10/14/09

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

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

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

"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! $\swarrow$ if $E_1 - E_0 > 0$

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

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

independent of x_f, x_i so true for Z

- 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

10/14/09

- 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 ∂_j: $e^{\frac{\lambda}{4}\xi^4} \Rightarrow e^{-\frac{\lambda}{4}(\frac{\partial}{\partial j})^4}[\;\;]$
- Here: analog is to add $f(\tau)$ to H in path integral:

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

- 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 $Z[f]$, $f(\tau) \to \{f(\tau_i)\} \equiv \{f_i\}$, $i = 1, \ldots, N_\tau$

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

So $\frac{1}{\epsilon}\frac{\partial Z[f]}{\partial f_j} = C\int \prod_k dx_k\; x_j\, e^{-\epsilon\sum_i[\qquad]}$ $\leftarrow$ 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

$\nwarrow$ "functional derivatives"

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

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

$\nwarrow \tau_i$ — 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 $\to \sum_{k=1}^{N_\tau}\epsilon\left(\frac{1}{\epsilon}\delta_{ik}\right) = \sum_k \delta_{ik} = 1$ $\checkmark$)

10/14/09

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

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

- 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):

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

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

- 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.

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

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

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

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

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

10/14/09

note the boundary conditions

or

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

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

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

How do we understand the continuum version?

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

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

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

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

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

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

⇒ $A^{-1}(\tau,\tau')$ 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 $\left(-\frac{m}{2}\frac{d^2}{d\tau^2} + \frac{1}{2}a\right) A^{-1}(\tau) = \delta(\tau)$ 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:

τ_1 τ_2

10/14/09

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)

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

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

- The completeness relation is

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

- 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.

10/14/09

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

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

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,

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

- When we simulate fermions with this form, $e^{-\beta H}$ filters out the lowest state of any symmetry $\Rightarrow$ 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:

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

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.

10/14/09

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, $a_\alpha^\dagger, a_\alpha$
- 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!