Pure states and mixtures

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Solution: *a. In this case, the system is in a pure state. Therefore, the density operator is,*

$$\rho = |\psi\rangle\langle\psi| = \alpha|1\rangle\langle 1| + \beta|2\rangle\langle 2| + \alpha\beta^*|1\rangle\langle 2| + \alpha^*\beta|2\rangle\langle 1| = \begin{pmatrix} |\alpha|^2 & \alpha^*\beta \\ \alpha\beta^* & |\beta|^2 \end{pmatrix}$$
$$= \begin{pmatrix} \langle 1|\rho|1\rangle & \langle 1|\rho|2\rangle \\ \langle 2|\rho|1\rangle & \langle 2|\rho|2\rangle \end{pmatrix} = \begin{pmatrix} \langle 1|\psi\rangle\langle\psi|1\rangle & \langle 1|\psi\rangle\langle\psi|2\rangle \\ \langle 2|\psi\rangle\langle\psi|1\rangle & \langle 2|\psi\rangle\langle\psi|2\rangle \end{pmatrix} \; .$$

Now the trace, which is the sum of the diagonal elements, must be normalized,

$$Tr\ \hat\rho = |\alpha|^2 + |\beta|^2 = 1 \; .$$

The square is,

$$\hat\rho^2 = \begin{pmatrix} |\alpha|^4 + \alpha^*\beta\alpha\beta^* & |\alpha|^2\alpha^*\beta + \alpha^*\beta|\beta|^2 \\ |\alpha|^2\alpha\beta^* + \alpha\beta^*|\beta|^2 & \alpha^*\beta\alpha\beta^* + |\beta|^4 \end{pmatrix} = \begin{pmatrix} |\alpha|^2 & \alpha^*\beta \\ \alpha\beta^* & |\beta|^2 \end{pmatrix} = \hat\rho \; .$$

The expectation value of the Hamiltonian is,

$$\langle\hat H\rangle = Tr\ \hat\rho\hat H = Tr\ \begin{pmatrix} |\alpha|^2 & \alpha^*\beta \\ \alpha\beta^* & |\beta|^2 \end{pmatrix}\begin{pmatrix} 0 & \Omega \\ \Omega & \omega_0 \end{pmatrix} = \alpha^*\beta\Omega + \alpha\beta^*\Omega + |\beta|^2\omega_0$$
$$= \langle\psi|\hat H|\psi\rangle = (\alpha^*\langle 1| + \beta^*\langle 2|)\,\hat H\,(\alpha|1\rangle + \beta|2\rangle)$$
$$= |\alpha|^2\langle 1|\hat H|1\rangle + |\beta|^2\langle 2|\hat H|2\rangle + \alpha^*\beta\langle 1|\hat H|2\rangle + \alpha\beta^*\langle 2|\hat H|1\rangle = |\beta|^2\omega_0 + \alpha^*\beta\Omega + \alpha\beta^*\Omega \; .$$

b. In the case of a mixture of eigenstates, the density operator is,

$$\hat\rho = \mu|1\rangle\langle 1| + \nu|2\rangle\langle 2| = \begin{pmatrix} \mu & 0 \\ 0 & \nu \end{pmatrix} \; .$$

The trace is always normalized,

$$Tr\ \hat\rho = Tr\ \begin{pmatrix} \mu & 0 \\ 0 & \nu \end{pmatrix} = \mu + \nu = 1 \; .$$

but the state is not pure, since,

$$\rho^2 = \begin{pmatrix} \mu^2 & 0 \\ 0 & \nu^2 \end{pmatrix} \neq \hat\rho \; .$$

The average value of the Hamiltonian is now,

$$\langle\hat H\rangle = Tr\ \hat\rho\hat H = Tr\ \begin{pmatrix} \mu & 0 \\ 0 & \nu \end{pmatrix}\begin{pmatrix} 0 & \Omega \\ \Omega & \omega_0 \end{pmatrix} = Tr\begin{pmatrix} 0 & \mu\Omega \\ \nu\Omega & \nu\omega_0 \end{pmatrix} = \nu\omega_0 \; .$$