PHY 304, II-Semester 2021/22, Assignment 1 solution

(1) Perturbed Hydrogen atoms [10pts]: Through interaction with light, a Hydrogen atom has ended up in an equal superposition of the states $|\,3s0\,\rangle$ (with $n=3$, $\ell=0$, $m=0$) and $|\,3p0\,\rangle$ (with $n=3$, $\ell=1$, $m=0$) at $t=0$:

$$\Psi(\mathbf{r}, t=0) = \frac{1}{\sqrt{2}}\left(\phi_{300}(\mathbf{r}) + \phi_{310}(\mathbf{r})\right). \tag{1}$$

(a) Find the explicit probability distribution of the position of the electron as a function of time. Try to visualize this as best you can and discuss. *Hint: You may want to look at / use Assignment 6Q3.* [2pts]
Solution: The normalised hydrogen states [from Eq. (4.91)(4.92)(4.97)]

$$\phi_{300}(\mathbf{r}) = \frac{1}{\sqrt{4\pi}}\frac{2}{3\sqrt{3}a_0^{3/2}}\left(1-\left(\frac{2r}{3a_0}\right)+\frac{2}{27}\left(\frac{r}{a_0}\right)^2\right)e^{-r/3a_0} \tag{2}$$

$$\phi_{310}(\mathbf{r}) = \frac{8}{27\sqrt{6}a_0^{3/2}}\left(1-\frac{r}{6a_0}\right)\frac{r}{a_0}e^{-r/(3a_0)}\sqrt{\frac{3}{4\pi}}\cos\theta \tag{3}$$

We find that both the states satisfy $\phi^* = \phi$. Let E_1 and E_2 be the energies of state ϕ_{300} and ϕ_{310} respectively. Then the time dependent wavefunction is given by

$$\Psi(\mathbf{r}, t) = \frac{1}{\sqrt{2}}\left(e^{-i\frac{E_1}{\hbar}t}\phi_{300}(\mathbf{r}) + e^{-i\frac{E_2}{\hbar}t}\phi_{310}(\mathbf{r})\right) \tag{4}$$

The probability distribution of the position of the electron is

$$|\Psi(\mathbf{r},t)|^2 = \frac{1}{2}(|\phi_{300}(\mathbf{r})|^2 + |\phi_{310}(\mathbf{r})|^2 + e^{\frac{it}{\hbar}(E_1-E_2)}\phi_{300}^*(\mathbf{r})\phi_{310}(\mathbf{r}) + \text{c.c}) \tag{5}$$

$$= \frac{1}{2}(|\phi_{300}(\mathbf{r})|^2 + |\phi_{310}(\mathbf{r})|^2 + 2\cos\left(\frac{t}{\hbar}(E_1-E_2)\right)\phi_{300}(\mathbf{r})\phi_{310}(\mathbf{r})) \tag{6}$$

$$= \frac{\left(\frac{2r^2}{27a_0^2}-\frac{2r}{3a_0}+1\right)^2 e^{-\frac{2r}{3a_0}}}{54\pi a_0^3} + \frac{4r^2\left(1-\frac{r}{6a_0}\right)^2\cos^2(\theta)e^{-\frac{2r}{3a_0}}}{729\pi a_0^5} + \frac{2\sqrt{\frac{2}{3}}r\left(\frac{2r^2}{27a_0^2}-\frac{2r}{3a_0}+1\right)\left(1-\frac{r}{6a_0}\right)\cos(\theta)e^{-\frac{2r}{3a_0}}}{81\pi a_0^4}\cos(\omega t) \tag{7}$$

where we have defined $\omega = (E_2 - E_1)/\hbar$
The radial distribution $P_r(r)$ is given by integrating $r^2\sin\theta|\Psi(\mathbf{r},t)|^2$ over angular vari-

ables

$$P_r(r) = \int_0^{\pi} \sin\theta \; d\theta \int_0^{2\pi} d\varphi \; r^2 \; |\Psi(\mathbf{r},t)|^2 \tag{8}$$

$$= r^2 \frac{\left(\frac{2r^2}{27a_0^2} - \frac{2r}{3a_0} + 1\right)^2 e^{-\frac{2r}{3a_0}}}{54\pi a_0^3} \underbrace{\int_0^{\pi} \sin\theta \; d\theta}_{=2} \int_0^{2\pi} d\varphi$$

$$+ \frac{4r^4 \left(1 - \frac{r}{6a_0}\right)^2 e^{-\frac{2r}{3a_0}}}{729\pi a_0^5} \underbrace{\int_0^{\pi} \sin\theta \cos^2\theta \; d\theta}_{-\frac{1}{3}[\cos^3\theta]_0^{\pi} = +\frac{2}{3}} \int_0^{2\pi} d\varphi$$

$$+ \frac{2\sqrt{\frac{2}{3}} r^3 \left(\frac{2r^2}{27a_0^2} - \frac{2r}{3a_0} + 1\right)\left(1 - \frac{r}{6a_0}\right) e^{-\frac{2r}{3a_0}}}{81\pi a_0^4} \cos(\omega t) \underbrace{\int_0^{\pi} \sin\theta \cos\theta \; d\theta}_{=0} \int_0^{2\pi} d\varphi$$

$$= \frac{2r^2 \left(\frac{2r^2}{27a_0^2} - \frac{2r}{3a_0} + 1\right)^2 e^{-\frac{2r}{3a_0}}}{27a_0^3} + \frac{16r^4 \left(1 - \frac{r}{6a_0}\right)^2 e^{-\frac{2r}{3a_0}}}{2187a_0^5} \tag{9}$$

