,\tau') = A^{-1}(\tau-\tau')$.)

- Can you solve this? Next week we'll look at diagrams: $\underset{\tau_1}{\circ}\!\!-\!\!-\!\!-\!\!\underset{\tau_2}{\bullet}$

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How do we generalize to a few- or many-body system?

· For the quantum mechanics approach with Hamiltonian:

$$\boxed{\hat{H} = \sum_{i=1}^{N} \frac{(\hat{p}^{(i)})^2}{2m} + \frac{1}{2}\sum_{i,j=1}^{N} V(\hat{x}^{(i)} - \hat{x}^{(j)}) + (\text{3-body } V) + \ldots}$$

For N particles with identical masses

· Since they are identical particles, the partition function has to be a sum (trace) over a complete basis that has the correct symmetry (bosons - symmetric, fermions - antisymmetric).

· So going from $|x\rangle$ to $|x^{(1)}\rangle|x^{(2)}\rangle \cdots |x^{(N)}\rangle$ as a direct product seems problematic because it is not a definite symmetry

[Note: The indices written as superscripts here label the different particles. These are typically written as $x_1, x_2, \ldots x_N$. However, this directly clashes with our use of subscripts to indicate the x's at different time steps. Negele and Orland just use the same notation for both!]

(note, actually it does work if the states in the trace are symmetrized)

(note the curly bracket)

· So we use

$$\boxed{|x^{(1)}\ x^{(2)} \cdots x^{(N)}\} \equiv \frac{1}{\sqrt{N!}} \sum_{P} \zeta^{P} |x^{(P1)}\rangle |x^{(P2)}\rangle |x^{(P3)}\rangle \cdots |x^{(PN)}\rangle}$$

where the P means a permutation of the particles and $\zeta^P$ fixes up bosons ($\zeta = 1$, all $\zeta^P$ have same sign) and fermions ($\zeta = -1$, $\zeta^P = \pm 1$ as P is even/odd).

· The completeness relation is

$$\boxed{\frac{1}{N!} \sum_{x^{(1)} \ldots x^{(N)}} |x^{(1)} \cdots x^{(N)}\}\{x^{(1)} \cdots x^{(N)}| = \mathbb{1}}$$

· More generally, let $x \to \alpha$ represent a single-particle basis.

· This is not a normalized basis as yet, but that is not important for us.

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- At this stage, we simply need this basis to define the trace:

$$\boxed{\begin{aligned} Z &= \frac{1}{N!}\int \prod_{i=1}^{N \leftarrow \text{particle }\#} dx^{(i)} \{x^{(1)} \ldots x^{(N)} | e^{-\beta \hat{H}} | x^{(1)} \ldots x^{(N)}\} \\ &= \frac{1}{N!}\sum_{P} \xi^{P} \langle x^{(P1)} \ldots x^{(PN)} | e^{-\beta \hat{H}} | x^{(1)} \ldots x^{(N)} \rangle \end{aligned}}$$

Just as before, the "time interval" from 0 to $\beta$ can be broken into $N_\tau$ pieces and we insert complete sets of states.

- We can actually use either (anti)symmetrized or just product states. In the latter case, the final states of correct symmetry imposes the correct Fermi or Bose statistics.

- In the direct product case,

$$\boxed{Z = \frac{1}{N!}\sum_{P}\xi^{P} \int_{\substack{x^{(1)}(\beta) = x^{(P1)}(0) \\ \vdots \\ x^{(N)}(\beta) = x^{(PN)}(0)}} \mathcal{D}[x^{(1)}(\tau)] \cdots \mathcal{D}[x^{(N)}(\tau)]\, e^{-\int_0^\beta d\tau \left[\sum_{i=1}^{N}\left(\frac{dx^{(i)}(\tau)}{d\tau}\right)^2 + \frac{1}{2}\sum_{i \neq j} V(x_i(\tau) - x_j(\tau))\right]}}$$

- When we simulate fermions with this form, $e^{-\beta H}$ filters out the lowest state of any symmetry ⇒ but the lowest symmetric will be lower than the antisymmetric ⇒ noise growing exponentially before projecting on antisymmetric states.
- Alternative is to project at each $\epsilon$ step:

$$\boxed{\begin{aligned} \{x^{(1)} \ldots x^{(N)} | e^{-\epsilon H} | y^{(1)} \ldots y^{(N)}\} &= \left(\frac{m}{2\pi\epsilon}\right)^{N/2} \sum_{P} (-1)^{P} e^{-\frac{m}{2\epsilon}\sum_i (x_{Pi} - y_i)^2 - \frac{\epsilon}{2}\sum_{i \neq j} V(y_i - y_j)} \\ &= \left(\frac{m}{2\pi\epsilon}\right)^{N/2} \operatorname{Det} M \, e^{-\frac{m}{2\epsilon}\sum_i (x_i - y_i)^2 - \frac{\epsilon}{2}\sum_{i \neq j} V(y_i - y_j)} \end{aligned}}$$

with $\boxed{M_{ij} = e^{-\frac{m}{2\epsilon}\left[(x_j - y_i)^2 - (x_i - y_i)^2\right]}}$ but Det M has minus signs! More later on why this is bad.

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Instead of continuing with this basis, we are going to switch to a path integral over fields, by considering a different complete set of states to use, which are built from the occupation number basis.

- This gives rise to Hamiltonians written in terms of creation and destruction operators, $a^\dagger_\alpha$, $a_\alpha$
- Then the states we want are eigenstates of these (instead of $\hat{p}, \hat{x}$ eigen states)
  $\Rightarrow$ coherent states

- So let's do a bit of 2nd quantized formalism!