# QUANTUM MECHANICS II

# PHYS 517

## Solutions to Problem Set # 4

## Distributed: May 13, 2015

## Reduced Density Matrices

In this problem you will have to use: Schrödinger's time evolution equation, angular momentum recoupling (Clebsch-Gordon) coefficients, density matrices, and you will learn about *reduced* density matrices.

**1. Reduced Density Matrices:** A $p$ electron is initially in a state with $m_l = 0$, $m_s = +\frac{1}{2}$.

**a.** Write down its density matrix $\rho_{i\alpha,j\beta}(t=0)$. Here $-1 \leq i, j \leq +1$ and $\alpha, \beta = \pm\frac{1}{2}$.

**Ans:**

$$\rho(0) = \begin{array}{cc} \left[\begin{array}{cccccc} 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \end{array}\right] & \begin{array}{rc} 1 & + \\ 0 & + \\ -1 & + \\ 1 & - \\ 0 & - \\ -1 & - \end{array} \end{array}$$

Only the two states with $m_j = m_l + m_s = \frac{1}{2}$ will occur in the computations below: $\left| \begin{array}{cc} l=1 & s=1/2 \\ m_l=0 & m_s=1/2 \end{array} \right\rangle$ and $\left| \begin{array}{cc} l=1 & s=1/2 \\ m_l=1 & m_s=-1/2 \end{array} \right\rangle$. For this reason we keep only those two rows/columns for the density matrix:

$$\rho(0) = \begin{array}{cc} \left[\begin{array}{cc} 1 & 0 \\ 0 & 0 \end{array}\right] & \begin{array}{cc} 0 & + \\ 1 & - \end{array} \end{array}$$

**b.** The electron state evolves in time under a spin-orbit hamiltonian $H = \lambda \mathbf{L} \cdot \mathbf{S}$. Set $\lambda = 1$ and compute the state at later time $t$: $\psi(t) = \sum_{i,\alpha} c_{i,\alpha}(t)|i,\alpha\rangle$.

**ANS:** The two eigenstates of the hamiltonian are the states with $j = \frac{3}{2}$ and $j = \frac{1}{2}$, both with $m_j = \frac{1}{2}$.

$$| \begin{smallmatrix} \frac{3}{2} \\ \frac{1}{2} \end{smallmatrix} \rangle = |\frac{3}{2}\rangle = +\sqrt{\frac{2}{3}}|0,+\rangle + \sqrt{\frac{1}{3}}|1,-\rangle$$

$$| \begin{smallmatrix} \frac{1}{2} \\ \frac{1}{2} \end{smallmatrix} \rangle = |\frac{1}{2}\rangle = -\sqrt{\frac{1}{3}}|0,+\rangle + \sqrt{\frac{2}{3}}|1,-\rangle$$

These are easily inverted:

$$|0,+\rangle = \sqrt{\frac{2}{3}}|3/2\rangle - \sqrt{\frac{1}{3}}|1/2\rangle$$

$$|1,-\rangle = \sqrt{\frac{1}{3}}|3/2\rangle + \sqrt{\frac{2}{3}}|1/2\rangle$$

The eigenvalue of the state with $j = \frac{3}{2}$ is $\frac{1}{2}\left(J^2 - L^2 - S^2\right) = \frac{1}{2}\left(\frac{3}{2}\cdot\frac{5}{2} - 1\cdot 2 - \frac{1}{2}\cdot\frac{3}{2}\right) = \frac{1}{2}$ and for $j = \frac{1}{2}$ the eigenvalue is $-1$. Therefore the wave function $\psi(t)$ is

$$|\psi(t)\rangle = \sqrt{\frac{2}{3}}\left(+\sqrt{\frac{2}{3}}|0,+\rangle + \sqrt{\frac{1}{3}}|1,-\rangle\right)e^{i\phi_3} - \sqrt{\frac{1}{3}}\left(-\sqrt{\frac{1}{3}}|0,+\rangle + \sqrt{\frac{2}{3}}|1,-\rangle\right)e^{i\phi_1}$$

$$= \left(\frac{2}{3}e^{i\phi_3} + \frac{1}{3}e^{i\phi_1}\right)|0,+\rangle + \frac{\sqrt{2}}{3}\left(e^{i\phi_3} - e^{i\phi_1}\right)|1,-\rangle = A|0,+\rangle + B|1,-\rangle$$

The phase factors are $\phi_3 = (E_{3/2}/\hbar)t = t/2$ and $\phi_1 = -t$.

