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Monday 880.05

Handout:
- PS#2 will be released on Tuesday.

Follow-ups:
- The rand and randn functions in MATLAB can be given a random seed by the statement: "randn('seed', 12345)" where 12345 is an example of an integer seed. Using randn('state',sum(100*clock)); will initial to a different state every time. (See PS#2)
- Calculating expm in MATLAB: in PS#2 we'll compare 3 methods.

Recap from last time:

① functional derivatives $\frac{1}{\epsilon}\frac{\partial}{\partial f_i} \xrightarrow{\epsilon\to 0} \frac{\delta}{\delta f(\tau)}$ [Recall $N_\tau \epsilon = \beta$]

- follow-up comments from "Aside: Functionals and Functional Derivatives" on next pages

② Perturbation theory by extracting interaction from integral:

$$Z[f] = e^{-\int_0^\beta d\tau' \frac{\lambda}{4}\left(\frac{\delta}{\delta f(\tau')}\right)^4} C \int_{x(\beta)=x(0)} \mathcal{D}x(\tau)\, e^{-\underbrace{\int_0^\beta d\tau \left[\frac{m}{2}\left(\frac{dx}{d\tau}\right)^2 + \frac{1}{2}ax^2 - xf(\tau)\right]}_{S_f}}$$

- In the discrete version, this is a Gaussian integral

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

$Z_0 \leftarrow C'[\det A]^{-1/2}$

- $\underline{\underline{A}}$ is just a matrix with 1's and 2's and $\frac{m}{\epsilon}$, ϵa factors.

- Now ⇒ start with continuum version ⇒ (89) [we repeat and update these pages]
  - make it look like a matrix problem.

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note the bounding 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?

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

make it look like a matrix $x(\tau) \to x_i$ as a vector

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

↖ like diagonal matrix

(what about surface term? Remember boundary condition! ⇒ surface term = 0)

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

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

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

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

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

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

- Can you solve this? Next week we'll look at diagrams: $\underset{\tau}{\uparrow} \overset{A^{-1}}{\longrightarrow} \underset{\tau'}{\uparrow}$

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Try the first couple of orders of

$$\frac{Z[f]}{Z_0} = e^{-\int_0^\beta d\tau\, \frac{\lambda}{4}\left(\frac{\delta}{\delta f(\tau)}\right)^4} e^{\frac{1}{2}\int_0^\beta d\tau_1 \int_0^\beta d\tau_2\, f(\tau_1) A^{-1}(\tau_1,\tau_2) f(\tau_2)}$$

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

$$\left[1 + \frac{1}{2}\int f(1) A^{-1}(1,2) f(2) + \frac{1}{2!}\,\frac{1}{2}\int f(1) A^{-1}(1,2) f(2)\, \frac{1}{2}\int f(3) A^{-1}(3,4) f(4) + \dots\right]$$

· Assume $A^{-1}(1,2) = A^{-1}(2,1)$ here. Take $f \to 0$ at end.

$\left(\frac{1}{2}\right)^3$ symmetry factor

$$\int_0^\beta d\tau \left(-\frac{\lambda}{4}\right)\cdot\left(\frac{1}{2}\right)^3 4!\; A^{-1}(\tau,\tau) A^{-1}(\tau,\tau) \Rightarrow$$

$\leftarrow A^{-1}(\tau,\tau')\big|_{\tau'=\tau}$

$-\frac{\lambda}{4}4!$

order in which to hit f's. (permutations of 1,2,3,4)

added rule: Integrate τ from 0 to β.

$O(\lambda^2)$: connected and disconnected for $Z[f]/Z_0\big|_{f=0}$.

Consider

τ τ'

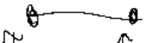
$$\int_0^\beta d\tau \int_0^\beta d\tau' \left(-\frac{\lambda}{4}4!\right)^2 \left[\left(\frac{1}{2}\right)^2 \frac{1}{2}\cdot\frac{1}{2}\right] A^{-1}(\tau,\tau) A^{-1}(\tau,\tau') A^{-1}(\tau',\tau) A^{-1}(\tau',\tau')$$

$$\int_0^\beta d\tau \int_0^\beta d\tau' \left(-\frac{\lambda}{4}4!\right)^2 \left[1\cdot\frac{1}{4!}\cdot\frac{1}{2}\right] \left(A^{-1}(\tau,\tau')\right)^4$$

and so on.

$$\langle X(\tau_a) X(\tau_b)\rangle = \frac{\left(\frac{\delta}{\delta f(\tau_a)}\frac{\delta}{\delta f(\tau_b)}\frac{Z[f]}{Z_0}\right)\Big|_{f=0}}{\left(Z[f]/f_0\right)\big|_{f=0}} = \frac{\delta}{\delta f(\tau_a)}\frac{\delta}{\delta f(\tau_b)}\,\frac{1}{2}\int f(1) A^{-1}(1,2) f(2) + \dots$$

$$= A^{-1}(\tau_a,\tau_b) + \dots$$



τ_a τ_b +

τ_a τ_b

$$\int_0^\beta d\tau \left(A^{-1}(\tau_a,\tau) A^{-1}(\tau,\tau) A^{-1}(\tau,\tau_b)\right)\left(-\frac{\lambda 4!}{4}\right)\left(\frac{1}{2}\cdot 1\cdot 1\right)$$

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

- For the quantum mechanics approach with Hamiltonian

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

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)

- So we use (note the curly bracket)

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

S or A symmetrizer or antisymmetrizer

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

- The completeness relation is

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

- 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:

$$\boxed{\begin{aligned} Z &= \frac{1}{N!}\int \prod_{i=1}^{N} dx^{(i)} \{x^{(1)}\cdots x^{(N)}| e^{-\beta \hat{H}} | x^{(1)} \cdots x^{(N)}\} \\ &= \frac{1}{N!}\sum_P \zeta^P \int \prod_{i=1}^{N} dx^{(i)} \langle x^{(P1)}\cdots x^{(PN)}| e^{-\beta\hat{H}} | x^{(1)}\cdots x^{(N)}\rangle \end{aligned}}$$

(i = particle #)

Just as before, the "time interval" from 0 to β can be broken into N_T 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,

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

When we simulate fermions with this form, $e^{-\beta H}$ filters out the lowest state of any symmetry $\Rightarrow$ but the lowest symmetric will be lower than the antisymmetric $\Rightarrow$ noise growing exponentially before projecting on antisymmetric states.

