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Wednesday 880.05

Handouts:

- Problem set #9.
- Print out of MATLAB codes for stochastic calculations.

Guide to PS#9

- Follow ups to some practical MATLAB issues — random numbers, algorithms for exponentiation.
  - introduce some more MATLAB features we will use, like histograms and displaying (printing to screen) variables.
  - address some questions like seeding of random numbers and how to create a normal distribution with any mean and width.
  - point of emphasis: "It matters how you do it!" In this case, how you calculate e^{A}. Issues are speed, accuracy, scaling, failure for some types of matrix.
- SVM demo program → mostly for cultural enrichment.
- Playing with the code in todays other handout → Metropolis example. Prototype we'll build on for stochastic calculations.

MATLAB stuff for next Tuesday

* • Discrete and continuum calculations of propagators (problems 4 and 5) step by step.

Today:

1st half
- Follow-up and recap to items from Monday.
- Extension to functional integral over fields.

2nd half
- Stochastic evaluation — Metropolis et al.

on board

Warm-up functional derivatives $\frac{\delta}{\delta j(x)}\frac{\delta}{\delta j(y)} e^{-\int [a\varphi(x)^2 + j(x)\varphi(x)]dx} = \varphi(y)\varphi(x)e^{-\int \ldots dx}$

$$\frac{\delta}{\delta f(x)}\int g(y)(f(y))^4 h(y)\,dy = \lim_{\Delta x \to 0} \frac{1}{\Delta x_i}\frac{\partial}{\partial f_i}\sum_j g_j f_j^4 h_j \Delta x_j$$
$$= 4\, g(x)(f(x))^3 h(x)$$

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Feynman rules for N=1 system, $H(p,x;\tau) = \frac{p^2}{2m} + V(x) - x f(\tau)$

Continuum version

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

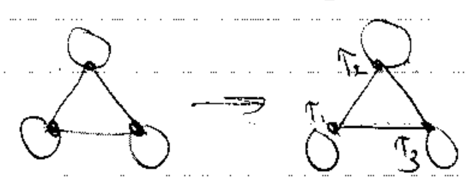
$$= \int \mathcal{D}x(\tau)\, e^{-\int_0^\beta d\tau \left[\frac{m}{2}\left(\frac{dx}{d\tau}\right)^2 + \frac{a}{2}x^2 - x f(\tau)\right]}$$

$x(\beta) = x(0)$ ← boundary condition on trajectories

calculate discrete and continuum versions in PS#2

Rules for $\log Z[f]/Z_0$ at order λ^n

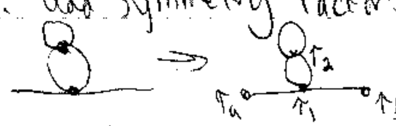
1. draw all connected diagrams with n "vertices" •
   (can you predict how many lines? $\Rightarrow (4\times n)/2 = 2n$ ← two ends to lines)
   # lines out ← will be important
2. label each vertex with a different τ variable
3. assign $(-\frac{\lambda}{4}\cdot 4!)$ for each vertex
4. assign $A^{-1}(\tau,\tau')$ for every line connecting τ and τ' vertices.
5. integrate each τ variable from 0 to βħ
6. apply a symmetry factor as in the model partition function

Try 

$$(-6\lambda)^3\underbrace{\left[\left(\frac{1}{2}\right)^3\cdot 1\cdot\frac{1}{3!}\right]}_{\text{symmetry factor}}\int_0^{\beta\hbar} d\tau_1 d\tau_2 d\tau_3\, A^{-1}(\tau_2,\tau_2)\, A^{-1}(\tau_1,\tau_1)\, A^{-1}(\tau_3,\tau_3)\, A^{-1}(\tau_1,\tau_2)\, A^{-1}(\tau_2,\tau_3)\, A^{-1}(\tau_3,\tau_1)$$

Rules for $\langle x(\tau_a)\, x(\tau_b)\rangle$ at order λ^n

1. draw all connected diagrams with two external points and n vertices
2. label each vertex with a τ variable and the external points with τ_a, τ_b
3. $(-\frac{\lambda}{4})\cdot 4!$ for each vertex
4. $A^{-1}(\tau,\tau')$ for lines connecting τ and τ' vertices.
5. integrate each internal τ variable from 0 to βħ
6. add symmetry factor.



