

Problem 1.

$$f(p_A, p_B, q_A, q_B) = f(p_A^{(0)}, p_B^{(0)}, q_A^{(0)}, q_B^{(0)})$$

$$e^{-i\hat{L}t} f = e^{-i(L_A + L_B)t} f$$

$$= e^{-i(L_A^{(p)} + L_B^{(p)})\frac{t}{2}} e^{-i(L_A^{(q)} + L_B^{(q)})t} e^{-i(L_A^{(p)} + L_B^{(p)})\frac{t}{2}} f$$

$$i\hat{L}_A f = -i\hat{L}_A f = \frac{\partial f}{\partial q_A} \frac{\partial H}{\partial p_A} - \frac{\partial f}{\partial p_A} \frac{\partial H}{\partial q_A}$$

$$-i\hat{L}_B f = \frac{\partial f}{\partial q_B} \frac{\partial H}{\partial p_B} - \frac{\partial f}{\partial p_B} \frac{\partial H}{\partial q_B}$$

$$-i\hat{L}_A^{(p)} f = -\frac{\partial f}{\partial p_A} \frac{\partial H}{\partial q_A}$$

$$-i\hat{L}_B^{(q)} f = -\frac{\partial f}{\partial p_B} \frac{\partial H}{\partial q_B}$$

$$-i\hat{L}_A^{(q)} f = -\frac{\partial f}{\partial q_A} \frac{\partial H}{\partial p_A}$$

$$-i\hat{L}_B^{(p)} f = -\frac{\partial f}{\partial q_B} \frac{\partial H}{\partial p_B}$$

$$= e^{-\frac{it}{2}(L_A^{(p)} + L_B^{(p)})} e^{-i\frac{t}{2}(L_A^{(q)} + L_B^{(q)})}$$

$$= e^{-\frac{it}{4}L_A^{(p)}} e^{-\frac{it}{2}L_A^{(q)}} e^{-\frac{it}{4}L_A^{(p)}} e^{-\frac{it}{4}L_B^{(p)}} e^{-\frac{it}{2}L_B^{(q)}} e^{-\frac{it}{4}L_B^{(p)}}$$

$$\times \left[e^{-\frac{i\delta}{2}L_B^{(q)}} e^{-i\delta L_B^{(p)}} e^{-\frac{i\delta}{2}L_B^{(q)}} \right]^n$$

$$\times e^{-\frac{it}{4}L_A^{(p)}} e^{-\frac{it}{2}L_A^{(q)}} e^{-\frac{it}{4}L_A^{(p)}} e^{-\frac{it}{4}L_B^{(p)}} e^{-\frac{it}{2}L_B^{(q)}} e^{-\frac{it}{4}L_B^{(p)}}$$

$$t = n\delta$$

$$f(p_A^{(0)}, p_B^{(0)}, q_A^{(0)}, q_B^{(0)})$$

Sequence:

start with $p_A(0), q_A(0), p_B(0), q_B(0)$

$$1.) p_A\left(\frac{t}{4}\right) = p_A(0) + F_A(q_A(0), q_B(0)) \frac{t}{4}$$

propagation of $p_A(0) \rightarrow p_A\left(\frac{t}{4}\right)$, using $q_A(0), q_B(0)$

$$2.) q_A\left(\frac{t}{2}\right) = q_A(0) + \frac{p_A\left(\frac{t}{4}\right)}{m} \frac{t}{2}$$

propagation of $q_A(0) \rightarrow q_A\left(\frac{t}{2}\right)$ using $p_A\left(\frac{t}{4}\right)$

$$3.) p_A\left(\frac{t}{2}\right) = p_A\left(\frac{t}{4}\right) + F_A(q_A\left(\frac{t}{2}\right), q_B(0)) \frac{t}{4}$$

propagation of $p_A\left(\frac{t}{4}\right) \rightarrow p_A\left(\frac{t}{2}\right)$ at this pt.
 $p_A\left(\frac{t}{2}\right), q_A\left(\frac{t}{2}\right), p_B(0), q_B(0)$