The radial probability distribution $P_r(r)$ is the probability density of finding an electron anywhere on a spherical surface of radius r

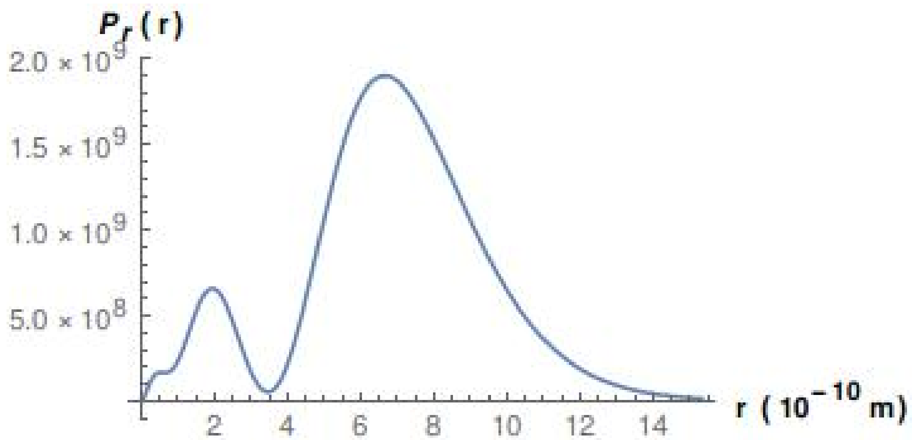

Figure 1: Radial probability distribution.

The angular probability distribution $P_{ang}(\theta, \varphi)$ is obtained by integrating $r^2|\Psi(\mathbf{r},t)|^2$ over the radial coordinate

$$P_{ang}(\theta, \varphi) = \int_0^{\infty} |\Psi(\mathbf{r},t)|^2 r^2 dr \tag{10}$$

$$= \int_0^{\infty} r^2 \frac{\left(\frac{2r^2}{27a_0^2} - \frac{2r}{3a_0} + 1\right)^2 e^{-\frac{2r}{3a_0}}}{54\pi a_0^3} dr \tag{11}$$

$$+\cos^2(\theta)\int_0^\infty \frac{4r^4\left(1-\frac{r}{6a_0}\right)^2 e^{-\frac{2r}{3a_0}}}{729\pi a_0^5}dr \tag{12}$$

$$+\cos(\omega t)\cos(\theta)\int_0^\infty \frac{2\sqrt{\frac{2}{3}}r^3\left(\frac{2r^2}{27a_0^2}-\frac{2r}{3a_0}+1\right)\left(1-\frac{r}{6a_0}\right)e^{-\frac{2r}{3a_0}}}{81\pi a_0^4}dr \tag{13}$$

Explicitly evaluating the radial integrals with Mathematica we obtain

$$P_{ang}(\theta,\varphi) = 0.0397887 + 0.119366\cos^2(\theta) + -0.129949\cos(\theta)\underbrace{\cos(\omega t)}_{=1,\text{since }\omega=0} \tag{14}$$

The angular distribution oscillates with a frequency given by $\omega = (E_2 - E_1)/\hbar$. This gives the time period of oscillations. For our case since $E_1 = E_2$, the frequency is zero. The resultant angular distribution is shown in Fig. 2

