TWO-STATE PROBLEMS

IN THIS PROJECT WE REVIEW A FAMOUS PROBLEM IN PHYSICS A TWO-STATE PROBLEM WITH A SINUSOIDAL POTENTIAL I BASE MY DISCUSSION UPON CHAPTER 5 FROM SAKURAI AND NAPOLITANO'S BOOK, AS WELL AS BARTON ZWEIBACH'S NOTES ON QUANTUM MECHANICS

FOLLOWING BARTON, WE WILL STUDY SPIN PRECESSION BOTH MATHEMATICALLY AND FROM A QUANTUM COMPUTING PERSPECTIVE WITH THE DEVELOPED INTUITION, WE WILL INTRODUCE A ROTATING MAGNETIC FIELD AND STUDY SPIN RESONANCE USING A DIRECT APPROACH FINALLY, WE WILL INTRODUCE ROTATING AXIS REPRESENTATION, AND USE IT TO SIMULATE SPIN RESONANCE

SPIN PRECESSION

FOR SAKE OF CLARITY, CONSIDER A SPIN 1/2 PARTICLE IN THE PRESENCE OF A CONSTANT EXTERNAL FIELD $\vec{B}_0$ POINTING AT $\hat{z}$ DIRECTION FOR CONSISTENCY, WE WILL IDENTIFY STATES

$$|\uparrow\rangle \equiv |0\rangle \qquad |\downarrow\rangle \equiv |1\rangle$$

WITH THIS CONVENTION, A QUBIT IS IDENTICAL TO A SPIN 1/2 PARTICLE MOREOVER, THE BLOCH VECTOR OF A QUBIT STATE IS A PRETTY GOOD REPRESENTATION OF THE "CLASSICAL" IMAGE OF SPIN

THE SPIN OPERATOR OF THE PARTICLE CAN BE IDENTIFIED WITH THE PAULI OPERATORS

$$\hat{S}_i \equiv \hat{\sigma}_i$$

$$\vec{S}_i = \sigma_x \hat{x} + \hat{\sigma}_y \hat{y} + \hat{\sigma}_z \hat{z}$$

NOTE IF YOU ARE NEW TO QUANTUM MECHANICHS, PLEASE TRUST ME WE WILL TALK MORE ABOUT SPIN IN FUTURE LESSONS

FOR NOW, IT IS ENOUGH TO POINT OUT THAT SPIN IS SORT OF AN INTRINSIC ANGULAR MOMENTUM FROM ELECTROMAGNETIC THEORY, IT CAN BE DEDUCED THAT A MAGNETIC FIELD INTERACTS WITH THE SPIN OF A PARTICLE SO AS TO PRODUCE A HAMILTONIAN (I E INTERACTION ENERGY)

$$\hat{\mathcal{H}}_0 = -\vec{B}_0 \vec{S} = -B_{0x}\hat{\sigma}_x - B_{0y}\hat{\sigma}_y - B_{0z}\hat{\sigma}_z$$

IF YOU ARE NEW TO PHYSICS, IT COULD BE A BIT USEFUL TO PICTURE THE PARTICLE'S SPIN AS A BLOCH VECTOR, AND THE MAGNETIC FIELD AS AN AXIS IN THE BLOCH SPHERE ALBEIT NOT COMPLETELY ACCURATE TO SAY, IF THE SPIN IS PARALLEL TO THE FIELD, THE ENERGY IS MINIMUM IN CONTRAST, IF THE SPIN IS ANTIPARALLEL, THE ENERGY IS MAXIMUM THOSE SPIN STATES ARE CALLED GROUND AND EXCITED STATES RESPECTIVELY.