- Alternative is to project at each ϵ step:

$$\boxed{\begin{aligned} \{x^{(1)}\cdots x^{(N)}| e^{-\epsilon H} | y^{(1)}\cdots y^{(N)}\} &= \left(\frac{m}{2\pi\epsilon}\right)^{3N/2} \sum_P \zeta^P e^{-\frac{m}{2\epsilon}\sum_{i=1}^{N}(x^{(Pi)}-y^{(i)})^2 - \frac{\epsilon}{2}\sum_{i\neq j}^{N} V(y^{(i)}-y^{(j)})} \\ &= \left(\frac{m}{2\pi\epsilon}\right)^{3N/2} \operatorname{Det} M\, e^{-\frac{m}{2\epsilon}\sum_{i=1}^{N}(x^{(i)}-y^{(i)})^2 - \frac{\epsilon}{2}\sum_{i\neq j}^{N} V(y^{(i)}-y^{(j)})} \end{aligned}}$$

$(-)$

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

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- Let's fill in some detail on the calculation of $\{x^{(1)}\cdots x^{(N)}|:e^{-\epsilon \hat{H}}:|y^{(1)}\cdots y^{(N)}\}$.

- With $\boxed{\hat{H} = \sum_{i=1}^{N} \frac{\hat{p}^{(i)2}}{2m} + \frac{1}{2}\sum_{i\neq j=1}^{N} V(\hat{x}^{(i)}-\hat{x}^{(j)})}$, the normal ordering simply puts all of the $\hat{p}^{(i)2}$ terms to the left and the V terms to the right. So insert a complete set of $|p^{(1)}\ldots p^{(N)}\rangle$ states between these two terms.

- The V's pick up the sum of terms with $(y^{(i)}-y^{(j)})$ arguments

$$\boxed{e^{-\frac{\epsilon}{2}\sum_{i\neq j} V(y^{(i)}-y^{(j)})}}$$

with no permutations in the end. (we count up the same terms when we sum over i and j if permuted).

- If we didn't have the permutations to account for, then we would just get $\left(\frac{m}{2\pi\epsilon}\right)^{3/2} e^{-\epsilon\frac{m}{2}\left(\frac{x^{(i)}-y^{(i)}}{\epsilon}\right)^2}$ for each $i=1$ to $N \Rightarrow$ just a summation in the exponent.

- But the permutations mean that we have to sum over all ways of mixing up the x's.

$$\boxed{\begin{aligned}\Rightarrow &\sum_P (-1)^P e^{-\frac{m}{2\epsilon}\sum_{i=1}^{N}(x^{(P_i)}-y^{(i)})^2} \\ &= e^{-\frac{m}{2\epsilon}\sum_{i=1}^{N}(x^{(i)}-y^{(i)})^2} \sum_P (-1)^P e^{-\frac{m}{2\epsilon}\sum_{i=1}^{N}\left[(x^{(P_i)}-y^{(i)})^2-(x^{(i)}-y^{(i)})^2\right]}\end{aligned}}$$

- we're assuming now we have fermions, so $\zeta^P \to (-1)^P$.
- Try the N=2 case for the sum over P:

$$e^{-\frac{m}{2\epsilon}\left[(x^{(1)}-y^{(1)})^2-(x^{(1)}-y^{(1)})^2\right]}\, e^{-\frac{m}{2\epsilon}\left[(x^{(2)}-y^{(2)})^2-(x^{(2)}-y^{(2)})^2\right]} - e^{-\frac{m}{2\epsilon}\left[(x^{(2)}-y^{(1)})^2-(x^{(1)}-y^{(1)})^2\right]}\, e^{-\frac{m}{2\epsilon}\left[(x^{(1)}-y^{(2)})^2-(x^{(2)}-y^{(2)})^2\right]}$$

If we introduce $\boxed{M_{ij} = e^{-\frac{m}{2\epsilon}\left[(x^{(i)}-y^{(j)})^2-(x^{(j)}-y^{(j)})^2\right]}}$, then this is $\det M$.

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- Considering general N, we see that this does match the definition of a determinant: $\det M_{ij} = \sum_P (-1)^P \prod_{i=1}^{N} M_{i,P(i)}$.

[In Wikipedia, this is called the "Leibniz Formula" for the determinant. They write it for $n\times n$ matrix $\underline{A}$ as

$$\det(A) = \sum_{\underset{\substack{\uparrow \\ \text{permutation} \\ \text{group of } n \text{ objects}}}{\sigma \in S_n}} \underbrace{\operatorname{sgn}(\sigma)}_{(-1)^P} \prod_{i=1}^{n} A_{i,\sigma(i)}$$
]

So we get that

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

which, except for the determinant, looks like a simple generalization of the $N=1$ result.
- The problem is that there are minus signs in $\det M$ that cause problems, "the sign problem".

- A description of the problem is given in Chapter 8 of Negele and Orland.
  $\Rightarrow$ we will probably return to this later.

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Aside: Finding Symmetrized States in Practice

- Suppose we have a single-particle basis $|\alpha\rangle$ that we use to form a direct product (ie unsymmetrized) basis. How do we construct symmetrized or anti-symmetrized basis states in practice?
  - We're particularly interested in implementing this on a computer.

- So how do we represent our Hilbert space?
  - We can see how it goes with a two level system and two particles. a,b
  - We have four possibilities: $|a\rangle, |b\rangle \otimes |a\rangle, |b\rangle$ or $|a\,a\rangle$, $|a\,b\rangle$, $|b\,a\rangle$, $|b\,b\rangle$, which we label: 1, 2, 3, 4

- Now any operator can be represented as the 16 matrix elements O_{ij} with $(i,j) = 1,2,3,4$.

- Two such operators are $S = \frac{1}{N!}\sum_P P$ and $A = \frac{1}{N!}\sum_P (-1)^P P$
  - each permutation takes a basis state (an i) to exactly one other one.
- We can label the $N=2$ P's as P_{12} and P_{21}.
  - P_{12} is the identity $\Rightarrow$ state of particle $1 \to 1$, state of particle $2 \to 2$
  - P_{21} takes state of particle $2 \to 1$ and state of particle $1 \to 2$.

$$\Rightarrow P_{12} = \begin{pmatrix} 1 & & & 0 \\ & 1 & & \\ & & 1 & \\ 0 & & & 1 \end{pmatrix} \qquad P_{21} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}$$

$$\Rightarrow \underline{\underline{S}} = \tfrac{1}{2}(P_{12}+P_{21}) = \begin{pmatrix} 1 & & & \\ & \frac{1}{2} & \frac{1}{2} & \\ & \frac{1}{2} & \frac{1}{2} & \\ & & & 1 \end{pmatrix} \qquad \underline{\underline{A}} = \tfrac{1}{2}(P_{12}-P_{21}) = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & \frac{1}{2} & -\frac{1}{2} & 0 \\ 0 & -\frac{1}{2} & \frac{1}{2} & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}$$

- Now we simply diagonalize to find the symmetric and antisymmetric combinations!