$$4.) p_B\left(\frac{t}{2}\right) = p_B(0) + F_B(q_A\left(\frac{t}{2}\right), q_B(0)) \frac{t}{2}$$

propagation of $p_B(0) \rightarrow p_B\left(\frac{t}{2}\right)$ using $q_A\left(\frac{t}{2}\right), q_B(0)$

$$5.) q_B(t) = q_B(0) + \frac{p_B\left(\frac{t}{2}\right)}{m} t$$

propagation of $q_B(0) \rightarrow q_B(t)$ using $p_B\left(\frac{t}{2}\right)$

$$6.) p_B(t) = p_B\left(\frac{t}{2}\right) + F_B(q_A\left(\frac{t}{2}\right), q_B(t)) \frac{t}{2}$$

at this pt.
 $p_A\left(\frac{t}{2}\right), q_A\left(\frac{t}{2}\right), p_B(t), q_B(t)$

$$7.) p_A\left(\frac{3t}{4}\right) = p_A\left(\frac{t}{2}\right) + F_A(q_A\left(\frac{t}{2}\right), q_B(t)) \frac{t}{4}$$

$p_A\left(\frac{t}{2}\right) \rightarrow p_A\left(\frac{3t}{4}\right)$ using $q_A\left(\frac{t}{2}\right), q_B(t)$

$$8.) q_A(t) = q_A\left(\frac{t}{2}\right) + \frac{p_A\left(\frac{3t}{4}\right)}{m} \frac{t}{2}$$

$q_A\left(\frac{t}{2}\right) \rightarrow q_A(t)$ using $p_A\left(\frac{3t}{4}\right)$

$$9.) p_A(t) = p_A\left(\frac{3t}{4}\right) + F_A(q_A(t), q_B(t)) \frac{t}{4}$$

$p_A\left(\frac{3t}{4}\right) \rightarrow p_A(t)$ using $q_A(t), q_B(t)$ at this pt.
 $p_B(t), q_B(t), p_A(t), q_A(t)$

operator in z -basis $O(z, z') \Rightarrow \begin{pmatrix} O(z+, z+) & O(z+, z-) \\ O(z-, z+) & O(z-, z-) \end{pmatrix} \quad (1)$

operator in x -basis $O(x, x') \Rightarrow \begin{pmatrix} O(x+, x+) & O(x+, x-) \\ O(x-, x+) & O(x-, x-) \end{pmatrix}$

Connection between the two

$$\begin{aligned} O(x, x') &\Rightarrow \langle \tilde{x} | \hat{O} | \tilde{x}' \rangle = O(x+, x+) \\ &= \langle \tilde{x}+ | \tilde{x}+ \rangle \langle x+ | z+ \rangle \langle z+ | \hat{O} | z+ \rangle \langle z+ | x+ \rangle \\ &\quad + \langle \tilde{x}+ | \tilde{x}+ \rangle \langle x+ | z- \rangle \langle z+ | \hat{O} | z- \rangle \langle z- | x+ \rangle \\ &\quad + \langle \tilde{x}+ | \tilde{x}- \rangle \langle z- | \hat{O} | z+ \rangle \langle z+ | x+ \rangle \\ &\quad + \langle \tilde{x}+ | \tilde{x}- \rangle \langle z- | \hat{O} | z- \rangle \langle z- | x+ \rangle \end{aligned}$$

$$= \begin{pmatrix} \langle \tilde{x}+ | \tilde{x}+ \rangle & \langle \tilde{x}+ | \tilde{x}- \rangle \\ \langle \tilde{x}- | \tilde{x}+ \rangle & \langle \tilde{x}- | \tilde{x}- \rangle \end{pmatrix} \begin{pmatrix} \langle z+ | \hat{O} | z+ \rangle & \langle z+ | \hat{O} | z- \rangle \\ \langle z- | \hat{O} | z+ \rangle & \langle z- | \hat{O} | z- \rangle \end{pmatrix} \begin{pmatrix} \langle z+ | x+ \rangle & \langle z+ | x- \rangle \\ \langle z- | x+ \rangle & \langle z- | x- \rangle \end{pmatrix}$$

to calculate $\langle z+ | x+ \rangle$ etc.

