# Solutions to problem set 4

### 4.1 Density operators

a) We have

$$\langle\sigma_i\rangle = \mathrm{Tr}\,\rho\sigma_i = \frac{1}{2}\,\mathrm{Tr}(\mathbb{1} + r_j\sigma_j)\sigma_i = \frac{1}{2}r_j\,\mathrm{Tr}(\mathbb{1}\delta_{ij} + i\epsilon_{jik}\sigma_k) = r_i \qquad (1)$$

b)

$$\hat{\rho} = p_1\hat{\rho}_1 + p_2\hat{\rho}_2 = \frac{1}{2}(\mathbb{1} + \mathbf{r}_1\cdot\boldsymbol{\sigma}) + \frac{1}{2}(\mathbb{1} + \mathbf{r}_2\cdot\boldsymbol{\sigma}) = \frac{1}{2}\left[\mathbb{1} + (p_1\mathbf{r}_1 + p_2\mathbf{r}_2)\cdot\boldsymbol{\sigma}\right]$$

c) We know that the pure states are on the surfae of the Bloch sphere. Any mixed state will have a Bloch vector of the form $\mathbf{r} = p_1\mathbf{r}_1 + p_2\mathbf{r}_2$ with $\mathbf{r}_1$ and $\mathbf{r}_2$ unit vectors. This means that $\mathbf{r}$ is on the line between $\mathbf{r}_1$ and $\mathbf{r}_2$, at a position given by the probabilities, and therefore it is inside the Bloch sphere.

d) We use the matrix representation:

$$\hat{\rho} = \frac{1}{2}\left(\mathbb{1} + \mathbf{r}\cdot\sigma\right) = \frac{1}{2}\left(\mathbb{1} + x\sigma_x + y\sigma_y + z\sigma_z\right) = \frac{1}{2}\begin{pmatrix} 1+z & x-iy \\ x+iy & 1-z \end{pmatrix} = \begin{pmatrix} \rho_{11} & \rho_{12} \\ \rho_{21} & \rho_{22} \end{pmatrix} \qquad (2)$$

e) The density matrix is given by:

$$\hat{\rho} = \sum_k p_k|\psi_k\rangle\langle\psi_k| = \frac{1}{3}\left(|\uparrow_x\rangle\langle\uparrow_x| + |\uparrow_y\rangle\langle\uparrow_y| + |\uparrow_z\rangle\langle\uparrow_z|\right) \qquad (3)$$

where $p_1 = p_2 = p_3 = 1/3$, is the (classical) probability of the state being up in x, y or z respectively. One can do the computation of $\hat{\rho}$ in two ways:

- Matrix representation:

$$\begin{aligned}
|\uparrow_x\rangle &= \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ 1 \end{pmatrix}, \quad \langle\uparrow_x| = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 1 \end{pmatrix} \\
|\uparrow_y\rangle &= \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ i \end{pmatrix}, \quad \langle\uparrow_y| = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & -i \end{pmatrix} \\
|\uparrow_z\rangle &= \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \quad \langle\uparrow_z| = \begin{pmatrix} 1 & 0 \end{pmatrix}
\end{aligned}$$

  Then:

$$\begin{aligned}
\hat{\rho} &= \frac{1}{3}\left[\frac{1}{2}\begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix} + \frac{1}{2}\begin{pmatrix} 1 & -i \\ i & 1 \end{pmatrix} + \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}\right] = \frac{1}{3}\frac{1}{2}\left[\begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix} + \begin{pmatrix} 1 & -i \\ i & 1 \end{pmatrix} + \begin{pmatrix} 2 & 0 \\ 0 & 0 \end{pmatrix}\right] \\
&= \frac{1}{3}\frac{1}{2}\begin{pmatrix} 4 & 1-i \\ 1+i & 2 \end{pmatrix} = \frac{1}{2}\begin{pmatrix} 1+\frac{1}{3} & \frac{1}{3}(1-i) \\ \frac{1}{3}(1+i) & 1-\frac{1}{3} \end{pmatrix}
\end{aligned}$$