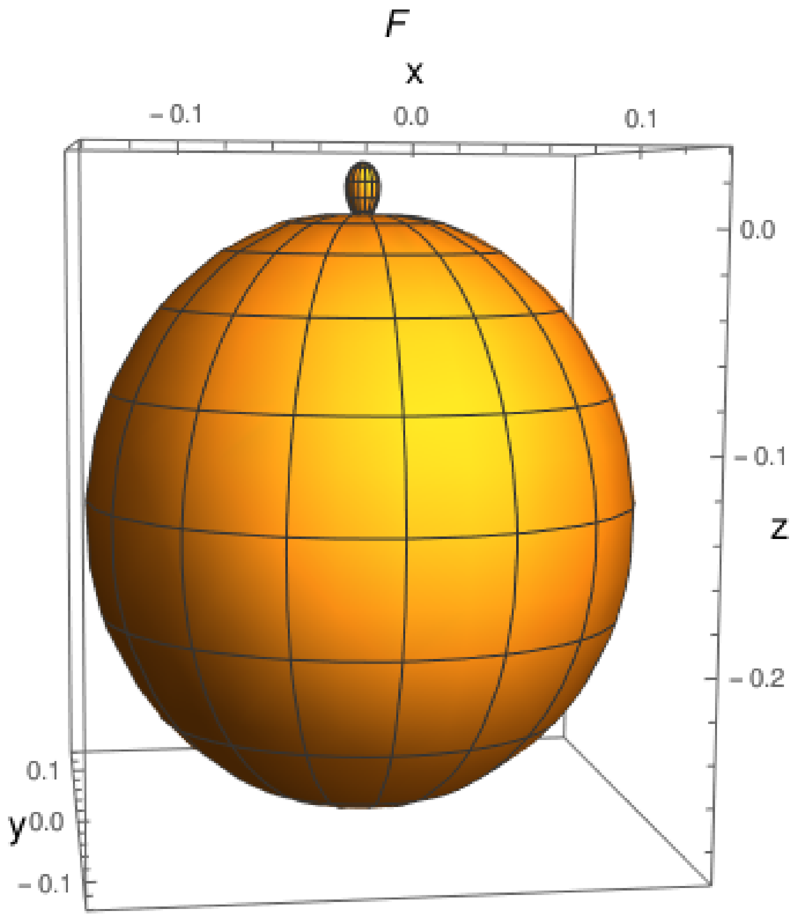

Figure 2: Angular probability distribution. The distance of the yellow surface from the origin in a direction of certain spherical angles θ, ϕ indicates $P_{ang}(\theta,\varphi)$.

(b) What are the possible outcomes of measuring the magnitude of angular momentum of the electron in the state (1), what are their probabilities, and how do those probabilities change in time? [2pt]

Solution: A measurement of angular momentum will give magnitude of angular momentum to be zero for ϕ_{300} (since $l = 0$) with 50% probability and $\hbar\sqrt{1(2)} = \sqrt{2}\hbar$ (since $l = 1$) with the other 50% for ϕ_{310}. In time, the state evolves as

$$\Psi(\mathbf{r}, t) = \frac{1}{\sqrt{2}} \left(e^{-i\frac{E_1}{\hbar}t} \phi_{300}(\mathbf{r}) + e^{-i\frac{E_2}{\hbar}t} \phi_{210}(\mathbf{r}) \right) \equiv c_1(t)\phi_{100}(\mathbf{r}) + c_2(t)\phi_{310}(\mathbf{r}). \tag{15}$$

Since $p_1 = |c_1|^2 = 1/2 = const$ and same for p_2, the probabilities do not change in time.

(c) What is the probability of finding the electron at $z > 0$ in the state (1), and how does this probability change in time? [2pts]
Solution: In terms of spherical polar coordinates the region $z > 0$ is given by $0 < \theta < \pi/2$. The probability to find the electron in the region $0 < \theta < \pi/2$ is given by

$$p_+ = \frac{1}{2} \int_0^\infty r^2 dr \int_0^{\pi/2} sin\theta d\theta \int_0^{2\pi} d\varphi \; |\Psi(\mathbf{r}, t)|^2 \tag{16}$$

$$= \frac{1}{2} \int_0^\infty r^2 dr \int_0^{\pi/2} sin\theta d\theta \underbrace{\int_0^{2\pi} d\varphi}_{=2\pi} \left(|\phi_{300}(\mathbf{r})|^2 + |\phi_{310}(\mathbf{r})|^2 + e^{\frac{it}{\hbar}(E_1 - E_2)} \phi^*_{300}(\mathbf{r})\phi_{310}(\mathbf{r}) + e^{\frac{it}{\hbar}(E_2 - E_1)} \phi^*_{310}(\mathbf{r})\phi_{300}(\mathbf{r}) \right) \tag{17}$$

Collecting the two hydrogen states required [from Eq. (4.91)(4.92)(4.97)] Using the expressions for the hydrogen states from Eq. (2) and Eq. (3), we get

$$p_+ = \pi \int_0^\infty r^2 dr \int_0^{\pi/2} sin\theta d\theta (|\phi_{300}(\mathbf{r})|^2 + |\phi_{310}(\mathbf{r})|^2 + \phi_{300}(\mathbf{r})\phi_{210}(\mathbf{r})) \tag{18}$$

There are three pieces to evaluate for which we use Mathematica.

(a) *1st piece:*

$$\pi \int_0^\infty r^2 dr \int_0^{\pi/2} sin\theta d\theta \; |\phi_{300}(\mathbf{r})|^2 = \pi \int_0^\infty r^2 \frac{\left(\frac{2r^2}{27a_0^2} - \frac{2r}{3a_0} + 1 \right)^2 e^{-\frac{2r}{3a_0}}}{27\pi a_0^3} \tag{19}$$

$$\times \underbrace{\int_0^{\pi/2} sin\theta d\theta}_{=1} \tag{20}$$

$$= 0.0397887\pi \times 2 \tag{21}$$

(b) *2nd piece:*

$$\pi \int_0^\infty r^2 dr \int_0^{\pi/2} sin\theta d\theta \; |\phi_{310}(\mathbf{r})|^2 = \pi \int_0^\infty \frac{8r^4 \left(1 - \frac{r}{6a_0}\right)^2 e^{-\frac{2r}{3a_0}}}{729\pi a_0^5} dr \tag{22}$$

$$\int_0^{\pi/2} \sin\theta \cos^2\theta \; d\theta_{= -\frac{1}{3}[\cos^3(\theta)]_0^\pi = +\frac{1}{3}} \tag{23}$$

$$= 0.0397867\pi \times 2 \tag{24}$$

(c) *Since $\omega = 0$ we put $\cos(\omega t) = 1$. We then get the 3rd piece:*

$$2\pi \int_0^\infty r^2 dr \int_0^{\pi/2} \sin\theta d\theta \; \phi_{300}(\mathbf{r})\phi_{310}(\mathbf{r}) \tag{25}$$