THE GROUND AND EXCITED STATES OF THE SYSTEM CORRESPOND TO

$$|\hat{n},+\rangle = \cos\frac{\theta_0}{2}|0\rangle + \sin\frac{\theta_0}{2}e^{i\phi_0}|1\rangle$$

$$|\hat{n},-\rangle = \sin\frac{\theta_0}{2}|0\rangle - \cos\frac{\theta_0}{2}e^{i\phi_0}|1\rangle$$

WHERE

$$\vec{B}_0 = B_0 \sin\theta_0 (\cos\phi_0 \hat{x} + \sin\phi_0 \hat{y}) + B_0 \cos\theta_0 \hat{z}$$

IT IS A POSTULATE OF QUANTUM MECHANICS THAT HAMILTONIAN PRODUCES UNITARY TIME EVOLUTION OF A QUANTUM SYSTEM'S STATE THIS HAS TO DO WITH THE NOTION THAT ENERGY OPERATORS ARE RELATED TO TIME TRANSLATIONS OF A SYSTEM'S COORDINATES

UNITARY EVOLUTION FOR THE PARTICLE IN A FIELD $\vec{B}_0$ IS PERFORMED BY OPERATOR

$$\hat{U}(t) = e^{-i\hat{\mathcal{H}}_0 t} = e^{-i(-B_0 t)\hat{n}\,\hat{\sigma}}$$

WITH $\hat{n} = \vec{B}_0 / B_0$ BEAR IN MIND THAT WE HAVE MAPPED THE SPIN STATES TO QUBIT STATES

UNITARY EVOLUTION OF THE PARTICLE CAN BE SIMULATED BY A ROTATION OPERATOR ACTING ON A QUBIT

$$\hat{U}(t) \equiv R_{\hat{n}}(-B_0 t)$$

GIVEN A INITIAL SPIN STATE $|\psi(0)\rangle$, THE STATE OF THE PARTICLE AT A LATER TIME IS GIVEN BY

$$|\psi(t)\rangle = \hat{U}(t)|\psi(0)\rangle = R_{\hat{n}}(-B_0 t)|\psi(0)\rangle$$

SPIN MAGNETIC RESONANCE

LETS ALLOW THE FIELD TO VARY IN TIME WE MAY CONSIDER A MAGNETIC FIELD SUCH THAT

$$\vec{B} = B_0\hat{z} + B_1(\cos\omega t\,\hat{x} - \sin\omega t\,\hat{y})$$

AGAIN, THE HAMILTONIAN THAT DRIVES TIME EVOLUTION IS GIVEN BY

$$\hat{\mathcal{H}} = -(B_0\hat{\sigma}_z + B_1\cos\omega t\,\hat{\sigma}_x - B_1\sin\omega t\,\hat{\sigma}_y)$$

LETS CONSIDER THE MATRIX REPRESENTATION OF THIS OPERATOR

$$\hat{\mathcal{H}} = -\begin{bmatrix} B_0 & B_1(\cos\omega t + i\sin\omega t) \\ B_1(\cos\omega t - i\sin\omega t) & -B_0 \end{bmatrix}$$

$$\hat{\mathcal{H}} = -\begin{bmatrix} B_0 & B_1 e^{i\omega t} \\ B_1 e^{-i\omega t} & -B_0 \end{bmatrix}$$

SCHRODINGER'S EQUATION FOR THIS SYSTEM IS

$$i\frac{d}{dt}\begin{bmatrix} C_0(t) \\ C_1(t) \end{bmatrix} = -\begin{bmatrix} B_0 & B_1 e^{i\omega t} \\ B_1 e^{-i\omega t} & -B_0 \end{bmatrix}\begin{bmatrix} C_0(t) \\ C_1(t) \end{bmatrix}$$

WITH THE DEFINITION

$$|\psi(t)\rangle = C_0(t)|0\rangle + C_1(t)|1\rangle$$

WE MAY SOLVE FOR $C_1(t)$ TO THAT END, LETS USE OUR MATHEMATICAL INTUITION IF $B_1 = 0$, THE SOLUTION IS

$$C_0(t) = C_0(0)e^{iB_0t}$$
$$C_1(t) = C_1(0)e^{-iB_0t}$$

LETS ASSUME THEN THAT

$$C_0(t) = \tilde{C}_0(t)e^{iB_0t}$$
$$C_1(t) = \tilde{C}_1(t)e^{-iB_0t}$$

WITH THE HOPES THAT $\tilde{C}_0(t) \xrightarrow[B_1\to 0]{} C_0(0)$, AND SIMILARLY FOR $\tilde{C}_1(t)$

