Problem 18:

a) $\hat{\rho}(0) = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}$ (2)

b) $\hat{S}_z^2 = \hbar^2 \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}$ $\quad \hat{S}_x^2 = \frac{\hbar^2}{2} \begin{pmatrix} 1 & 0 & 1 \\ 0 & 2 & 0 \\ 1 & 0 & 1 \end{pmatrix}$ $\quad \hat{S}_y^2 = -\frac{\hbar^2}{2} \begin{pmatrix} -1 & 0 & 1 \\ 0 & -2 & 0 \\ 1 & 0 & -1 \end{pmatrix}$

$$\Rightarrow \hat{H} = \hbar^2 \begin{pmatrix} A & 0 & B \\ 0 & 0 & 0 \\ B & 0 & A \end{pmatrix} \quad (2)$$

eigenvalues: $\hbar^2(A+B), 0, \hbar^2(A-B)$ (1)

eigenvectors: $\hbar^2(A+B): \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ 0 \\ 1 \end{pmatrix}$ $\quad 0: \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}$ $\quad \hbar^2(A-B): \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ 0 \\ -1 \end{pmatrix}$

$$U = \begin{pmatrix} \frac{1}{\sqrt{2}} & 0 & \frac{1}{\sqrt{2}} \\ 0 & 1 & 0 \\ \frac{1}{\sqrt{2}} & 0 & -\frac{1}{\sqrt{2}} \end{pmatrix} \Rightarrow U^{-1} = \begin{pmatrix} \frac{1}{\sqrt{2}} & 0 & \frac{1}{\sqrt{2}} \\ 0 & 1 & 0 \\ \frac{1}{\sqrt{2}} & 0 & -\frac{1}{\sqrt{2}} \end{pmatrix} = U \quad (1)$$

$$\cancel{e^{\frac{i}{\hbar}\hat{H}t}} = \quad \hat{H} = \hbar^2 U \begin{pmatrix} A+B & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & A-B \end{pmatrix} U^{-1}$$

$$\Rightarrow e^{\frac{i}{\hbar}\hat{H}t} = U \begin{pmatrix} e^{i\hbar(A+B)t} & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & e^{i\hbar(A-B)t} \end{pmatrix} U^{-1}$$

$$\begin{pmatrix} e^{i\hbar(A+B)t} & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & e^{i\hbar(A-B)t} \end{pmatrix} \begin{pmatrix} \frac{1}{\sqrt{2}} & 0 & \frac{1}{\sqrt{2}} \\ 0 & 1 & 0 \\ \frac{1}{\sqrt{2}} & 0 & -\frac{1}{\sqrt{2}} \end{pmatrix}$$

$$= \begin{pmatrix} \frac{1}{\sqrt{2}} & 0 & \frac{1}{\sqrt{2}} \\ 0 & 1 & 0 \\ \frac{1}{\sqrt{2}} & 0 & -\frac{1}{\sqrt{2}} \end{pmatrix} \begin{pmatrix} \frac{1}{\sqrt{2}} e^{i\hbar(A+B)t} & 0 & \frac{1}{\sqrt{2}} e^{i\hbar(A+B)t} \\ 0 & 1 & 0 \\ \frac{1}{\sqrt{2}} e^{i\hbar(A-B)t} & 0 & -\frac{1}{\sqrt{2}} e^{i\hbar(A-B)t} \end{pmatrix} \begin{pmatrix} e^{i\hbar At} \cos \hbar Bt & 0 & i e^{i\hbar At} \sin \hbar Bt \\ 0 & 1 & 0 \\ i e^{i\hbar At} \sin \hbar Bt & 0 & e^{i\hbar At} \cos \hbar Bt \end{pmatrix} \quad (2)$$

$$\hat\rho(t) = e^{-\frac{i}{\hbar}\hat H t}\,\hat\rho(0)\,e^{\frac{i}{\hbar}\hat H t}$$