$$= 2\pi \int_0^\infty \frac{4\sqrt{\frac{2}{3}} r^3 \left(\frac{2r^2}{27a_0^2} - \frac{2r}{3a_0} + 1\right)\left(1 - \frac{r}{6a_0}\right) e^{-\frac{2r}{3a_0}}}{81\pi a_0^4} dr \underbrace{\int_0^{\pi/2} \sin\theta\cos\theta \; d\theta}_{=\frac{1}{2}[\sin^2\theta]_0^{\pi/2}=\frac{1}{2}} \tag{26}$$

$$= -\,0.129949 \times \pi \tag{27}$$

Collecting all the pieces Eq. (21), Eq. (24) and Eq. (27) we get

$$p_+ = 0.0917517 \tag{28}$$

(d) What is the expectation value of the electronic dipole operator $\hat{\mathbf{d}} = -e\hat{\mathbf{r}}$ as function of time? [2pts]
Solution: The expectation value is

$$\langle \hat{d}(t) \rangle = -\frac{e}{2} \int d^3\mathbf{r} (\mathbf{r}|\phi_{300}(\mathbf{r})|^2 + \mathbf{r}|\phi_{310}(\mathbf{r})|^2 + \mathbf{r} e^{\frac{it}{\hbar}(E_1-E_2)} \phi_{300}^*(\mathbf{r})\phi_{310}(\mathbf{r}) + \mathbf{r} e^{\frac{it}{\hbar}(E_2-E_1)} \phi_{310}^*(\mathbf{r})\phi_{300}(\mathbf{r})) \tag{29}$$

From the expressions of hydrogen states Eq. (2) and Eq. (3) we see that $|\phi_{300}(\mathbf{r})|^2$ and $|\phi_{310}(\mathbf{r})|^2$ are symmetric under $\mathbf{r} \to -\mathbf{r}$. Thus the first two terms in Eq. (29) vanish when integrated over. Also both ϕ_{300} and ϕ_{310} satisfy $\phi^* = \phi$. These arguments results in

$$\langle \hat{d}(t) \rangle = -e \int d^3\mathbf{r} \; \mathbf{r} \; \phi_{310}(\mathbf{r})\phi_{300}(\mathbf{r}) \tag{30}$$

$$= -e \int_0^\infty dr r^2 \int_0^\pi d\theta \sin\theta \int_0^{2\pi} d\varphi \; \phi_{300}(\mathbf{r}) \begin{bmatrix} r\sin\theta cos\varphi \\ r\sin\theta\sin\varphi \\ r\cos\theta \end{bmatrix} \phi_{310}(\mathbf{r}) \tag{31}$$

$$= -\hat{\mathbf{e}}_z e \int_0^\infty \frac{2\sqrt{\frac{2}{3}} r^4 \left(\frac{2r^2}{27a_0^2} - \frac{2r}{3a_0} + 1\right)\left(1 - \frac{r}{6a_0}\right) \cos(\theta) e^{-\frac{2r}{3a_0}}}{81\pi a_0^4} dr \underbrace{\int_0^\pi \cos^2\theta \sin\theta d\theta}_{=-\frac{1}{3}[\cos^3(\theta)]_0^\pi=+\frac{2}{3}} \underbrace{\int_0^{2\pi} d\varphi}_{=2\pi} \tag{32}$$

$$= 9.28034 \times 10^{-11} \times \frac{4\pi}{3} \times e\hat{\mathbf{e}}_z = 7.3484 e\hat{\mathbf{e}}_z \tag{33}$$

(e) From your knowledge of waves, optics and electro-magnetism, discuss the expected interplay between an atom in this state and electro-magnetic waves. [2pts]
Solution: The above result does not have an oscillating dipole and therefore there will be no electromagnetic radiation emitted. Though, if the above state is subjected to an oscillating electromagnetic field, the dipole will start oscillating and then start emitting electromagnetic radiation.

(2) Entanglement [10pts]:

(a) For the following two-particle states, identify which are entangled and which are not [3pts]
Solution:

(i) $\Psi(x,y) = \frac{1}{\sqrt{2}}[\phi_0(x-x_0)\phi_3(y-y_0) + \phi_2(x-x_0)\phi_1(y-y_0)]$ *(position of particle 1 is* x*, position of particle 2 is* y*,* $\phi_n(x)$ *are normalised eigenstates of the simple harmonic oscillator)*
This is an entangled state since it cannot be expressed as a product of two single-particle states.

(ii) $\Psi(x,y) = \phi_0(x-x_0)\phi_3(y-y_0)$
This is a separable state since it can be expressed as a product of two single-particle states.

(iii) $\Psi(x,y) = \frac{1}{2}[\phi_0(x)\phi_0(y) - \phi_0(x)\phi_1(y) - \phi_1(x)\phi_0(y) + \phi_1(x)\phi_1(y)]$
This is a separable state since it can be expressed as a product of two single-particle states.

$$\Psi(x,y) = \frac{1}{2}[\phi_0(x)\phi_0(y) - \phi_0(x)\phi_1(y) - \phi_1(x)\phi_0(y) + \phi_1(x)\phi_1(y)] \tag{34}$$

$$= \frac{1}{\sqrt{2}}[\phi_0(x) - \phi_1(x)]\frac{1}{\sqrt{2}}[\phi_0(y) - \phi_1(y)] \tag{35}$$

(iv) $\Psi(x,y) = \frac{1}{2}[\phi_0(x)\phi_0(y) - \phi_0(x)\phi_1(y) + \phi_1(x)\phi_0(y) + \phi_1(x)\phi_1(y)]$
This is an entangled state since it cannot be expressed as a product of two single-particle states.

