Physics 443, Solutions to PS 7

1. Griffiths 4.50

The singlet configuration state is

$$\begin{aligned} \mid \chi\rangle = & \frac{1}{\sqrt{2}}\left(\mid \frac{1}{2}\frac{1}{2}\rangle_1 \mid \frac{1}{2} - \frac{1}{2}\rangle_2 - \mid \frac{1}{2} - \frac{1}{2}\rangle_1 \mid \frac{1}{2}\frac{1}{2}\rangle_2\right) \\ = & \frac{1}{\sqrt{2}}(\mid \chi_+^1\rangle \mid \chi_-^2\rangle - \mid \chi_-^1\rangle \mid \chi_+^2\rangle) \end{aligned}$$

where that second equation defines the abbreviated notation $\mid \chi_+\rangle$ and $\mid \chi_-\rangle$.

$$\langle S_a^{(1)} S_b^{(2)}\rangle = \left\langle \chi \mid \hat{a}\cdot\vec{S}^{(1)}\hat{b}\cdot S^{(2)} \mid \chi\right\rangle$$

In spherical coordinates the unit vector in the θ, ϕ direction is $\hat{r} = \sin\theta\cos\phi\hat{i} + \sin\theta\cos\phi\hat{j} + \cos\theta\hat{k}$ Let's choose $\hat{a}$ to be along the z-direction. Then $\theta = \phi = 0$ and $\hat{a} = \hat{k}$. And choose $\hat{b}$ to be in the x-y plane at an angle θ with respect to the z-direction so that $\phi = 0$. Then $\hat{b} = \sin\theta\hat{i} + \cos\theta\hat{k}$. Now

$$\begin{aligned} & \langle S_a^{(1)} S_b^{(2)}\rangle = \left\langle \chi \mid \hat{a}\cdot\vec{S}^{(1)}\hat{b}\cdot\vec{S}^{(2)} \mid \chi\right\rangle \\ = & \left\langle \chi \mid S_z^{(1)}(\sin\theta S_x^{(2)} + \cos\theta S_z^{(2)}) \mid \chi\right\rangle \\ = & \frac{1}{\sqrt{2}}\left(\langle\chi_+^1 \mid\langle\chi_-^2 \mid - \langle\chi_-^1 \mid\langle\chi_+^2 \mid\right)\mid S_z^{(1)}(\sin\theta S_x^{(2)} + \cos\theta S_z^{(2)})\mid \frac{1}{\sqrt{2}}\left(\mid \chi_+^1\rangle\mid \chi_-^2\rangle - \mid \chi_-^1\rangle\mid \chi_+^2\rangle\right) \\ = & \frac{1}{2}\sin\theta\left(\langle\chi_+^1 \mid\langle\chi_-^2 \mid - \langle\chi_-^1 \mid\langle\chi_+^2 \mid\right)\mid S_z^{(1)} S_x^{(2)}\mid\left(\mid \chi_+^1\rangle\mid \chi_-^2\rangle - \mid \chi_-^1\rangle\mid \chi_+^2\rangle\right) \\ & + \frac{1}{2}\cos\theta\left(\langle\chi_+^1 \mid\langle\chi_-^2 \mid - \langle\chi_-^1 \mid\langle\chi_+^2 \mid\right)\mid S_z^{(1)} S_z^{(2)}\mid\left(\mid \chi_+^1\rangle\mid \chi_-^2\rangle - \mid \chi_-^1\rangle\mid \chi_+^2\rangle\right) \\ = & -\frac{1}{2}\cos\theta\left(2\frac{\hbar^2}{4}\right) = -\frac{\hbar^2}{4}\cos\theta \end{aligned}$$

We have used the fact that $\langle\chi_\pm \mid S_z \mid \chi_\pm\rangle = \pm\hbar/2$ and $\langle\chi_\pm \mid S_x \mid \chi_\pm\rangle = \left\langle\chi_\pm \mid \frac{\hbar}{2} \mid \chi_\mp\right\rangle = 0$.