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For this simple case, give it to MATLAB:

$$[V,D] = \mathrm{eig}(S) \Rightarrow V = \begin{pmatrix} 0 & 0 & 1 & 0 \\ \frac{-1}{\sqrt{2}} & 1/\sqrt{2} & 0 & 0 \\ 1/\sqrt{2} & 1/\sqrt{2} & 0 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} \quad D = \begin{pmatrix} 0 & & & \\ & 1 & & \\ & & 1 & \\ & & & 1 \end{pmatrix}$$

The symmetric states are those with eigenvalue $+1$ $(S|\psi\rangle = +1|\psi\rangle)$

Read off eigenvectors $\frac{1}{\sqrt{2}}(|ab\rangle + |ba\rangle)$, $|aa\rangle$, $|bb\rangle$.

For A:

$$[V,D] = \mathrm{eig}(A) \Rightarrow V = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & -\frac{1}{\sqrt{2}} & 0 & -1/\sqrt{2} \\ 0 & -1/\sqrt{2} & 0 & 1/\sqrt{2} \\ 0 & 0 & 1 & 0 \end{pmatrix} \quad D = \begin{pmatrix} 0 & & & \\ & 0 & & \\ & & 0 & \\ & & & 1 \end{pmatrix}$$

so one antisymmetric state: $\frac{1}{\sqrt{2}}(-|ab\rangle + |ba\rangle)$

(the normalization is undetermined up to a sign).

- These are exactly what you would have written down.
- Note that $\mathcal{H} = \mathcal{H}_S \oplus \mathcal{H}_A \Rightarrow$ they fill the Hilbert space.
- We can use these matrices to project onto the subspaces.

- The key point is that the generalization of this trivial example works just the same way.
  - But there will generally be states that are neither symmetric or antisymmetric.
  - Try a two-level system with 3 particles

1 aaa $\quad \binom{S}{A} = \frac{1}{3!}\left(P_{123} + P_{312} + P_{231} \pm P_{132} \pm P_{213} \pm P_{321}\right)$

2 aab

3 aba $\quad$ What is P_{123}? (identity)

4 abb

5 baa $\quad$ Try P_{321}

6 bab

7 bba $\quad aab \to baa$

8 bbb $\quad 2 \to 5$

$\Rightarrow (P_{321})_{2,5} = 1$

$$P_{321} = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \end{pmatrix}$$

$$P_{312} = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ & & & & 1 & & & 0 \\ & 1 & & & & & & 0 \\ & & & & & 1 & & 0 \\ & & 1 & & & & & 0 \\ & & & & & & 1 & 0 \\ & & & 1 & & & & 0 \\ & & & & & & & 1 \end{pmatrix}$$

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- Now we diagonalize and find 4 unit eigenvalues for S and 0 unit eigenvalues for A.
  - Why? (3 particle and 2 states for fermions means $\rightarrow$)
  - Where are the 4 "missing" states?
  - You should be able to write down the symmetric states by inspection, but it's nice to see this work out automagically with MATLAB.

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

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Aside: Functionals and Functional Derivatives

Ref.: Appendix B in the text by N. Nagaosa is the source for much of this presentation. Most field theory books have an introduction to functionals in their discussions of path integrals.

- First let's contrast functions and functionals:
  - i) function f: you give me a real number $x \in \mathbb{R}$ and I'll give you another real number:

$$\boxed{f: x \in \mathbb{R} \to f(x) \in \mathbb{R}}$$

  - generalizations include different domains and ranges (e.g. complex numbers)

  - ii) Functional F: rather than a single x, give me an entire function f(x) in an interval $\alpha \leq x \leq \beta$ and I'll give you a single real number back:

$$\boxed{F: f(x) \in \mathcal{H} \to F(\{f(x)\}) \equiv F[f] \equiv F[f(x)] \in \mathbb{R}}$$

  - we've indicated a variety of notations you might find in the literature
  - $\mathcal{H}$ signifies a Hilbert space
  - Note that when we use the notation $F[f(x)]$, there is no particular value of x involved; the entire function (in a relevant interval) is the input.

- It is useful (as usual) to imagine putting a functional on a computer.
  - We can represent a function f(x) as breaking up the interval $\alpha < x < \beta$ into a discrete mesh (set) of points $\{x_i\}$ with $\boxed{\alpha \equiv x_1 < x_2 < \cdots < x_{N-1} < x_N \equiv \beta}$

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- These numbers might be stored in an array, x[i], for example, with $i = 1$ to N.
- The function $f(x)$ is the set of N numbers $f_i \equiv f(x_i)$, (which we can also store as f[i].

$\Rightarrow$ A functional F is a function of the N numbers $\{f_i\}$ (not of the N numbers $\{x_i\}$!)

- A functional derivative tells us about what happens to the value of a functional when we let $f(x)$ become $f(x) + \delta f(x) \Rightarrow$ a slightly different function.
  - In the discrete version, we take $f_i \to f_i + \delta f_i$ (just like one takes $x_i \to x_i + \Delta x_i$ in an ordinary derivative).

- Suppose
$$\boxed{F[f(x)] = \int_a^b f(x)\, g(x)\, dx}$$
where $g(x)$ is some other fixed function of x.
  - Note that we integrate over x, so there is no free $x \Rightarrow F$ is not a function of x!
  - Let's make the simplest discrete version:

$$\boxed{F[f(x)] \to \sum_i f(x_i)\, g(x_i)\, \Delta x_i \equiv \sum_i f_i g_i \Delta x_i}$$

[we called this ϵ for breaking up the time interval]

Now let $f_i \to f_i + \delta f_i$:

$$\boxed{\begin{aligned}\delta F &= F(f_1 + \delta f_1, \ldots, f_N + \delta f_N) - F(f_1, \ldots, f_N)\\ &\doteq \sum_{i=1}^{N} \frac{\partial F(f_1, \ldots, f_N)}{\partial f_i}\, \delta f_i + O(\delta f_i^2)\end{aligned}}$$

- Notice the δ's instead of ∂'s.

