Zhi Chen HW#4 PHY 540

15) a) $$dE = \sum_i (E_i dp_i + p_i dE_i)$$

use Gibbs entropy formula at T, show

$$TdS = \text{đ}Q)_{rev} = \sum_i (E_i dp_i)$$

$\Rightarrow$ Gibbs: $$S = -k_B \sum_i p_i \ln p_i$$

$$dS = -k_B \sum_i \left(dp_i \ln p_i + \frac{p_i}{p_i} dp_i \right)$$

$$dS = -k_B \sum_i (\ln p_i + 1) dp_i$$

$\hookrightarrow$ $$TdS = -k_B T \sum_i (\ln p_i + 1) dp_i$$

With well-defined temperature implies canonical ensemble:

$$p_i = \exp\{-\beta E_i\} / Q$$

$$\ln p_i = -\beta E_i - \ln Q \qquad \text{where } \beta = \frac{1}{k_B T}$$

$\Rightarrow$ $$TdS = -k_B T \sum_i (-\beta E_i - \ln Q + 1) dp_i$$

$$\overset{!}{=} -\cancel{k_B T}(\cancel{-\beta}) \sum_i E_i dp_i - k_B T(-\ln Q + 1) \underbrace{\cancel{\sum_i dp_i}}_{=0}$$

note that $\sum_i dp_i = 0$ since probability always sum to 1, so the overall sum in the change of probability must be 0, i.e. $\sum_i dp_i = 0$

$$\boxed{\therefore TdS = \sum_i E_i dp_i = \text{đ}Q}$$

b) At const T and N: $dA)_{T,N} = \text{đ}W$

use. $A = \frac{-1}{\beta} \ln Q$, show $dA)_{T,N} = \text{đ}W = \sum_i P_i \, dE_i$

$$A = \frac{-1}{\beta} \ln \left(\sum_i e^{-\beta E_i} \right)$$

$$dA)_{T,N} = \cancel{\frac{-1}{\beta}} \frac{1}{Q} (\cancel{-\beta}) \sum_i e^{-\beta E_i} \, dE_i$$

$$= \frac{1}{Q} \sum_i e^{-\beta E_i} \, dE_i$$

but we know that $P_i = \frac{1}{Q} \sum_i e^{-\beta E_i}$ for canonical ensemble.

$$\boxed{\therefore \; dA)_{T,N} = \sum_i P_i \, dE_i = \text{đ}W}$$

Consider particle mass m in 1D box, length L, with $E_n = \hbar^2 \pi^2 n^2/(2mL^2)$, in thermal equilibrium with heat bath at low temp, so $\beta E_{n=1} \gg 1$, only consider first 2 quantum states

c) Find $C_L(T)$, explain result at $T=0$ in context of thermodynamic 3rd law.

heat Bath: Canonical Ensemble:

$$C_L(T) = \left(\frac{dQ}{dT}\right)_L = T\left(\frac{dS}{dT}\right)_L = \sum_n E_n \left(\frac{dP_n}{dT}\right)_L$$

$$C_L(T) = \sum_{n=1}^{2} E_n \left(\frac{\partial P_n}{\partial T}\right)_L$$

$$\stackrel{1}{=} \sum E_n \left(\frac{\partial P_n}{\partial \beta}\right)_L \left(\frac{d\beta}{dT}\right)_L$$

$$\stackrel{1}{=} \sum E_n \left(\frac{\partial P_n}{\partial \beta}\right)_L \frac{-1}{k_B T^2}$$

$$\stackrel{1}{=} \sum E_n \left(\frac{\partial}{\partial \beta} \frac{e^{-\beta E_n}}{Q}\right)_L \frac{-1}{k_B T^2}$$

$$\stackrel{1}{=} \sum E_n \left(\frac{-E_n e^{-\beta E_n}}{Q} - \frac{1}{Q^2} e^{-\beta E_n} \left(\frac{dQ}{dT}\right)_L\right) \frac{-1}{k_B T^2}$$

$$\hookrightarrow = \sum E_n \left(-E_n P_n - P_n \frac{1}{Q}\left(\frac{\partial Q}{\partial \beta}\right)_L\right) \frac{-1}{k_B T^2}$$

$$\stackrel{1}{=} \left[\sum E_n^2 P_n + E_n P_n \left(\frac{\partial}{\partial \beta} \ln Q\right)_L\right] \frac{1}{k_B T^2}$$

$$\langle E \rangle = \left(\frac{-\partial}{\partial \beta} \ln Q\right)_L$$

$$\stackrel{1}{=} \sum \left[E_n^2 P_n - E_n P_n \langle E \rangle\right] \frac{1}{k_B T^2}$$

$$\boxed{C_L(T) \stackrel{1}{=} \left(\langle E^2 \rangle - \langle E \rangle^2\right) \frac{1}{k_B T^2}}$$

For our specific system:

$$P_n = \frac{e^{-\beta E_n}}{Q} = \frac{e^{-\beta E_n}}{e^{-\beta E_1} + e^{-\beta E_2}}$$