2. Griffiths 4.59

To determine the time rate of change of expectation values we use

$$\frac{d\langle Q\rangle}{dt} = \frac{i}{\hbar}\langle[H, Q]\rangle + \left\langle\frac{\partial Q}{\partial t}\right\rangle$$

(a) We have that

$$H = \frac{1}{2m}(\mathbf{p} - q\mathbf{A})^2 - q\phi = \frac{1}{2m}(p^2 - q\mathbf{p}\cdot\mathbf{A} - q\mathbf{A}\cdot\mathbf{p} + q^2A^2) + q\phi$$

Then

$$\frac{d\langle \mathbf{r}\rangle}{dt} = \frac{i}{\hbar}\langle [H,\mathbf{r}]\rangle$$

$$= \langle \frac{1}{2m}\Big([p^2,\mathbf{r}] - q[\mathbf{p}\cdot\mathbf{A},\mathbf{r}] - q[\mathbf{A}\cdot\mathbf{p},\mathbf{r}] + q^2[A^2,\mathbf{r}]) + q[\phi,\mathbf{r}]\Big)\rangle$$

Let's look at the commutators one at a time. (Sum over pairs of indices)

$$\begin{aligned}[p^2,\mathbf{r}] &= [p_i p_i, x_j]\hat{x}_j = p_i[p_i,x_j]\hat{x}_j + [p_i,x_j]p_i\hat{x}_j \\ &= -2i\hbar p_i\delta_{ij}\hat{x}_j = -2i\hbar\mathbf{p} \end{aligned} \tag{1}$$

$$\begin{aligned}[\mathbf{p}\cdot\mathbf{A},\mathbf{r}] &= [p_iA_i,x_j]\hat{x}_j = p_i[A_i,x_j]\hat{x}_j + [p_i,x_j]A_i\hat{x}_j \\ &= -i\hbar\delta_{ij}A_i\hat{x}_j = -i\hbar\mathbf{A}\end{aligned} \tag{2}$$

$$\begin{aligned}[\mathbf{A}\cdot\mathbf{p},\mathbf{r}] &= [A_ip_i,x_j]\hat{x}_j = A_i[p_i,x_j]\hat{x}_j + [A_i,x_j]p_i\hat{x}_j = \\ &\quad -i\hbar A_i\delta_{ij}\hat{x}_j = -i\hbar\mathbf{A}\end{aligned} \tag{3}$$

$$[A^2,\mathbf{r}] = A_i[A_i,x_j]\hat{x}_j + [A_i,x_j]A_i\hat{x}_j = 0 \tag{4}$$

$$[\phi,\mathbf{r}] = 0 \tag{5}$$

Putting the pieces together we get

$$\frac{i}{\hbar}[H,\mathbf{r}] = \frac{i}{2m\hbar}\left(-2i\hbar\mathbf{p} + qi\hbar\mathbf{A} + qi\hbar\mathbf{A}\right)$$

$$= \frac{1}{m}(\mathbf{p} - q\mathbf{A})$$

(b)

$$\frac{d\langle \mathbf{v}\rangle}{dt} = \frac{i}{\hbar}\langle [H,\frac{1}{m}(\mathbf{p}-q\mathbf{A})]\rangle + \frac{1}{m}\langle\frac{\partial}{\partial t}(\mathbf{p}-q\mathbf{A})\rangle$$

$$= \frac{i}{2m^2\hbar}\Big([p^2,\mathbf{p}] - q[\mathbf{p}\cdot\mathbf{A},\mathbf{p}] - q[\mathbf{A}\cdot\mathbf{p},\mathbf{p}] + q^2[A^2,\mathbf{p}]$$

$$+ \quad -q[p^2,\mathbf{A}] + q^2[\mathbf{p}\cdot\mathbf{A},\mathbf{A}] + q^2[\mathbf{A}\cdot\mathbf{p},\mathbf{A}] - q^3[A^2,\mathbf{A}]\Big) - \frac{iq}{m\hbar}\left([\phi,\mathbf{p}] - q[\phi,\mathbf{A}]\right)$$

Let's collect terms and write

$$\frac{i}{\hbar}[H,\frac{1}{m}(\mathbf{p}-q\mathbf{A})] = \frac{i}{2m^2\hbar}\Big(-qI_1 + q^2I_2\Big) - \frac{iq}{m\hbar}I_3$$

i I_1 includes the terms with one power of $\mathbf{A}$ and 2 powers of $\mathbf{p}$

$$I_1 = [p^2, \mathbf{A}] + [\mathbf{p} \cdot \mathbf{A}, \mathbf{p}] + [\mathbf{A} \cdot \mathbf{p}, \mathbf{p}]$$

ii I_2 has the terms with 2 powers of $\vec{A}$ and one power of $\mathbf{p}$

$$I_2 = [\mathbf{A}^2, \mathbf{p}] + [\mathbf{p} \cdot \mathbf{A}, \mathbf{A}] + [\mathbf{A} \cdot \mathbf{p}, \mathbf{A}]$$

iii And finally I_3 is the term with ϕ and $\mathbf{p}$

$$I_3 = [\phi, \mathbf{p}]$$

All of the other terms are zero.