  Comparing with (2), we see that $\mathbf{r} = \left(\frac{1}{3}, \frac{1}{3}, \frac{1}{3}\right)$

- Bra-ket formalism:
  We start of by expressing $|\uparrow_x\rangle$ and $|\uparrow_y\rangle$ in the $|\pm\rangle$ basis by solving the eigenvector equations:

$$\sigma_x|\uparrow_x\rangle = |\uparrow_x\rangle \Rightarrow (\sigma_+ + \sigma_-)(a|+\rangle + b|-\rangle) = a|+\rangle + b|-\rangle$$

We see that the only terms surviving $\sigma_\pm|\mp\rangle$, our equation becomes:

$$b|+\rangle + a|-\rangle = a|+\rangle + b|-\rangle$$

Then choosing $a = b = \frac{1}{\sqrt{2}}$ gives

$$|\uparrow_x\rangle = \frac{1}{\sqrt{2}}(|+\rangle + |-\rangle)$$

Next up:

$$\sigma_y|\uparrow_y\rangle = |\uparrow_y\rangle \Rightarrow i(\sigma_- - \sigma_+)(a|+\rangle + b|-\rangle) = a|+\rangle + b|-\rangle$$

By the same argument as earlier, we arrive at:

$$ai|-\rangle + bi|+\rangle = a|+\rangle + b|-\rangle$$

This gives: $ai = b \Rightarrow \frac{b}{a} = i \Rightarrow a = \frac{1}{\sqrt{2}}, b = \frac{1}{\sqrt{2}}i$ and

$$|\uparrow_y\rangle = \frac{1}{\sqrt{2}}(|+\rangle + i|-\rangle)$$

Inserting this into (3):

$$\begin{aligned}
\hat{\rho} &= \frac{1}{3}\frac{1}{2}(|+\rangle + |-\rangle)(\langle+| + \langle-|) + \frac{1}{3}\frac{1}{2}(|+\rangle + i|-\rangle)(\langle+| - i\langle-|) + \frac{1}{3}\frac{1}{2}2|+\rangle\langle+| \\
&= \frac{1}{2}\frac{1}{3}((3+1)|+\rangle\langle+| + (1-i)|+\rangle\langle-| + (1+i)|-\rangle\langle+| + (3-1)|-\rangle\langle-|) \\
&= \frac{1}{2}\left(\left(1+\frac{1}{3}\right)|+\rangle\langle+| + \frac{1}{3}(1-i)|+\rangle\langle-| + \frac{1}{3}(1+i)|-\rangle\langle+| + \left(1-\frac{1}{3}\right)|-\rangle\langle-|\right)
\end{aligned}$$

This can be read of as:

$$\hat{\rho} = \frac{1}{2}\left(\mathbb{1} + \frac{1}{3}(1,1,1)\cdot\sigma\right)$$

where $\mathbf{r} = \left(\frac{1}{3}, \frac{1}{3}, \frac{1}{3}\right)$

The Von Neuman entropy is given by equation 2.24 in the lecture notes, which reads:

$$S = -\frac{1}{2}\log\left[(1+r)^{1+r}(1-r)^{1-r}\right] + \log 2$$

where $r = |\mathbf{r}| = \frac{1}{\sqrt{3}}$.

$$\begin{aligned}
S &= -\frac{1}{2}\log\left[\left(1+\frac{1}{\sqrt{3}}\right)^{1+\frac{1}{\sqrt{3}}}\left(1-\frac{1}{\sqrt{3}}\right)^{1-\frac{1}{\sqrt{3}}}\right] + \log 2 \\
&\approx 0.744
\end{aligned}$$

when choosing $\log = \log_2$.

