Solution to Problem Set 9 Physics 480 / Fall 1999 Prof. Klaus Schulten / Prepared by Pinaki Sengupta

Problem 1: An important relationship

1a. Since $A = diag(\lambda_1, \lambda_2, \lambda_3)$ implies $A^n = diag(\lambda_1^n, \lambda_2^n, \lambda_3^n)$ $U = exp(iA) = diag(e^{i\lambda_1}, e^{i\lambda_2}, e^{i\lambda_3})$ and $detU = exp(i(\lambda_1 + \lambda_2 + \lambda_3))$ Hence detU = 1 implies $(\lambda_1 + \lambda_2 + \lambda_3) = 0 \mod 2\pi$ i.e. $tr(A) = 0 \mod 2\pi$.

Hence detU = 1 implies $(\lambda_1 + \lambda_2 + \lambda_3) = 0 \mod 2\pi$ i.e. $tr(A) = 0 \mod 2\pi$. 1b. Let h(1), h(2), h(3) be the 3 eigenvectors of A. i.e. $\sum_{m=1}^{3} A_m^n h^m(i) = \epsilon_i h^n(i), n = 1, 2, 3$ Orthogonality of the eigenvectors give,

$$\sum_{m} h_m(i)h^m(j) = \delta_{ij}$$

Let us define the matrix R as

$$T_k^m = h_k(m)$$

It follows from the above orthogonality condition that

$$(T^{-1})_m^l = h^l(m)$$

Let us consider the matrix

$$A' = TAT^{-1}$$

The matrix elements of A' are

$$(A')_n^m = T_k^m A_L^k (T^{-1})_n^l$$

= $h_k(m) A_l^k h^l(n)$
= $h_k(m) \epsilon_n h^k(n)$
= $\epsilon_n \delta_{mn}$

Hence A' is diagonal.

1c.

$$\begin{aligned} TUT^{-1} &= Te^{iA}T^{-1} \\ &= 1\sum_{n=0}^{\infty} \frac{i^n}{n!}TA^nT^{-1} \\ &= \sum_{n=0}^{\infty} \frac{i^n}{n!}TAT^{-1}TAT^{-1}.....TAT^{-1} \\ &= exp[iTAT^{-1}] \end{aligned}$$

1d.

implies
$$B^n = \begin{pmatrix} \lambda_1^n & 0\\ 0 & \lambda_2^n \end{pmatrix}$$

Hence, $e^B = \begin{pmatrix} e^{\lambda_1} & 0\\ 0 & e^{\lambda_2} \end{pmatrix}$
1e.

$$Tr(AB) = A_{ij}B_{ji}$$
$$= B_{ji}A_{ij}$$
$$= Tr(BA)$$

 $B = \left(\begin{array}{cc} \lambda_1 & 0\\ 0 & \lambda_2 \end{array}\right)$

Therefore, $Tr(TAT^{-1}) = Tr(T^{-1}TA) = Tr(A)$ 1f.

$$U = e^{iTA}$$
$$TUT^{-1} = e^{iTAT^{-1}}$$
$$detTUT^{-1} = det(e^{iTAT^{-1}})$$

but, $detTUT^{-1} = det(U)$ therefore, det(U) = 1 implies

$$det(e^{iTAT^{-1}}) = 1$$

which implies

$$Tr(TAT^{-1}) = 0mod2\pi$$

But since Tr(AB) = Tr(BA) $Tr(TAT^{-1}) = 0$ imples $Tr(A) = 0mod2\pi$

Problem 2: Spin along x_1 axis

2a. Taylor expanding the operator (3) we get

$$e^{i\theta\sigma_1/2} = \sum_{n=0}^{\infty} \frac{i^n}{n!} (\frac{\theta_1}{2})^n \sigma_1^n$$

Using the fact that

$$\sigma_1 = \left(\begin{array}{cc} 0 & 1\\ 1 & 0 \end{array}\right)$$

 $\sigma_1^2 = I$ and $i^2 = -1$ we get,

$$e^{i\theta\sigma_1/2} = \sum_{n=0}^{\infty} \frac{(-1)^n}{2n!} (\frac{\theta_1}{2})^{2n} \cdot I + i \sum_{n=0}^{\infty} \frac{(-1)^n}{(2n+1)!} (\frac{\theta_1}{2})^{2n+1} \cdot \sigma_1$$
$$e^{i\theta\sigma_1/2} = \cos\frac{\theta_1}{2} I + i \sin\frac{\theta_1}{2} \sigma_1$$
$$= \begin{pmatrix} \cos\frac{\theta_1}{2} & i \sin\frac{\theta_1}{2} \\ i \sin\frac{\theta_1}{2} & \cos\frac{\theta_1}{2} \end{pmatrix}$$