$$\begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} e^{i\hbar At}\cos\hbar Bt & 0 & ie^{i\hbar At}\sin\hbar Bt \\ 0 & 1 & 0 \\ ie^{i\hbar At}\sin\hbar Bt & 0 & e^{i\hbar At}\cos\hbar Bt \end{pmatrix}$$

$$= \begin{pmatrix} e^{-i\hbar At}\cos\hbar Bt & 0 & -ie^{-i\hbar At}\sin\hbar Bt \\ 0 & 1 & 0 \\ -ie^{-i\hbar At}\sin\hbar Bt & 0 & e^{-i\hbar At}\cos\hbar Bt \end{pmatrix}\begin{pmatrix} e^{-i\hbar At}\cos\hbar Bt & 0 & 0 \\ 0 & 0 & 0 \\ -ie^{-i\hbar At}\sin\hbar Bt & 0 & 0 \end{pmatrix}$$

$$= \begin{pmatrix} \cos^2\hbar Bt & 0 & i\cos\hbar Bt\sin\hbar Bt \\ 0 & 0 & 0 \\ -i\cos\hbar Bt\sin\hbar Bt & 0 & \sin^2\hbar Bt \end{pmatrix} \quad (2)$$

c) $\langle\hat S_z(t)\rangle = \mathrm{Tr}\,\hat S_z\hat\rho(t) = \hbar\,\mathrm{Tr}\begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix}\begin{pmatrix} \cos^2\hbar Bt & 0 & i\cos\hbar Bt\sin\hbar Bt \\ 0 & 0 & 0 \\ -i\cos\hbar Bt\sin\hbar Bt & 0 & \sin^2\hbar Bt \end{pmatrix}$

$$= \hbar\left[\cos^2\hbar Bt - \sin^2\hbar Bt\right] = \hbar\cos 2\hbar Bt \quad (2)$$

Problem 19:

Since $\mathrm{Tr}\, AB^+ = \langle A, B\rangle$ is a scalar product, it fulfils the Cauchy-Schwarz inequality

$$|\langle A,B\rangle| \le \|A\|\,\|B\| = \sqrt{\langle A,A\rangle}\sqrt{\langle B,B\rangle}$$

$$\Rightarrow |\mathrm{Tr}\, AB^+| \le \sqrt{\mathrm{Tr}\, AA^+}\sqrt{\mathrm{Tr}\, BB^+}$$

a) $A = \hat\varrho_1^{1/2}$ $\quad B = \hat\varrho_2^{1/2}$ $\quad B^+ = B$ (ϱ_2 hermitian)

$$\Rightarrow \left|\mathrm{Tr}\, \hat\varrho_1^{1/2}\hat\varrho_2^{1/2}\right| \le \sqrt{\mathrm{Tr}\, \hat\varrho_1^{1/2}\hat\varrho_1^{1/2}}\sqrt{\mathrm{Tr}\, \hat\varrho_2^{1/2}\hat\varrho_2^{1/2}}$$

$$= \sqrt{\mathrm{Tr}\, \hat\varrho_1}\sqrt{\mathrm{Tr}\, \hat\varrho_2} = 1\cdot 1 = 1$$

$$\langle \hat\varrho_1^{1/2}, \hat\varrho_2^{1/2}\rangle = \mathrm{Tr}\, \hat\varrho_1^{1/2}(\hat\varrho_2^{1/2})^+ = \mathrm{Tr}\, \hat\varrho_1^{1/2}\hat\varrho_2^{1/2} = \mathrm{Tr}\, (\hat\varrho_1^{1/2})^+\hat\varrho_2^{1/2} = \mathrm{Tr}\, \hat\varrho_2^{1/2}(\hat\varrho_1^{1/2})^+$$
$$= \langle \hat\varrho_2^{1/2}, \hat\varrho_1^{1/2}\rangle$$