Since $E_n = n^2 E_1 = n^2 \frac{\hbar^2 \pi^2}{2mL^2}$

$E_2 \overset{!}{=} 4E_1$

$$P_n = \frac{e^{-\beta E_n}}{e^{-\beta E_1} + e^{-4\beta E_1}}$$

$\hookrightarrow$ $$\langle E^2 \rangle = \sum E_n^2 P_n = \frac{E_1^2 e^{-\beta E_1} + (4E_1)^2 e^{-4\beta E_1}}{e^{-\beta E_1} + e^{-4\beta E_1}}$$

$$\langle E \rangle = \sum E_n P_n = \frac{E_1 e^{-\beta E_1} + 4E_1 e^{-4\beta E_1}}{e^{-\beta E_1} + e^{-4\beta E_1}}$$

$$C_L(T) = \frac{1}{k_B T^2}\left(\langle E^2\rangle - \langle E\rangle^2\right)$$

$$\overset{!}{=} \frac{1}{k_B T^2}\left\{\frac{E_1^2 e^{-\beta E_1} + 16E_1^2 e^{-4\beta E_1}}{e^{-\beta E_1} + e^{-4\beta E_1}} - \left(\frac{E_1 e^{-\beta E_1} + 4E_1 e^{-4\beta E_1}}{e^{-\beta E_1} + e^{-4\beta E_1}}\right)^2\right\}$$

$$\boxed{C_L(T) \overset{!}{=} \frac{E_1^2}{k_B T^2}\left\{\frac{1 + 16e^{-3\beta E_1}}{1 + e^{-3\beta E_1}} - \left(\frac{1 + 4e^{-3\beta E_1}}{1 + e^{-3\beta E_1}}\right)^2\right\}}$$

At low T, $\beta E_1 \gg 1$, then $e^{-\beta E_1}$ and $e^{-3\beta E_1} \to \frac{1}{e^{\infty}} \Rightarrow 0$

$$\lim_{T \to 0} C_L(T) = \frac{E_1^2}{k_B T^2}(1 - 1) = 0$$

Third law states that entropy of the system must be minimized at $T=0$

know $\quad C_L = T\left(\frac{\partial S}{\partial T}\right)_L$

$= \left(\frac{\partial S}{\partial \ln T}\right)_L$

as $T \to 0$, we know $\ln T \to -\infty$, and due to third law S must be minimized, so $S \to 0$,

then $\quad C_L \sim \frac{0}{-\infty} \Rightarrow 0$

d) Find pressure, $\left(\frac{-\partial A}{\partial L}\right)_T$, at $T=0$, show its the same as $\frac{-dE_1}{dL}$. Interpret Result

$$A = \frac{-1}{\beta}\ln Q$$
$$\stackrel{!}{=} \frac{-1}{\beta}\ln \sum e^{-\beta E_n}$$

$$\left(\frac{-\partial A}{\partial L}\right)_T = \frac{1}{\beta}\frac{1}{Q}\left(\frac{\partial Q}{\partial L}\right)_L$$
$$\stackrel{!}{=} \frac{1}{\beta}\frac{1}{Q}\left(\frac{\partial Q}{\partial E_n}\right)_L\left(\frac{\partial E_n}{\partial L}\right)_L$$
$$\stackrel{!}{=} \frac{1}{\beta}\frac{1}{Q}\,{-\beta}\, e^{-\beta E_n}\left(\frac{(n\hbar\pi)^2}{2mL^2}\frac{(-2)}{L}\right)$$
$$\stackrel{!}{=} \frac{1}{Q}e^{-\beta E_n}\frac{2}{L}E_n$$
$$\stackrel{!}{=} \sum P_n E_n \frac{2}{L}$$

For our system:

$$\left(\frac{-\partial A}{\partial L}\right)_T = \left(\frac{E_1 e^{-\beta E_1} + 4E_1 e^{-4\beta E_1}}{e^{-\beta E_1} + e^{-4\beta E_1}}\right)\frac{2}{L}$$
$$\stackrel{!}{=} \frac{2E_1}{L}\left(\frac{1+4e^{-3\beta E_1}}{1+e^{-3\beta E_1}}\right)$$

as $T \to 0$, $e^{-3\beta E_1} \to \frac{1}{\infty} \to 0$.

$$\lim_{T\to 0}\left(\frac{-\partial A}{\partial L}\right)_T = \frac{2E_1}{L}$$

Same result

and $\left(\frac{-\partial E_1}{\partial L}\right)_T = -\frac{\partial}{\partial L}\left(\frac{(n\hbar\pi)^2}{2mL^2}\right) = (-)\left(\frac{-2}{L}\right)\left(\frac{(n\hbar\pi)^2}{2mL^2}\right) = \frac{2}{L}E_1$

since $A = E - TS$, as $T \to 0$, $A \to E$. And since $T \to 0$, all states go to the lowest energy state, E_1, so $A = E = E_1$

e) Relate two meaning of adiabatic, no heat transfer and slowly varying Hamiltonian.

Consider non-adiabatic:

$\Rightarrow$ First consider suddenly $L \to 2L$:

$$E_{n,old} = \frac{(n\pi\hbar)^2}{2mL^2} \xRightarrow{L\to 2L} E_{n,new} = \frac{(n\pi\hbar)^2}{2mL^2}\left(\frac{1}{4}\right) = \frac{1}{4}E_{n,old}.$$

Since most particles occupy the lowest energy state E_1, when $E_{n,old} \to E_{n,new} = \frac{1}{4}E_{n,old}$, and $E_{1,old} = E_{2,new}$.

This means that most particles are no longer in the lowest energy state immediately after the expansion. So there will be an overall shift as particle go to the new lowest energy state, or $dp_i \neq 0$.

If $dp_i \neq 0$, and $TdS = E_i dp_i$, then there is also a change in the entropy after expansion.

$\Rightarrow$ Now, consider expansion slowly:

If expand slowly, particles can adjust their energy state accordingly and so most particles are still always in the lowest energy level. Therefore, as $L \to 2L$, all particles are still in equilibrium, which means $dp_i = 0$, and therefore entropy remains constant, then $dQ = TdS = E_i dp_i = 0$
If $dQ = 0$, we recover the same meaning of no heat transfer.

