Exercise 1. ***Density Operator Overdose.***

Write out the density matrices of the following systems in the standard $|\uparrow\rangle$, $|\downarrow\rangle$ basis (or the relevant basis for the system).

(i) A spin $1/2$ particle in its "down" state $|\downarrow\rangle$;

(ii) A spin $1/2$ particle in the superposition state $|\psi\rangle = \frac{1}{\sqrt{2}}\left(|\uparrow\rangle - i\,|\downarrow\rangle\right)$;

(iii) A spin $1/2$ particle, randomly produced with probability $1/2$ in either state $|\uparrow\rangle$ or $|\downarrow\rangle$.

Suppose you are given either many copies of system (ii) or many copies of system (iii). Devise a procedure to distinguish both cases.

(iv) A spin $1/2$ particle in the superposition state $|\phi\rangle = \frac{\sqrt{3}}{2}|\uparrow\rangle + \frac{1}{2}|\downarrow\rangle$;

(v) The particle described in (iv), after having measured it and observed it in the state $|\uparrow\rangle$;

(vi) The particle described in (iv), after someone else measured it in the basis $\{|\uparrow\rangle, |\downarrow\rangle\}$ but didn't tell you the measurement result ;

(vii) The particle described in (iv), after someone else measured it in the basis $\{|+\rangle, |-\rangle\}$ (where $|\pm\rangle = \frac{1}{\sqrt{2}}\left(|\uparrow\rangle \pm |\downarrow\rangle\right)$) but didn't tell you the measurement result ;

(viii) The spin state of an electron coming out of a source that produces particles with uniformly random spin. Assume that the spins are created in a random direction given by the spherical angles θ, ϕ, evenly distributed on the surface of the sphere. The state with "spin in direction θ, ϕ" is given by

$$|\theta,\phi\rangle = \cos\frac{\theta}{2}\,|\uparrow\rangle + \mathrm{e}^{i\phi}\sin\frac{\theta}{2}\,|\downarrow\rangle\ . \tag{1}$$

(This representation is known as the Bloch sphere, or Poincaré sphere for photon polarizations.)

(ix) Two (distinguishable) spin $1/2$ particles in the entangled state

$$|\Psi^-\rangle = \frac{1}{\sqrt{2}}\left(|\uparrow\rangle_1|\downarrow\rangle_2 - |\downarrow\rangle_1|\uparrow\rangle_2\right)\ ; \tag{2}$$

(x) The two particles of system (ix), after particle #1 was measured in the basis $|\pm\rangle = \frac{1}{\sqrt{2}}\left(|\uparrow\rangle \pm |\downarrow\rangle\right)$, and was found in the $|+\rangle$ state. In particular, what is the state of particle #2?

(xi) Two (distinguishable) spin $1/2$ particles with their state chosen at random between $|\uparrow\rangle_1|\downarrow\rangle_2$ and $|\downarrow\rangle_1|\uparrow\rangle_2$ with probability $1/2$;

(xii) The two particles of system (xi), after particle #1 was measured in the basis $|\pm\rangle = \frac{1}{\sqrt{2}}\left(|\uparrow\rangle \pm |\downarrow\rangle\right)$, and was found in the $|+\rangle$ state. In particular, what is the state of particle #2?

(xiii) A harmonic oscillator in thermodynamic equilibrium at temperature T.

Hint. At thermodynamic equilibrium, each Hamiltonian eigenstate $|n\rangle$ of energy ϵ_n is populated with probability proportional to $\mathrm{e}^{-\epsilon_n/kT}$.

Solution. We will use the convention $|\uparrow\rangle = \left(\begin{smallmatrix}1\\0\end{smallmatrix}\right)$, $|\downarrow\rangle = \left(\begin{smallmatrix}0\\1\end{smallmatrix}\right)$.