LETS SUBSTITUTE OUR TEST SOLUTION AND SEE IF IT SIMPLIFIES THE EQUATIONS

THE FIRST EQUATION IS

$$i\dot{\tilde{C}}_0(t) - B_0\tilde{C}_0(t) = -B_0\tilde{C}_0(t) - B_1 e^{i(\omega-2B_0)}\tilde{C}_1(t)$$

$$i\dot{\tilde{C}}_0(t) = -B_1 e^{i(\omega-2B_0)t}\tilde{C}_1(t)$$

THE SECOND EQUATION RESULTS

$$i\dot{\tilde{C}}_1(t) + B_0\tilde{C}_1(t) = B_0\tilde{C}_1(t) - B_1 e^{-i(\omega-2B_0)t}\tilde{C}_0(t)$$

$$i\dot{\tilde{C}}_1(t) = -B_1 e^{-i(\omega-2B)t}\tilde{C}_0(t)$$

THIS IS A BIT SIMPLER, BUT NOT ENOUGH FURTHER SIMPLIFICATION IS OBTAINED IF A CHANGE OF VARIABLE

$$\tilde{C}_1(t) = e^{-i(\omega-2B_0)t/2}a_1(t)$$
$$\tilde{C}_0(t) = e^{i(\omega-2B_0)t/2}a_0(t)$$

IS MADE THIS PRODUCES

$$-\frac{\omega-2B_0}{2}a_0(t) + i\dot{a}_0(t) = -B_1 a_1(t)$$

$$\frac{\omega-2B_0}{2}a_1(t) + i\dot{a}_1(t) = -B_1 a_0(t)$$

NOW, ASSUME $a_i(t) = \tilde{a}_i e^{-i\Omega t}$ FOR SOME CONSTANTS $\Omega, \tilde{a}_i$ THIS YIELDS

$$\begin{bmatrix} \Omega - \frac{\omega-2B_0}{2} & B_1 \\ B_1 & \Omega + \frac{\omega-2B_0}{2} \end{bmatrix} \begin{bmatrix} a_0 \\ a_1 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix}$$

THIS EQUATION HAS SOLUTION ONLY FOR

$$\Omega^2 = B_1^2 + \left(\frac{\omega - 2B_0}{2}\right)^2$$

WHICH IMPLIES

$$\Omega = \pm \left[B_1^2 + \left(\frac{\omega - 2B_0}{2}\right)^2 \right]^{1/2}$$

LET US DEFINE

$$\Omega_0 = \left[B_1^2 + \left(\frac{\omega - 2B_0}{2}\right)^2 \right]^{1/2}$$

$$\Delta\omega = \frac{\omega - 2B_0}{2}$$

NOW, IT IS SO THAT

$$a_0(t) = \tilde{a}_0^+ e^{i\Omega_0 t} + \tilde{a}_0^- e^{-i\Omega_0 t}$$

$$a_1(t) = \tilde{a}_1^+ e^{i\Omega_0 t} + \tilde{a}_1^- e^{-i\Omega_0 t}$$

FOR SIMPLICITY, ASSUME $C_1(0) = 0$ THIS IMPLIES $\tilde{a}_1^+ = -\tilde{a}_1^-$ AND THUS

$$a_1(t) = 2i\,\tilde{a}_1^+ \sin \Omega_0 t$$

WE MAY NOTICE THAT

$$\tilde{a}_0^- = \frac{B_1}{\Omega_0 + \Delta\omega}\tilde{a}_1^- \qquad \tilde{a}_0^+ = -\frac{B_1}{\Omega_0 - \Delta\omega}\tilde{a}_1^+$$