$$(-6\lambda)^2\left(\frac{1}{2}\cdot\frac{1}{2}\cdot 1\right)\int_0^{\beta} d\tau_1 d\tau_2\, A^{-1}(\tau_a,\tau_1)\, A^{-1}(\tau_1,\tau_b)\, A^{-1}(\tau_1,\tau_2)\, A^{-1}(\tau_2,\tau_1)\, A^{-1}(\tau_2,\tau_2)$$

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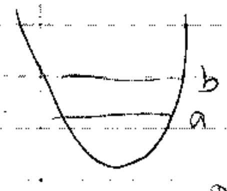
- For many particles, either symmetrized basis or number basis.
  $\Rightarrow$ both are in use in "real-life" physics calculations.

- Quick recap of symmetrized states.



Suppose two level and 3 particles (bosons)
Hilbert space is $|a \text{ or } b\rangle \otimes |a \text{ or } b\rangle \otimes |a \text{ or } b\rangle$
particle: 1 2 3

What are the symmetrized possibilities for wave functions?

$|aaa\rangle$,
$|bbb\rangle$
if normalized $\frac{1}{\sqrt{3}}\left(|aab\rangle + |aba\rangle + |baa\rangle\right)$
$\frac{1}{\sqrt{3}}\left(|abb\rangle + |bab\rangle + |bba\rangle\right)$

eigenstates of $S = \frac{1}{N!}\sum_P P = \frac{1}{6}(P_{123} + P_{132} + \ldots)$

mixing up by any permutation of the states of the 3 particles.

- We designate the coordinate representation states as:
$$|x^{(1)}\, x^{(2)} \cdots x^{(N)}\} = \frac{1}{\sqrt{N!}}\sum_P \xi^P |x^{(P1)}\rangle \cdots |x^{(PN)}\rangle$$

which is a complete set, so when evaluating $\mathrm{tr}\, e^{-\beta\hat{H}}$ we can do the usual splitting into $e^{-\epsilon\hat{H}} = :e^{-\epsilon\hat{H}}: + O(\epsilon^2)$

So what do we get? $\Rightarrow$ jump to 91ab to show

NOT N_T, but $N =$ # of particles

$$\{x^{(1)} \cdots x^{(N)}| :e^{-\epsilon\hat{H}}: |y^{(1)} \cdots y^{(N)}\} = \left(\frac{m}{2\pi\epsilon}\right)^{3N/2} \mathrm{Det}\, M\, e^{-\frac{m}{2\epsilon}\sum_{i=1}^{N}(x^{(i)}-y^{(i)})^2 - \frac{\epsilon}{2}\sum_{i\neq j}^{N} V(y^{(i)}-y^{(j)})}$$

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Alternative to inserting $|x^{(1)} \cdots x^{(N)}\}$ states is to insert coherent states built on $|n_1 n_2 \cdots n_\infty\rangle$ states

$$\underset{a}{\uparrow}\ \underset{b}{\uparrow}\ \underset{c}{\uparrow}$$

$\Rightarrow$ complete and orthonormal. Use $a_k, a_k^\dagger$ to change numbers.

$$|n_1 \cdots n_\infty\rangle \equiv (a_1^\dagger)^{n_1} \cdots (a_\alpha^\dagger)^{n_\alpha}|0\rangle$$

$$a_k^\dagger a_k |n_1 \cdots n_\infty\rangle = n_k |n_1 \cdots n_\infty\rangle$$

0, 1 fermions
0, 1, 2, … bosons

$$\hat{H} = \sum_{\alpha\beta} a_\alpha^\dagger \langle\alpha|T|\beta\rangle a_\beta + \frac{1}{2}\sum_{\alpha\beta\gamma\delta} a_\alpha^\dagger a_\beta^\dagger \langle\alpha\beta|V|\gamma\delta\rangle a_\delta a_\gamma + \ldots$$

· Now $|\alpha\rangle$ states unspecified here. Could be hydrogen wf's, harmonic oscillators, $\vec{k}$ states.

