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Ensembles for spin one half

Mixed ensemble averages In [1], Sakurai leaves it to the reader to verify that knowledge of the three ensemble averages [S_x], [S_y],[S_z] is sufficient to reconstruct the density operator for a spin one half system.

I'll do this in two parts, the first using a spin-up/down ensemble to see what form this has, then the general case. The general case is a bit messy algebraically. After first attempting it the hard way, I did the grunt work portion of that calculation in Mathematica, but then realized it's not so bad to do it manually.

Consider first an ensemble with density operator

$$\rho = w_+ \left|+\right\rangle \left\langle+\right| + w_- \left|-\right\rangle \left\langle-\right|, \tag{1.1}$$

where these are the $\mathbf{S} \cdot (\pm\hat{\mathbf{z}})$ eigenstates. The traces are

$$\begin{aligned}
\mathrm{Tr}(\rho\sigma_x) &= \left\langle+\right| \rho\sigma_x \left|+\right\rangle + \left\langle-\right| \rho\sigma_x \left|-\right\rangle \\
&= \left\langle+\right| \rho \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \left|+\right\rangle + \left\langle-\right| \rho \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \left|-\right\rangle \\
&= \left\langle+\right| \left(w_+ \left|+\right\rangle \left\langle+\right| + w_- \left|-\right\rangle \left\langle-\right|\right) \left|-\right\rangle + \left\langle-\right| \left(w_+ \left|+\right\rangle \left\langle+\right| + w_- \left|-\right\rangle \left\langle-\right|\right) \left|+\right\rangle \\
&= \left\langle+\right| w_- \left|-\right\rangle + \left\langle-\right| w_+ \left|+\right\rangle \\
&= 0,
\end{aligned} \tag{1.2}$$

$$\begin{aligned}
\mathrm{Tr}(\rho\sigma_y) &= \left\langle+\right| \rho\sigma_y \left|+\right\rangle + \left\langle-\right| \rho\sigma_y \left|-\right\rangle \\
&= \left\langle+\right| \rho \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix} \left|+\right\rangle + \left\langle-\right| \rho \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix} \left|-\right\rangle \\
&= i \left\langle+\right| \left(w_+ \left|+\right\rangle \left\langle+\right| + w_- \left|-\right\rangle \left\langle-\right|\right) \left|-\right\rangle - i \left\langle-\right| \left(w_+ \left|+\right\rangle \left\langle+\right| + w_- \left|-\right\rangle \left\langle-\right|\right) \left|+\right\rangle \\
&= i \left\langle+\right| w_- \left|-\right\rangle - i \left\langle-\right| w_+ \left|+\right\rangle \\
&= 0,
\end{aligned} \tag{1.3}$$

and

$$\begin{aligned}
\mathrm{Tr}(\rho\sigma_z) &= \left\langle+\right| \rho\sigma_z \left|+\right\rangle + \left\langle-\right| \rho\sigma_z \left|-\right\rangle \\
&= \left\langle+\right| \rho \left|+\right\rangle - \left\langle-\right| \rho \left|-\right\rangle \\
&= \left\langle+\right| \left(w_+ \left|+\right\rangle \left\langle+\right| + w_- \left|-\right\rangle \left\langle-\right|\right) \left|+\right\rangle - \left\langle-\right| \left(w_+ \left|+\right\rangle \left\langle+\right| + w_- \left|-\right\rangle \left\langle-\right|\right) \left|-\right\rangle \\
&= \left\langle+\right| w_+ \left|+\right\rangle - \left\langle-\right| w_- \left|-\right\rangle \\
&= w_+ - w_-.
\end{aligned} \tag{1.4}$$

Since $w_+ + w_- = 1$, this gives

$$\boxed{\begin{aligned} w_+ &= \frac{1 + \mathrm{Tr}(\rho\sigma_z)}{2} \\ w_- &= \frac{1 - \mathrm{Tr}(\rho\sigma_z)}{2} \end{aligned}} \tag{1.5}$$

Attempting to do a similar set of trace expansions this way for a more general spin basis turns out to be a really bad idea and horribly messy. So much so that I resorted to Mathematica to do this symbolic work. However, it's not so bad if the trace is done completely in matrix form.