THEREFORE, SINCE $\tilde{a}_0^- + \tilde{a}_0^+ = 1$

$$1 = \tilde{a}_1^+ \left(\frac{-2B_1\Omega_0}{\Omega_0^2 - \Delta\omega^2}\right) = -2\tilde{a}_1^+ \frac{\Omega_0}{B_1}$$

AS A RESULT

$$a_1(t) = \frac{B_1}{i\Omega_0}\sin\Omega_0 t$$

SINCE $|C_1(t)|^2 = |a_1(t)|^2 = \frac{B_1^2}{\Omega_0^2}\sin^2\Omega_0 t$

$$|C_0(t)|^2 = 1 - |C_1(t)|^2$$

WE SEE THAT THE EXTERNAL FIELD INDUCES CYCLES OF EXCITATION FROM GROUND STATE AND DECAY TO GROUND STATE THE PERIOD OF EACH CYCLE IS $T = 2\pi/\omega_0$ THE PROBABILITY OF FINDING THE SPIN PARTICLE ON THE EXCITED STATE PEAKS WITH A VALUE

$$P_{MAX,1} = \frac{B_1}{\Omega_0} = \frac{B_1}{\left[B_1^2 + \left(\frac{\omega - 2B_0}{2}\right)\right]^{1/2}}$$

IF $\omega = 2B_0$, WE CAN ASSERT FOR SURE THAT AT $t = \pi/2\Omega_0$, THE SPIN IS ON THE EXCITED STATE AT THIS FREQUENCY, THE EXTERNAL FIELD IS THE MOST EFFICIENT AT PUMPING ENERGY TO THE SYSTEM THE DECAY PROCESS WOULD CONSTITUTE THE MOST EFFICIENT WAY FOR COHERENT RADIATION EMISSION

ROTATING FRAME

FOLLOWING BARTON, WE MAY CONSIDER A FRAME OF REFERENCE THAT ROTATES WITH THE MAGNETIC FIELD ANY FIXED SPIN ON THIS FRAME IS ACTUALLY ROTATING ON THE ORIGINAL FRAME THE RATE OF ROTATION IS $-\omega$, SINCE THE FIELD IS ROTATING CLOCKWISE

LETS DENOTE THE SPIN STATE ON THE ROTATING FRAME BY $|\psi_R\rangle$ THE CLAIM IS THAT $|\psi_R\rangle$ RELATES TO $|\psi\rangle$ (NON-ROTATING-FRAME STATE) BY

$$R_{\hat{z}}(-\omega t)|\psi_R\rangle = |\psi\rangle$$

WE WILL DERIVE THE EQUATION OF MOTION FOR THE ROTATING FRAME STATE WE THEN PROCEED TO SOLVE IT EXACTLY, AND ANALYSE THE RESULTS

THE SCHRODINGER EQUATION IN THE NON-ROTATING FRAME IS

$$i\frac{d}{dt}|\psi\rangle = \hat{H}|\psi\rangle$$

SUBSTITUTE THE ROTATING STATE IN THIS EQUATION TO OBTAIN

$$i\frac{d}{dt}\left(e^{i\omega t\hat{\sigma}_z}|\psi_R\rangle\right) = \hat{H}e^{i\omega t\hat{\sigma}_z}|\psi_R\rangle$$

FROM THE PRODUCT RULE, WE OBTAIN

$$e^{i\omega t\hat{\sigma}_z}\left(-\omega\hat{\sigma}_z + i\frac{d}{dt}|\psi_R\rangle\right) = \hat{H}e^{i\omega t\hat{\sigma}_z}|\psi_R\rangle$$

WHICH YIELDS

$$i\frac{d}{dt}|\psi_R\rangle = \left(\omega\hat{\sigma}_z + \hat{H}_{1R}\right)|\psi_R\rangle$$

