

Problem 1: Matrix representation of the density matrix

The completeness relation

$$\sum_n |n\rangle \langle n| = 1 \quad (1)$$

tells us that the set of vectors $\{|n\rangle\}$ spans its vector space, and that any vector in that space can be defined as some linear combination of them. There is, however, something else useful that comes with this relation. Let us consider an operator \hat{A} and apply the relation twice like so:

$$\hat{A} = \sum_{m,n} |m\rangle \langle m| \hat{A} |n\rangle \langle n| \quad (2)$$

If N is the dimensionality of the vector space, then we have N^2 terms in the summation. We can arrange the $\langle m| \hat{A} |n\rangle$ into a $N \times N$ square matrix, forming the matrix representation of the operator. Formally,

$$\hat{A}_{mn} = \langle m| \hat{A} |n\rangle \quad (3)$$

We can use this to compute the elements of the density matrix in any given basis. The density matrix for the general case of a mixed state is given by

$$\rho = \sum_i p_i |\psi_i\rangle \langle \psi_i| \quad (4)$$

Expanding $|\psi_i\rangle$ in some basis $\{|i\rangle\}$, we write

$$\begin{aligned} \rho &= \sum_i p_i \left(\sum_u c_u^i |u\rangle \right) \left(\sum_v (c_v^i)^* \langle v| \right) \\ &= \sum_{u,v} \left(\sum_i p_i c_u^i (c_v^i)^* \right) |u\rangle \langle v| \end{aligned} \quad (5)$$

The matrix elements in that basis is thus

$$\begin{aligned} \rho_{ab} &= \langle a| \rho |b\rangle \\ &= \langle a| \sum_{u,v} \left(\sum_i p_i c_u^i (c_v^i)^* \right) |u\rangle \langle v| b\rangle \\ &= \sum_i p_i c_a^i (c_b^i)^* \\ &\equiv \overline{c_a c_b^*} \end{aligned} \quad (6)$$

That is, the matrix element of a mixed-state density matrix is given by the mixture average of the projection of each component state onto the given basis.

Problem 2: Expectation value in terms of the density matrix

We again make use of the completeness relation:

$$\begin{aligned} \langle A \rangle &= \langle \psi | \hat{A} | \psi \rangle \\ &= \langle \psi | \left(\sum_j |j\rangle \langle j| \right) \hat{A} \left(\sum_i |i\rangle \langle i| \right) | \psi \rangle \\ &= \sum_{i,j} \langle \psi | j \rangle \langle j | \hat{A} | i \rangle \langle i | \psi \rangle \end{aligned} \quad (7)$$

But note that

$$\begin{aligned} \langle j | \hat{A} | i \rangle &= A_{ji} \\ \langle i | \psi \rangle \langle \psi | j \rangle &= \rho_{ij} \end{aligned} \quad (8)$$

Thus,

$$\langle A \rangle = \sum_{i,j} \rho_{ij} \hat{A}_{ji} = \sum_i (\rho \hat{A})_{ii} = \text{tr}(\rho \hat{A}) \quad (9)$$

This is for a pure state. For a mixed state, we have

$$\begin{aligned}\overline{\langle A \rangle} &= \sum_i p_i \langle \psi_i | \hat{A} | \psi_i \rangle \\ &= \sum_{i,j,k} p_i \langle \psi_i | j \rangle \langle j | \hat{A} | k \rangle \langle k | \psi_i \rangle\end{aligned}\quad (10)$$

But

$$\begin{aligned}\langle k | \left(\sum_i p_i | \psi_i \rangle \langle \psi_i | \right) | j \rangle &= \rho_{kj}^{(\text{mixed state})} \\ \langle j | A | k \rangle &= A_{jk}\end{aligned}\quad (11)$$

so we obtain (not quite) the same expression

$$\overline{\langle A \rangle} = \text{tr} \left(\rho^{(\text{mixed state})} \hat{A} \right) \quad (12)$$

Problem 3: Miller's QM Problem 14.3.1

We have

$$\begin{aligned}| \psi_1 \rangle &= | H \rangle \rightarrow 20\% \text{ chance} \\ | \psi_2 \rangle &= 0.6 | H \rangle + 0.8i | V \rangle \rightarrow 80\% \text{ chance}\end{aligned}\quad (13)$$

where $| H \rangle$ and $| V \rangle$ are the orthonormal polarization basis state vectors.