(v) $|\,\Psi\,\rangle = |\,s=1; m_s=-1\,\rangle \otimes |\,s=1; m_s=+1\,\rangle$ *(two different spin-1 particles)*
This is a separable state since it can be expressed as a product of two single-particle states.

(vi)

$$\begin{aligned}|\,\Psi\,\rangle = \frac{1}{2}\Big[&|\,s=1; m_s=-1\,\rangle \otimes |\,s=1; m_s=-1\,\rangle \\ &+ |\,s=1; m_s=+1\,\rangle \otimes |\,s=1; m_s=-1\,\rangle \\ &+ |\,s=1; m_s=-1\,\rangle \otimes |\,s=1; m_s=0\,\rangle \\ &+ |\,s=1; m_s=+1\,\rangle \otimes |\,s=1; m_s=+1\,\rangle \Big]\end{aligned} \tag{36}$$

This is an entangled state since it cannot be expressed as a product of two single-particle states.

(b) Give another 2 examples of entangled and 2 examples of separable states involving <u>three</u> particles and discuss [2 pts].
Solution:

(a) *Examples of entangled states*

i. $|\Psi\rangle = \frac{1}{\sqrt{2}}(|\uparrow\downarrow\downarrow\rangle + |\downarrow\uparrow\uparrow\rangle)$

ii. $|\Psi\rangle = \frac{1}{\sqrt{3}}(|001\rangle + |010\rangle + |100\rangle$

(b) *Examples of separable states*

i. $|\Psi\rangle = |\uparrow\rangle \otimes \left(\frac{1}{\sqrt{2}}(|\uparrow\rangle + |\downarrow\rangle)\right) \otimes \left(\frac{1}{\sqrt{2}}(|\uparrow\rangle - |\downarrow\rangle)\right) = \frac{1}{2}(|\uparrow\uparrow\uparrow\rangle - |\uparrow\uparrow\downarrow\rangle + |\uparrow\downarrow\uparrow\rangle - |\uparrow\downarrow\downarrow\rangle)$

ii. $\Psi(x, y) = \mathcal{N}\sin(x)\sin(y)\sin z$

(c) Einstein-Podolsky-Rosen correlations: Consider the entangled state for two spin-1/2 particles: $|\Psi\rangle = (|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle)/\sqrt{2}$. Show that the correlation of the spin projection onto axis **a** for particle one, with that onto axis **b** for particle two is:

$$\langle(\mathbf{a}\cdot\hat{\mathbf{S}}^{(1)})(\mathbf{b}\cdot\hat{\mathbf{S}}^{(2)})\rangle = -\frac{\hbar^2}{4}\mathbf{a}\cdot\mathbf{b}, \tag{37}$$

where $\hat{\mathbf{S}}^{(k)}$ is the spin-operator for particle k. [5pts]
Solution: Let us first expand the dot products

$$(\mathbf{a}\cdot\hat{\mathbf{S}}^{(1)})(\mathbf{b}\cdot\hat{\mathbf{S}}^{(2)}) = (a_x\hat{\mathbf{S}}^{(1)}_x + a_y\hat{\mathbf{S}}^{(1)}_y + a_z\hat{\mathbf{S}}^{(1)}_z)(b_x\hat{\mathbf{S}}^{(2)}_x + b_y\hat{\mathbf{S}}^{(2)}_y + b_z\hat{\mathbf{S}}^{(2)}_z) \tag{38}$$

$$\begin{aligned} &= a_xb_x\hat{\mathbf{S}}^{(1)}_x\hat{\mathbf{S}}^{(2)}_x + a_xb_y\hat{\mathbf{S}}^{(1)}_x\hat{\mathbf{S}}^{(2)}_y + a_xb_z\hat{\mathbf{S}}^{(1)}_x\hat{\mathbf{S}}^{(2)}_z \\ &+ a_yb_x\hat{\mathbf{S}}^{(1)}_y\hat{\mathbf{S}}^{(2)}_x + a_yb_y\hat{\mathbf{S}}^{(1)}_y\hat{\mathbf{S}}^{(2)}_y + a_yb_z\hat{\mathbf{S}}^{(1)}_y\hat{\mathbf{S}}^{(2)}_z \\ &+ a_zb_x\hat{\mathbf{S}}^{(1)}_z\hat{\mathbf{S}}^{(2)}_x + a_zb_y\hat{\mathbf{S}}^{(1)}_z\hat{\mathbf{S}}^{(2)}_y + a_zb_z\hat{\mathbf{S}}^{(1)}_z\hat{\mathbf{S}}^{(2)}_z \end{aligned} \tag{39}$$