(i) This state is pure, so

$$\rho = |\downarrow\rangle\langle\downarrow| = \begin{pmatrix}0 & 0\\ 0 & 1\end{pmatrix} . \tag{L.1}$$

(ii) This state is also pure, so we can calculate

$$\rho = |\psi\rangle\langle\psi| = \frac{1}{2}\big(|\uparrow\rangle - i\,|\downarrow\rangle\big)\big(\langle\uparrow| + i\,\langle\downarrow|\big) = \begin{pmatrix}1/2 & i/2\\ -i/2 & 1/2\end{pmatrix} . \tag{L.2}$$

(Notice that $|\uparrow\rangle\langle\downarrow| = \left(\begin{smallmatrix}1\\0\end{smallmatrix}\right)\left(\begin{smallmatrix}0 & 1\end{smallmatrix}\right) = \left(\begin{smallmatrix}0 & 1\\ 0 & 0\end{smallmatrix}\right)$.)

(iii) The electron is in state $|\uparrow\rangle$ with probability $1/2$, or in state $|\downarrow\rangle$ with probability $1/2$. Thus

$$\rho = \frac{1}{2}|\uparrow\rangle\langle\uparrow| + \frac{1}{2}|\downarrow\rangle\langle\downarrow| = \begin{pmatrix}1/2 & 0\\ 0 & 1/2\end{pmatrix} .$$

Notice how the off-diagonal terms have dissapeared, compared to (ii). This is the manifestation of the fundamental difference between **quantum superposition** and **statistical mixture** of quantum states. In the first case, you may have quantum effects with interference between the two superposed states (for example, interference pattern resulting from superposition of a particle taking two different paths in presence of Young slits). The second case exhibits no quantum behavior, and would correspond to someone else measuring which path a particle took in presence of Young slits, which would destroy the interference pattern even if they don't tell you where the particle passed.

You can distinguish the two cases by measuring in the superposition basis. If you measure your system in the $\{|\psi\rangle, |\psi^\perp\rangle\}$ basis ($|\psi^\perp\rangle$ may be any state orthogonal to $|\psi\rangle$), then if your system was in the state $|\psi\rangle$ you will always measure the outcome $|\psi\rangle$. If, however, your system was in a statistical mixture of $|\uparrow\rangle$ and $|\downarrow\rangle$, the total probability that you get $|\psi\rangle$ is $\frac{1}{2}|\langle\psi|\uparrow\rangle|^2 + \frac{1}{2}|\langle\psi|\downarrow\rangle|^2 = 1/2$ and the total probability that you get $|\psi^\perp\rangle$ is $1 - 1/2 = 1/2$ (since probabilities add up to one). So if you're given many copies of either system, you will notice when measuring them if all outcomes are $|\psi\rangle$ or if half of them give $|\psi\rangle$ and the other half $|\psi^\perp\rangle$.

(iv) This is a pure state, so we simply have

$$\rho = |\phi\rangle\langle\phi| = \big(\tfrac{\sqrt{3}}{2}|\uparrow\rangle + \tfrac{1}{2}|\downarrow\rangle\big)\big(\tfrac{\sqrt{3}}{2}\langle\uparrow| + \tfrac{1}{2}|\downarrow\rangle\big) = \begin{pmatrix}3/4 & \sqrt{3}/4\\ \sqrt{3}/4 & 1/4\end{pmatrix} . \tag{L.3}$$

(v) After the measurement, the electron is projected onto the state $|\uparrow\rangle$, so its density operator is simply

$$\rho = |\uparrow\rangle\langle\uparrow| = \begin{pmatrix}1 & 0\\ 0 & 0\end{pmatrix} .$$

(vi) The measurement either projected the system onto $|\uparrow\rangle$ with probability $|\langle\phi|\uparrow\rangle|^2 = 3/4$, or onto $|\downarrow\rangle$ with probability $|\langle\phi|\downarrow\rangle| = 1/4$. Then

$$\rho = \frac{3}{4}|\uparrow\rangle\langle\uparrow| + \frac{1}{4}|\downarrow\rangle\langle\downarrow| = \begin{pmatrix}3/4 & 0\\ 0 & 1/4\end{pmatrix} . \tag{L.4}$$

One can see that even though you do not know the measurement result, the system will have *decohered*, i.e. it will have lost all its quantum behavior, and you won't be able to see e.g. any interference patterns.