16) $\hat{\rho} = \frac{1}{Q} \sum e^{-\beta E_i} |\psi_i\rangle\langle\psi_i|$

$$= \frac{1}{Q} \begin{pmatrix} e^{-\beta E_1} & & 0 \\ & e^{-\beta E_2} & \\ 0 & & \ddots \end{pmatrix}$$

$\hat{H} = -\mu B \hat{\sigma}_z$, $\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$ $\sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$ $\sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$

a) Show $\hat{\rho} = \frac{1}{Q_1}\left[\cosh(x)\mathbb{1} + \hat{\sigma}_z \sinh(x)\right]$

$x = \beta \mu B$ $Q_1 = e^{x} + e^{-x}$

Consider 2 level system: $\hat{H} = -\mu B \hat{\sigma}_z$

$$\hat{\rho} = \frac{e^{-\beta \hat{H}}}{Q} = \frac{e^{-\beta \hat{H}}}{\mathrm{Tr}(e^{-\beta \hat{H}})}$$

$$e^{-\beta \hat{H}} = e^{\beta \mu B \hat{\sigma}_z} = e^{x \hat{\sigma}_z}$$

Taylor expand $e^{x\hat{\sigma}_z} = \sum_{n=0}^{\infty} \frac{1}{n!} (x\sigma_z)^n = \left(\sum_{n=\text{even}}^{\infty} + \sum_{n=\text{odd}}^{\infty}\right)\left(\frac{1}{n!}(x\sigma_z)^n\right)$

Split to even and odd cases:

For even case: $n = 2k$

$$\sum_{k=0}^{\infty} \frac{1}{(2k)!} (x\sigma_z)^{2k} = \sum_{k=0}^{\infty} \frac{1}{(2k)!} (x)^{2k} \underbrace{(\hat{\sigma}_z \cdot \sigma_z)^k}_{=1}$$

$$= \sum_{k=0}^{\infty} \frac{1}{(2k)!} x^{2k}$$

Same as taylor expand of $\cosh x$

$$= \cosh x$$

For odd case:

$$\sum_{k=0}^{\infty} \frac{1}{(2k+1)!} (x\hat{\sigma}_z)^{2k+1} = \sum_{k=0}^{\infty} \frac{1}{(2k+1)!} x^{2k+1} \sigma_z \underbrace{(\hat{\sigma}_z \cdot \hat{\sigma}_z)}_{=1}^{k}$$

$$= \underbrace{\sum_{k=0}^{\infty} \frac{1}{(2k+1)!} x^{2k+1}}_{=\sinh x} \sigma_z$$

$$= \hat{\sigma}_z \sinh x$$

All together $\quad e^{-\beta\hat{H}} = \sum_{k=0}^{\infty} \frac{1}{(2k)!} (x\hat{\sigma}_z)^{2k} + \sum_{k=0}^{\infty} \frac{1}{(2k+1)!} (x\hat{\sigma}_z)^{2k+1}$

$$= \mathbb{1} \cosh x + \hat{\sigma}_z \sinh x$$

$$Q = \mathrm{Tr}(e^{-\beta\hat{H}}) = \mathrm{Tr}\begin{pmatrix} \cosh x + \sinh x & 0 \\ 0 & \cosh x - \sinh x \end{pmatrix}$$

$$= \cosh x + \cancel{\sinh x} + \cosh x - \cancel{\sinh x}$$

$$= 2\cosh x$$

$\cosh x = \frac{e^{x} + e^{-x}}{2}$

$$= e^{x} + e^{-x}$$

$$\boxed{\therefore \quad \hat{\rho} = \frac{e^{-\beta\hat{H}}}{\mathrm{Tr}(e^{-\beta\hat{H}})} = \frac{1}{e^{x}+e^{-x}} \left[\mathbb{1} \cosh x + \hat{\sigma}_z \sinh x\right]}$$

b) Pure state: $\hat{\rho}^2 = \hat{\rho}$ or $Tr(\hat{\rho}^2) = 1$

Mixed state: $\hat{\rho}^2 \neq \hat{\rho}$ or $Tr(\hat{\rho}^2) < 1$

$$\hat{\rho}^2 = \left(\frac{1}{e^x + e^{-x}}\right)^2 \begin{pmatrix} \cosh x + \sinh x & 0 \\ 0 & \cosh x - \sinh x \end{pmatrix}^2$$

$$= \frac{1}{(e^x + e^{-x})^2} \begin{pmatrix} (\cosh x + \sinh x)^2 & 0 \\ 0 & (\cosh x - \sinh x)^2 \end{pmatrix}$$

$$= \frac{1}{e^{2x} + e^{-2x} + 2} \begin{pmatrix} \cosh^2 x + \sinh^2 x + 2\cosh x \sinh x & 0 \\ 0 & \cosh^2 x + \sinh^2 x - 2\cosh x \sinh x \end{pmatrix}$$

$$\cosh(2x) = \cosh^2 x + \sinh^2 x = \frac{e^{2x} + e^{-2x}}{2}$$

$$\sinh(2x) = 2\cosh x \sinh x$$

$$\boxed{\hat{\rho}^2 = \frac{1}{2(1 + \cosh 2x)} \begin{pmatrix} \cosh 2x + \sinh 2x & 0 \\ 0 & \cosh 2x - \sinh 2x \end{pmatrix}}$$

we see $\hat{\rho}^2 \neq \hat{\rho}$, so mixed state.