It is convenient to handle the computations here using the matrix representations for spin operators and spin states as given in Eq. (4.107) and Eq. (4.111) from the Griffiths Book[GR]. The entangled state written in matrix representation reads:

$$|\Psi\rangle = \frac{1}{\sqrt{2}}\left(\begin{pmatrix}1\\0\end{pmatrix}\otimes\begin{pmatrix}0\\1\end{pmatrix} - \begin{pmatrix}0\\1\end{pmatrix}\otimes\begin{pmatrix}1\\0\end{pmatrix}\right) \tag{40}$$

Let us find the action of each spin operator on the state $|\,\Psi\,\rangle$ in matrix representation:

$$\hat{\mathbf{S}}_x^{(1)}|\,\Psi\,\rangle = \frac{\hbar}{2\sqrt{2}}\left(\begin{pmatrix}0\\1\end{pmatrix}\otimes\begin{pmatrix}0\\1\end{pmatrix}-\begin{pmatrix}1\\0\end{pmatrix}\otimes\begin{pmatrix}1\\0\end{pmatrix}\right) \tag{41}$$

$$\hat{\mathbf{S}}_x^{(2)}|\,\Psi\,\rangle = \frac{\hbar}{2\sqrt{2}}\left(\begin{pmatrix}1\\0\end{pmatrix}\otimes\begin{pmatrix}1\\0\end{pmatrix}-\begin{pmatrix}0\\1\end{pmatrix}\otimes\begin{pmatrix}0\\1\end{pmatrix}\right) \tag{42}$$

$$\hat{\mathbf{S}}_y^{(1)}|\,\Psi\,\rangle = \frac{i\hbar}{2\sqrt{2}}\left(\begin{pmatrix}0\\1\end{pmatrix}\otimes\begin{pmatrix}0\\1\end{pmatrix}+\begin{pmatrix}1\\0\end{pmatrix}\otimes\begin{pmatrix}1\\0\end{pmatrix}\right) \tag{43}$$

$$\hat{\mathbf{S}}_y^{(2)}|\,\Psi\,\rangle = \frac{-i\hbar}{2\sqrt{2}}\left(\begin{pmatrix}1\\0\end{pmatrix}\otimes\begin{pmatrix}1\\0\end{pmatrix}+\begin{pmatrix}0\\1\end{pmatrix}\otimes\begin{pmatrix}0\\1\end{pmatrix}\right) \tag{44}$$

$$\hat{\mathbf{S}}_z^{(1)}|\,\Psi\,\rangle = \frac{\hbar}{2\sqrt{2}}\left(\begin{pmatrix}1\\0\end{pmatrix}\otimes\begin{pmatrix}0\\1\end{pmatrix}+\begin{pmatrix}0\\1\end{pmatrix}\otimes\begin{pmatrix}1\\0\end{pmatrix}\right) \tag{45}$$

$$\hat{\mathbf{S}}_z^{(2)}|\,\Psi\,\rangle = \frac{-\hbar}{2\sqrt{2}}\left(\begin{pmatrix}1\\0\end{pmatrix}\otimes\begin{pmatrix}0\\1\end{pmatrix}+\begin{pmatrix}0\\1\end{pmatrix}\otimes\begin{pmatrix}1\\0\end{pmatrix}\right) \tag{46}$$

Now the correlation for a typical term for example in Eq. (39) can be written as:

$$\langle\hat{\mathbf{S}}_x^{(1)}\hat{\mathbf{S}}_x^{(2)}\rangle = \langle\Psi|\hat{\mathbf{S}}_x^{(1)}\hat{\mathbf{S}}_x^{(2)}|\Psi\rangle \tag{47}$$

$$= (\langle\Psi|\hat{\mathbf{S}}_x^{(1)})(\hat{\mathbf{S}}_x^{(2)}|\Psi\rangle) \tag{48}$$

$$= (\hat{\mathbf{S}}_x^{(1)}|\Psi\rangle)^\dagger(\hat{\mathbf{S}}_x^{(2)}|\Psi\rangle) \tag{49}$$

$$= -\frac{\hbar^2}{8}\left(\begin{pmatrix}0 & 1\end{pmatrix}\otimes\begin{pmatrix}0 & 1\end{pmatrix}-\begin{pmatrix}1 & 0\end{pmatrix}\otimes\begin{pmatrix}1 & 0\end{pmatrix}\right)\left(\begin{pmatrix}1\\0\end{pmatrix}\otimes\begin{pmatrix}1\\0\end{pmatrix}-\begin{pmatrix}0\\1\end{pmatrix}\otimes\begin{pmatrix}0\\1\end{pmatrix}\right) \tag{50}$$

$$= -\frac{\hbar^2}{8}\Bigg\{\underbrace{\begin{pmatrix}0 & 1\end{pmatrix}\begin{pmatrix}1\\0\end{pmatrix}}_{=0}\times\underbrace{\begin{pmatrix}0 & 1\end{pmatrix}\begin{pmatrix}1\\0\end{pmatrix}}_{=0}-\underbrace{\begin{pmatrix}0 & 1\end{pmatrix}\begin{pmatrix}0\\1\end{pmatrix}}_{=1}\times\underbrace{\begin{pmatrix}0 & 1\end{pmatrix}\begin{pmatrix}0\\1\end{pmatrix}}_{=1} \tag{51}$$

$$-\underbrace{\begin{pmatrix}1 & 0\end{pmatrix}\begin{pmatrix}1\\0\end{pmatrix}}_{=1}\otimes\underbrace{\begin{pmatrix}1 & 0\end{pmatrix}\begin{pmatrix}1\\0\end{pmatrix}}_{=1}+\underbrace{\begin{pmatrix}1 & 0\end{pmatrix}\begin{pmatrix}0\\1\end{pmatrix}}_{=0}\times\underbrace{\begin{pmatrix}1 & 0\end{pmatrix}\begin{pmatrix}0\\1\end{pmatrix}}_{=0}\Bigg\} = -\frac{\hbar^2}{4} \tag{52}$$