Using the basis

$$\begin{aligned} |\mathbf{S}\cdot\hat{\mathbf{n}};+\rangle &= \begin{bmatrix} \cos(\theta/2) \\ \sin(\theta/2)e^{i\phi} \end{bmatrix} \\ |\mathbf{S}\cdot\hat{\mathbf{n}};-\rangle &= \begin{bmatrix} \sin(\theta/2)e^{-i\phi} \\ -\cos(\theta/2) \end{bmatrix}, \end{aligned} \tag{1.6}$$

the projector matrices are

$$\begin{aligned} |\mathbf{S}\cdot\hat{\mathbf{n}};+\rangle\langle\mathbf{S}\cdot\hat{\mathbf{n}};+| &= \begin{bmatrix} \cos(\theta/2) \\ \sin(\theta/2)e^{i\phi} \end{bmatrix} \begin{bmatrix} \cos(\theta/2) & \sin(\theta/2)e^{-i\phi} \end{bmatrix} \\ &= \begin{bmatrix} \cos^2(\theta/2) & \cos(\theta/2)\sin(\theta/2)e^{-i\phi} \\ \sin(\theta/2)\cos(\theta/2)e^{i\phi} & \sin^2(\theta/2) \end{bmatrix}, \end{aligned} \tag{1.7}$$

$$\begin{aligned} |\mathbf{S}\cdot\hat{\mathbf{n}};-\rangle\langle\mathbf{S}\cdot\hat{\mathbf{n}};-| &= \begin{bmatrix} \sin(\theta/2)e^{-i\phi} \\ -\cos(\theta/2) \end{bmatrix} \begin{bmatrix} \sin(\theta/2)e^{i\phi} & -\cos(\theta/2) \end{bmatrix} \\ &= \begin{bmatrix} \sin^2(\theta/2) & -\cos(\theta/2)\sin(\theta/2)e^{-i\phi} \\ -\cos(\theta/2)\sin(\theta/2)e^{i\phi} & \cos^2(\theta/2) \end{bmatrix} \end{aligned} \tag{1.8}$$

With $C = \cos(\theta/2)$, $S = \sin(\theta/2)$, a general density operator in this basis has the form

$$\begin{aligned} \rho &= w_+ \begin{bmatrix} C^2 & CSe^{-i\phi} \\ SCe^{i\phi} & S^2 \end{bmatrix} + w_- \begin{bmatrix} S^2 & -CSe^{-i\phi} \\ -CSe^{i\phi} & C^2 \end{bmatrix} \\ &= \begin{bmatrix} w_+C^2 + w_-S^2 & (w_+ - w_-)CSe^{-i\phi} \\ (w_+ - w_-)SCe^{i\phi} & w_+S^2 + w_-C^2 \end{bmatrix}. \end{aligned} \tag{1.9}$$

The products with the Pauli matrices are

$$\begin{aligned} \rho\sigma_x &= \begin{bmatrix} w_+C^2 + w_-S^2 & (w_+ - w_-)CSe^{-i\phi} \\ (w_+ - w_-)SCe^{i\phi} & w_+S^2 + w_-C^2 \end{bmatrix} \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \\ &= \begin{bmatrix} (w_+ - w_-)CSe^{-i\phi} & w_+C^2 + w_-S^2 \\ w_+S^2 + w_-C^2 & (w_+ - w_-)SCe^{i\phi} \end{bmatrix} \end{aligned} \tag{1.10}$$

$$\begin{aligned}\rho\sigma_y &= \begin{bmatrix} w_+ C^2 + w_- S^2 & (w_+ - w_-) C S e^{-i\phi} \\ (w_+ - w_-) S C e^{i\phi} & w_+ S^2 + w_- C^2 \end{bmatrix} \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix} \\ &= i \begin{bmatrix} (w_+ - w_-) C S e^{-i\phi} & -w_+ C^2 - w_- S^2 \\ w_+ S^2 + w_- C^2 & -(w_+ - w_-) S C e^{i\phi} \end{bmatrix}\end{aligned} \tag{1.11}$$

$$\begin{aligned}\rho\sigma_z &= \begin{bmatrix} w_+ C^2 + w_- S^2 & (w_+ - w_-) C S e^{-i\phi} \\ (w_+ - w_-) S C e^{i\phi} & w_+ S^2 + w_- C^2 \end{bmatrix} \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} \\ &= \begin{bmatrix} w_+ C^2 + w_- S^2 & -(w_+ - w_-) C S e^{-i\phi} \\ (w_+ - w_-) S C e^{i\phi} & -(w_+ S^2 + w_- C^2) \end{bmatrix}\end{aligned} \tag{1.12}$$