c) Find $\langle E \rangle$, $\langle M_z \rangle$, and $\langle M_x \rangle$

$$\langle E \rangle = \mathrm{Tr}(\hat{\rho}\hat{H}) \qquad \text{where } \hat{H} = -uB\hat{\sigma}_z = -uB\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

$$\overset{!}{=} \frac{1}{Q}\mathrm{Tr}\left\{\begin{pmatrix} \cosh x + \sinh x & 0 \\ 0 & \cosh x - \sinh x \end{pmatrix}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}\right\}(-uB)$$

$$\overset{|}{=} \frac{-uB}{Q_1}\mathrm{Tr}\left\{\begin{pmatrix} \cosh x + \sinh x & 0 \\ 0 & -\cosh x + \sinh x \end{pmatrix}\right\}$$

$$\overset{|}{=} \frac{-uB}{Q_1}\left[\cosh x + \sinh x - \cosh x + \sinh x\right]$$

$$\overset{!}{=} \frac{-uB}{Q_1} 2\sinh x$$

$$\overset{!}{=} -uB \frac{2\sinh x}{2\cosh x}$$

$$\boxed{\langle E \rangle \overset{!}{=} -uB\tanh x \text{ for 1 particle}, \quad \langle E \rangle \overset{!}{=} -NuB\tanh x}$$

for N particles

$$\langle M_z \rangle = \mathrm{Tr}\{\hat{\rho}\, u\hat{\sigma}_z\}$$

$$\overset{!}{=} \frac{\langle E \rangle}{-B}$$

$$\boxed{\langle M_z \rangle \overset{!}{=} u\tanh x \quad \Rightarrow \langle M_z \rangle \overset{!}{=} Nu\tanh x}$$

for N particles

$$\langle M_x \rangle = \mathrm{Tr}\{\hat{\rho}\, u\hat{\sigma}_x\}$$

$$\overset{!}{=} \frac{u}{Q_1}\mathrm{Tr}\Big\{\underbrace{\begin{pmatrix} \cosh x + \sinh x & 0 \\ 0 & \cosh x - \sinh x \end{pmatrix}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}}_{\mathrm{Tr}\left\{\begin{pmatrix} 0 & \cosh x + \sinh x \\ \cosh x - \sinh x & 0 \end{pmatrix}\right\} = 0}\Big\}$$

$$\boxed{\langle M_x \rangle \overset{|}{=} 0}$$

d) Find entropy of the system:

$$S = -k_B P_i \ln P_i = -\mathrm{Tr}\{\hat{\rho}\ln\hat{\rho}\}$$

What happens when $T \to \infty$? Does the result make sense

$$\hat{\rho} = \frac{1}{Q_1}\begin{pmatrix} \cosh x + \sinh x & 0 \\ 0 & \cosh x - \sinh x \end{pmatrix}$$

then $P_1 = \dfrac{\cosh x + \sinh x}{Q_1}$

$P_2 = \dfrac{\cosh x - \sinh x}{Q_1}$

$$S = -k_B\left[\frac{\cosh x + \sinh x}{Q_1}\ln\left(\frac{\cosh x + \sinh x}{Q_1}\right) + \frac{\cosh - \sinh x}{Q_1}\ln\left(\frac{\cosh - \sinh x}{Q_1}\right)\right]$$

$$\cosh x + \sinh x = \frac{1}{2}\left(e^{x} + e^{-x} + e^{x} - e^{-x}\right) = e^{x}$$

$$\cosh x - \sinh x = \frac{1}{2}\left(e^{x} + e^{-x} - e^{x} + e^{-x}\right) = e^{-x}$$

$$\stackrel{!}{=} -k_B\left[\frac{e^{x}}{Q_1}\ln\left(\frac{e^{x}}{Q_1}\right) + \frac{e^{-x}}{Q_1}\ln\left(\frac{e^{-x}}{Q_1}\right)\right]$$

$$\stackrel{!}{=} -k_B\left[\frac{e^{x}}{Q_1}(x - \ln Q_1) + \frac{e^{-x}}{Q_1}(-x - \ln Q_1)\right]$$

$Q_1 = e^{x} + e^{-x} = 2\cosh x$

$$\stackrel{!}{=} -k_B\left[x\left(\frac{e^{x} - e^{-x}}{Q_1}\right) - \ln Q_1\left(\frac{e^{x} + e^{-x}}{Q_1}\right)\right]$$

$$\stackrel{!}{=} \frac{-k_B}{2\cosh x}\left[2x\sinh x - 2\ln Q_1 \cosh x\right]$$

$$S \stackrel{!}{=} -Nk_B\left[x\tanh(x) - \ln Q_1\right]$$

extra factor of N to account for N-particles as $T \to \infty$, $x = \beta \mu B \propto \frac{1}{T} \to 0$

$$S = -k_B[x\tanh(x) - \ln Q_1] = -k_B[x\tanh x - \ln(2\cosh x)]$$

$$\lim_{x \to 0} S = k_B \ln Q_1$$

$$\stackrel{!}{=} k_B \ln(e^{-0} + e^{0})$$

$$\stackrel{!}{=} k_B \ln(2)$$

For N particles:

$$\lim_{T \to \infty} S = N k_B \ln 2$$

It makes sense since as $T \to \infty$, it becomes equal likely for the particle to occupy both energy levels. Thus we shift from canonical to microcanical ensemble. where $S = k_B \ln \Omega$. For two level system $\Omega = 2$

hence $S = k_B \ln 2$ for a single particle.