Similarly we can evaluate all other pieces in Eq. (39)

$$\langle(\mathbf{a}\cdot\hat{\mathbf{S}}^{(1)})(\mathbf{b}\cdot\hat{\mathbf{S}}^{(2)})\rangle = -\frac{\hbar^2}{4}\mathbf{a}\cdot\mathbf{b} \tag{53}$$

(d) (Bonus) Read and understand the proof of Bell's theorem in Griffith (page 446), that shows that Eq. (37) cannot be explained by a classical local hidden variable theory.
Solution: See Griffith

(3) (Pseudo) Spin-1/2 particle [10pts]: Let the Hamiltonian of a spin-1/2 particle (or any other two-level system that we can map onto a pseudo spin-1/2) be:

$$\hat{H} = \kappa\sigma_y + E(\sigma_z + 1), \tag{54}$$

where σ_k are Pauli matrices.

(a) Write the most general time-dependent state and then the TDSE in terms of its coefficients. [2pts]

Solution: The most general time-dependent state can be written as:

$$|\Psi(t)\rangle = a(t)\begin{pmatrix}1\\0\end{pmatrix} + b(t)\begin{pmatrix}0\\1\end{pmatrix} \tag{55}$$

The TDSE for $|\Psi(t)\rangle$ *is then given by:*

$$i\hbar\frac{\partial|\Psi(t)\rangle}{\partial t} = \hat{H}|\Psi(t)\rangle \tag{56}$$

Substituting the most general expression for time dependent wavefunction Eq. (55) in the TDSE Eq. (56) and using the Pauli matrices we get:

$$\begin{aligned} i\hbar\frac{da(t)}{dt}\begin{pmatrix}1\\0\end{pmatrix} + i\hbar\frac{db(t)}{dt}\begin{pmatrix}0\\1\end{pmatrix} &= \kappa a(t)\begin{pmatrix}0 & -i\\ i & 0\end{pmatrix}\begin{pmatrix}1\\0\end{pmatrix} + \kappa b(t)\begin{pmatrix}0 & -i\\ i & 0\end{pmatrix}\begin{pmatrix}0\\1\end{pmatrix} \\ &+ Ea(t)\begin{pmatrix}2 & 0\\ 0 & 0\end{pmatrix}\begin{pmatrix}1\\0\end{pmatrix} + Eb(t)\begin{pmatrix}2 & 0\\ 0 & 0\end{pmatrix}\begin{pmatrix}0\\1\end{pmatrix} \qquad (57) \\ &= (2Ea(t) - i\kappa b(t))\begin{pmatrix}1\\0\end{pmatrix} + i\kappa a(t)\begin{pmatrix}0\\1\end{pmatrix} \qquad (58) \end{aligned}$$

This gives us a set of two coupled differential equations:

$$i\hbar\frac{da(t)}{dt} = 2Ea(t) - i\kappa b(t) \tag{59}$$

$$i\hbar\frac{db(t)}{dt} = i\kappa a(t) \tag{60}$$

(b) Solve the TDSE for the initial state $|\Psi(0)\rangle = |\uparrow\rangle$. *You may use mathematica.* [5 pts]

Solution: The initial state can be expressed as the following initial condition for the coupled differential equations Eq. (59) and Eq. (60):

$$a(0) = 1 \qquad\qquad b(0) = 0 \tag{61}$$

Solving the above differential equation using Mathematica gives:

$$a(t) = e^{-\frac{iEt}{\hbar}}\left(\cos\left(\frac{\gamma t}{\hbar}\right) + \frac{E\sin\left(\frac{\gamma t}{\hbar}\right)}{i\gamma}\right) \tag{62}$$

$$b(t) = \frac{\kappa e^{-\frac{iEt}{\hbar}}\sin\left(\frac{\gamma t}{\hbar}\right)}{\gamma} \tag{63}$$

where $\gamma = \sqrt{E^2 + \kappa^2}$

(c) Make drawings or plots of the probability to be in state $|\downarrow\rangle$ as a function of time, for $E = 0$, $E \approx \kappa$ and $E \gg \kappa$, discuss your results. [3pts]

Solution: The probability of finding the state in $|\downarrow\rangle$ *is* $|b(t)|^2 = b^*(t)b(t) = \frac{\kappa^2 \sin^2\left(\frac{\gamma t}{\hbar}\right)}{\gamma^2}$

(a) $\Delta E = 0$

The probability to find the state in $|\downarrow\rangle$ *from Eq. (63) is*

$$|b(t)|^2 = \left(\sin\left(\frac{t\kappa}{\hbar}\right)\right)^2 \tag{64}$$

where κ *sets the oscillation frequency which makes sense as it is the coefficient of the operator* σ_y *that evolves* $|\uparrow\rangle$ *to* $|\downarrow\rangle$ *and vice-versa.*