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We define the functional derivative $\frac{\delta F}{\delta f(x)}$ as

$$\boxed{\frac{\delta F[f]}{\delta f(x)} = \lim_{\Delta x_i \to 0} \frac{1}{\Delta x_i} \frac{\partial F(f_1, \ldots, f_N)}{\partial f_i}}$$ where $f_i = f(x_i)$

this x matters!

- The x on the left corresponds to x_i on the right; in the limit that we make the mesh very fine.

$\Rightarrow$ We look how much the functional changes when we change the function at the i^{th} mesh point.

- Apply this definition to the example:

$$\frac{\delta F[f(x)]}{\delta f(x)} = \lim_{\Delta x_i \to 0} \frac{1}{\Delta x_i} \frac{\partial}{\partial f_i}\left(\sum_j f_j g_j \Delta x_j\right)$$

$$= \lim_{\Delta x_i \to 0} \frac{1}{\Delta x_i} \sum_j \delta_{ij} g_j \Delta x_j$$

$$= \lim_{\Delta x_i \to 0} \frac{1}{\cancel{\Delta x_i}} g_i \cancel{\Delta x_i} = \lim_{\Delta x_i \to 0} g_i = g(x)$$

- Rewriting this:

$$\boxed{\frac{\delta}{\delta f(x)} \int f(x') g(x') \, dx' = g(x)}$$

- note again that the "x" argument on the left is not a dummy argument.

- Special case: $F[f(x)] = \int f(x) \, dx$ (or $g(x) = 1$)

$$\Rightarrow \boxed{\frac{\delta}{\delta f(x)} \int f(x') \, dx' = 1}$$

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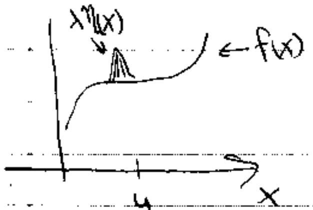
- For completeness, we present an alternative definition of the functional derivative that is more common in the literature.



As in the picture at the left we add a "bump" at y, which we take to be a delta function with strength λ, and see how much the functional changes!

$$\boxed{\frac{\delta F[f]}{\delta f(y)} = \lim_{\lambda\to 0} \frac{F[f(x)+\lambda\delta(x-y)] - F[f(x)]}{\lambda}}$$

Try it out on the example:

$$\frac{\delta}{\delta f(y)} \int f(x)\, g(x)\, dx = \lim_{\lambda\to 0} \frac{1}{\lambda}\left[\int [f(x)+\lambda\delta(x-y)]\, g(x)\, dx - \int f(x) g(x)\, dx\right]$$

$$= \lim_{\lambda\to 0} \frac{1}{\lambda}\lambda \int \delta(x-y) g(x)\, dx = g(y)$$

as before.

- Another special case, which can be used as the definition of the functional derivative as well: $g(x) = \delta(x-z)$

$$\Rightarrow \boxed{\frac{\delta}{\delta f(x)} \int f(x')\,\delta(x'-z)\, dx' = \frac{\delta f(z)}{\delta f(x)} = \delta(x-z)}$$

where the last equality is what we want.

- Note that this is the analog of $\frac{\partial}{\partial j_i} j = 1$, which we used repeatedly in the model problem.
  - Here, if we let $f(x) \Rightarrow f_i \Rightarrow j_i$, then the equivalent formula is

$$\boxed{\frac{\partial j_i}{\partial j_k} = \delta_{jk} \Rightarrow \frac{\delta j(x)}{\delta j(y)} = \delta(x-y)}$$

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Let's try another example we'll come across

$$\boxed{\begin{aligned}&\frac{\delta}{\delta f(x)}\int f(x_1)C(x_1,x_2)f(x_2)\,dx_1dx_2 \quad \text{with } C(x_2,x_1)=C(x_1,x_2)\\ &=\lim_{\Delta x_i\to 0}\frac{1}{\Delta x_i}\frac{\partial}{\partial f_i}\sum_{jk} f_j C_{jk} f_k \Delta x_j \Delta x_k\\ &=\lim_{\Delta x_i\to 0}\frac{1}{\Delta x_i}\sum_{jk}\left(\delta_{ij}C_{jk}f_k + f_j C_{jk}\delta_{ik}\right)\Delta x_j\Delta x_k\\ &=\lim_{\Delta x_i\to 0}\frac{2}{\Delta x_i}\sum_k C_{ik}f_k \Delta x_i \Delta x_k = 2\int C(x,x_2)f(x_2)\,dx_2\end{aligned}}$$

- More generally, if $C_n(x_1, x_2, \cdots, x_n)$ is totally symmetric under interchange of any two x_i, then

$$\boxed{\frac{\delta^n F[f]}{\delta f(x_1)\cdots\delta f(x_n)} = n!\, C_n(x_1,\dots,x_n)}$$

- We get the special case of $n=2$ by taking another functional derivative of the example up top.

- Exercise for the diligent reader: rederive these results using the alternative definition of a functional derivative.

- The familiar properties of ordinary (partial) derivatives, such as the product and chain rules, carry over to functional derivatives in a natural way.

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So consider

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

$$= \lim_{\Delta x_i \to 0} \frac{1}{\Delta x_i} \sum_j 3(f_j)^2 \delta_{ij} g_j \Delta x_j$$

$$= \lim_{\Delta x_i \to 0} 3(f_i)^3 g_i = 3(f(x))^2 g(x)$$

and so we have the chain rule:

$$\boxed{\frac{\delta}{\delta f(x)} \int g[f(y)]\, dy = g'[f(x)]}$$

where g' means to take the derivative of g with respect to f as if it were a partial derivative.