f) The unit vector in the direction of $\mathbf{r}$ is $\mathbf{n} = \frac{\mathbf{r}}{|\mathbf{r}|} = \frac{1}{\sqrt{3}}(1,1,1)$. According to Eq (2.22) of the lecture notes we have that

$$\hat{\rho} = \frac{1}{2}(1+r)|\Psi_n\rangle\langle\Psi_n| + \frac{1}{2}(1-r)|\Psi_{-n}\rangle\langle\Psi_{-n}|$$

where $|\Psi_{\pm n}\rangle$ are the eigenstates of $\sigma_{\mathbf{n}} = \mathbf{n}\cdot\boldsymbol{\sigma}$. If we want the explicit form of these states we can recall that (Eq (1.136)in the lecture notes)

$$|\Psi_n\rangle = \begin{pmatrix} \cos\theta/2 \\ e^{i\phi}\sin\theta/2 \end{pmatrix} \qquad |\Psi_{-n}\rangle = \begin{pmatrix} -e^{-i\phi}\sin\theta/2 \\ \cos\theta/2 \end{pmatrix}$$

where $(\theta,\phi)$ are the polar coordinates for $\mathbf{n}$. With $\mathbf{n}\frac{1}{\sqrt{3}}(1,1,1)$ we have $\cos\theta = 1/\sqrt{3}$ and $\phi = \pi/4$. Using

$$\cos\theta/2 = \frac{1}{\sqrt{2}}\sqrt{1+\cos\theta} = \sqrt{\frac{\sqrt{3}+1}{2\sqrt{3}}}$$
$$\sin\theta/2 = \frac{1}{\sqrt{2}}\sqrt{1-\cos\theta} = \sqrt{\frac{\sqrt{3}-1}{2\sqrt{3}}}$$

we get

$$|\Psi_n\rangle = \frac{1}{\sqrt{2\sqrt{3}}}\begin{pmatrix} \sqrt{\sqrt{3}+1} \\ e^{i\pi/4}\sqrt{\sqrt{3}-1} \end{pmatrix} \qquad |\Psi_{-n}\rangle = \begin{pmatrix} -e^{-i\pi/4}\sqrt{\sqrt{3}-1} \\ \sqrt{\sqrt{3}+1} \end{pmatrix}.$$

## 4.2 Entropy of a thermal state

a)

$$\hat{\rho} = \frac{1}{Z}e^{-\beta\hat{H}}, \qquad Z = \mathrm{Tr}\left(e^{-\beta\hat{H}}\right), \qquad \frac{dZ}{d\beta} = -\,\mathrm{Tr}\left(e^{-\beta\hat{H}}\hat{H}\right)$$

The Von Neumann entropy is given in the lecture notes as:

$$S = -\mathrm{Tr}\left(\hat{\rho}\ln\hat{\rho}\right) = -\frac{1}{Z}\,\mathrm{Tr}\left[e^{-\beta\hat{H}}(-\beta\hat{H} - \ln Z)\right] = \frac{\beta}{Z}\,\mathrm{Tr}\left[e^{-\beta\hat{H}}\hat{H}\right] + \frac{1}{Z}\ln Z)\,\mathrm{Tr}\left[e^{-\beta\hat{H}}\right]$$
$$= -\frac{\beta}{Z}\frac{dZ}{d\beta} + \ln Z = -\beta\frac{d}{d\beta}\ln Z + \ln Z. \tag{4}$$

b)

$$\hat{H} = \hbar\omega\sum_{n=0}^{\infty}\left(n+\frac{1}{2}\right)|n\rangle\langle n|, \quad E_n = \hbar\omega\left(n+\frac{1}{2}\right)$$

$$N(\beta)^{-1} = \sum_{n=0}^{\infty} e^{-\beta E_n} \sum_{n=0}^{\infty} e^{-\beta\hbar\omega/2}e^{-\beta\hbar\omega n} = e^{-\beta\hbar\omega/2}\sum_{n=0}^{\infty} e^{-\beta\hbar\omega n}$$

We recognize $\sum_{n=0}^{\infty} e^{-\beta\hbar\omega n}$ as a konvergent sum of a geometric series.

$$\sum_{n=0}^{\infty} e^{-\beta\hbar\omega n} = \frac{1}{1-e^{-\beta\hbar\omega}}$$