2b. The required probability is given by

$$P = |M|^2$$

where,

$$M = y^T A X$$

where

$$y = \frac{1}{\sqrt{2}} \begin{pmatrix} 1\\1 \end{pmatrix}$$
$$A = \begin{pmatrix} \cos(\theta_1/2) & i\sin(\theta_1/2)\\ i\sin(\theta_1/2) & \cos(\theta_1/2) \end{pmatrix}$$
$$X = \begin{pmatrix} 1\\0 \end{pmatrix}$$

It follows $M = \frac{1}{\sqrt{2}} (\cos(\theta_1/2) + i\sin(\theta_1/2))$ Therefore, P = 1/2

Problem 3: Spin in a magnetic field

If the axis of quantization is chosen to be along the magnetic field, then

$$H = -\frac{e}{2mc}\vec{\sigma}.\vec{B}$$
$$H = -\frac{e}{2mc}B_0 \begin{pmatrix} 1 & 0\\ 0 & -1 \end{pmatrix}$$

The time dependence of an arbitrary spin state $\begin{pmatrix} a \\ b \end{pmatrix}$ is given by

$$\psi(t) = e^{-iHt}\psi(0)$$
$$= \begin{pmatrix} e^{i\frac{e}{2mc}Bt} & a\\ e^{-i\frac{e}{2mc}Bt} & b \end{pmatrix}$$

which is the same as a rotation of the spin about the z-axis by an angle $\frac{eBt}{2mc}$

3b. For
$$\psi(0) = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$$

$$\psi(t) = \begin{pmatrix} e^{i\frac{e}{2mc}Bt} \\ 0 \end{pmatrix}$$

Problem 4: Spin Dynamics

4a.

$$H = \frac{g\mu_B\hbar}{2}(B_x\sigma_x + B_y\sigma_y + B_z\sigma_z) + a(\frac{\hbar}{2})^2(\sigma_x^e\sigma_x^n + \sigma_y^e\sigma_y^n + \sigma_z^e\sigma_z^n)$$

Using the fact that

$$\sigma_x |\pm\rangle = |\mp\rangle$$

$$\sigma_y |\pm\rangle = \pm i |\mp\rangle$$

$$\sigma_z |\pm\rangle = \pm 1 |\pm\rangle$$

for both electronic and nuclear spins, we get the Hamiltonian in a matrix form in the given basis $(\hbar = 1)$

$$H = \begin{pmatrix} \frac{g\mu_B}{2}B_3 + \frac{a}{4} & 0 & \frac{g\mu_B}{2}(B_1 - iB_2) & 0\\ 0 & \frac{g\mu_B}{2}B_3 - \frac{a}{4} & \frac{a}{2} & \frac{g\mu_B}{2}(B_1 - iB_2)\\ \frac{g\mu_B}{2}(B_1 + iB_2) & \frac{a}{2} & -\frac{g\mu_B}{2}B_3 - \frac{a}{4} & 0\\ 0 & \frac{g\mu_B}{2}(B_1 + iB_2) & 0 & -\frac{g\mu_B}{2}B_3 + \frac{a}{4} \end{pmatrix}$$

For $\vec{B} = (0, 0, b)$ the eigenvalues are $\frac{a}{4} \pm 8.8b, -\frac{a}{4} \pm \frac{1}{2}\sqrt{a^2 + (g\mu_B B_3)^2}$ 4c. The time evolution of a wave function is given by

$$\psi(t) = e^{-iHt}\psi(0)$$

Here $\psi(0) = |2\rangle$ We expand it in the basis of eigenvectors of H

$$|2> = \sum_{n=1}^{4} C_n |n>$$

Therefore

$$|\psi(t)\rangle = \sum_{n} C_{n} e^{-iE_{n}t} |n\rangle$$

$$<2|\psi(t)>=\sum_{n}C_{n}^{*}C_{n}e^{-iE_{n}t}$$

Therefore, Probability of finding it in another state,

$$P = 1 - |<2|\psi(t)>|^2$$