- Another form of the chain rule we'll use a lot is:

$$\boxed{\frac{\delta}{\delta j(y)} e^{-\int dx\,(a\varphi(x)^2 + j(x)\varphi(x))} = -\varphi(y)\, e^{-\int dx\,(a\varphi(x)^2 + j(x)\varphi(x))}}$$

- What if we have a function of $\vec{x}$ or $\vec{x}$ and t (or τ)?
  - We can combine $\vec{x}$ and t into a "four-vector" x^μ, so it is sufficient to consider an n-vector $\vec{x} = (x_1, \dots, x_n)$
  - Consider

$$F[f(\vec{x})] = \int_a^b f(\vec{x})\, g(\vec{x})\, dx_1 \cdots dx_n$$

$$\Rightarrow F[f(\vec{x})] \to \sum_{i_1, i_2, \dots, i_n} f_{i_1,\dots,i_n}\, g_{i_1,\dots,i_n}\, \Delta x_{i_1} \cdots \Delta x_{i_n}$$

where we now have n-dimensional arrays $x[i_1, \dots, i_n]$ and $f[i_1, \dots, i_n]$, where i_1 runs over the mesh for x_1, i_2 runs over the mesh for i_2, and so on.

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Let's take $n=2$ for clarity. Then our mesh is a two-dimensional grid and the function value is defined at each grid point (i,j) to be f_{ij}.

$$\Rightarrow F[f(\vec{x})] = \sum_{i,j} f_{ij}\, g_{ij}\, \Delta x_i\, \Delta y_j \qquad \text{with } \vec{x}=(x,y)$$

and the functional derivative

$$\boxed{\begin{aligned} \frac{\delta F[f]}{\delta f(\vec{x})} &= \lim_{\substack{\Delta x_i \to 0 \\ \Delta y_j \to 0}} \frac{1}{\Delta x_i \Delta y_j} \frac{\partial}{\partial f_{ij}} \sum_{i',j'} f_{i'j'}\, g_{i'j'}\, \Delta x_{i'}\, \Delta y_{j'} \\ &= \lim_{\substack{\Delta x_i \to 0 \\ \Delta y_j \to 0}} \frac{1}{\Delta x_i \Delta y_j} \sum_{i',j'} \delta_{ii'}\, \delta_{jj'}\, g_{i'j'}\, \Delta x_{i'}\, \Delta y_{j'} \\ &= \lim_{\substack{\Delta x_i \to 0 \\ \Delta y_j \to 0}} g_{ij} = g(\vec{x}) \end{aligned}}$$

Similarly,

$$\boxed{\frac{\delta f(\vec{x})}{\delta f(\vec{x}')} = \delta^n(\vec{x}-\vec{x}')}$$

and so on.

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· What if there is a derivative in the functional?

$$\frac{\delta}{\delta f(x)} \int \frac{df(x')}{dx'} g(x')\, dx' \;?$$

· We can do this several ways. Here are two:

i) partially integrate

$$\boxed{\begin{aligned} \frac{\delta}{\delta f(x)} \int \frac{df(x')}{dx'} g(x')\, dx' &= \frac{\delta}{\delta f(x)}\left[-\int f(x')\frac{dg(x')}{dx'}\, dx' + \text{surface term}\right] \\ &= -\frac{dg(x)}{dx} \quad \text{[if the surface term doesn't contribute]} \end{aligned}}$$

or

ii) discrete version:

$$\boxed{\begin{aligned} \frac{\delta}{\delta f(x)} \int \frac{df(x')}{dx'} g(x')\, dx' &= \lim_{\Delta x_i \to 0} \frac{1}{\Delta x_i}\frac{\partial}{\partial f_i}\sum_j \frac{f_{j+1}-f_j}{\cancel{\Delta x_j}}\, g_j \cancel{\Delta x_j} \\ &= \lim_{\Delta x_i \to 0} \frac{1}{\Delta x_i}\sum_j (\delta_{i,j+1} - \delta_{ij})\, g_j \\ &= \frac{1}{\Delta x_i}(g_{i-1} - g_i) = -\frac{dg}{dx} \end{aligned}}$$

· note that the possible surface terms in this case are left over from taking $\sum_j f_{j+1} g_j - \sum_j f_j g_j$ and changing dummy indices in the first.

· Ok, that's it for now ⇒ more later!

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In generalizing the path integral to many-particle systems (by which we mean more than a few particles to of order 10^{23} particles – effectively infinity) there are two choices:

i) Work with many particle states built from a basis for each particle ⇒ path integral is direct generalization of the example of one-particle quantum mechanics we've been discussing.

- main complication is dealing with properly symmetrized states (which means antisymmetrizing for fermions, which leads to sign problems.)

ii) Work with fields that operate in the space spanned by the number basis.

- Let's pursue this second option.

- We will give a very brief introduction now and backfill details as needed.

- We'll assume our building blocks for the basis is a set of orthonormal single-particle states labeled $|\alpha\rangle$
  - not necessary for most results that orthogonal, but easier.
  - Basis for Hilbert space $\mathcal{H}_1$:

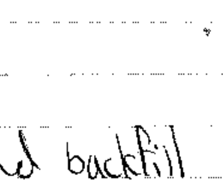
$$\sum_\alpha |\alpha\rangle\langle\alpha| = 1 \qquad \langle\alpha|\beta\rangle = \delta_{\alpha\beta}$$

- Then $\mathcal{H}_N$ is tensor product $\underbrace{\mathcal{H}_1^{(1)} \otimes \mathcal{H}_1^{(2)} \otimes \cdots \otimes \mathcal{H}_1^{(N)}}_{N \text{ copies}} \equiv \mathcal{H}_N$

and

means not symmetrized

$$|\alpha_1\alpha_2\ldots\alpha_N) \equiv |\alpha_1\rangle|\alpha_2\rangle\cdots|\alpha_N\rangle$$



- order of kets refers to particle 1, 2, ..

$|a\,c\,c\,b\,a\,c)$

Even outside of symmetrizing, this seems like a pain!

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Issues:

i) Different $\hat{H}$ for each N, or $\hat{H}$ refers specifically to N

ii) awkward at best for identical particles → permutations

iii) with one, two, three-body operators, only one, two, three states affected → rest are bystanders

e.g. $\hat{H} = \sum_i T_i + \sum_{i<j} V_{ij} + \ldots = \ldots + V_{12} + V_{13} + V_{23} + \ldots$

so $\langle \alpha_1' \alpha_2' \alpha_3' \alpha_4' \alpha_5' \alpha_6' \cdots | \hat{H} | \alpha_1\, \alpha_2\, \alpha_3\, \alpha_4\, \alpha_5\, \alpha_6 \cdots \rangle$

$= \langle \alpha_1' \alpha_2' | V_{12} | \alpha_1 \alpha_2 \rangle \delta_{\alpha_3' \alpha_3} \delta_{\alpha_4' \alpha_4} \cdots + \langle \alpha_1' \alpha_3' | V_{13} | \alpha_1 \alpha_3 \rangle \delta_{\alpha_2' \alpha_2} \delta_{\alpha_4' \alpha_4} + \ldots$

but they are identical!