Thus:

$$\begin{aligned} N(\beta) &= \frac{1-e^{-\beta\hbar\omega}}{e^{-\beta\hbar\omega/2}} \\ &= e^{\beta\hbar\omega/2} - e^{-\beta\hbar\omega+\beta\hbar\omega/2} \\ &= e^{\beta\hbar\omega/2} - e^{-\beta\hbar\omega/2} \\ &= 2\sinh\frac{\beta\hbar\omega}{2} \end{aligned}$$

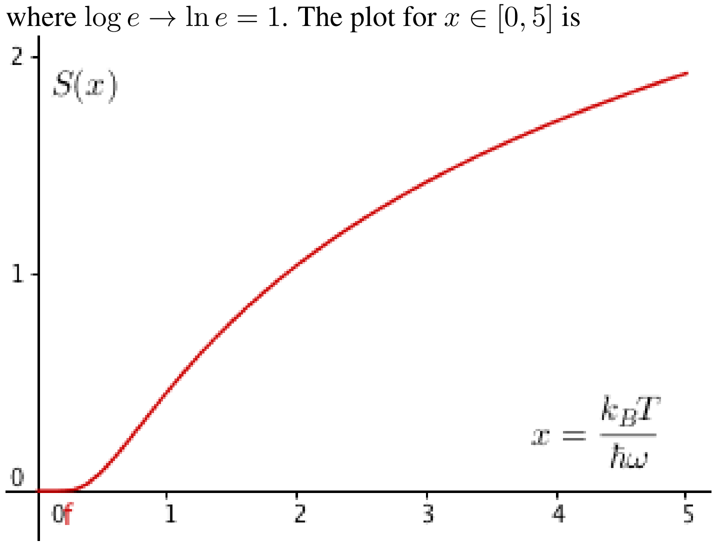
Inserting this into (4) gives:

$$\begin{aligned} S(\beta) &= \beta\frac{d}{d\beta}\ln\left(2\sinh\frac{\beta\hbar\omega}{2}\right) - \ln\left(2\sinh\frac{\beta\hbar\omega}{2}\right) \\ &= \beta\frac{\frac{d}{d\beta}\left(2\sinh\frac{\beta\hbar\omega}{2}\right)}{2\sinh\frac{\beta\hbar\omega}{2}} - \ln\left(2\sinh\frac{\beta\hbar\omega}{2}\right) = \frac{\beta\hbar\omega}{2}\frac{2\cosh\frac{\beta\hbar\omega}{2}}{2\sinh\frac{\beta\hbar\omega}{2}} - \ln\left(2\sinh\frac{\beta\hbar\omega}{2}\right) \\ &= \frac{\beta\hbar\omega}{2}\coth\frac{\beta\hbar\omega}{2} - \ln\left(2\sinh\frac{\beta\hbar\omega}{2}\right) \end{aligned}$$

c) We now write the entropy as a function of $x = \frac{2k_BT}{\hbar\omega} = \frac{2}{\beta\hbar\omega}$ so we get:

$$S(x) = \frac{1}{x}\coth\frac{1}{x} - \ln\left(2\sinh\frac{1}{x}\right)$$

where $\log e \to \ln e = 1$. The plot for $x \in [0,5]$ is



Evaluating the limit $T \to 0 \Rightarrow x \to 0$

$$\begin{aligned}
\lim_{x\to 0^+} S(x) &= \lim_{x\to 0^+} \left(\frac{1}{x}\coth\frac{1}{x} - \ln\left(2\sinh\frac{1}{x}\right)\right) \\
&= \lim_{x\to 0^+} \frac{1}{x}\left(\coth\frac{1}{x} - \frac{\ln\left(2\sinh\frac{1}{x}\right)}{\frac{1}{x}}\right) \\
&= \lim_{x\to 0^+} \left(\frac{1}{x}\right)\left(\lim_{x\to 0^+}\coth\frac{1}{x} - \lim_{x\to 0^+}\frac{\ln\left(2\sinh\frac{1}{x}\right)}{\frac{1}{x}}\right) \\
&= \lim_{x\to 0^+} \left(\frac{1}{x}\right)\left(\lim_{x\to 0^+}\coth\frac{1}{x} - \lim_{x\to 0^+}\frac{\ln\left(2\sinh\frac{1}{x}\right)}{\frac{1}{x}}\right)
\end{aligned}$$