$$\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \begin{pmatrix} 1 \\ 0 \end{pmatrix} \Rightarrow \begin{pmatrix} 1 \\ 0 \end{pmatrix} \quad |z+\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$$

$$|z-\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

$$\sigma_x = \sum_{i,j} \langle i | \sigma_x | j \rangle \begin{pmatrix} i \\ j \end{pmatrix} = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} x \\ y \end{pmatrix} = \begin{pmatrix} y \\ x \end{pmatrix}$$

$$\lambda^2 - 1 = 0 \quad \lambda = \pm 1 \Rightarrow |x+\rangle = \begin{pmatrix} 1/\sqrt{2} \\ 1/\sqrt{2} \end{pmatrix} \quad |x-\rangle = \begin{pmatrix} 1/\sqrt{2} \\ -1/\sqrt{2} \end{pmatrix}$$

$$\langle z+ | x+ \rangle = (1 \ 0) \begin{pmatrix} 1/\sqrt{2} \\ 1/\sqrt{2} \end{pmatrix} = 1/\sqrt{2}$$

$$\langle z+ | x- \rangle = (1 \ 0) \begin{pmatrix} 1/\sqrt{2} \\ -1/\sqrt{2} \end{pmatrix} = 1/\sqrt{2} \Rightarrow$$

$$\langle z- | x+ \rangle = -1/\sqrt{2}$$

$$\langle z- | x- \rangle = 1/\sqrt{2}$$

$$\begin{pmatrix} 1/\sqrt{2} & 1/\sqrt{2} \\ -1/\sqrt{2} & 1/\sqrt{2} \end{pmatrix}$$

transform $\hat{S}$

$$\hat{S} = \frac{1}{2Q} \begin{pmatrix} 1 & -1 \\ 1 & 1 \end{pmatrix} \begin{pmatrix} e^{\beta\mu_B B} & 0 \\ 0 & e^{-\beta\mu_B B} \end{pmatrix} \begin{pmatrix} 1 & 1 \\ -1 & 1 \end{pmatrix}$$

$$Q = 2 \cosh(\beta\mu_B B)$$

$$= \frac{1}{2Q} \begin{pmatrix} 1 & -1 \\ 1 & 1 \end{pmatrix} \begin{pmatrix} e^{\beta\mu_B B} & e^{\beta\mu_B B} \\ -e^{-\beta\mu_B B} & e^{-\beta\mu_B B} \end{pmatrix}$$

$$= \frac{1}{2Q} \begin{pmatrix} 2 \cosh(\beta\mu_B B) & 2 \sinh(\beta\mu_B B) \\ 2 \sinh(\beta\mu_B B) & 2 \cosh(\beta\mu_B B) \end{pmatrix}$$

$$= \frac{1}{2} \begin{pmatrix} 1 & \tanh(\beta\mu_B B) \\ \tanh(\beta\mu_B B) & 1 \end{pmatrix}$$

transform σ_z

$$\sigma_z \text{ in } \times \text{ basis: } \frac{1}{2} \begin{pmatrix} 1 & -1 \\ 1 & 1 \end{pmatrix} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \begin{pmatrix} 1 & 1 \\ -1 & 1 \end{pmatrix}$$

$$= \frac{1}{2} \begin{pmatrix} 1 & -1 \\ 1 & 1 \end{pmatrix} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}$$

$$= \frac{1}{2} \begin{pmatrix} 0 & 2 \\ 2 & 0 \end{pmatrix} = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$

