Topics in Quantum Many-Body Theory

Week III/IV 2025.III.13/20

Coherent states: summary

(Now consider both fermions and bosons).

$$\zeta = \begin{cases} +1 & \text{bosons} \\ -1 & \text{fermions} \end{cases} \qquad [a_\alpha, a_\beta^+]_{-\zeta} = \delta_{\alpha\beta}$$

$$|\xi\rangle = e^{\zeta \sum_\alpha \xi_\alpha a_\alpha^+}|0\rangle \qquad a_\alpha|\xi\rangle = \xi_\alpha|\xi\rangle \qquad \left\{ \langle\xi|a_\alpha^+ = \langle\xi|\xi_\alpha^* \right.$$

$$\xi, \xi^* - \begin{cases} \text{complex numbers for boson} \\ \text{Grassmann numbers for fermions} \end{cases} \qquad a_\alpha^+|\xi\rangle = \zeta \frac{\partial}{\partial \xi_\alpha}|\xi\rangle$$

$$\langle\xi|A(a_\alpha^+, a_\alpha)|\xi'\rangle = e^{\sum_\alpha \xi_\alpha^* \xi_\alpha'} A(\xi_\alpha^*, \xi_\alpha') \qquad (A \text{ normal ordered})$$

$$1 = \int d\mu(\xi)\, e^{-\sum_\alpha \xi_\alpha^* \xi_\alpha} |\xi\rangle\langle\xi|$$

$$d\mu(\xi) = \prod_\alpha \left(\frac{d\xi_\alpha^* d\xi_\alpha}{\mathcal{N}} \right)$$

$$\mathcal{N} = \begin{cases} 2\pi i & \text{bosons} \\ 1 & \text{fermions} \end{cases} \qquad \mathrm{Tr}\, A = \int d\mu(\xi)\, e^{-\sum_\alpha \xi_\alpha^* \xi_\alpha} \langle \zeta\xi|A|\xi\rangle$$

Propagator in QM vs partition function (case of a single particle)

$$|\psi(t)\rangle = \mathcal{U}(t)|\psi(t=0)\rangle$$

$\hookrightarrow$ evolution operator (Schrödinger picture) $\quad \mathcal{U}(t) = e^{-\frac{i\hat{H}}{\hbar}t}$ (for time-independent $\hat{H}$)

Probability amplitude to find a particle at position q_f at time t_f:

$$\psi(q_f, t_f) = \langle q_f|\psi(t_f)\rangle = \langle q_f|\hat{\mathcal{U}}(t_f - t_i)|\psi(t_i)\rangle = \int dq_i \underbrace{\mathcal{U}(q_f, q_i, t_f - t_i)}_{= \langle q_f|\hat{\mathcal{U}}(t_f - t_i)|q_i\rangle} \psi(q_i, t_i)$$

– propagator (probability amplitude for a particle to propagate from q_i to q_f in a time $t_f - t_i$)

$$\hat{H}|n\rangle = \epsilon_n|n\rangle$$

$$\mathcal{U}(q_f, q_i, t_f - t_i) = \langle q_f| e^{-\frac{i\hat{H}}{\hbar}(t_f - t_i)}|q_i\rangle = \sum_n \langle q_f|n\rangle e^{-\frac{i\epsilon_n}{\hbar}(t_f - t_i)} \langle n|q_i\rangle$$

$$= \sum_n e^{-\frac{i}{\hbar}\epsilon_n(t_f - t_i)} \varphi_n(q_f)\varphi_n^*(q_i)$$

if we know $\{|n\rangle, \epsilon_n\}$, we can calculate $\mathcal{U}$

$\mathcal{U}(q_f, q_i, t)$ can also be represented as a path integral $\rightarrow$ see the exercise class

- Consider first an infinitesimal time ϵ and recall the Baker-Campbell-Hausdorff formula $e^X e^Y = e^{X+Y+\frac{1}{2}[X,Y]+\frac{1}{12}([X,[X,Y]]-[Y,[X,Y]])+\dots}$