- We know the "wave function" in x space is $|\alpha\rangle = \int dx\, |x\rangle\langle x|\alpha\rangle$ (insert 1)
$= \int dx\, \varphi_\alpha(x)|x\rangle$

We can do this with the operators as well

$$\sum_\alpha \varphi_\alpha(x)\, a_\alpha = \hat{\psi}(x) \qquad \sum_\alpha a_\alpha^\dagger \varphi_\alpha^*(x) = \hat{\psi}^\dagger(x)$$

weighted sum → wave function $\Rightarrow$ "field operators"

$\hat{\psi}^\dagger(x)$ creates and $\hat{\psi}(x)$ destroys a particle at x. Spin: $\hat{\psi}(\vec{x}) \to \hat{\psi}_\alpha(\vec{x})$

$$\hat{H} \to \int d^3x\, \hat{\psi}_\alpha^\dagger(\vec{x})\left(-\frac{\nabla^2}{2m}\right)\hat{\psi}_\alpha(\vec{x}) + \int d^3x\, d^3x'\, \hat{\psi}_\alpha^\dagger(\vec{x})\hat{\psi}_\beta^\dagger(\vec{x}')V(\vec{x}-\vec{x}')\hat{\psi}_\beta(\vec{x}')\hat{\psi}_\alpha(\vec{x})$$

$$\xrightarrow{V(\vec{x}-\vec{x}') = \lambda\delta(\vec{x}-\vec{x}')} \int d^3x\, \hat{\psi}_\alpha^\dagger(x)\hat{\psi}_\beta^\dagger(\vec{x})\hat{\psi}_\beta(\vec{x})\hat{\psi}_\alpha(\vec{x})$$

looks like what we're been doing!

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Revisit coherent states and then continue with functional integral

- Some more on how to interpret bosonic coherent states. (From Negele + Orland, problem 1.5).

- What is the wave function of a (classical) pendulum? Answer: a coherent state!

- Consider a (1 dof) harmonic oscillator:

$$\hat{H} = \tfrac{1}{2}\hat{p}^2 + \tfrac{1}{2}\omega^2\hat{x}^2 = \hbar\omega\left(a^\dagger a + \tfrac{1}{2}\right) \quad (\overset{\text{mass}}{m}=1 \text{ here})$$

$$\Rightarrow \hat{x} = \left(\frac{\hbar}{2\omega}\right)^{1/2}(a^\dagger + a) \qquad \hat{p} = i\left(\frac{\hbar\omega}{2}\right)^{1/2}(a^\dagger - a)$$

- We can look at the coherent state

In our earlier discussion ϕ was called z complex!

$$|\phi\rangle = e^{a^\dagger\phi}|0\rangle = \sum_n \frac{\phi^n}{\sqrt{n!}}|n\rangle \xrightarrow[\text{derive and solve equation.}]{\text{coordinate space}} \langle x|\phi\rangle = \phi(x) = C e^{-\left[\left(\frac{\omega}{2\hbar}\right)^{1/2}x - \phi\right]^2}$$

ϕ labels both the wavefunction and the value. Confusing!

This is Heisenberg rep. Schrödinger time dependent wf is

claim: $$|\phi_{sch}(x,t)|^2 = \sqrt{\frac{\omega}{\pi\hbar}}\, e^{-2\left[\sqrt{\frac{\omega}{2\hbar}}x - |\phi|\cos\omega t\right]^2}$$

This is the same as a "minimum uncertainty wave packet". [Solution to S-eqn with $\Delta x \Delta p$ minimum]

- We can calculate $\langle\hat{x}\rangle = \left(\frac{2\hbar}{\omega}\right)^{1/2}|\phi|\cos\omega t$, $\langle\hat{p}\rangle = (2\hbar\omega)^{1/2}|\phi|\sin\omega t$ and $\langle\hat{H}\rangle = \frac{1}{2}(\langle\hat{p}\rangle^2 + \omega^2\langle\hat{x}^2\rangle) = \hbar\omega(|\phi|^2 + 1/2)$

so $\langle\hat{x}\rangle$ and $\langle\hat{p}\rangle$ satisfy in coherent state the classical equations of motion.

- amplitude is proportional to $|\phi|$!

- $|\phi\rangle$ mixes all $|n\rangle$'s. Most probable has $n = |\phi|^2$ and $E_n = \hbar\omega(n + 1/2) = \hbar\omega(|\phi|^2 + \tfrac{1}{2}) = \langle H\rangle$