

# TEAS - SHEET 3

WICK ROTATION:

$$4. a) \quad i \frac{\partial}{\partial t} |\psi\rangle = H |\psi\rangle \xrightarrow{t = -i\tau} - \frac{\partial}{\partial \tau} |\psi(\tau)\rangle = H |\psi(\tau)\rangle$$

$\Rightarrow \left( \frac{\partial}{\partial t} \mapsto i \frac{\partial}{\partial \tau} \right)$  (CLASSICAL DIFFUSION EQUATION)

b)  $\langle \psi_{\text{init}} | \psi_{\text{GS}} \rangle \neq 0, |\psi_{\text{init}}\rangle = |\psi(0)\rangle$

FORMAL SOLUTION TO SEQ IN IMAGINARY TIME:  $\psi(\tau) = e^{-\tau H} \psi(0)$

$\langle \psi_{\text{GS}} | H | \psi_{\text{GS}} \rangle = E_{\text{GS}}(H)$

BASIS REPRESENTATION WITH  $|\psi_n\rangle$ 's FULFILLING  $H\psi_n = E\psi_n, n \in \mathbb{N}$

$$\begin{aligned} \rightarrow \psi(\tau) &= \sum_{n=0}^{\infty} c_n e^{-\tau E_n} \psi_n, \quad c_n = \langle \psi_n | \psi(0) \rangle \\ &= c_0 e^{-\tau E_0} \psi_{\text{GS}} + \sum_{n=1}^{\infty} c_n e^{-\tau E_n} \psi_n \quad (\psi_0 = \psi_{\text{GS}}) \\ (\langle \psi_{\text{GS}} | \psi(0) \rangle = c_0 \neq 0) & \quad \left| \begin{aligned} &= e^{-\tau E_0} \left( c_0 \psi_{\text{GS}} + \sum_{n=1}^{\infty} c_n e^{-\tau(E_n - E_0)} \psi_n \right) \end{aligned} \right. \end{aligned}$$

NORMALIZE  $\psi(\tau)$ :

$$\frac{\psi(\tau)}{|\psi(\tau)|} = \frac{e^{-\tau E_0} (c_0 \psi_{\text{GS}} + \sum c_n e^{-\tau(E_n - E_0)} \psi_n)}{|e^{-\tau E_0} (c_0 \psi_{\text{GS}} + \sum c_n e^{-\tau(E_n - E_0)} \psi_n)|}$$

for  $\tau \rightarrow \infty$ :

$$\begin{aligned} \lim_{\tau \rightarrow \infty} \frac{|\psi(\tau)|}{|\psi(\tau)|} &= \frac{c_0 \psi_{\text{GS}} + \sum c_n e^{-\tau(E_n - E_0)} \psi_n}{|c_0 \psi_{\text{GS}} + \sum c_n e^{-\tau(E_n - E_0)} \psi_n|} \\ &\quad (E_n \geq E_0 \forall n) \\ &= \frac{c_0 \psi_{\text{GS}}}{|c_0 \psi_{\text{GS}}|} = \frac{c_0}{|c_0|} \psi_{\text{GS}} \Leftrightarrow \psi(\tau) = \frac{c_0}{|c_0|} \frac{\psi_{\text{GS}}}{|\psi(\tau)|} \end{aligned}$$

4.] c)  $|\psi_{GS}| \neq |e^{-\tau H} \psi_{GS}| = |e^{-\tau E_0} \psi_{GS}| \rightarrow e^{-\tau H} \text{ is not unitary}$

$\Rightarrow$  CONSERVATION OF PROBABILITY NOT AUTOMATICALLY  
GIVEN IN IMAGINARY TIME PROPAGATION

$\Rightarrow$  PERIODIC RENORMALIZATION NEEDED  
TO OBTAIN WAVE FUNCTIONS AFTER  
EVERY APPLICATION OF  $e^{-\tau H}$  (HERE:  $\tau$  TIMESTEP)