Alternative: number basis

- Line up single-particle states in some order and just say how many in each state

$$|n_1\, n_2\, n_3\, \cdots\, n_\infty\rangle = |n_1\rangle |n_2\rangle \cdots |n_\infty\rangle$$

$$\begin{array}{ccc} \uparrow & \uparrow & \uparrow \\ a & b & c \\ 2 & 1 & 3 \end{array}$$

e.g. 2 1 3 in example

separate harmonic oscillator for each "mode"

- complete and orthonormal: $\langle n_1' n_2' \cdots n_\infty' | n_1 n_2 \cdots n_\infty \rangle = \delta_{n_1 n_1'} \cdots \delta_{n_\infty n_\infty'}$

$$\sum_{n_1, n_2, \cdots n_\infty} |n_1\, n_2 \cdots n_\infty\rangle \langle n_1\, n_2 \cdots n_\infty| = 1$$

- bosons $n_i = 0, 1, 2, \cdots \infty$
- fermions $n_i = 0, 1$

- Use raising and lowering operators to change n_i (creation and destruction)

$$[a_\alpha, a_\beta]_\mp = [a_\alpha^\dagger, a_\beta^\dagger]_\mp = 0 \qquad [a_\alpha, a_\beta^\dagger]_\mp = \delta_{\alpha\beta}$$

where $\mp \Rightarrow$ bosons $[a,b]_- = ab - ba$

fermions $[a,b]_+ = ab + ba \Rightarrow [a,a]_- = 0$

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$$a_k|n_k\rangle = (n_k)^{1/2}|n_k - 1\rangle$$ "destruction operator"

$$a_k^\dagger|n_k\rangle = (n_k+1)^{1/2}|n_{k+1}\rangle$$ "creation operator.

For fermions, $a_k|0\rangle = |1\rangle$ $\quad a_k|1\rangle = 0$
$a_k^\dagger|1\rangle = 0$ $\quad a|0\rangle = 0$

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

$a_k^\dagger a_k \underline{|n_1\cdots n_\infty\rangle = n_k|n_1\cdots} n_\infty\rangle \Rightarrow a_k^\dagger a_k \equiv n_k$ "number operator"

Key point: $\quad i\hbar\frac{\partial}{\partial t}|\Psi(t)\rangle = \hat{H}|\Psi(t)\rangle$

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

+ [what does 3-body look like?]

- The (anti) symmetrization is taken care of by the a's and $a^\dagger$'s.
- $\hat{H}$ doesn't reference N
- only the relevant orbitals play a role — don't worry about the other 10^{23}!

Can switch to x-representation $|\alpha\rangle = \int dx\, |x\rangle\langle x|\alpha\rangle = \int dx\, \varphi_\alpha(x)|x\rangle$
also with these operators:

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

"field operators" create and destroy at x.

- We'll use these a lot!

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<u>Boson</u> Coherent states: What are the eigenstates of $a_\alpha, a_\alpha^\dagger$?

- Start with a one-level system (one dof.)

$$|n\rangle = \frac{(a^\dagger)^n}{\sqrt{n!}}|0\rangle \quad n=0,1,2,\ldots$$

$$a|n\rangle = \sqrt{n}|n-1\rangle \quad \text{and} \quad a^\dagger|n\rangle = \sqrt{n+1}\,|n+1\rangle$$

so not eigenstates of either.

- But now superpose the $|n\rangle$'s so that the factorials work out.
  - Let z be a complex number (<u>any</u> one — like x representation)

$$\Rightarrow |z\rangle = e^{a^\dagger z}|0\rangle = \left(1 + a^\dagger z + \tfrac{1}{2}(a^\dagger z)(a^\dagger z) + \ldots\right)|0\rangle$$

$$= \sum_{n=0}^{\infty} \frac{z^n}{\sqrt{n!}}|n\rangle$$

Then
$$a|z\rangle = a|0\rangle + a\frac{z}{\sqrt{1!}}|1\rangle + a\frac{z^2}{\sqrt{2!}}|2\rangle + a\frac{z^3}{\sqrt{3!}}|3\rangle + \ldots$$

$$= 0 + \frac{z}{\sqrt{1!}}\sqrt{1}\,|0\rangle + \frac{z^2}{\sqrt{2!}}\sqrt{2}\,|1\rangle + \frac{z^3}{\sqrt{3!}}\sqrt{3}\,|2\rangle + \ldots$$

$$= z\left(|0\rangle + \frac{z}{\sqrt{1!}}|1\rangle + \frac{z^2}{\sqrt{2!}}|2\rangle + \ldots\right)$$

$$= z|z\rangle \; ! \quad \text{eigenstate}$$

Further, $\langle z| = \langle 0|e^{z^* a} = \sum_{n=0}^{\infty} \langle n|\frac{z^{*n}}{\sqrt{n!}}$ and $\langle z|a^\dagger = \langle z|z^*$.

Now $\langle z|z'\rangle = e^{z^* z'}$ $\Rightarrow$ <u>not</u> orthogonal.

key $\Rightarrow$
$$\frac{\langle z|:A(a^\dagger,a):|z'\rangle}{\langle z|z'\rangle} = A(z^*,z')$$
just what we need!

- note $\langle 0|z\rangle = 1$, $|z=0\rangle = |n=0\rangle = |0\rangle$

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Claim: close relation is

$$\int \frac{dz\,dz^*}{2\pi i} e^{-z^* z} |z)\langle z| = 1$$

This means $z = x+iy$, $\int \frac{dx\,dy}{\pi}$ $\quad -\infty < x, y < +\infty$

Proof: Substitute $|z\rangle$, $\langle z|$ definitions:

$$\int \frac{dz\,dz^*}{2\pi i} e^{-z^* z} |z\rangle\langle z| \overset{z=re^{i\theta}}{=} \int \frac{dz\,dz^*}{2\pi i} \sum_{nm} \frac{z^n z^{*m}}{\sqrt{n!\,m!}} |n\rangle\langle m| e^{-z^* z}$$

$$= \sum_{mn} |n\rangle\langle m| \frac{1}{\sqrt{n!\,m!}} \int_0^\infty \frac{r\,dr}{\pi} \int_0^{2\pi} d\theta\, r^{n+m} e^{i(n-m)\theta} e^{-r^2}$$

$$= \sum_n |n\rangle\langle n| = 1.$$

- For fermions, $\Rightarrow$ grassmann numbers
  - More later. For now, works the same except no 2π.