Let's see what we can do with I_1

$$\begin{aligned} I_1 &= [p^2, \mathbf{A}] + [\mathbf{p} \cdot \mathbf{A}, \mathbf{p}] + [\mathbf{A} \cdot \mathbf{p}, \mathbf{p}] \\ &= [p_i p_i, A_j]\hat{x}_j + [p_i A_i, p_j]\hat{x}_j + [A_i p_i, p_j]\hat{x}_j \\ &= (p_i[p_i, A_j] + [p_i, A_j]p_i + p_i[A_i, p_j] + [A_i, p_j]p_i)\, \hat{x}_j \end{aligned}$$

Now we need

$$\begin{aligned} [p_i, A_j]\psi &= (p_i A_j - A_j p_i)\psi \\ &= (p_i A_j)\psi + A_j p_i \psi - A_j p_i \psi \\ &= (p_i A_j)\psi \\ &= -i\hbar \frac{\partial A_j}{\partial x_i}\psi \end{aligned}$$

Then I_1 becomes

$$\begin{aligned} I_1 &= -\hbar^2 \left(\frac{\partial}{\partial x_i}\frac{\partial A_j}{\partial x_i} + \frac{\partial A_j}{\partial x_i}\frac{\partial}{\partial x_i} - \frac{\partial}{\partial x_i}\frac{\partial A_i}{\partial x_j} - \frac{\partial A_i}{\partial x_j}\frac{\partial}{\partial x_i} \right) \hat{x}_j \\ &= -\hbar^2 \left(\nabla^2 A_j - \frac{\partial}{\partial x_j}(\vec{\nabla} \cdot \mathbf{A}) + (\vec{\nabla} A_j) \cdot \vec{\nabla} - \frac{\partial \mathbf{A}}{\partial x_j} \cdot \vec{\nabla} \right) \hat{x}_j \\ &= -\hbar^2 \left(-\vec{\nabla} \times (\vec{\nabla} \times \mathbf{A}) + (\vec{\nabla} \times \mathbf{A}) \times \vec{\nabla} \right) \hat{x}_j \\ &= i\hbar(\mathbf{p} \times \mathbf{B} - \mathbf{B} \times \mathbf{p})\hat{x}_j \end{aligned}$$

In the last step we used the vector identity

$$\vec{\nabla} \times (\vec{\nabla} \times \mathbf{A}) = -\nabla^2 \mathbf{A} + \vec{\nabla}(\vec{\nabla} \cdot \mathbf{A})$$

and note that

$$\left((\vec{\nabla} A_j)\cdot\vec{\nabla} - \frac{\partial \mathbf{A}}{\partial x_j}\cdot\vec{\nabla}\right)\hat{x}_j = \left((\vec{\nabla}\times\mathbf{A})\times\vec{\nabla}\right)\hat{x}_j$$

Next we evaluate I_2

$$\begin{aligned}
I_2 &= [\mathbf{A}^2, \mathbf{p}] + [\mathbf{p}\cdot\mathbf{A}, \mathbf{A}] + [\mathbf{A}\cdot\mathbf{p}, \mathbf{A}] \\
&= (A_i[A_i, p_j] - [p_j, A_i]A_i - [A_j, p_i]A_i - A_i[p_i, A_j])\,\hat{x}_j \\
&= -i\hbar\left(-A_i\frac{\partial A_i}{\partial x_j} - \frac{\partial A_i}{\partial x_j}A_i + \frac{\partial A_j}{\partial x_i} + A_i\frac{\partial A_j}{\partial x_i}\right)\hat{x}_j \\
&= -i\hbar\left(A_i(\frac{\partial A_j}{\partial x_i} - \frac{\partial A_i}{\partial x_j}) + (\frac{\partial A_j}{\partial x_i} - \frac{\partial A_i}{\partial x_j})A_i\right)\hat{x}_j \\
&= -i\hbar\left(\mathbf{A}\times(\vec{\nabla}\times\mathbf{A}) - (\vec{\nabla}\times\mathbf{A})\times\mathbf{A}\right)\hat{x}_j \\
&= i\hbar(\mathbf{A}\times\mathbf{B} - \mathbf{B}\times\mathbf{A}) = 2i\hbar\mathbf{A}\times\mathbf{B}
\end{aligned}$$