$\Rightarrow \langle \hat\varrho_1^{1/2}, \hat\varrho_2^{1/2}\rangle = \mathrm{Tr}\, \hat\varrho_1^{1/2}\hat\varrho_2^{1/2}$ real

$$\Rightarrow \mathrm{Tr}\, \hat\varrho_1^{1/2}\hat\varrho_2^{1/2} \le 1$$

b) $\mathrm{Tr}\, \hat\varrho_1^{1-2^{-n}}\hat\varrho_2^{2^{-n}}$ real for the same reason

$n=1$: see part a)

$n-1 \to n$: $\mathrm{Tr}\, \hat\varrho_1^{1-2^{-n}}\hat\varrho_2^{2^{-n}} = \mathrm{Tr}\, \hat\varrho_1^{1/2}\hat\varrho_1^{\frac12-2^{-n}}\hat\varrho_2^{2^{-n}} = \mathrm{Tr}\, \hat\varrho_1^{1/2}\left(\hat\varrho_2^{2^{-n}}\hat\varrho_1^{\frac12-2^{-n}}\right)^+$

$$= \langle \hat\varrho_1^{1/2}, \hat\varrho_2^{2^{-n}}\hat\varrho_1^{\frac12-2^{-n}}\rangle \le \left|\langle \hat\varrho_1^{1/2}, \hat\varrho_2^{2^{-n}}\hat\varrho_1^{\frac12-2^{-n}}\rangle\right|$$

$$\le \sqrt{\mathrm{Tr}\, \hat\varrho_1^{1/2}(\hat\varrho_1^{1/2})^+}\sqrt{\mathrm{Tr}\, \hat\varrho_2^{2^{-n}}\hat\varrho_1^{\frac12-2^{-n}}\left(\hat\varrho_2^{2^{-n}}\hat\varrho_1^{\frac12-2^{-n}}\right)^+}$$

$$= \sqrt{\mathrm{Tr}\, \hat\varrho_1}\sqrt{\mathrm{Tr}\, \hat\varrho_2^{2^{-n}}\hat\varrho_1^{\frac12-2^{-n}}\hat\varrho_1^{\frac12-2^{-n}}\hat\varrho_2^{2^{-n}}} = 1\cdot\sqrt{\mathrm{Tr}\, \hat\varrho_1^{1-2^{-(n-1)}}\hat\varrho_2^{2^{-(n-1)}}}$$

$$\le 1$$

$\uparrow$ by induction for $n-1$

c) $\mathrm{Tr}\, \hat{\varrho}_1^{\,1-2^{-n}} \hat{\varrho}_2^{\,2^{-n}} \leq 1$

$$\mathrm{Tr}\, \hat{\varrho}_1 \exp(-2^{-n} \log \hat{\varrho}_1) \exp(2^{-n} \log \hat{\varrho}_2) \leq 1 \quad 1$$

$$n \to \infty: \quad \mathrm{Tr}\, \hat{\varrho}_1 (1 - 2^{-n} \log \hat{\varrho}_1)(1 + 2^{-n} \log \hat{\varrho}_2) + O(2^{-2n}) \leq 1 \quad 1$$

$$\underbrace{\mathrm{Tr}\, \hat{\varrho}_1}_{=1} - 2^{-n}\, \mathrm{Tr}\, \hat{\varrho}_1 \log \hat{\varrho}_1 + 2^{-n}\, \mathrm{Tr}\, \hat{\varrho}_1 \log \hat{\varrho}_2 + O(2^{-2n}) \leq 1$$

$$2^{-n}\, \mathrm{Tr}\, \hat{\varrho}_1 (\ln \hat{\varrho}_2 - \ln \hat{\varrho}_1) + O(2^{-2n}) \leq 0$$

$$\mathrm{Tr}\, \hat{\varrho}_1 (\ln \hat{\varrho}_2 - \ln \hat{\varrho}_1) + O(2^{-n}) \leq 0 \quad 1$$

$$\xrightarrow[n \to \infty]{} \quad \mathrm{Tr}\, \hat{\varrho}_1 (\ln \hat{\varrho}_2 - \ln \hat{\varrho}_1) \leq 0 \quad 1$$