In particular

$$\frac{\langle z| :A(a^\dagger, a): |z'\rangle}{\langle z|z'\rangle} = A(z^*, z)$$

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Coherent State Functional Integral: First Pass

- This discussion is based largely on Negele and Orland, chapters 1 and 2.

- We want to use the same procedure for evaluating the partition function (or, more generally, an evolution operator) by splitting the interval from 0 to β into little steps of size ϵ for which

$$\boxed{e^{\epsilon \hat{H}} = :e^{\epsilon \hat{H}}: + O(\epsilon^2)}$$

and we can insert intermediate states to evaluate $:e^{\epsilon \hat{H}}:$. Except now we want $\hat{H}$ to be expressed in 2nd quantized form: $a^\dagger$'s and a's.
  - normal ordering in this case will mean that a's appear to the right of $a^\dagger$'s.
  - It won't help to use the number basis in general, because we need the analog of $\langle p_n|\hat{H}(\hat{p},\hat{x})|x_n\rangle = H(p_n,x_n)\langle p_n|x_n\rangle \Rightarrow$ we need states that are eigenstates of the annihilation operators — these are the coherent states.

- The steps are the same as before, only now we have $\hat{H} \to \hat{H}(a_\alpha^\dagger, a_\alpha)$ (and we assume it is normal ordered $\Rightarrow$ $a^\dagger$'s to left, a's to right).
  - We break up $[0,\beta]$ into N_τ steps of width ϵ.

- The partition function we want to use now is the grand partition function $Z = \mathrm{Tr}\, e^{-\beta(\hat{H}-\mu\hat{N})}$ (note that coherent states do not have a definite number of particles, so we really need μ!).

- Our starting expression is (up to an overall constant)

$$Z = \mathrm{Tr}\, e^{-\beta(\hat{H}-\mu\hat{N})}$$

+ for bosons
− for fermions

$$= \int \frac{1}{c}\prod_\alpha d\phi_\alpha^* d\phi_\alpha\, e^{-\sum_\alpha \phi_\alpha^*\phi_\alpha} \langle \zeta\phi| e^{-\beta(\hat{H}-\mu\hat{N})}|\phi\rangle$$

$\frac{d(\mathrm{Re}\,\phi_\alpha)\, d(\mathrm{Im}\,\phi_\alpha)}{\pi}$

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- For bosons, this comes from inserting $\hat{1} = \int \prod_\alpha \frac{d\phi_\alpha^* d\phi_\alpha}{2\pi i} e^{-\sum_\alpha \phi_\alpha^* \phi_\alpha} |\phi\rangle\langle\phi|$

$$\mathrm{Tr}\, A = \sum_n \langle n|A|n\rangle = \int \prod_\alpha \frac{d\phi_\alpha^* d\phi_\alpha}{2\pi i} e^{-\sum_\alpha \phi_\alpha^* \phi_\alpha} \sum_n \langle n|\phi\rangle\langle\phi|A|n\rangle$$
$$= \int \prod_\alpha \frac{d\phi_\alpha^* d\phi_\alpha}{2\pi i} e^{-\sum_\alpha \phi_\alpha^* \phi_\alpha} \langle\phi|A\left(\sum_n |n\rangle\langle n|\right)|\phi\rangle$$
$$= \int \prod_\alpha \frac{d\phi_\alpha^* d\phi_\alpha}{2\pi i} e^{-\sum_\alpha \phi_\alpha^* \phi_\alpha} \langle\phi|A|\phi\rangle.$$

- For fermions it is the same except no $2\pi i$ factors and we get a minus sign (hence $\langle\zeta\phi|$) when moving A through $|\phi\rangle\langle\phi|$.

- So now we insert at each time step $k = 1, \ldots, N_\tau$

$$1 = \frac{1}{C} \prod_\alpha d\phi_{\alpha,k}^* d\phi_{\alpha,k} e^{-\sum_\alpha \phi_{\alpha,k}^* \phi_{\alpha,k}} |\phi_{\alpha,k}\rangle\langle\phi_{\alpha,k}|$$

(constant) $\rightarrow C$

- We have
$$e^{\epsilon \hat{H}(a_\alpha^\dagger, a_\alpha)} = :e^{\epsilon H(a_\alpha^\dagger, a_\alpha)}: + O(\epsilon^2)$$

normal ordered

and
$$\langle\phi|A(a_\alpha^\dagger, a_\alpha)|\phi'\rangle = A(\phi_\alpha^*, \phi_\alpha')\, e^{\sum_\alpha \phi_\alpha^* \phi_\alpha'}$$

from $\langle\phi|\phi'\rangle$

(either side)

$\Rightarrow$
$$Z = \lim_{N_\tau \to \infty} \int \prod_\alpha \frac{1}{C} d\phi_\alpha^* d\phi_\alpha\, e^{-\sum_\alpha \phi_\alpha^* \phi_\alpha} \prod_{k=1}^{N_\tau - 1} \prod_\alpha \frac{1}{C} d\phi_{\alpha,k}^* d\phi_{\alpha,k}\, e^{-\sum_{k=1}^{N_\tau-1} \sum_\alpha \phi_{\alpha,k}^* \phi_{\alpha,k}}$$
$$\times \prod_{k=1}^{N_\tau} \langle\phi_k| :e^{-\epsilon \hat{H}'(a_\alpha^\dagger, a_\alpha)}: + O(\epsilon^2)|\phi_{k-1}\rangle$$

Here $H' = H - \mu N$

Now $\langle\phi_k| :e^{-\epsilon \hat{H}'(a_\alpha^\dagger, a_\alpha)}: |\phi_{k-1}\rangle = e^{\sum_\alpha \phi_{\alpha,k}^* \phi_{\alpha,k-1} - \epsilon H'(\phi_{\alpha,k}^*, \phi_{\alpha,k-1})}$

So we get another sum on k and α. We can also combine with the trace bc's that $\phi_{\alpha,0} = \phi_\alpha$, $\phi_{\alpha, N_\tau}^* = \zeta \phi_\alpha^*$ to get: (with $\phi_\alpha \equiv \zeta \phi_{\alpha,N_\tau}$)