To first order in ϵ: $\mathcal{U}(q_f, q_i, \epsilon) = \langle q_f | e^{-i\frac{\hat{H}}{\hbar}\epsilon} | q_i \rangle \simeq \langle q_f | e^{-i\epsilon\frac{\hat{p}^2}{2m}\frac{1}{\hbar}} e^{-i\frac{\epsilon}{\hbar}V(\hat{q})} | q_i \rangle$

$\left(\hat{H} = \frac{\hat{p}^2}{2m} + V(\hat{q})\right)$

$1 = \sum_p |p\rangle\langle p|$ allows for evaluating $\mathcal{U}(q_f, q_i, \epsilon)$

$$\mathcal{U}(q_f, q_i, \epsilon) = \left(\frac{m}{2\pi i \epsilon}\right)^{\frac{1}{2}} e^{i \overbrace{S(q_f, q_i, \epsilon)}^{\epsilon \frac{m}{2}\frac{(q_f-q_i)^2}{\epsilon^2} - V(q_i)} + \mathcal{O}(\epsilon^2)}$$

$\left\{ e^{\epsilon\hat{X}+\epsilon\hat{Y}} = 1 + \epsilon(\hat{X}+\hat{Y}) + \mathcal{O}(\epsilon^2) = e^{\epsilon\hat{X}} e^{\epsilon\hat{Y}} e^{\mathcal{O}(\epsilon^2)} \right\}$

- $\mathcal{U}(q_f, q_i, t_f - t_i) = \langle q_f | \underbrace{e^{-i\hat{H}\frac{\epsilon}{\hbar}} e^{-i\hat{H}\frac{\epsilon}{\hbar}} \dots e^{-i\hat{H}\frac{\epsilon}{\hbar}}}_{N \text{ times}} | q_i \rangle$, $N \cdot \epsilon = t_f - t_i$.

At the end send $N \to \infty$ $(\epsilon \to 0)$

At each time step insert $\int_q |q\rangle\langle q|$

$$\mathcal{U}(q_f, q_i, t_f - t_i) = \int \left(\prod_{k=1}^{N-1} dq_k\right) \langle q_f | e^{-i\frac{\hat{H}}{\hbar}\epsilon} | q_{N-1}\rangle \langle q_{N-1} | e^{-i\frac{\hat{H}}{\hbar}\epsilon} | q_{N-2}\rangle \dots \langle q_1 | e^{-i\frac{\hat{H}}{\hbar}\epsilon} | q_i \rangle =$$

$\left(\begin{matrix} q_0 = q_i \\ q_N = q_f \end{matrix}\right)$ $$= \int \prod_{k=1}^{N-1} dq_k \prod_{k=1}^{N} \mathcal{U}(q_k, q_{k-1}, \epsilon)$$

{EACH TIME STEP INTRODUCES AN ERROR OF ORDER ϵ^2 $\rightarrow$ THE TOTAL ERROR IS OF ORDER $N\epsilon^2 = \epsilon$ AND VANISHES FOR $\epsilon \to 0$}

... $\rightarrow$ see the exercise class.

$$\left\{ \mathcal{U}(q_f, q_i, t) = \lim_{N\to\infty} \left(\frac{mN}{2\pi i t}\right)^{\frac{N}{2}} \prod_{k=1}^{N-1} dq_k \, e^{i\frac{1}{\hbar}S[q]} \qquad S[q] = \sum_{k=1}^{N} S(q_k, q_{k-1}, \epsilon) = \epsilon \sum_{k=1}^{N} \left[\frac{m}{2}\frac{(q_k - q_{k-1})^2}{\epsilon^2} - V(q_{k-1})\right] \right.$$

NOTATION: $\mathcal{U}(q_f, q_i, t_f - t_i) = \int_{q(t_i)=q_i}^{q(t_f)=q_f} \mathcal{D}[q] \, e^{\frac{i}{\hbar}S[q]}$

$S[q] = \int_{t_i}^{t_f} dt \, L(q, \dot{q})$

<u>Partition function</u> $\rightarrow$ $Z = \mathrm{Tr}\, e^{-\beta\hat{H}} = \int dq \underbrace{\langle q | e^{-\beta\hat{H}} | q \rangle}_{}$ (single particle as above)

$\left(e^{-i\frac{\hat{H}}{\hbar}t} \xrightarrow{t \to -i\beta\hbar} e^{-\beta\hat{H}} \right)$ Matrix element of the evolution operator in imaginary time!