Problem 20:

a) $\mathrm{Tr}\,\hat\varrho_1(\ln\hat\varrho_2 - \ln\hat\varrho_1) \le 0$

$$\mathrm{Tr}\,\hat\varrho_1 \ln \frac{e^{-\beta\hat H}}{\mathrm{Tr}\,e^{-\beta\hat H}} \le \mathrm{Tr}\,\hat\varrho_1\ln\hat\varrho_1$$

$$\underbrace{-k_B\,\mathrm{Tr}\,\hat\varrho_1\ln\hat\varrho_1}_{S'} \le -k_B\,\mathrm{Tr}\,\hat\varrho_1 \ln e^{-\beta\hat H}\,(1) + k_B \ln \mathrm{Tr}\,e^{-\beta \hat H}\,\underbrace{\mathrm{Tr}\,\hat\varrho_1}_{=1}$$

$$= \frac{1}{T}\mathrm{Tr}\,\hat\varrho_1\hat H - \frac{E}{T} + \frac{1}{T}\mathrm{Tr}\,\hat\varrho_2\hat H + k_B\ln\mathrm{Tr}\,e^{-\beta\hat H}\,\underbrace{\mathrm{Tr}\,\hat\varrho_2}_{=1}$$

$$= \frac{E'-E}{T} - k_B\,\mathrm{Tr}\,\hat\varrho_2 \ln e^{-\beta\hat H}\,(1) + k_B\ln\mathrm{Tr}\,e^{-\beta\hat H}\,\mathrm{Tr}\,\hat\varrho_2$$

$$= \frac{E'-E}{T} - k_B\,\mathrm{Tr}\,\hat\varrho_2\ln\hat\varrho_2 = \frac{E'-E}{T} + S$$

$$\Rightarrow S \ge S + \frac{1}{T}(E-E') \quad (2)$$

(or $E - TS \ge E' - TS'$ $\Rightarrow$ the free energy is maximized)

b) $$\mathrm{Tr}\,\hat\varrho_1\ln\frac{e^{-\beta\hat H+\beta\mu'\hat N}}{\mathrm{Tr}\,e^{-\beta\hat H+\beta\mu'\hat N}} \le \mathrm{Tr}\,\hat\varrho_1\ln\hat\varrho_1$$

$$\Rightarrow S' = -k_B\,\mathrm{Tr}\,\hat\varrho_1\ln\hat\varrho_1 \le -k_B\,\mathrm{Tr}\,\hat\varrho_1\ln\frac{e^{-\beta\hat H+\beta\mu'\hat N}}{\mathrm{Tr}\,e^{-\beta\hat H+\beta\mu'\hat N}}$$

$$= \frac{1}{T}\mathrm{Tr}(\hat\varrho_1\hat H - \mu'\hat\varrho_1\hat N)\,(1) + k_B\ln\mathrm{Tr}\,e^{-\beta\hat H+\beta\mu'\hat N}\,\underbrace{\mathrm{Tr}\,\hat\varrho_1}_{=1}$$

$$= \frac{1}{T}(E'-\mu'N') - \frac{1}{T}(E-\mu'N) + \frac{1}{T}\mathrm{Tr}(\hat\varrho_2\hat H - \mu'\hat\varrho_2\hat N)$$

$$+ k_B\ln\mathrm{Tr}\,e^{-\beta\hat H+\beta\mu'\hat N}\,(1)\,\underbrace{\mathrm{Tr}\,\hat\varrho_2}_{=1}$$

$$= -\frac{1}{T}\left[(E-E') - \mu'(N-N')\right] - k_B\,\mathrm{Tr}\,\hat\varrho_2\ln\hat\varrho_2$$

$$= -\frac{1}{T}\left[(E-E') - \mu'(N-N')\right] + S \quad (2)$$