Looking at the last limit, we see that it approaches "$\infty/\infty$" and we need to apply L'Hôpital's rule.

$$\lim_{x\to 0^+}\frac{\ln\left(2\sinh\frac{1}{x}\right)}{\frac{1}{x}} \stackrel{L'H}{=} \lim_{x\to 0^+}\frac{-\frac{2\cosh\frac{1}{x}}{2\sinh\frac{1}{x}}\frac{1}{x^2}}{-\frac{1}{x^2}} = \lim_{x\to 0^+}\coth\frac{1}{x}$$

Inserting back into the limit of $S(x)$:

$$\lim_{x\to 0^+} S(x) = \lim_{x\to 0^+}\frac{1}{x}\left(\coth\frac{1}{x} - \coth\frac{1}{x}\right) = 0$$

Onto the limit $T \to \infty \Rightarrow x \to \infty$

$$\lim_{x\to\infty} S(x) = \lim_{x\to\infty}\left(\frac{1}{x}\coth\frac{1}{x} - \ln\left(2\sinh\frac{1}{x}\right)\right) = \lim_{x\to\infty}\frac{1}{x}\coth\frac{1}{x} - \lim_{x\to\infty}\ln\left(2\sinh\frac{1}{x}\right)$$

Looking at the first limit:

$$\lim_{x\to\infty}\frac{1}{x}\coth\frac{1}{x} = \lim_{y\to 0^+} y\coth y = \lim_{y\to 0^+}\frac{y\cosh y}{\sinh y}$$

This is a limit that approaches 0/0, and we may use L'Hôpital's rule:

$$\lim_{y\to 0^+}\frac{y\cosh y}{\sinh y} \stackrel{L'H}{=} \lim_{y\to 0^+}\frac{\cosh y + y\sinh y}{\cosh y} = \lim_{y\to 0^+}(1 + y\tanh y) = 1$$

Then,

$$\lim_{x\to\infty} S(x) = 1 + -\underbrace{\lim_{x\to\infty}\ln\left(2\sinh\frac{1}{x}\right)}_{=-\infty} = \infty$$

So the entropy approaches 0 for $T \to 0$, which makes sense since there is only one possible state the system can be in the limit, and the system is therefore ordered. In the other limit, there is an infinite number of states available, so the system has an infinite number of states to "choose" from, meaning that the entropy approaches infinity.

## 4.3 Bloch-Siegert shift

This problem was adapted from Y. Yan *et al.*, Bloch-Siegert shift of the Rabi model, Phys. Rev. A 91, 053834 (2015) where you can read more details and background material.

a) If $|\psi\rangle$ is the state of the system in the laboratory frame, the state in the rotating frame is $|psi'\rangle = T|\psi\rangle$ with the time-dependent unitary transformation

$$T = e^{i\frac{\omega t}{2}\sigma_z}$$

The Hamiltonian in the rotating frame is given by

$$H' = THT^\dagger + \frac{dT}{dt}T^\dagger$$

We use the relation

$$e^{-i\phi\sigma_i} = \cos\phi\,\mathbb{1} - i\sin\phi\,\sigma_i.$$

to get

$$e^{i\frac{\omega t}{2}\sigma_z}\sigma_x e^{-i\frac{\omega t}{2}\sigma_z} = \cos(\omega t)\,\sigma_x - \sin(\omega t)\,\sigma_y$$
$$e^{i\frac{\omega t}{2}\sigma_z}\sigma_y e^{-i\frac{\omega t}{2}\sigma_z} = \cos(\omega t)\,\sigma_y + \sin(\omega t)\,\sigma_x$$

Combining, we get

$$H' = \frac{\hbar}{2}(\omega_0 - \omega)\sigma_z + \frac{\hbar}{2}A\sigma_x$$

which is time-independent. The resonance condition is $\omega = \omega_0$ irrespective of the driving amplitude $A$. Then we get Rabi oscillations between the ground and excited state.