Real-time dynamics connected to (equilibrium) statistical mechanics by $t \to -i\tau$

$\{q_0 = q_i, \; q_N = q_f\}$ (so called Wick rotation)

$$\mathcal{U}(q_f, q_i, -i\tau) = \langle q_f | e^{-\frac{\hat{H}\tau}{\hbar}} | q_i \rangle = \lim_{N\to\infty} \left(\frac{mN}{2\pi\tau\hbar}\right)^{\frac{N}{2}} \int \prod_{k=1}^{N-1} dq_k \, e^{-\frac{\epsilon}{\hbar}\sum_{k=1}^{N}\left[\frac{m}{2}\frac{(q_k - q_{k-1})^2}{\epsilon^2} + V(q_{k-1})\right]} =$$

$$= \int_{q(0)=q_i}^{q(\tau)=q_f} \mathcal{D}[q]\, e^{-S_E[q]\frac{1}{\hbar}} \qquad S_E(q) = \int_0^\tau d\tau' \left[\frac{m}{2}\dot{q}^2 + V(q)\right]$$

("symbolic" notation — the paths are not differentiable)

{ paths which are not continuous are exponentially suppressed since $\frac{q_u - q_{u-1}}{\epsilon} \to \infty$. }

$$Z = \int dq\, \mathcal{U}(q, q, -i\beta\hbar) = \int_{q(\beta\hbar) = q(0)} \mathcal{D}[q]\, e^{-S_E[q]\frac{1}{\hbar}} \qquad (\text{no operators} \ldots)$$

Classical limit: $\beta\hbar \to 0^+$ → the time interval becomes "infinitesimal" and can be calculated with a single time step ($N=1$)

$$Z_{cl} = \left(\frac{m}{2\pi\beta\hbar^2}\right)^{\frac{1}{2}} \int dq\, e^{-\beta\hbar\left[\frac{m}{2}\frac{(q-q)^2}{(\beta\tau)^2} + V(q)\right]/\hbar} = \left(\frac{m}{2\pi\beta\hbar^2}\right)^{\frac{1}{2}} \int dq\, e^{-\beta V(q)} =$$

$$= \int dq\, e^{-\beta V(q)} \underbrace{\int dp\, e^{-\beta\frac{p^2}{2m}}}_{\frac{\sqrt{\pi}}{\sqrt{\beta/2m}}} \underbrace{\sqrt{\frac{\beta/2m}{\pi}}\sqrt{\frac{m}{2\pi\beta\hbar^2}}}_{\frac{1}{2\pi\hbar}} = \int \frac{dp}{h} \int dq\, e^{-\beta\left(\frac{p^2}{2m} + V(q)\right)}$$

(Further on $\hbar = 1$).

Path integral for the many-body systems

Recall:

$d\mu(\xi) = \prod_\alpha \left(\frac{d\xi_\alpha^* d\xi_\alpha}{\mathcal{N}}\right) \qquad 1 = \int d\mu(\xi)\, e^{-\sum_\alpha \xi_\alpha^* \xi_\alpha} |\xi\rangle\langle\xi|$

$\mathcal{N} = \begin{cases} 2\pi i & \text{bosons} \\ 1 & \text{fermions} \end{cases} \qquad \operatorname{Tr} A = \int d\mu(\xi)\, e^{-\sum_\alpha \xi_\alpha^* \xi_\alpha} \langle \zeta\xi | A | \xi\rangle$

$$Z = \operatorname{Tr} e^{-\beta\hat{H}} = \int d\mu(\xi)\, e^{-\sum_\alpha \xi_\alpha^* \xi_\alpha} \langle \zeta\xi | e^{-\beta\hat{H}} | \xi\rangle$$

Here GCE ($-\beta\hat{H} \leftrightarrow -\beta(\hat{H} - \mu\hat{N})$) !!