And

$$I_3 = i\hbar\vec{\nabla}\phi$$

Putting the pieces together we get

$$\begin{aligned}
\frac{i}{\hbar}\langle[H, \frac{1}{m}(\mathbf{p} - q\mathbf{A})]\rangle &= \frac{i}{2m^2\hbar}\left(-qI_1 + q^2 I_2\right) - \frac{iq}{m\hbar}I_3 \\
&= \frac{i}{2m^2\hbar}\left(-qi\hbar(\mathbf{p}\times\mathbf{B} - \mathbf{B}\times\mathbf{p}) + q^2(2i\hbar\mathbf{A}\times\mathbf{B})\right) + \frac{q}{m}\vec{\nabla}\phi \\
&= \frac{q}{2m^2}(\mathbf{p}\times\mathbf{B} - \mathbf{B}\times\mathbf{p}) - \frac{q^2}{m^2}(\mathbf{A}\times\mathbf{B}) + \frac{q}{m}\vec{\nabla}\phi
\end{aligned}$$

And finally

$$\begin{aligned}
\frac{d\langle\mathbf{v}\rangle}{dt} &= \frac{q}{2m^2}\langle(\mathbf{p}\times\mathbf{B} - \mathbf{B}\times\mathbf{p}) - \frac{q^2}{m^2}(\mathbf{A}\times\mathbf{B})\rangle + \frac{q}{m}(\langle\vec{\nabla}\phi - \frac{\partial\mathbf{A}}{\partial t}\rangle) \\
&= \frac{q}{2m^2}\langle(\mathbf{p}\times\mathbf{B} - \mathbf{B}\times\mathbf{p}) - \frac{q^2}{m^2}(\mathbf{A}\times\mathbf{B})\rangle + \frac{q}{m}\langle\mathbf{E}\rangle
\end{aligned}$$

(c) If **E** and **B** are uniform over the volume where the wave function is non zero then, **p** and **B** commute and there is a sign change due to reversing the order of the cross product. That is:

$$\mathbf{p}\times(\mathbf{B}\psi) = \frac{\hbar}{i}\vec{\nabla}\times(\mathbf{B}\psi) = -\frac{\hbar}{i}\left((\vec{\nabla}\times\mathbf{B})\psi - \mathbf{B}\times(\vec{\nabla}\psi)\right) = -\mathbf{B}\times\mathbf{p}\psi$$

Then

$$
\begin{aligned}
m\frac{d\langle \mathbf{v}\rangle}{dt} &= \frac{q}{m}\langle \mathbf{p}\times\mathbf{B}\rangle - \frac{q^2}{m}(\mathbf{A}\times\mathbf{B})\rangle + \frac{q}{m}\langle \mathbf{E}\rangle \\
&= \frac{q}{m}\left(\langle(\mathbf{p}-q\mathbf{A})\times\mathbf{B}\rangle + \mathbf{E}\rangle\right) \\
&= q(\langle \mathbf{v}\rangle \times \mathbf{B} + \mathbf{E})
\end{aligned}
$$

3. Griffiths 4.61

(a) The effect of the gauge transformation on the electric field is

$$
\begin{aligned}
\mathbf{E} &= -\nabla\phi - \frac{\partial \mathbf{A}}{\partial t} \\
\mathbf{E}' &= -\nabla\phi' - \frac{\partial \mathbf{A}'}{\partial t} \\
&= -\nabla(\phi - \frac{\partial \Lambda}{\partial t}) - \frac{\partial \mathbf{A}}{\partial t} - \frac{\partial \nabla\Lambda}{\partial t} \\
&= -\nabla\phi - \frac{\partial \mathbf{A}}{\partial t} \\
&= \mathbf{E}
\end{aligned}
$$

The effect of the gauge transformation on the magnetic field is

$$
\begin{aligned}
\mathbf{B} &= \nabla\times\mathbf{A} \\
\mathbf{B}' &= \nabla\times\mathbf{A}' \\
&= \nabla\times(\mathbf{A}+\nabla\Lambda) \\
&= \nabla\times\mathbf{A} \\
&= \mathbf{B}
\end{aligned}
$$

where we use the fact that $\nabla\times(\nabla\Lambda) = 0$.