e) Verify $dE = TdS - M_z dB$

from previous parts

$$\langle E \rangle = E = -N\mu B \tanh x$$
$$\langle M_z \rangle = N\mu \tanh x$$
$$S = -Nk_B [x \tanh x - \ln(2\cosh x)]$$

$$dE = TdS - M_z\, dB$$

then $T = \frac{\partial E}{\partial S}$ and $-M_z = \frac{\partial E}{\partial B}$

$$x = \beta\mu B = \frac{\mu B}{k_B T}$$

Rewrite E: $E = -N\mu B \tanh x = -N k_B T x \tanh x$

know $S = -Nk_B x \tanh x + Nk_B \ln(2\cosh x)$

$$T\left(S - Nk_B \ln(2\cosh x)\right) = -Nk_B T\, x \tanh x$$

$$E = TS - Nk_B T \ln\left(2\cosh \frac{\mu B}{k_B T}\right)$$

$$\boxed{\left(\frac{\partial E}{\partial S}\right)_B = T \quad \checkmark}$$

$$\boxed{\begin{aligned}\left(\frac{\partial E}{\partial B}\right)_S &= -Nk_B T \frac{1}{2\cosh\left(\frac{\mu B}{k_B T}\right)} 2\sinh\left(\frac{\mu B}{k_B T}\right)\frac{\mu}{k_B T} \\ &\stackrel{!}{=} -N\mu \tanh\left(\frac{\mu B}{k_B T}\right) \\ &\stackrel{!}{=} -M_z \quad \checkmark\end{aligned}}$$

f) $|\phi\rangle = \sqrt{\frac{e^{x}}{Q_1}}\,|\uparrow\rangle + \sqrt{\frac{e^{-x}}{Q_1}}\,|\downarrow\rangle$

$$\hat{\rho} = 1\,|\phi\rangle\langle\phi|$$

$$= \frac{1}{Q_1}\begin{pmatrix} e^{\frac{x}{2}} \\ e^{-\frac{x}{2}} \end{pmatrix}\begin{pmatrix} e^{\frac{x}{2}} & e^{-\frac{x}{2}} \end{pmatrix}$$

$$\boxed{\hat{\rho} = \frac{1}{Q_1}\begin{pmatrix} e^{x} & 1 \\ 1 & e^{-x} \end{pmatrix}}$$

$$\hat{\rho}^2 = \frac{1}{Q_1^2}\begin{pmatrix} e^{x} & 1 \\ 1 & e^{-x} \end{pmatrix}\begin{pmatrix} e^{x} & 1 \\ 1 & e^{-x} \end{pmatrix}$$

$$= \frac{1}{Q_1^2}\begin{pmatrix} e^{2x}+1 & e^{x}+e^{-x} \\ e^{x}+e^{-x} & 1+e^{-2x} \end{pmatrix}$$

$$= \frac{1}{Q_1^2}\underbrace{(e^{x}+e^{-x})}_{=Q_1}\begin{pmatrix} \frac{e^{2x}+1}{e^{x}+e^{-x}} & 1 \\ 1 & \frac{1+e^{-2x}}{e^{x}+e^{-x}} \end{pmatrix}$$

$$= \frac{1}{Q_1}\begin{pmatrix} e^{x}\left(\cancel{\frac{e^{x}+e^{-x}}{e^{x}+e^{-x}}}\right) & 1 \\ 1 & e^{-x}\left(\cancel{\frac{e^{x}+e^{-x}}{e^{x}+e^{-x}}}\right) \end{pmatrix}$$

$$\boxed{\hat{\rho}^2 = \underbrace{\frac{1}{Q_1}\begin{pmatrix} e^{x} & 1 \\ 1 & e^{-x} \end{pmatrix}}_{\hat{\rho}} \quad \text{so} \quad \hat{\rho}^2 = \hat{\rho}}$$

g) Find $\sigma = -\mathrm{Tr}(\hat{\rho}\ln\hat{\rho}) = -\lambda_i \ln \lambda_i$

$$\hat{\rho} = \frac{1}{Q_1}\begin{pmatrix} e^{x} & 1 \\ 1 & e^{-x} \end{pmatrix}$$

Find eigenvalues of $\hat{\rho}$:

$$|\hat{\rho} - \lambda \mathbb{1}| = \frac{1}{Q_1}\begin{vmatrix} e^{x}-\lambda & 1 \\ 1 & e^{-x}-\lambda \end{vmatrix} = 0$$

$\hookrightarrow (e^{x}-\lambda)(e^{-x}-\lambda) - 1 = 0$

$\hookrightarrow 1 - \lambda e^{-x} - \lambda e^{x} + \lambda^2 - 1 = 0$

$$\lambda^2 - \lambda(\underbrace{e^{-x} + e^{x}}_{Q_1}) = 0$$

$$\lambda(\lambda - Q_1) = 0$$

$$\lambda = 0, Q_1$$

$$\hat{\rho} = \frac{1}{Q_1}\begin{pmatrix} Q_1 & 0 \\ 0 & 0 \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}$$

$$\sigma = -\lambda_i \ln \lambda_i = \underbrace{\cancel{0\ln 0} - 1\ln(1)}_{\boxed{\sigma = 0}}$$

h) Find $\langle M_z \rangle$ and $\langle M_x \rangle$

$$\langle M_z \rangle = \mathrm{Tr}\{\hat{\rho}\, u \hat{\sigma}_z\}$$

$$\stackrel{!}{=} \frac{u}{Q_1}\mathrm{Tr}\left\{\begin{pmatrix} e^x & 1 \\ 1 & e^{-x}\end{pmatrix}\begin{pmatrix} 1 & 0 \\ 0 & -1\end{pmatrix}\right\}$$

$$\stackrel{!}{=} \frac{u}{Q_1}\mathrm{Tr}\left\{\begin{pmatrix} e^x & -1 \\ 1 & -e^{-x}\end{pmatrix}\right\}$$

$$\stackrel{!}{=} \frac{u}{Q_1}\left(e^x - e^{-x}\right)$$

$$\stackrel{!}{=} u\,\frac{2\sinh x}{2\cosh x}$$

$$\langle M_z \rangle \stackrel{!}{=} u \tanh x$$

get same answer for $\langle M_z \rangle$ compared to part c, since pure state and mixed state have the same diagonal terms