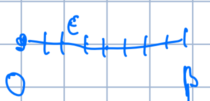
$\hat{H}$ is normal-ordered

{ ($\hat{H} = :\hat{H}:$)

→ $e^{-\epsilon\hat{H}} = :e^{-\epsilon\hat{H}}: + \mathcal{O}(\epsilon^2)$ } (normal-ordered exponential)

$$Z = \int d\mu(\xi)\, e^{-\sum_\alpha \xi_\alpha^* \xi_\alpha} \langle \zeta\xi | \underbrace{e^{-\epsilon\hat{H}} e^{-\epsilon\hat{H}} \ldots e^{-\epsilon\hat{H}}}_{M \gg 1 \text{ times}} | \xi\rangle \qquad \left(M = \frac{\beta}{\epsilon}\right)$$

insert the coherent-state unity between each $e^{-\beta\epsilon\hat{H}}\, e^{-\beta\epsilon\hat{H}}$ (M−1 times)



$$\langle \xi_u | e^{-\epsilon\hat{H}(a^\dagger_\alpha, a_\alpha)} | \xi_{u-1}\rangle = \underbrace{\langle \xi_u | \xi_{u-1}\rangle}_{= e^{\sum_\alpha \xi^*_{u\alpha}\xi_{u-1\alpha}}} e^{-\epsilon H(\xi^*_{u\alpha}, \xi_{u-1\alpha})} + \mathcal{O}(\epsilon^2).$$

Introduce $\xi_0 = \zeta \xi_M$ $\quad \xi \to \xi_0$

$\xi_0^* = \zeta \xi_M^*$

No operators!

$$\boxed{\mathcal{Z} = \int \prod_{k=1}^{M} d\mu_{(k)}(\xi_{(k)})\, e^{-\epsilon \sum_{k=1}^{M}\left[\sum_\alpha \xi^*_{(k)\alpha} \frac{(\xi_{(k)\alpha} - \xi_{(k-1)\alpha})}{\epsilon} + H(\xi^*_{(k)\alpha}, \xi_{(k-1)\alpha})\right]}}$$

for $\epsilon \to 0$
$M \to \infty$
$\epsilon M = \beta$

$\{\xi_{(0)\alpha}, \xi_{(1)\alpha} \dots \xi_{(M)\alpha}\} \longrightarrow \xi_\alpha(\tau)$ ("continuous trajectory")

$\tau \in]0, \beta] \to$ imaginary time

boundary conditions: $\xi_\alpha(\beta) = \zeta \xi_\alpha(0)$
$\xi_\alpha^*(\beta) = \zeta \xi_\alpha^*(0)$

Symbolic notation: $\epsilon \sum_{k=1}^{M} \longrightarrow \int_0^\beta d\tau$

$$\xi^*_{(k)\alpha} \frac{\xi_{(k)\alpha} - \xi_{(k-1)\alpha}}{\epsilon} \longrightarrow \xi^*_\alpha(\tau)\, \partial_\tau \xi_\alpha(\tau)$$

$$H(\xi^*_{(k)\alpha}, \xi_{(k-1)\alpha}) \longrightarrow H(\xi^*_\alpha(\tau), \xi_\alpha(\tau))$$

$$\mathcal{Z} = \int_{\substack{\xi(\beta) = \zeta \xi(0) \\ \xi^*(\beta) = \zeta \xi^*(0)}} \mathcal{D}[\xi^*, \xi]\, e^{-S[\xi^*, \xi]} \quad (*)$$

$$S[\xi^*, \xi] = \int_0^\beta d\tau \left[\sum_\alpha \xi^*_\alpha(\tau) \partial_\tau \xi_\alpha(\tau) + H(\xi^*_\alpha(\tau), \xi_\alpha(\tau))\right]$$

$$\mathcal{D}[\xi^*, \xi] = \lim_{M \to \infty} \prod_{k=0}^{M} d\mu_{(k)}(\xi_{(k)})$$