**c.** Write down its density matrix $\rho_{i\alpha,j\beta}(t)$.

**ANS:** Take the outer product of the last expression above:

$$\rho(t) = \begin{array}{cc} \begin{bmatrix} AA^* & AB^* \\ BA^* & BB^* \end{bmatrix} & \begin{array}{cc} 0 & + \\ 1 & - \end{array} \end{array}$$

**d.** What is its entropy?

**ANS:** 0. The density matrix is that of a pure state, so its eigenvalues are $+1$ (one) and 0 (all the rest).

**e.** Compute the *reduced* spin density matrix

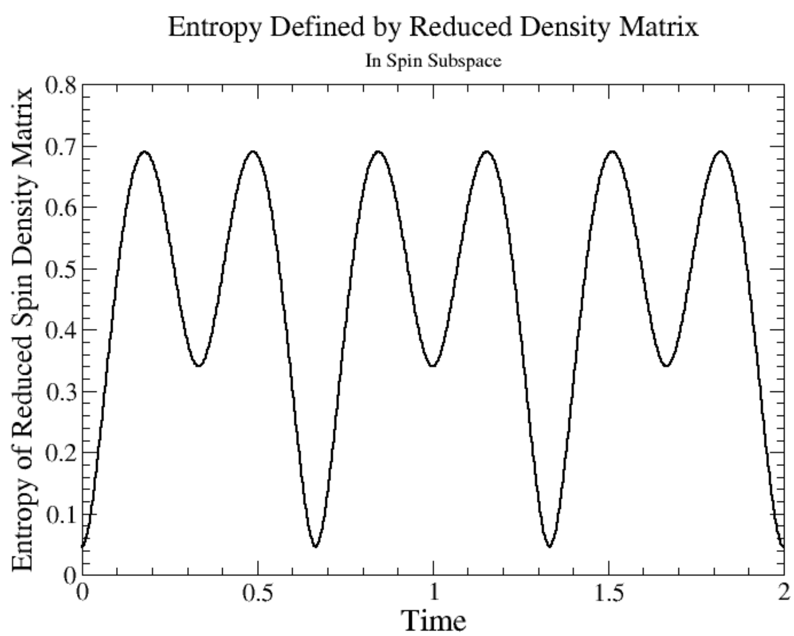
$$\rho^{\text{red}}_{\alpha,\beta}(t) = \sum_{i=j}\rho_{i\alpha,j\beta}(t)$$

**ANS:**

$$\rho^{\mathrm{red}}_{\alpha,\beta}(t) = \begin{array}{c} \left[\begin{array}{cc} AA^* & 0 \\ 0 & BB^* \end{array}\right] \end{array} \begin{array}{c} + \\ - \end{array}$$

**f.** Plot the entropy determined by this reduced density matrix as a function of time.

**ANS:** $AA^* = \frac{5}{9} + \frac{4}{9}\cos(\phi_3 - \phi_1)$ and $BB^* = \frac{4}{9} - \frac{4}{9}\cos(\phi_3 - \phi_1)$. These are the probabilities that enter into $S = -\sum p_i \log p_i$.



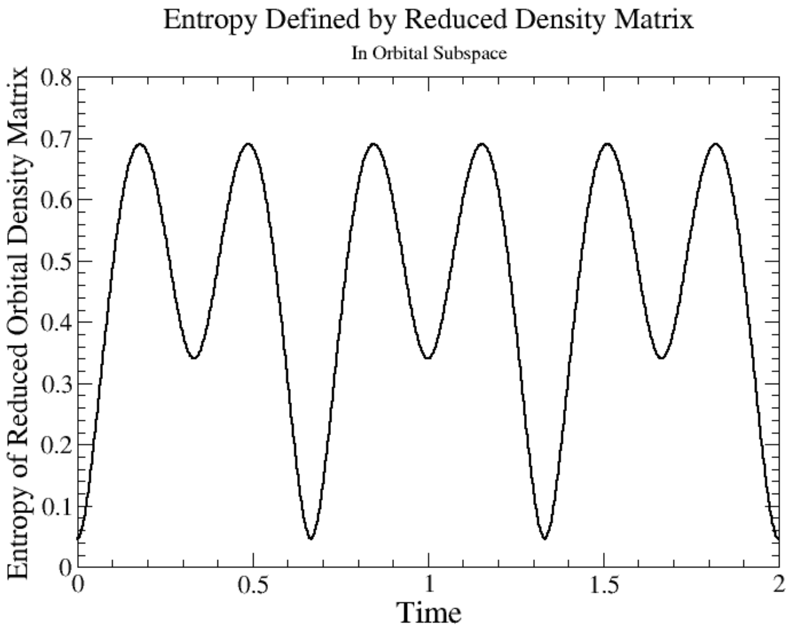

**g.** Compute the *reduced* orbital density matrix

$$\rho^{\mathrm{red}}_{i,j}(t) = \sum_{\alpha=\beta} \rho_{i\alpha,j\beta}(t)$$

**ANS:**

$$\rho^{\mathrm{red}}_{i,j}(t) = \left[\begin{array}{ccc} BB^* & 0 & 0 \\ 0 & AA^* & 0 \\ 0 & 0 & 0 \end{array}\right] \begin{array}{c} + \\ 0 \\ - \end{array}$$

**h.** Plot the entropy determined by this reduced density matrix as a function of time.




**i.** Explain (in words) what this computation has taught you.

**ANS:** Entropy of a combined quantum system is conserved under time evolution. If only a subsystem is available for measurement, the density matrix describing this subsystem will indicate that the entropy *of that subsystem* is not conserved.