The respective traces can be read right off the matrices

$$\begin{aligned}\mathrm{Tr}(\rho\sigma_x) &= (w_+ - w_-) \sin\theta \cos\phi \\ \mathrm{Tr}(\rho\sigma_y) &= (w_+ - w_-) \sin\theta \sin\phi \, . \\ \mathrm{Tr}(\rho\sigma_z) &= (w_+ - w_-) \cos\theta\end{aligned} \tag{1.13}$$

This gives

$$(w_+ - w_-)\hat{\mathbf{n}} = \left(\mathrm{Tr}(\rho\sigma_x), \mathrm{Tr}(\rho\sigma_y), \mathrm{Tr}(\rho\sigma_z)\right), \tag{1.14}$$

or

$$\boxed{w_\pm = \frac{1 \pm \sqrt{\mathrm{Tr}^2(\rho\sigma_x) + \mathrm{Tr}^2(\rho\sigma_y) + \mathrm{Tr}^2(\rho\sigma_z)}}{2}.} \tag{1.15}$$

So, as claimed, it's possible to completely describe the ensemble weight factors using the ensemble averages of $[S_x], [S_y], [S_z]$. I used the Pauli matrices instead, but the difference is just an $\hbar/2$ scaling adjustment.

Pure ensemble It turns out that doing the above is also pr. 3.10(b). Part (a) of that problem is to show how the expectation values $\langle S_x \rangle, \langle S_y \rangle, \langle S_x \rangle$ fully determine the spin orientation for a pure ensemble.

Suppose that the system is in the state $|\mathbf{S} \cdot \hat{\mathbf{n}}; +\rangle$ as defined in eq. (1.6), then the expectation values of $\sigma_x, \sigma_y, \sigma_z$ with respect to this state are

$$\begin{aligned}\langle \sigma_x \rangle &= \begin{bmatrix} \cos(\theta/2) & \sin(\theta/2) e^{-i\phi} \end{bmatrix} \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \begin{bmatrix} \cos(\theta/2) \\ \sin(\theta/2) e^{i\phi} \end{bmatrix} \\ &= \begin{bmatrix} \cos(\theta/2) & \sin(\theta/2) e^{-i\phi} \end{bmatrix} \begin{bmatrix} \sin(\theta/2) e^{i\phi} \\ \cos(\theta/2) \end{bmatrix} \\ &= \sin\theta \cos\phi,\end{aligned} \tag{1.16}$$

$$
\begin{aligned}
\langle \sigma_y \rangle &= \begin{bmatrix}\cos(\theta/2) & \sin(\theta/2)e^{-i\phi}\end{bmatrix} \begin{bmatrix}0 & -i \\ i & 0\end{bmatrix} \begin{bmatrix}\cos(\theta/2) \\ \sin(\theta/2)e^{i\phi}\end{bmatrix} \\
&= i \begin{bmatrix}\cos(\theta/2) & \sin(\theta/2)e^{-i\phi}\end{bmatrix} \begin{bmatrix}-\sin(\theta/2)e^{i\phi} \\ \cos(\theta/2)\end{bmatrix} \\
&= \sin\theta \sin\phi,
\end{aligned} \tag{1.17}
$$

$$
\begin{aligned}
\langle \sigma_z \rangle &= \begin{bmatrix}\cos(\theta/2) & \sin(\theta/2)e^{-i\phi}\end{bmatrix} \begin{bmatrix}1 & 0 \\ 0 & -1\end{bmatrix} \begin{bmatrix}\cos(\theta/2) \\ \sin(\theta/2)e^{i\phi}\end{bmatrix} \\
&= \begin{bmatrix}\cos(\theta/2) & \sin(\theta/2)e^{-i\phi}\end{bmatrix} \begin{bmatrix}\cos(\theta/2) \\ -\sin(\theta/2)e^{i\phi}\end{bmatrix} \\
&= \cos\theta.
\end{aligned} \tag{1.18}
$$

So we have

$$
\boxed{\hat{\mathbf{n}} = \left(\langle \sigma_x \rangle, \langle \sigma_y \rangle, \langle \sigma_z \rangle\right).} \tag{1.19}
$$

The spin direction is completely determined by this vector of expectation values (or equivalently, the expectation values of S_x, S_y, S_z).

Bibliography

[1] Jun John Sakurai and Jim J Napolitano. *Modern quantum mechanics*. Pearson Higher Ed, 2014. 1