(vii) The measurement either projected the system onto $|+\rangle$ with probability $|\langle\phi|+\rangle|^2$, or onto $|-\rangle$ with probability $|\langle\phi|-\rangle|^2$. So calculate the overlaps

$$|\langle\phi|+\rangle|^2 = \left|\frac{\sqrt{3}}{2}\langle+|\uparrow\rangle + \frac{1}{2}\langle+|\downarrow\rangle\right|^2 = \left|\frac{\sqrt{3}+1}{2\sqrt{2}}\right|^2 = \frac{2+\sqrt{3}}{4} \approx 0.93\ ;$$

$$|\langle\phi|-\rangle|^2 = \left|\frac{\sqrt{3}}{2}\langle-|\uparrow\rangle + \frac{1}{2}\langle-|\downarrow\rangle\right|^2 = \left|\frac{\sqrt{3}-1}{2\sqrt{2}}\right|^2 = \frac{2-\sqrt{3}}{4} \approx 0.07\ ,$$

and then

$$\begin{aligned}\rho &= |\langle\phi|+\rangle|^2|+\rangle\langle+| \ + \ |\langle\phi|-\rangle|^2|-\rangle\langle-| = |\langle\phi|+\rangle|^2\begin{pmatrix}1/2 & 1/2\\ 1/2 & 1/2\end{pmatrix} + |\langle\phi|-\rangle|^2\begin{pmatrix}1/2 & -1/2\\ -1/2 & 1/2\end{pmatrix}\\ &= \begin{pmatrix}\frac{1}{2}|\langle\phi|+\rangle|^2 + \frac{1}{2}|\langle\phi|-\rangle|^2 & \frac{1}{2}|\langle\phi|+\rangle|^2 - \frac{1}{2}|\langle\phi|-\rangle|^2\\ \frac{1}{2}|\langle\phi|+\rangle|^2 - \frac{1}{2}|\langle\phi|-\rangle|^2 & \frac{1}{2}|\langle\phi|+\rangle|^2 + \frac{1}{2}|\langle\phi|-\rangle|^2\end{pmatrix} = \begin{pmatrix}1/2 & \sqrt{3}/4\\ \sqrt{3}/4 & 1/2\end{pmatrix} \approx \begin{pmatrix}0.5 & 0.43\\ 0.43 & 0.5\end{pmatrix}\end{aligned} \tag{L.5}$$

Here, the system has only slightly decohered. It is no longer pure (it doesn't have rank 1), yet it still has off-diagonal terms.

(viii) The source produces randomly the states $|\theta,\phi\rangle$, evenly distributed on the surface of the sphere. By definition, ρ is the average of $|\theta,\phi\rangle\langle\theta,\phi|$ on the surface of the sphere,

$$\begin{aligned}\rho &= \frac{1}{4\pi}\int \sin\theta\,\mathrm{d}\theta\mathrm{d}\phi\,|\theta,\phi\rangle\langle\theta,\phi| = \frac{1}{4\pi}\int \mathrm{d}\theta\mathrm{d}\phi\,\sin\theta\,\Big(\cos\tfrac{\theta}{2}\,|\!\uparrow\rangle + \mathrm{e}^{i\phi}\sin\tfrac{\theta}{2}\,|\!\downarrow\rangle\Big)\Big(\cos\tfrac{\theta}{2}\,\langle\uparrow\!| + \mathrm{e}^{-i\phi}\sin\tfrac{\theta}{2}\,\langle\downarrow\!|\Big)\\ &= \frac{1}{4\pi}\int \mathrm{d}\theta\mathrm{d}\phi\,\sin\theta\,\Big[\cos^2\tfrac{\theta}{2}\,|\!\uparrow\rangle\langle\uparrow\!| + \cos\tfrac{\theta}{2}\sin\tfrac{\theta}{2}\,\mathrm{e}^{-i\phi}\,|\!\uparrow\rangle\langle\downarrow\!| + \cos\tfrac{\theta}{2}\sin\tfrac{\theta}{2}\,\mathrm{e}^{+i\phi}\,|\!\downarrow\rangle\langle\uparrow\!| + \sin^2\tfrac{\theta}{2}\,|\!\downarrow\rangle\langle\downarrow\!|\Big]\;. \qquad (L.6)\end{aligned}$$