(b) We aim to show that if

$$
i\hbar\frac{\partial\Psi}{\partial t} = \left[\frac{1}{2m}\left(\frac{\hbar}{i}\nabla - q\mathbf{A}\right)^2 + q\phi\right]\Psi \tag{6}
$$

then

$$
i\hbar\frac{\partial\Psi'}{\partial t} = \left[\frac{1}{2m}\left(\frac{\hbar}{i}\nabla - q\mathbf{A}'\right)^2 + q\phi'\right]\Psi'
$$

where

$$\Psi' - e^{q\Lambda/\hbar}\Psi$$

and

$$\phi' \equiv \phi - \frac{\partial\lambda}{\partial t}, \quad \mathbf{A}' = \mathbf{A} + \nabla\Lambda$$

Substitution into Schodinger's equation gives

$$LHS = \left[\frac{1}{2m}\left(\frac{\hbar}{i}\nabla - q(\mathbf{A}+\nabla\Lambda)\right)^2 + q(\phi - \frac{\partial\Lambda}{\partial t})\right]\Psi e^{iq\Lambda/\hbar} \tag{7}$$

Taking the derivative on the left hand side of Equation 1 we get

$$i\hbar\frac{\partial}{\partial t}\Psi e^{iq\Lambda/\hbar} = e^{iq\Lambda/\hbar}\left(-q\frac{\partial\Lambda}{\partial t} + i\hbar\frac{\partial}{\partial t}\right)\Psi \tag{8}$$

On the right hand side we get

$$\begin{aligned}
RHS &= \frac{1}{2m}\left(\frac{\hbar}{i}\nabla - q(\mathbf{A}+\nabla\Lambda)\right)e^{iq\Lambda/\hbar}\left(\frac{\hbar}{i}\nabla + q\nabla\Lambda - q(\mathbf{A}+\nabla\Lambda)\right)\Psi \\
&\qquad + q(\phi - \frac{\partial\Lambda}{\partial t})\Psi e^{iq\Lambda/\hbar} \\
&= \frac{1}{2m}\left(\frac{\hbar}{i}\nabla - q(\mathbf{A}+\nabla\Lambda)\right)e^{iq\Lambda/\hbar}\left(\frac{\hbar}{i}\nabla + -q\mathbf{A}\right)\Psi + q(\phi - \frac{\partial\Lambda}{\partial t})\Psi e^{iq\Lambda/\hbar} \\
&= e^{iq\Lambda/\hbar}\left[\frac{1}{2m}\left(\frac{\hbar}{i}\nabla + q\nabla\Lambda - q(\mathbf{A}+\nabla\Lambda)\right)\left(\frac{\hbar}{i}\nabla + -q\mathbf{A}\right)\Psi + q(\phi - \frac{\partial\Lambda}{\partial t})\Psi\right] \\
&= e^{iq\Lambda/\hbar}\left[\frac{1}{2m}\left(\frac{\hbar}{i}\nabla - q\mathbf{A}\right)\left(\frac{\hbar}{i}\nabla + -q\mathbf{A}\right)\Psi + q(\phi - \frac{\partial\Lambda}{\partial t})\Psi\right]
\end{aligned}$$

Setting the LHS equal to the RHS we recover Equation 6.