b) The same transformation gives now the Hamiltonian

$$H' = \frac{\hbar}{2}(\omega_0 - \omega)\sigma_z + \frac{\hbar}{4}A\sigma_x + \frac{\hbar}{4}A(\cos(2\omega t)\,\sigma_x - \sin(2\omega t)\,\sigma_y).$$

We see that we get an additional term which describes a field rotating at the frequency $2\omega$. To understand this, we can decompose the oscillating field in two counterrotating fields

$$\cos(\omega t)\,\sigma_x = \frac{1}{2}(\cos\omega t\,\sigma_x + \sin\omega t\,\sigma_y) + \frac{1}{2}(\cos\omega t\,\sigma_x - \sin\omega t\,\sigma_y).$$

The first term is rotating as the field in question a) and is transformed to a constant field. The second term is rotating in the opposite direction, and when seen in the rotating frame is rotating twice as fast. We can neglect the rotating term when $A$ is sufficiently small because it changes rapidly in time and its effect on the state does not have time to build up before the field changes direction. On the average, it does not have large effect, and the true state will wiggle around the approximate state that we find useing the rotating wave approximation.

c) Since the operator $S(t)$ commutes with $\sigma_x$, we only need to consider the transformation of $\sigma_z$. We write $\tilde{A} = \frac{A}{2\omega}\xi\sin(\omega t)$ and get

$$e^{iS}\sigma_z e^{-iS} = e^{i\tilde{A}\sigma_x}\sigma_z e^{-i\tilde{A}\sigma_x} = \cos(2\tilde{A})\,\sigma_z + \sin(2\tilde{A})\,\sigma_y.$$

This gives the transformed Hamiltonian

$$H' = \frac{\hbar}{2}\omega_0\left\{\cos\left[\frac{A}{\omega}\xi\sin(\omega t)\right]\sigma_z + \sin\left[\frac{A}{\omega}\xi\sin(\omega t)\right]\sigma_y\right\} + \frac{\hbar}{2}A(1-\xi)\cos(\omega t)\,\sigma_x.$$

d) If we choose

$$J_1\left(\frac{A}{\omega}\xi\right)\omega_0 = \frac{1}{2}A(1-\xi) = \frac{1}{2} \tag{5}$$

the Hamiltonian will be (when neglecting the terms from $H_2'$)

$$H = \frac{\hbar}{2}\omega_0 J_0\left(\frac{A}{\omega}\xi\right)\sigma_z + \frac{\hbar}{2}A'(\cos(\omega t)\,\sigma_x + \sin(\omega t)\,\sigma_y)$$

With this choice of $\xi$, the $x$- and $y$-components of the field have the same amplitude, and we have a rotating field similar to the one in question a) but with $\omega_0$ rescaled by the Bessel function. The resonance condition is therefore

$$\omega = \omega_0 J_0\left(\frac{A}{\omega}\xi\right). \tag{6}$$

e) We determine $\xi$ to lowest order in $A$ we expand the Bessel function in (5) to get

$$J_1\left(\frac{A}{\omega}\xi\right)\omega_0 \approx \frac{A}{2\omega}\xi\omega_0.$$

From (5) we then get

$$\xi = \frac{\omega}{\omega_0+\omega}.$$

We insert this in (6) and expand the Bessel function

$$\omega = \omega_0 J_0\left(\frac{A}{\omega}\xi\right) \approx \omega_0 J_0\left(\frac{A}{\omega_0\omega}\right) \approx \omega_0\left(1-\frac{A^2}{4(\omega_0+\omega)^2}\right).$$

For $A \to 0$, we recover the resonance at $\omega = \omega_0$ as we had using the rotating wave approximation. To next order, we must have $\omega = \omega_0 + cA^2$, and we can replace $\omega_0+\omega$ with $2\omega_0$ in the denominator to get

$$\omega = \omega_0 - \frac{A^2}{16\omega_0}.$$