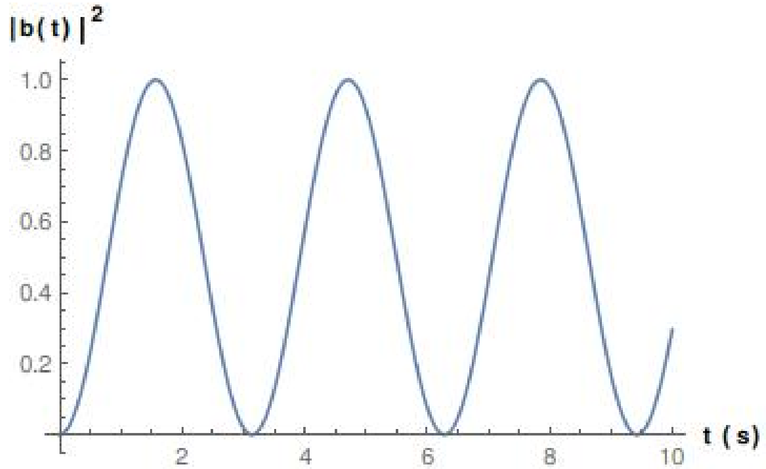

Figure 3: $|b|^2$ v/s t for the case $E = 0$. ($\frac{\kappa}{\hbar}$ *taken to be unity for simplicity*)

(b) $E = \kappa$

The probability to find the state in $|\downarrow\rangle$ *from Eq. (63) is*

$$|b(t)|^2 = \frac{\sin^2\left(\frac{\sqrt{2}\kappa t}{\hbar}\right)}{2} \tag{65}$$

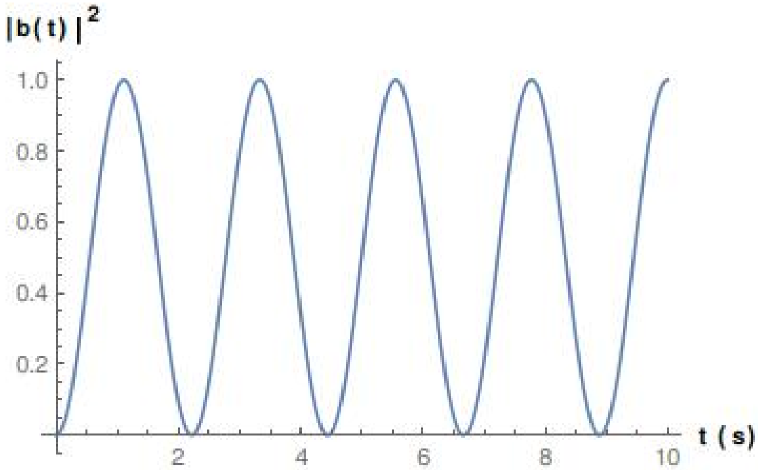

Figure 4: $|b|^2$ v/s t for the case $E = \kappa$. *(again $\frac{\kappa}{\hbar}$ is taken to be unity for simplicity)*

(c) $E >> \kappa$
The probability to find the state in $|\downarrow\rangle$ from Eq. (63) is

$$|b(t)|^2 = \frac{\kappa^2 \sin^2\left(\frac{Et}{\hbar}\right)}{E^2} \tag{66}$$

Note that since $\sin^2\left(\frac{Et}{\hbar}\right)$ is bounded by 1, for $E >> \kappa$, $|b(t)|^2$ will always stay negligibly small. This makes sense since for a very large E compared to κ the first term in the Hamiltonian that causes evolution from up spin state to down can be neglected.

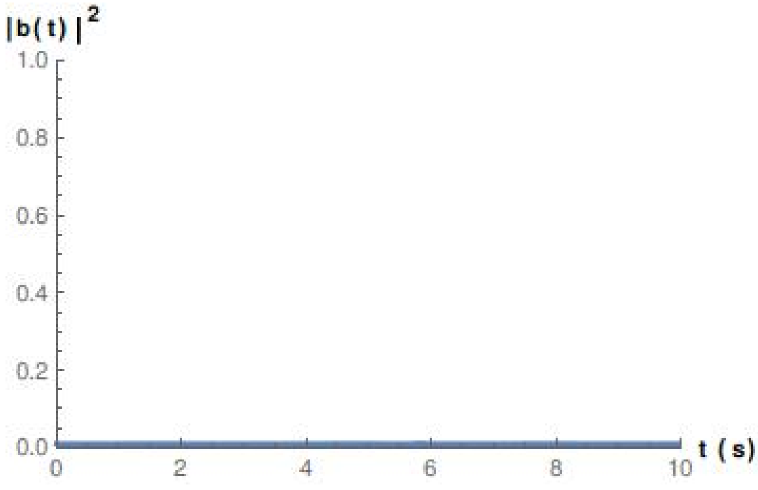

Figure 5: $|b|^2$ v/s t for the case $E >> \kappa$.*(plotted for $\frac{\kappa}{E} = 10^{-2}$ and the plot line made thick to show that it's non-zero but very small; of the order of* 10^{-4})