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$$Z = \lim_{N_\tau \to \infty} \int \prod_{k=1}^{N_\tau} \prod_\alpha \frac{1}{c}\, d\phi^*_{\alpha,k}\, d\phi_{\alpha,k}\, e^{-S(\phi^*,\phi)}$$

where

$$S(\phi^*,\phi) = \epsilon \sum_{k=2}^{N_\tau} \left[\sum_\alpha \phi^*_{\alpha k} \left\{ \frac{(\phi_{\alpha,k} - \phi_{\alpha,k-1})}{\epsilon} - \mu \phi_{\alpha,k-1} \right\} + H(\phi^*_{\alpha,k}, \phi_{\alpha,k-1}) \right]$$

$$+ \epsilon \left[\sum_\alpha \phi^*_{\alpha,1} \left\{ \frac{\phi_{\alpha,1} - \zeta\phi_{\alpha,N_\tau}}{\epsilon} - \mu\zeta \phi_{\alpha,N_\tau} \right\} + H(\phi^*_{\alpha,1}, \zeta\phi_{\alpha,N_\tau}) \right]$$

boundary condition $\Rightarrow$

· With $H \to H_0 = \sum_\alpha \epsilon_\alpha a^\dagger_\alpha a_\alpha$, we can (and will!) show that we reproduce

$$Z_0 = \prod_\alpha \left(1 - \zeta e^{-\beta(\epsilon_\alpha - \mu)}\right)^{-\zeta}$$

· The trajectory notation is

$$\{\phi_{\alpha,1}, \ldots, \phi_{\alpha,N_\tau}\} \longrightarrow \phi_\alpha(\tau)$$

and

$$\phi^*_{\alpha,k} \frac{(\phi_{\alpha,k} - \phi_{\alpha,k-1})}{\epsilon} \equiv \phi^*_\alpha(\tau) \frac{\partial}{\partial\tau} \phi_\alpha(\tau)$$

$$H(\phi^*_{\alpha,k}, \phi_{\alpha,k-1}) \equiv H(\phi^*_\alpha(\tau), \phi_\alpha(\tau))$$

$$\Rightarrow Z = \int_{\phi_\alpha(\beta) = \zeta\phi_\alpha(0)} \mathcal{D}(\phi^*_\alpha(\tau)\, \phi_\alpha(\tau))\, e^{-\int_0^\beta d\tau \left\{ \sum_\alpha \phi^*_\alpha(\tau) \left(\frac{\partial}{\partial\tau} - \mu\right) \phi_\alpha(\tau) + H(\phi^*_\alpha(\tau), \phi_\alpha(\tau)) \right\}}$$

- integrations are over complex variables satisfying periodic BC's for bosons and Grassman variables satisfying antiperiodic BC's for fermions

· We can now do perturbation theory as before (with some generalizations!)

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Rather than general α, let's go to the $\vec{x}$ representation so $\phi_\alpha(\tau) \to \psi_\alpha(\vec{x},\tau)$ where now α is just a spin index and x means $(\vec{x},\tau)$ where used. Assume a spin-independent potential for now.

$$\Rightarrow \quad Z = \mathrm{Tr}\, e^{-\beta(\hat{H}-\mu\hat{N})}$$

$$= \int \mathcal{D}[\psi^\dagger(\vec{x},\tau)\psi(\vec{x},\tau)]\, e^{-\frac{1}{\hbar}\int_0^{\beta\hbar} d\tau \int d^3x\, \psi^\dagger_\alpha(\vec{x},\tau)\left(\frac{\partial}{\partial\tau} - \frac{\nabla^2}{2m} - \mu\right)\psi_\alpha(\vec{x},\tau)}$$

$$\times\, e^{-\frac{1}{2}\int_0^{\beta\hbar} d\tau \int d^3x\, d^3x'\, \psi^\dagger_\beta(\vec{x},\tau)\psi^\dagger_\alpha(\vec{x}',\tau)\, V(\vec{x}-\vec{x}')\, \psi_\alpha(\vec{x}',\tau)\psi_\beta(\vec{x},\tau)}$$

$\psi(\vec{x},\beta) = \pm\psi(\vec{x},0)$ (boson / fermion)

$V \to -\lambda\delta(\vec{x}-\vec{x}')$

$$\longrightarrow \int \mathcal{D}[\psi^\dagger(x)\psi(x)]\, e^{-\frac{1}{\hbar}\int_0^{\beta\hbar} d\tau \int d^3x\, \psi^\dagger_\alpha(x)\left(\frac{\partial}{\partial\tau} - \frac{\nabla^2}{2m} - \mu\right)\psi_\alpha(x)}$$

$$\times\, e^{\frac{\lambda}{2}\int_0^{\beta\hbar} d\tau \int d^3x\, \psi^\dagger_\alpha(x)\psi^\dagger_\beta(x)\psi_\beta(x)\psi_\alpha(x)}$$

$\psi(\vec{x},\beta) = \pm\psi(\vec{x},0)$

- Now this is suitable for perturbation theory, and we'll do that, but what about stochastic simulations?
  - Neither the boson nor fermion form is suitable here.

$\Rightarrow$ introduce an auxiliary field:

$$Z = \int \mathcal{D}(\psi^\dagger\psi)\mathcal{D}\sigma(x)\, e^{-\int d\tau\, d\tau' \int d\vec{x}\, d\vec{x}'\, \psi^\dagger(x\tau)\left[\left(\frac{\partial}{\partial\tau} - \mu - \frac{\nabla^2}{2m} + \frac{1}{2}\int dy\, V(x-y)\sigma(y,\tau)\right)\right]_{x\tau,x'\tau'}\psi(x',\tau')}$$

integrate $\psi^\dagger\psi$

$$= \int \mathcal{D}\sigma(x)\left[\mathrm{Det}\, M(\sigma)\right]^2 e^{-\frac{1}{2}\int d\tau \int dx\, dx'\, \sigma(x,\tau)V(x-x')\sigma(x',\tau)}$$

where $M_{x\tau;x'\tau'} \equiv \left[\frac{\partial}{\partial\tau} - \mu - \frac{\nabla^2}{2m} + \frac{1}{2}\int dy\, V(x-y)\,\sigma(y,\tau)\right]_{x\tau,x'\tau'}$

- Much simplified if $V(x-y) \to -\lambda\delta(x-y)$