$$\text{Tr} \{ \hat{S} \sigma_z \hat{S} \} = \frac{\text{Tr}}{2} \begin{pmatrix} 1 & \tanh(\beta\mu_B B) \\ \tanh(\beta\mu_B B) & 1 \end{pmatrix} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$

$$= \frac{\text{Tr}}{2} \begin{pmatrix} \tanh(\beta\mu_B B) & 1 \\ 1 & \tanh(\beta\mu_B B) \end{pmatrix}$$

$$= \tanh(\beta\mu_B B)$$

5.2

$$\langle q | e^{-\beta \hat{H}} | q' \rangle = \exp[-\beta \hat{H}(-i\hbar \partial_q, q)] \delta(q - q')$$

$$\delta(q - q') = \sum_i \langle q | \psi_i \rangle \langle \psi_i | q' \rangle$$

$$\hat{H} | \psi_i \rangle = E_i | \psi_i \rangle$$

$$\text{L.H.S.} \Rightarrow \sum_i \langle q | \psi_i \rangle e^{-\beta E_i} \langle \psi_i | q' \rangle$$

e q i
f n d
t d e

$$\text{R.H.S.} \Rightarrow \exp[-\beta \hat{H}(-i\hbar \partial_q, q)] \sum_i \langle q | \psi_i \rangle \langle \psi_i | q' \rangle$$

expand exponential

$$\exp[-\beta \hat{H}(-i\hbar \partial_q, q)] = 1 - \beta \hat{H} + \frac{\beta^2}{2} \hat{H}^2 + \dots$$

$$\hat{H}(-i\hbar \partial_q, q) \psi_i(q) = E_i \psi_i(q)$$

$$[\hat{H}(-i\hbar \partial_q, q)]^2 \psi_i(q) = E_i^2 \psi_i(q)$$

$$\exp(-\beta \hat{H}(-i\hbar \partial_q, q)) \sum_i \langle q | \psi_i \rangle \langle \psi_i | q' \rangle$$

$$= \sum_i \exp(-\beta \hat{H}(-i\hbar \partial_q, q)) \langle q | \psi_i \rangle \langle \psi_i | q' \rangle$$

$$= \sum_i \exp(-\beta E_i) \langle q | \psi_i \rangle \langle \psi_i | q' \rangle \quad \checkmark$$

$$\text{Free particle:} \quad \langle q | e^{-\beta \left(-\frac{\hbar^2}{2m} \frac{\partial^2}{\partial q^2} \right)} | q' \rangle = e^{-\beta \left(-\frac{\hbar^2}{2m} \frac{\partial^2}{\partial q^2} \right)} \int dq e^{ik(q-q')}$$

$$= \int dk e^{-\beta \left(-\frac{\hbar^2}{2m} \frac{\partial^2}{\partial q^2} \right)} e^{ik(q-q')} = \int dk e^{-\left(\frac{\hbar^2 k^2}{2m} + ik(q-q') \right)}$$

$$= \int dk e^{-\frac{\hbar^2 k^2}{2m} - \frac{2m}{\hbar^2} ik(q-q')} = \int dk e^{-\frac{\hbar^2 k^2}{2m} - \frac{m^2}{\hbar^2} (q-q')^2} = \sqrt{\frac{2m\hbar^2}{\beta}} e^{-\frac{m}{\hbar^2 \beta} (q-q')^2}$$

$$= \frac{-\xi^2 + 2\xi\xi' e^{-\beta\hbar\omega} - \xi'^2 + \xi\xi' e^{-\beta\hbar\omega}}{1 - e^{-\beta\hbar\omega}}$$

$$= e^{-\frac{\beta\hbar\omega}{2}} \left(\frac{m\omega}{\hbar}\right)^{1/2} e^{\frac{\xi\xi' e^{-\frac{\beta\hbar\omega}{2}}}{\sinh(\frac{\beta\hbar\omega}{2})}}$$