WITH THE DEFINITION

$$\hat{H}_{1R} = \hat{R}_{\hat{z}}(\omega t)\,\hat{H}\,R_{\hat{z}}(-\omega t)$$

AT FIRST, THIS MAY APPEAR DAUNTING HOWEVER, IT IS ACTUALLY QUITE SIMPLE, GIVEN THAT

THE ROTATION OPERATORS MERELY TRANSFORM THE HAMILTONIAN TO THE ROTATING FRAME IN THIS ONE, THE FIELD IS STATIC AND MAY BE DESCRIBED BY THE VECTOR

$$\vec{B}_R = B_0 \hat{z} + B_1 \hat{x}$$

COMO CONSECUENCIA, LA EVOLUCIÓN TEMPORAL DEL ESTADO DE ESPÍN ESTÁ DETERMINADA POR LA ECUACIÓN

$$i \frac{d}{dt} |\psi_R\rangle = -(\vec{B}' \, \vec{\sigma}) |\psi_R\rangle$$

CON $\vec{B}' = (B_0 - \omega)\hat{z} + B_1 \hat{x}$ LETS DEFINE

$$\cos \phi_0 = \frac{B_0 - \omega}{(B_1^2 + (B_0 - \omega)^2)^{1/2}}$$

$$\sin \phi_0 = \frac{B_1}{(B_1^2 + (B_0 - \omega)^2)^{1/2}}$$

SUCH THAT

$$\vec{B}' = B(\cos\phi_0 \hat{z} + \sin\phi_0 \hat{x})$$
$$\vec{B}' = B\hat{n}'$$

AS A RESULT, WE OBTAIN

$$|\psi_R(t)\rangle = R_{\hat{n}}(-Bt) |\psi_R(0)\rangle$$

AND THUS IT IS SO THAT

$$|\psi(t)\rangle = R_{\hat{z}}(-\omega t) R_{\hat{n}}(-Bt) |\psi(0)\rangle$$

SINCE $|\psi_R(0)\rangle = |\psi(0)\rangle$ FOR COMPLETENESS, LETS LOOK AT THE MATRIX REPRESENTATION OF THE OPERATOR $R_{\hat{n}}(\theta)$

$$R_{\hat{n}}(\theta) = \cos\frac{\theta}{2} + i\sin\frac{\theta}{2}\left(\cos\phi_0\hat{\sigma}_z + \sin\phi_0\hat{\sigma}_x\right)$$

$$\begin{bmatrix} \cos\frac{\theta}{2} + i\sin\frac{\theta}{2}\cos\phi_0 & i\sin\frac{\theta}{2}\sin\phi_0 \\ i\sin\frac{\theta}{2}\sin\phi_0 & \cos\frac{\theta}{2} - i\sin\frac{\theta}{2}\cos\phi_0 \end{bmatrix}$$

CONSIDERING THAT

$$\cos^2\frac{\theta}{2} + \sin^2\frac{\theta}{2}\cos^2\phi_0 + \sin^2\frac{\theta}{2}\sin^2\phi_0 = 1$$

WE MAY DEFINE

$$\sin\frac{\theta}{2}\sin\phi_0 = \sin\frac{\Upsilon}{2}$$

$$\tan\frac{\theta}{2}\cos\phi_0 = \tan\delta$$

SUCH THAT

$$R_{\hat{n}}(\theta) = \begin{bmatrix} e^{i\delta}\cos\frac{\Upsilon}{2} & i\sin\frac{\Upsilon}{2} \\ i\sin\frac{\Upsilon}{2} & e^{-i\delta}\cos\frac{\Upsilon}{2} \end{bmatrix}$$

$$R_{\hat{n}}(\theta) = e^{i\delta}\begin{bmatrix} \cos\frac{\Upsilon}{2} & -e^{i(-\delta-\pi/2)}\sin\frac{\Upsilon}{2} \\ e^{i(-\delta+\pi/2)}\sin\frac{\Upsilon}{2} & e^{-i2\delta}\cos\frac{\Upsilon}{2} \end{bmatrix}$$