for N particles: $\langle M_z \rangle_{tot} = N\langle M_z \rangle = N u \tanh x$

$$\langle M_x \rangle = \mathrm{Tr}\{\rho\, u \hat{\sigma}_x\}$$

$$\stackrel{!}{=} \frac{u}{Q_1}\mathrm{Tr}\left\{\begin{pmatrix} e^x & 1 \\ 1 & e^{-x}\end{pmatrix}\begin{pmatrix} 0 & 1 \\ 1 & 0\end{pmatrix}\right\}$$

$$\stackrel{!}{=} \frac{u}{Q_1}\mathrm{Tr}\left\{\begin{matrix} 1 & e^x \\ e^{-x} & 1\end{matrix}\right\}$$

$$= \frac{u}{2\cosh x}(1+1)$$

$$\langle M_x \rangle \stackrel{!}{=} \frac{u}{\cosh x}$$

Here, we have a nonzero $\langle M_x \rangle$, compared to $\langle M_x \rangle = 0$ in part c. This is because in this pure state, we have non-zero off diagonal terms that are associated with σ_x, whereas the mix state is purely in $+z$ or $-z$ spin.

For N particles:

$$\langle M_x \rangle_{tot} = N\langle M_x \rangle = \frac{Nu}{\cosh x}$$

17) a) $$H(X) = -\sum_{x \in \mathcal{X}} P_x \log_2 P_x$$

vs. $$S = -k_B P_n \ln P_n$$

Show using $\log_2$ vs. $\ln$ is equivalent to changing the definition of k_B or T.

$$S = -k_B P_n \ln P_n = -k_B P_n \log_e (P_n)$$

know $$\log_b x = \frac{\log_y x}{\log_y b}$$

then $$\log_e x = \frac{\log_2 x}{\log_2 e} = \log_2 x \ln 2$$

$$\boxed{\begin{array}{l} \hookrightarrow S = -k_B \ln 2 \, P_n \log_2 P_n \\ \text{So here we change } k_B \Rightarrow k_B \ln 2 = k_B' \\ \text{or: } \frac{1}{T} = \left(\frac{\partial S}{\partial E}\right)_{N,V} = -k_B \ln 2 \frac{\partial}{\partial E}\left(P_n \log_2 P_n\right)_{N,V} \\ \left.\begin{array}{l} \frac{1}{\ln(2) T} = -k_B \frac{\partial}{\partial E}\left(P_n \log_2 P_n\right)_{N,V} \\ \text{vs. } \frac{1}{T} = -k_B \frac{\partial}{\partial E}\left(P_n \ln P_n\right)_{N,V} \end{array}\right\} T \to T' = \ln(2) T \\ \qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad \uparrow \\ \qquad\qquad\qquad\qquad\qquad\qquad\qquad \text{new Temp} \end{array}}$$

For 2 level microcanonical ensemble, $P_n = \frac{1}{\Omega} = \frac{1}{2}$

$$S = -\underbrace{k_B \ln(2)}_{k_B'} \frac{1}{2} \log_2 \frac{1}{2} = k_B \ln(2)$$

$\nearrow$ Same answer.

b) Show Shanon's entropy scales linearly with # of symbols sent, which means it is extensive.

For a single symbol X from alphabet $\mathcal{X}$:

$$H(X) = -\sum_{x \in \mathcal{X}} P_x \log_2 P_x$$

Now if we have a second symbol y from $\mathcal{Y}$:

$$H = -\sum_{x \in \mathcal{X}} \sum_{y \in \mathcal{Y}} P_x P_y \log_2 (P_x P_y)$$

$$= -\sum_{x \in \mathcal{X}} \sum_{y \in \mathcal{Y}} P_x P_y \log_2 P_x - \sum_{x \in \mathcal{X}} \sum_{y \in \mathcal{Y}} P_x P_y \log_2 P_y$$

if we sum over P_y in $P_x P_y \log_2 P_x$, or sum over P_x in $P_x P_y \log_2 P_y$, we get 1, since probability sum to 1:

$$= \underbrace{-\sum_{x \in \mathcal{X}} P_x \log_2 P_x}_{H(X)} \underbrace{- \sum_{y \in \mathcal{Y}} P_y \log_2 P_y}_{H(Y)}$$

Similarly for N different symbols we just sum over all entropy for each symbol

$$\boxed{H = \sum_{i=1}^{N} H_i}$$ ← which means shannons entropy is extensive.

So $H \propto N$

c) Show H is maximized when all symbols have equal possibility.

$$H(x) = \sum_{x \in \mathcal{X}} -P_x \log_2 P_x$$

Subject to the constraint that $\sum_{x \in X} P_x = 1$, possibility sum to 1.

$$H(X, \lambda) = \sum_{x \in X} -P_x \log_2 P_x - \lambda\left(\sum_{x \in X} P_x - 1\right)$$

$$\frac{\partial H}{\partial \lambda} = \sum_{x \in X} P_x - 1 = 0$$

$$\frac{\partial H}{\partial P_x} = \sum_{x \in X} \left(\underbrace{-\log_2 P_x - \cancel{P_x}\frac{1}{\cancel{P_x}\ln(2)} - \lambda}_{0}\right) = 0$$

$$\log_2 P_x = -(\log_2 e - \lambda)$$

$$\text{or} \quad P_x = 2^{-\log_2 e - \lambda} = \frac{1}{e} 2^{-\lambda}$$

$$\text{Then} \quad \sum_{x \in X} P_x = \sum_{x \in X} \frac{1}{e} 2^{-\lambda}$$