$$- \frac{4}{2(1 - e^{-\beta\hbar\omega})} + \frac{\xi(1 - e^{-\beta\hbar\omega})}{2(1 - e^{-\beta\hbar\omega})} = \frac{-2 + 1 - e^{-\beta\hbar\omega}}{2(1 - e^{-\beta\hbar\omega})}$$

$$= \frac{-1 - e^{-\beta\hbar\omega}}{2(1 - e^{-\beta\hbar\omega})} = -\frac{1}{2} \frac{(1 + e^{-\beta\hbar\omega})}{(1 - e^{-\beta\hbar\omega})}$$

$$= -\frac{1}{2} \frac{\cosh(\frac{\beta\hbar\omega}{2})}{\sinh(\frac{\beta\hbar\omega}{2})} = -\frac{1}{2} \coth(\frac{\beta\hbar\omega}{2})$$

$$= e^{-\frac{\beta\hbar\omega}{2}} \left(\frac{m\omega}{\hbar}\right)^{1/2} e^{-\frac{1}{2} \coth(\frac{\beta\hbar\omega}{2}) (\xi^2 + \xi'^2) + \frac{\xi\xi' e^{-\frac{\beta\hbar\omega}{2}}}{\sinh(\frac{\beta\hbar\omega}{2})}}$$

S. 4

$$\psi_{\mathcal{E}}(\vec{q}) = \prod_i u_{q_i}(q_i)$$

density matrix:

$$\begin{aligned} & \sum_E \langle \vec{r}_1, \dots, \vec{r}_N | E \rangle e^{-\beta E} \langle E | \vec{r}'_1, \dots, \vec{r}'_N \rangle \\ &= \sum_{\vec{p}_1, \dots, \vec{p}_N} \langle \vec{r}_1, \dots, \vec{r}_N | \vec{p}_1, \dots, \vec{p}_N \rangle e^{-\beta \frac{(\vec{p}_1^2 + \dots + \vec{p}_N^2)}{2m}} \langle \vec{p}_1, \dots, \vec{p}_N | \vec{r}'_1, \dots, \vec{r}'_N \rangle \\ &= \sum_{\vec{p}_1, \dots, \vec{p}_N} \langle \vec{r}_1, \dots, \vec{r}_N | \vec{p}_1, \dots, \vec{p}_N \rangle e^{-\frac{\beta}{2m} (\vec{p}_1^2 + \dots + \vec{p}_N^2)} e^{i\vec{p}_1 \cdot \vec{r}_1} \dots e^{i\vec{p}_N \cdot \vec{r}_N} e^{-\frac{\beta}{2m} (\vec{p}_1^2 + \dots + \vec{p}_N^2)} e^{-i\vec{p}_1 \cdot \vec{r}'_1} \dots e^{-i\vec{p}_N \cdot \vec{r}'_N} \\ &= \sum_{\vec{p}_1, \dots, \vec{p}_N} \frac{e^{i\vec{p}_1 \cdot \vec{r}_1} \dots e^{i\vec{p}_N \cdot \vec{r}_N} e^{-\frac{\beta}{2m} (\vec{p}_1^2 + \dots + \vec{p}_N^2)} e^{-i\vec{p}_1 \cdot \vec{r}'_1} \dots e^{-i\vec{p}_N \cdot \vec{r}'_N}}{(2\pi)^N} \\ &= \prod_{i=1}^N \int d\vec{p}_i \frac{e^{-\frac{\beta}{2m} \vec{p}_i^2}}{(2\pi)^N} e^{i\vec{p}_i \cdot (\vec{r}_i - \vec{r}'_i)} = \left(\sqrt{\frac{2m}{\beta}} \right)^N e^{-\frac{m}{2\beta} \sum_{i=1}^N (\vec{r}_i - \vec{r}'_i)^2} \end{aligned}$$

- different particles are uncorrelated since $\hat{Q}$ is a product $\Rightarrow \prod_i \delta(\vec{r}_i, \vec{r}'_i)$
- no Gibbs correction factor