4. **Griffiths 5.1**

(a) If

$$\mathbf{r} = \mathbf{r}_1 - \mathbf{r}_2 \quad \text{and} \tag{9}$$

$$\mathbf{R} = \frac{m_1\mathbf{r}_1 + m_2\mathbf{r}_2}{m_1 + m_2} \tag{10}$$

then solving for $\mathbf{r}_1$ in terms of $\mathbf{R}$ and $\mathbf{r}$ gives $\mathbf{r}_1 = \mathbf{R} + (\mu/m)1)\mathbf{r}$ and solving for $\mathbf{r}_2$ gives $\mathbf{r}_2 = \mathbf{R} - (\mu/m_2)\mathbf{r}$. If

$$\begin{aligned} \nabla_1 &= = \hat{i}\frac{\partial}{\partial x_1} + \hat{j}\frac{\partial}{\partial y_1} + \hat{k}\frac{\partial}{\partial z_1} \\ \nabla_r &= = \hat{i}\frac{\partial}{\partial x} + \hat{j}\frac{\partial}{\partial y} + \hat{k}\frac{\partial}{\partial z} \\ \nabla_R &= = \hat{i}\frac{\partial}{\partial X} + \hat{j}\frac{\partial}{\partial Y} + \hat{k}\frac{\partial}{\partial Z} \end{aligned}$$

then

$$\nabla_{1x} = \frac{\partial X}{\partial x_1}\frac{\partial}{\partial X} + \frac{\partial x}{\partial x_1}\frac{\partial}{\partial x}$$

From Equation 9 we get that $\frac{\partial x}{\partial x_1} = 1$ and from 10 that $\frac{\partial X}{\partial x_1} = \frac{m_1}{m_1+m_2}$ so that

$$\begin{aligned} \nabla_{1x} &= \frac{m_1}{m_1+m_2}\nabla_{Rx} + \nabla_{rx} \\ &= \frac{\mu}{m_2}\nabla_{Rx} + \nabla_{rx} \end{aligned}$$

and similarly for the y and z components. And so

$$\nabla_1 = \frac{\mu}{m_2}\nabla_R + \nabla_r$$

Meanwhile Equation 9 gives $\frac{\partial x}{\partial x_2} = -1$, and 10 that $\frac{\partial X}{\partial x_2} = \frac{m_1}{m_1+m_2}$ so that

$$\begin{aligned} \nabla_{2x} &= \frac{m_1}{m_1+m_2}\nabla_{Rx} - \nabla_{rx} \\ &= \frac{\mu}{m_1}\nabla_{Rx} - \nabla_{rx} \\ &\rightarrow \nabla_2 = \frac{\mu}{m_1}\nabla_R - \nabla_r \end{aligned}$$

(b) The two particle Schrodinger equation is

$$\left[-\frac{\hbar^2}{2m_1}\nabla_1^2 - \frac{\hbar^2}{2m_2}\nabla_2^2 + V(\mathbf{r}_1 - \mathbf{r}_2)\right]\psi = E\psi$$

$$\left[-\frac{\hbar^2}{2m_1}(\frac{\mu}{m_2}\nabla_R + \nabla_r)^2 - \frac{\hbar^2}{2m_2}(\frac{\mu}{m_1}\nabla_R - \nabla_r)^2 + V(\mathbf{r})\right]\psi = E\psi$$
$$\left[-\frac{\hbar^2}{2m_1}(\left(\frac{\mu}{m_2}\right)^2\nabla_R^2 + \nabla_r^2) - \frac{\hbar^2}{2m_2}(\left(\frac{\mu}{m_1}\right)^2\nabla_R^2 + \nabla_r^2) + V(\mathbf{r})\right]\psi = E\psi$$
$$\left[-\frac{\hbar^2\mu^2}{2m_1m_2}\left(\frac{1}{m_2} + \frac{1}{m_1}\right)\nabla_R^2 - \frac{\hbar^2}{2}\left(\frac{1}{m_1} + \frac{1}{m_2}\right)\nabla_r^2 + V(\mathbf{r})\right]\psi = E\psi$$
$$\left[-\frac{\hbar^2}{2(m_1+m_2)}\nabla_R^2 - \frac{\hbar^2}{2\mu}\nabla_r^2 + V(\mathbf{r})\right]\psi = E\psi$$

(c) Separate the variables so that $\psi(\mathbf{R}, \mathbf{r}) = \psi_R(\mathbf{R})\psi_r\mathbf{r}$, substitute into the Schrodinger equation and divide by ψ and we get

$$-\frac{\hbar^2}{2(m_1+m_2)}\frac{\nabla_R^2\psi_R}{\psi_R} - \frac{\hbar^2}{2\mu}\frac{\nabla_r^2\psi_r}{\psi_r} + V(\mathbf{r}) = E$$