① Suppose there are m different symbols

② and use constraint $\sum_{x \in X} P_x = 1$

$$\sum_{x \in X} P_x = 1 = m \frac{1}{e} 2^{-\lambda}$$

but we know $P_x = \frac{1}{e} 2^{-\lambda}$

then $1 = m P_x$

$$\boxed{P_x = \frac{1}{m}} \leftarrow \text{Equal Probability}$$

d) Consider 4 symbols: A, B, C, D.
with $P_A = 1/2$, $P_B = 1/4$, $P_C = P_D = 1/8$

Derive an unambiguous binary coding scheme that accomplish this optimum encoding.

use 7/4 bits per symbol

let

$A \Leftrightarrow 0$
$B \Leftrightarrow 10$
$C \Leftrightarrow 110$
$D \Leftrightarrow 111$

so that we use less bits to represent symbols that occur more frequently to reduce the average symbols per bit.

then

$$\langle bits \rangle = \sum P_i (bits)$$
$$= \left(\tfrac{1}{2}\right)(1) + \left(\tfrac{1}{4}\right)(2) + \tfrac{1}{8}(3) + \tfrac{1}{8}(3)$$
$$= 1.75 \text{ bits per symbol}$$

e) Estimate energy required to charge a 7nm MOSFET transistor gate to 1V, compare to Landauer limit: 2.9×10^{-21} J at RT

Energy required to charge MOSFET is given by:

$$E = \tfrac{1}{2} C V^2 \qquad \text{where } C \cong \varepsilon \tfrac{A}{d}$$

For a 7nm MOSFET, approximate $\frac{A}{d} \sim 10^{-8}$ m, and due to the material used, $\varepsilon \sim 30\,\varepsilon_0$

$$E = \tfrac{1}{2}(30)(8.85 \times 10^{-12})(10^{-8})(1V)^2 \approx 10^{-18} J$$

which is much greater than Landauer limit at room temperature which is 2.9×10^{-21} J.

f) Calculate the reduced density matrix for the qubit and the entanglement entropy :

$$|\Psi\rangle = \frac{1}{\sqrt{2}}|0\rangle \otimes \left(\sum_i c_i |\Phi_i^{(0)}\rangle\right) + \frac{1}{\sqrt{2}}|1\rangle \otimes \left(\sum_i d_i |\Phi_i^{(1)}\rangle\right)$$

$$\stackrel{!}{=} \frac{1}{\sqrt{2}} \sum_i c_i |0, \Phi_i^{(0)}\rangle + \frac{1}{\sqrt{2}} \sum_i d_i |1, \Phi_i^{(1)}\rangle$$

$$\hat{\rho}_{tot} = |\Psi\rangle\langle\Psi|$$

$$\stackrel{!}{=} \frac{1}{2}\Big\{ \sum_i \sum_j c_i c_j^* |0, \Phi_i^{(0)}\rangle\langle 0, \Phi_j^{(0)}|$$

$$+ \sum_i \sum_j c_i d_j^* |0, \Phi_i^{(0)}\rangle\langle 1, \Phi_j^{(1)}|$$

$$+ \sum_i \sum_j d_i c_j^* |1, \Phi_i^{(1)}\rangle\langle 0, \Phi_j^{(0)}|$$

$$+ \sum_i \sum_j d_i d_j^* |1, \Phi_i^{(1)}\rangle\langle 1, \Phi_j^{(1)}| \Big\}$$

$$\hat{\rho}_{qubit} = \mathrm{Tr}_{apparatus}\{\rho_{tot}\}$$

$$\stackrel{!}{=} \left(\mathbb{1}_{qubit} \otimes \langle\Phi_k^{(0)}|\right) \hat{\rho}_{tot} \left(\mathbb{1}_{qubit} \otimes |\Phi_k^{(0)}\rangle\right)$$

$$+ \left(\mathbb{1}_{qubit} \otimes \langle\Phi_k^{(1)}|\right) \hat{\rho}_{tot} \left(\mathbb{1}_{qubit} \otimes |\Phi_k^{(1)}\rangle\right)$$

$$\stackrel{!}{=} \hat{\rho}_{qubit}^{(0)} + \hat{\rho}_{qubit}^{(1)}$$

$$\mathbb{1}_{qubit} = |0\rangle\langle 0| + |1\rangle\langle 1|$$

$$\Rightarrow \mathbb{1}_{qubit} \otimes \langle \Phi_k| = (|0\rangle\langle 0| + |1\rangle\langle 1|) \otimes \langle \Phi_k|$$

$$\overset{!}{=} |0\rangle\langle 0| \otimes \langle \Phi_k| + |1\rangle\langle 1| \otimes \langle \Phi_k|$$

$$\overset{!}{=} |0\rangle\langle 0, \Phi_k| + |1\rangle\langle 1, \Phi_k|$$

$$\Rightarrow \mathbb{1}_{qubit} \otimes |\Phi_k\rangle = (|0\rangle\langle 0| + |1\rangle\langle 1|) \otimes |\Phi_k\rangle$$

$$\overset{!}{=} |0\rangle\langle 0| \otimes |\Phi_k\rangle + |1\rangle\langle 1| \otimes |\Phi_k\rangle$$

$$\overset{!}{=} |0\rangle \otimes |\Phi_k\rangle \langle 0| + |1\rangle \otimes |\Phi_k\rangle \langle 1|$$

$$\overset{!}{=} |0, \Phi_k\rangle\langle 0| + |1, \Phi_k\rangle\langle 1|$$

$$\hat{\rho}_{qubit}^{(0)} = (|0\rangle\langle 0, \Phi_k^{(0)}| + |1\rangle\langle 1, \Phi_k^{(0)}|)$$