Notice now that $\int_0^{2\pi}\mathrm{e}^{i\phi} = \int_0^{2\pi}\mathrm{e}^{-i\phi} = 0$, killing the two cross-terms. Recall also that $\cos^2\frac{\theta}{2} = \frac{1}{2} + \frac{1}{2}\cos\theta$ and $\sin^2\frac{\theta}{2} = \frac{1}{2} - \frac{1}{2}\cos\theta$. This gives us

$$(\text{L.6}) = \frac{1}{2}\int_0^{\pi}\mathrm{d}\theta\,\sin\theta\,\big[\big(\tfrac{1}{2}+\tfrac{1}{2}\cos\theta\big)\,|\!\uparrow\rangle\langle\uparrow\!| + \big(\tfrac{1}{2}-\tfrac{1}{2}\cos\theta\big)\,|\!\downarrow\rangle\langle\downarrow\!|\big]\;. \qquad (L.7)$$

Recall that $\int_0^{\pi}\sin\theta\,\mathrm{d}\theta = 2$ and notice that $\int_0^{\pi}\sin\theta\cos\theta\,\mathrm{d}\theta = \frac{1}{2}\int_0^{\pi}\sin 2\theta\,\mathrm{d}\theta = 0$. We thus obtain

$$\rho = \frac{1}{2}|\!\uparrow\rangle\langle\uparrow\!| + \frac{1}{2}|\!\downarrow\rangle\langle\downarrow\!|\;, \qquad (L.8)$$

which is the same as if the source were randomly producing one of the two pure states $|\!\uparrow\rangle$ and $|\!\downarrow\rangle$.

(ix) Let's use the basis vectors

$$|\!\uparrow\rangle_1|\!\uparrow\rangle_2 = \begin{pmatrix}1\\0\\0\\0\end{pmatrix}\;;\quad |\!\uparrow\rangle_1|\!\downarrow\rangle_2 = \begin{pmatrix}0\\1\\0\\0\end{pmatrix}\;;\quad |\!\downarrow\rangle_1|\!\uparrow\rangle_2 = \begin{pmatrix}0\\0\\1\\0\end{pmatrix}\;;\quad |\!\downarrow\rangle_1|\!\downarrow\rangle_2 = \begin{pmatrix}0\\0\\0\\1\end{pmatrix}\;.$$

This system is again a pure state, so we simply have

$$\rho = |\Psi^-\rangle\langle\Psi^-| = \frac{1}{2}\big(|\!\uparrow\rangle_1|\!\downarrow\rangle_2 - |\!\downarrow\rangle_1|\!\uparrow\rangle_2\big)\big(\langle\uparrow\!|_1\langle\downarrow\!|_2 - \langle\downarrow\!|_1\langle\uparrow\!|_2\big) = \begin{pmatrix}0&0&0&0\\0&1/2&-1/2&0\\0&-1/2&1/2&0\\0&0&0&0\end{pmatrix}\;.$$

(x) One can rewrite the state $|\Psi^-\rangle$ of the system in the $|\pm\rangle$ basis, using the basis transformation

$$|+\rangle = \frac{1}{\sqrt{2}}\,(|\!\uparrow\rangle + |\!\downarrow\rangle)\;;\quad |-\rangle = \frac{1}{\sqrt{2}}\,(|\!\uparrow\rangle - |\!\downarrow\rangle)\;. \qquad (L.9)$$