The first term depends only on $\mathbf{R}$ and the second and third only on $\mathbf{r}$ so

$$\begin{aligned} - & \frac{\hbar^2}{2(m_1+m_2)}\nabla_R^2\psi_R = E_R\psi_R \\ - & \frac{\hbar^2}{2\mu}\nabla_r^2\psi_r + V(\mathbf{r})\psi_r = E_r\psi_r \\ & \text{and} \quad E = E_R + E_r \end{aligned}$$

5. Entangled States

(a)

$$\begin{aligned} \langle 1G2G \mid \psi\rangle &= 0 \\ \to 0 &= \langle 1G2G \mid 1R1G\rangle\alpha + \langle 1G2G \mid 1G1R\rangle\beta + \langle 1G2G \mid 1G1G\rangle\gamma \\ 0 &= \langle 1G \mid 1R\rangle\langle 2G \mid 1G\rangle\alpha + \langle 1G \mid 1G\rangle\langle 2G \mid 1R\rangle\beta + \langle 1G \mid 1G\rangle\langle 2G \mid 1G\rangle\gamma \\ \Rightarrow 0 &= \langle 2G \mid 1R\rangle\beta + \langle 2G \mid 1G\rangle\gamma \end{aligned}$$

where we use the fact that $\langle 1G \mid 1G\rangle = 1$, and $\langle 1G \mid 1R\rangle = 0$. Similarly

$$\begin{aligned}
\langle 2G1G \mid \psi\rangle &= 0 \\
\rightarrow 0 &= \langle 2G1G \mid 1R1G\rangle\alpha + \langle 2G1G \mid 1G1R\rangle\beta + \langle 2G1G \mid 1G1G\rangle\gamma \\
0 &= \langle 2G \mid 1R\rangle\langle 1G \mid 1G\rangle\alpha + \langle 2G \mid 1G\rangle\langle 1G \mid 1R\rangle\beta + \langle 2G \mid 1G\rangle\langle 1G \mid 1G\rangle\gamma \\
\Rightarrow 0 &= \langle 2G \mid 1R\rangle\alpha + \langle 2G \mid 1G\rangle\gamma
\end{aligned}$$

For future reference, we have that

$$\alpha = \beta = -\gamma\frac{\langle 2G \mid 1G\rangle}{\langle 2G \mid 1R\rangle} \tag{11}$$

(b)

$$\begin{aligned}
\sqrt{p} &= \langle 2G2G \mid \psi\rangle \\
&= \langle 2G \mid 1R\rangle\langle 2G \mid 1G\rangle\alpha + \langle 2G \mid 1G\rangle\langle 2G \mid 1R\rangle\beta + \langle 2G \mid 1G\rangle\langle 2G \mid 1G\rangle\gamma \\
&= -\gamma\langle 2G \mid 1G\rangle^2 - \gamma\langle 2G \mid 1G\rangle^2 + \gamma\langle 2G \mid 1G\rangle^2 \\
&= -\gamma\langle 2G \mid 1G\rangle^2
\end{aligned}$$

where we have used Equation 11. Finally, since $|\alpha|^2 + |\beta|^2 + |\gamma|^2 = 1$ we have that

$$\begin{aligned}
1 &= \gamma^2\left[2\left|\frac{\langle 2G \mid 1G\rangle}{\langle 2G \mid 1R\rangle}\right|^2 + 1\right] \\
\Rightarrow \gamma^2 &= \frac{|\langle 2G \mid 1R\rangle|^2}{2|\langle 2G \mid 1G\rangle|^2 + |\langle 2G \mid 1R\rangle|^2}
\end{aligned}$$

And

$$\begin{aligned}
p &= \gamma^2\left(|\langle 2G \mid 1G\rangle|^2\right)^2 \\
&= \frac{|\langle 2G \mid 1R\rangle|^2\left(|\langle 2G \mid 1G\rangle|^2\right)^2}{2|\langle 2G \mid 1G\rangle|^2 + |\langle 2G \mid 1R\rangle|^2}
\end{aligned} \tag{12}$$

Since (we are given)

$$\begin{aligned}
\mid 2G\rangle &= q^{\frac{1}{2}}\mid 1G\rangle + \sqrt{1-q}\mid 1R\rangle \\
\mid 2R\rangle &= q^{\frac{1}{2}}\mid 1R\rangle - \sqrt{1-q}\mid 1G\rangle
\end{aligned}$$

we get that

$$
\begin{aligned}
\langle 1G \mid 2G \rangle &= \sqrt{q} && (13)\\
\langle 1R \mid 2G \rangle &= \sqrt{1-q} && (14)\\
\langle 1G \mid 2R \rangle &= -\sqrt{1-q} && (15)\\
\langle 1R \mid 2R \rangle &= q^{\frac{1}{2}} && (16)
\end{aligned}
$$