As we are asked to put $\langle H | \rho | H \rangle$ as the top left element of the density matrix, we shall use

$$| H \rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \quad | V \rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix} \quad (14)$$

Our density matrix is

$$\begin{aligned}\rho &= 0.2 | \psi_1 \rangle \langle \psi_1 | + 0.8 | \psi_2 \rangle \langle \psi_2 | \\ &= 0.2 \begin{pmatrix} 1 \\ 0 \end{pmatrix} \begin{pmatrix} 1 & 0 \end{pmatrix} + 0.8 \begin{pmatrix} 0.6 \\ 0.8i \end{pmatrix} \begin{pmatrix} 0.6 & 0.8i \end{pmatrix} \\ &= \begin{pmatrix} 0.488 & 0.384i \\ 0.384i & -0.512 \end{pmatrix}\end{aligned}\quad (15)$$

Problem 4: Miller's QM Problem 14.3.2

(a) & (b)

With the z -axis as the axis of quantization, and the usual convention that

$$|\uparrow\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \quad |\downarrow\rangle = \begin{pmatrix} 0 \\ i \end{pmatrix} \quad (16)$$

we have

$$\begin{aligned} \rho &= 0.5 |s_x\rangle \langle s_x| + 0.5 |s_y\rangle \langle s_y| \\ &= 0.5 \frac{1}{\sqrt{2}} (|\uparrow\rangle + |\downarrow\rangle) (\langle\uparrow| + \langle\downarrow|) + 0.5 (|\uparrow\rangle + i|\downarrow\rangle) (\langle\uparrow| + i\langle\downarrow|) \\ &= 0.5 \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 1 \end{pmatrix} \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \end{pmatrix} + 0.5 \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ i \end{pmatrix} \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & -i \end{pmatrix} \\ &= \frac{1}{4} \begin{pmatrix} 2 & 1-i \\ 1+i & 2 \end{pmatrix} \end{aligned} \quad (17)$$

(c)

This one is easy, since we are already familiar with the Pauli matrices in this basis. If $\mathbf{x}, \mathbf{y}, \mathbf{z}$ are the Cartesian basis vectors, then

$$\begin{aligned} \hat{\mu} &= g\mu_B (\sigma_x \mathbf{x} + \sigma_y \mathbf{y} + \sigma_z \mathbf{z}) \\ &= g\mu_B \begin{pmatrix} \mathbf{z} & \mathbf{x} - i\mathbf{y} \\ \mathbf{x} + i\mathbf{y} & -\mathbf{z} \end{pmatrix} \end{aligned} \quad (18)$$

(d)

$$\begin{aligned} \langle \mu \rangle &= \text{tr}(\rho \hat{\mu}) \\ &= \frac{g\mu_B}{4} \text{tr} \left(\begin{pmatrix} 2 & 1-i \\ 1+i & 2 \end{pmatrix} \begin{pmatrix} \mathbf{z} & \mathbf{x} - i\mathbf{y} \\ \mathbf{x} + i\mathbf{y} & -\mathbf{z} \end{pmatrix} \right) \\ &= \frac{g\mu_B}{4} (2\mathbf{z} + (1-i)(\mathbf{x} + i\mathbf{y}) + (1+i)(\mathbf{x} - i\mathbf{y}) + 2(-\mathbf{z})) \\ &= \frac{g\mu_B}{4} (2, 2, 0) \end{aligned} \quad (19)$$

It is exactly what we found in problem 14.1.1.