This gives us

$$\begin{aligned}|\Psi^-\rangle &= \frac{1}{\sqrt{2}}\,(|\!\uparrow\rangle_1|\!\downarrow\rangle_2 - |\!\downarrow\rangle_1|\!\uparrow\rangle_2)\\ &= \frac{1}{2\sqrt{2}}\Big[|+\rangle_1|+\rangle_2 - |+\rangle_1|-\rangle_2 + |-\rangle_1|+\rangle_2 + |-\rangle_1|-\rangle_2\Big]\\ &\quad - \frac{1}{2\sqrt{2}}\Big[|+\rangle_1|+\rangle_2 + |+\rangle_1|-\rangle_2 - |-\rangle_1|+\rangle_2 + |-\rangle_1|-\rangle_2\Big]\\ &= \frac{1}{\sqrt{2}}\Big[|-\rangle_1|+\rangle_2 - |+\rangle_1|-\rangle_2\Big]\;. \qquad (L.10)\end{aligned}$$

If the first particle projects onto state $|+\rangle$, then the full state of the system is projected onto the second term of (L.10), and the (normalized) post-measurement state is $|+\rangle_1|-\rangle_2$.
This means that by measuring the first particle in the $|+\rangle$ state, we force the state of the second particle to $|-\rangle$.
(Written out explicitly in the $|\!\uparrow / \downarrow\rangle$ basis,

$$\rho' = |+\rangle_1|-\rangle_2\langle+|_1\langle-|_2 = \begin{pmatrix}1/2&-1/2&1/2&-1/2\\-1/2&1/2&-1/2&1/2\\1/2&-1/2&1/2&-1/2\\-1/2&1/2&-1/2&1/2\end{pmatrix}\;.) \qquad (L.11)$$

(xi) This gives us an even mixture between $|\!\uparrow\rangle_1|\!\downarrow\rangle_2$ and $|\!\downarrow\rangle_1|\!\uparrow\rangle_2$, that is

$$\rho = \frac{1}{2}|\!\uparrow\rangle_1|\!\downarrow\rangle_2\langle\uparrow\!|_1\langle\downarrow\!|_2 + \frac{1}{2}|\!\downarrow\rangle_1|\!\uparrow\rangle_2\langle\downarrow\!|_1\langle\uparrow\!|_2 = \begin{pmatrix}0&0&0&0\\0&1/2&0&0\\0&0&1/2&0\\0&0&0&0\end{pmatrix}\;.$$

Notice again how the off-diagnoal terms have vanished compared to (ix).

(xii) We know that the two particles are with probability 1/2 in the $|\uparrow\rangle_1|\downarrow\rangle_2$ state, and with probability 1/2 in the $|\downarrow\rangle_1|\uparrow\rangle_2$ state.

First suppose the system is in the $|\uparrow\rangle_1|\downarrow\rangle_2$ state. In order to find the post-measurement state, we will use the basis transformation (L.9) to rewrite $|\uparrow\rangle_1|\downarrow\rangle_2$ in the $|\pm\rangle$ basis,

$$|\uparrow\rangle_1|\downarrow\rangle_2 = \frac{1}{2}\Big[|+\rangle_1|+\rangle_2 - |+\rangle_1|-\rangle_2 + |-\rangle_1|+\rangle_2 + |-\rangle_1|-\rangle_2\Big] \ . \tag{L.12}$$

If the first particle is measured in the $|+\rangle$ state, then the system is projected onto the first two terms of (L.12) and the system is left in the state (normalized again to have norm 1)

$$\frac{1}{\sqrt{2}}\left(|+\rangle_1|+\rangle_2 - |+\rangle_1|-\rangle_2\right) = |+\rangle_1|\downarrow\rangle_2 \ . \tag{L.13}$$

Now if the initial system were in the state $|\downarrow\rangle_1|\uparrow\rangle_2$ instead, then following a similar reasoning, we obtain for the initial state in the $|\pm\rangle$ basis,

$$|\downarrow\rangle_1|\uparrow\rangle_2 = \frac{1}{2}\Big[|+\rangle_1|+\rangle_2 + |+\rangle_1|-\rangle_2 - |-\rangle_1|+\rangle_2 + |-\rangle_1|-\rangle_2\Big] \ . \tag{L.14}$$