(supplemented with the b.c. $(*)$)

EXAMPLE Non-interacting particles

$$\hat{H} = \sum_\alpha (\epsilon_\alpha - \mu)\, a_\alpha^\dagger a_\alpha \qquad \{\xi \Longleftrightarrow \phi\}$$

$$\mathcal{Z}_0 = \lim_{M \to \infty} \int \prod_{k=1}^{M} \prod_\alpha \frac{1}{\mathcal{N}} d\phi^*_{\alpha k}\, d\phi_{\alpha k} \exp\left\{-\epsilon \sum_{k=2}^{M}\left[\sum_\alpha \phi^*_{\alpha k} \frac{\phi_{\alpha k} - \phi_{\alpha, k-1}}{\epsilon} + \sum_\alpha (\epsilon_\alpha - \mu)\, \phi^*_{\alpha k} \phi_{\alpha k-1}\right] + \right.$$
$$\left. - \epsilon \sum_\alpha \phi^*_{\alpha,1} \frac{\phi_{\alpha 1} - \zeta \phi_{\alpha M}}{\epsilon} + \sum_\alpha (\epsilon_\alpha - \mu)\, \phi^*_{\alpha 1} \phi_{\alpha M} \zeta \right\} =$$

$\left\{ \epsilon = \frac{\beta}{M} \right.$ $\quad a := 1 - \frac{\beta}{M}(\epsilon_\alpha - \mu) \Big\}$ $\quad$ GAUSSIAN INTEGRAL!

THIS TERM ENCODES STATISTICS

$$Z_0 = \lim_{M\to\infty} \int \prod_{k=1}^{M} \prod_{\alpha} \frac{1}{N}\, d\phi^*_{\alpha k}\, d\phi_{\alpha k}\, \exp\left\{ -\sum_{\alpha} \left[\phi^*_{\alpha 1} \cdots \phi^*_{\alpha M}\right] \underbrace{\begin{bmatrix} 1 & 0 & \cdots & \cdots & -\zeta a \\ -a & 1 & 0 & \cdots & \vdots \\ 0 & -a & \ddots & \ddots & \vdots \\ \vdots & \vdots & \ddots & \ddots & \vdots \\ 0 & \cdots & \cdots & -a & 1 \end{bmatrix}}_{S^{(\alpha)}} \begin{bmatrix} \phi_{\alpha 1} \\ \vdots \\ \vdots \\ \phi_{\alpha M} \end{bmatrix} \right\}$$

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{ GAUSSIAN INTEGRATIONS ! }

$$Z_0 = \lim_{M\to\infty} \prod_{\alpha} \left[\det S^{(\alpha)}\right]^{-\zeta}$$

$$\det S^{(\alpha)} = \left(\text{LAPLACE EXPANSION WITH RESPECT TO 1ST ROW.} \right)$$

$$= \det\begin{pmatrix} 1 & 0 & 0 & & \\ -a & 1 & 0 & & \\ 0 & -a & 1 & & \\ \vdots & 0 & -a & \ddots & \\ \vdots & \vdots & 0 & \ddots & \\ 0 & 0 & 0 \cdots 0 & -a & 1 \end{pmatrix} + (-\zeta a)(-1)^{M+1} \det\begin{pmatrix} -a & 1 & 0 & & \\ 0 & -a & 1 & & \\ \vdots & 0 & -a & \ddots & 0 \\ \vdots & \vdots & 0 & \ddots & 1 \\ 0 & 0 & 0 \cdots 0 & & -a \end{pmatrix} =$$

$$= 1 - \zeta a (-1)^{M+1} (-a)^{M-1} = 1 - \zeta a^M (-1)^{2M} = 1 - \zeta a^M = 1 - \zeta\left[1 - \frac{\beta}{M}(\epsilon_\alpha - \mu)\right]^M$$

$$\left\{ \left(1 + \frac{x}{n}\right)^n \xrightarrow{n\to\infty} e^x \right\}$$

$$\xrightarrow{M\to\infty} 1 - \zeta e^{-\beta(\epsilon_\alpha - \mu)}$$

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

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