$$\frac{1}{2}\Big(c_i c_j^* |0, \Phi_i^{(0)}\rangle\langle 0, \Phi_j^{(0)}| + c_i d_j^* |0, \Phi_i^{(0)}\rangle\langle 1, \Phi_j^{(1)}|$$

$$+ d_i c_j^* |1, \Phi_i^{(1)}\rangle\langle 0, \Phi_j^{(0)}| + d_i d_j^* |1, \Phi_i^{(1)}\rangle\langle 1, \Phi_j^{(1)}| \Big)$$

$$(|0, \Phi_k^{(0)}\rangle\langle 0| + |1, \Phi_k^{(0)}\rangle\langle 1|)$$

note: $\langle 0, \Phi_k^{(0)} | 0, \Phi_i^{(0)}\rangle = \delta_{ki}$

$$= \frac{1}{2}\Big(c_k c_j^* |0\rangle\langle 0, \Phi_j^{(0)}| + c_k d_j^* |0\rangle\langle 1, \Phi_j^{(1)}| \Big)\Big(|0, \Phi_k^{(0)}\rangle\langle 0| + |1, \Phi_k^{(0)}\rangle\langle 1| \Big)$$

note: $\langle 0, \Phi_j^{(0)} | 0\, \Phi_k^{(0)}\rangle = \delta_{jk}$

$$\Rightarrow \hat{\rho}_{qubit}^{(0)} = \frac{1}{2}\left(|c_k|^2 |0\rangle\langle 0| \right)$$

$$\rho^{(1)}_{qubit} = \left(|0\rangle\langle 0, \Phi^{(1)}_K| + |1\rangle\langle 1, \Phi^{(1)}_K| \right)$$

$$\frac{1}{2}\Big(c_i c_j^* |0, \Phi_i^{(0)}\rangle\langle 0, \Phi_j^{(0)}| + c_i d_j^* |0, \Phi_i^{(0)}\rangle\langle 1, \Phi_j^{(1)}|$$

$$+ d_i c_j^* |1, \Phi_i^{(1)}\rangle\langle 0, \Phi_j^{(0)}| + d_i d_j^* |1, \Phi_i^{(1)}\rangle\langle 1, \Phi_j^{(1)}| \Big)$$

$$\left(|0, \Phi^{(1)}_K\rangle\langle 0| + |1, \Phi^{(1)}_K\rangle\langle 1| \right)$$

$$\overset{!}{=} \frac{1}{2}\left(d_K c_j^* |1\rangle\langle 0, \Phi_j^{(0)}| + d_K d_j^* |1\rangle\langle 1, \Phi_j^{(1)}| \right)$$

$$\left(|0, \Phi^{(1)}_K\rangle\langle 0| + |1, \Phi^{(1)}_K\rangle\langle 1| \right)$$

$$\hat{\rho}^{(1)}_{qubit} \overset{!}{=} \frac{1}{2}\left(|d_K|^2 |1\rangle\langle 1| \right)$$

$$\boxed{\begin{aligned} \hat{\rho}_{qubit} &= \hat{\rho}^{(0)}_{qubit} + \hat{\rho}^{(1)}_{qubit} \\ &\overset{!}{=} \frac{1}{2}\left(|c_K|^2 |0\rangle\langle 0| + |d_K|^2 |1\rangle\langle 1| \right) \\ &\overset{!}{=} \frac{1}{2}\begin{pmatrix} |c_K|^2 & 0 \\ 0 & |d_K|^2 \end{pmatrix} \end{aligned}}$$

$$S(\hat{\rho}_{qubit}) = -\mathrm{Tr}\left(\rho_{qubit} \ln \rho_{qubit}\right) = -\sum_j \lambda_j \ln \lambda_j$$

clearly eigenvalues are $\frac{|c_K|^2}{2}$ and $\frac{|d_K|^2}{2}$

so $$\boxed{S(\hat{\rho}_{qubit}) = -\frac{|c_K|^2}{2} \ln\left(\frac{|c_K|^2}{2}\right) - \frac{|d_K|^2}{2} \ln\left(\frac{|d_K|^2}{2}\right)}$$

18) $V(z) = \begin{cases} mgz & z \geq 0 \\ \infty & z < 0 \end{cases}$

with eigenstate:

$$\psi_n(z') = \begin{cases} N_n A_i(z' - |z_n|) & z \geq 0 \\ 0 & z < 0 \end{cases}$$

a)

$$|\psi\rangle = \sum_n \underbrace{\sqrt{\frac{e^{-\beta E_n}}{Q}}}_{c_n} |\psi_n\rangle$$

$$\stackrel{!}{=} \sqrt{\frac{e^{-\beta E_n}}{Q}} N_n A_i(z' - |z_n|)$$

$$\langle E_n \rangle = \langle \psi_n | E | \psi_n \rangle = \sum P_n E_n$$

$$\stackrel{!}{=} \sum \frac{e^{-\beta E_n}}{Q} E_n$$

let $\frac{k_B T}{mg l_g} = X$

$$-\beta E_n = \frac{-E_n}{mg l_g} \frac{mg l_g}{k_B T} = \frac{z_n}{X}$$

see graph from code

then $\langle E_n \rangle = \sum \frac{e^{z_n/X}}{Q} E_n$

b) $\langle z \rangle = \langle \psi_n | z | \psi_n \rangle$

$$\stackrel{!}{=} \int_0^\infty z' |N_n|^2 A_i(z' - |z_n|)^2 dz' \sum \frac{e^{z_n/X}}{Q}$$

c) $P(z') = \sum \frac{e^{z_n/X}}{Q} |N_n|^2 A_i(z' - |z_n|)^2$

where $|N_n|^2 = \frac{1}{\int_0^\infty A_i(z' - |z_n|)^2}$