Projecting again the first particle onto the $|+\rangle$ state again yields

$$\frac{1}{\sqrt{2}}\left(|+\rangle_1|+\rangle_2 + |+\rangle_1|-\rangle_2\right) = |+\rangle_1|\uparrow\rangle_2 \ . \tag{L.15}$$

Both sequences may occur with probability 1/2, so we can write our full final density matrix as

$$\begin{aligned}\rho' &= \frac{1}{2}\ |+\rangle_1|\downarrow\rangle_2\langle+|_1\langle\downarrow|_2 \ + \ \frac{1}{2}\ |+\rangle_1|\uparrow\rangle_2\langle+|_1\langle\uparrow|_2 \\ &= |+\rangle\langle+|_1 \otimes \left(\frac{1}{2}|\uparrow\rangle\langle\uparrow|_2 + \frac{1}{2}|\downarrow\rangle\langle\downarrow|_2\right) \\ &= |+\rangle\langle+|_1 \otimes \begin{pmatrix} 1/2 & 0 \\ 0 & 1/2 \end{pmatrix} \ .\end{aligned} \tag{L.16}$$

One can see that the state of particle #2 is either $\uparrow$ or $\downarrow$ with probability 1/2. This means that in contrast to the case where the two particles are initially entangled, like in point (ix), measuring the first particle in an arbitrary state does **not** correspondingly project the second particle, but "randomizes" it.

Note also that since the identity matrix is invariant under any basis transformation, one can see the second particle as simply "random", i.e. it can be described as being randomly either $|\uparrow\rangle$ or $|\downarrow\rangle$, or it can be described as being randomly $|+\rangle$ or $|-\rangle$, or as having a completely random spin as in point (viii). In quantum information terms, such states are known as **fully mixed**.

(xiii) A system in thermodynamical equilibrium is found in the state $|n\rangle$, of energy ϵ_n, with probability $\frac{1}{Z}\mathrm{e}^{-\epsilon_n/kT}$, where $Z = \sum_n \mathrm{e}^{-\epsilon_n/kT}$ is a normalization factor.

The density operator is then simply

$$\rho = \sum_n \frac{1}{Z}\,\mathrm{e}^{-\epsilon_n/kT}\,|n\rangle\langle n| = \frac{1}{Z}\,\mathrm{e}^{-H/kT} \ , \tag{L.17}$$

where H is the Hamiltonian of the system. (Here we noticed that $|n\rangle$ are the eigenvectors of $\mathrm{e}^{-H/kT}$ with corresponding eigenvalues $\mathrm{e}^{-\epsilon_n/kT}$.)

In the case of a harmonic oscillator, we have $H = \hbar\omega\left(n + \frac{1}{2}\right)$, and

$$Z = \sum_n \mathrm{e}^{-\frac{\hbar\omega}{kT}\left(n+\frac{1}{2}\right)} = \mathrm{e}^{-\frac{1}{2}\frac{\hbar\omega}{kT}} \cdot \frac{1}{1-\mathrm{e}^{-\frac{\hbar\omega}{kT}}} = \frac{1}{2\sinh\left[\frac{1}{2}\frac{\hbar\omega}{kT}\right]} \ . \tag{L.18}$$

Now the density operator is given by

$$\rho = 2\,\sinh\left[\frac{1}{2}\frac{\hbar\omega}{kT}\right]\sum_n \mathrm{e}^{-\frac{\hbar\omega}{kT}\left(n+\frac{1}{2}\right)}\,|n\rangle\langle n| \ . \tag{L.19}$$

So the components of the density matrix are

$$\rho_{nn} = 2\,\sinh\left[\frac{1}{2}\frac{\hbar\omega}{kT}\right]\,\mathrm{e}^{-\frac{\hbar\omega}{kT}\left(n+\frac{1}{2}\right)} \ ; \qquad \rho_{nm} = 0 \quad (n \neq m) \ . \tag{L.20}$$