Then substitution of Equations 13 - 16 into 12 gives

$$p = \frac{(1-q)q^2}{2q+1-q} = \frac{(1-q)^2q^2}{1-q^2}$$

(c) To maximize p with respect to q set

$$
\begin{aligned}
0 &= \frac{d}{dq}\left(\frac{(1-q)^2q^2}{1-q^2}\right)\\
&= \left(2q(1-q)^2 - 2q^2(1-q) + \frac{q^2(1-q)^2(2q)}{1-q^2}\right)\frac{1}{1-q^2}\\
\Rightarrow 0 &= \left((1-q) - q + \frac{q^2}{1+q}\right)\\
\Rightarrow 0 &= (1-2q)(1+q) + q^2 = 1 - q - q^2 && (17)\\
\Rightarrow q &= -\frac{1}{2}(1 \pm \sqrt{5})
\end{aligned}
$$

But $q > 0$ so we choose the $+$ sign and the q that minimizes p is $q \equiv z = \frac{1}{2}(\sqrt{5}-1)$. For future reference note that

$$
\begin{aligned}
\gamma^2 &= \frac{|\langle 2G \mid 1R \rangle|^2}{2|\langle 2G \mid 1G \rangle|^2 + |\langle 2G \mid 1R \rangle|^2}\\
&= \frac{1-q}{2q+1-q} = \frac{1-q}{1+q}\\
\alpha^2 &= \beta^2 = \gamma^2 \left|\frac{\langle 2G \mid 1G \rangle}{\langle 2G \mid 1R \rangle}\right|^2 = \frac{1-q}{1+q}\frac{q}{1-q}
\end{aligned}
$$

Then when p is maximized so that $z = q$ and $1 - z = z^2$ and $1 + z = z/(1-z)$ (which follows from Equation 17)

$$|\langle 1G1G \mid \psi \rangle = |\alpha\langle 1G \mid 1R \rangle\langle 1G \mid 1G \rangle + \beta\langle 1G \mid 1G \rangle\langle 1G \mid 1R \rangle + \gamma\langle 1G \mid 1G \rangle\langle 1G \mid 1G \rangle|^2$$

$$
\begin{aligned}
&= \gamma^2 = \frac{1-z}{1+z} = z^3 \\
|\langle 1G1R \mid \psi\rangle &= |\alpha\langle 1G \mid 1R\rangle\langle 1R \mid 1G\rangle + \beta\langle 1G \mid 1G\rangle\langle 1R \mid 1R\rangle + \gamma\langle 1G \mid 1G\rangle\langle 1R \mid 1G\rangle|^2 \\
&= \beta^2 = \frac{z}{1+z} = z^2 \\
|\langle 1R1G \mid \psi\rangle &= |\alpha\langle 1R \mid 1R\rangle\langle 1G \mid 1G\rangle + \beta\langle 1R \mid 1G\rangle\langle 1G \mid 1R\rangle + \gamma\langle 1R \mid 1G\rangle\langle 1G \mid 1G\rangle|^2 \\
&= \alpha^2 = z^2 \\
|\langle 1R1R \mid \psi\rangle &= |\alpha\langle 1R \mid 1R\rangle\langle 1R \mid 1G\rangle + \beta\langle 1R \mid 1G\rangle\langle 1R \mid 1R\rangle + \gamma\langle 1R \mid 1G\rangle\langle 1R \mid 1G\rangle|^2 \\
&= 0 \\
|\langle 1G2G \mid \psi\rangle &= |\alpha\langle 1G \mid 1R\rangle\langle 2G \mid 1G\rangle + \beta\langle 1G \mid 1G\rangle\langle 2G \mid 1R\rangle + \gamma\langle 1G \mid 1G\rangle\langle 2G \mid 1G\rangle|^2 \\
&= |\beta\sqrt{1-z} + \gamma\sqrt{z}|^2 \\
&= |-\gamma\sqrt{\frac{z}{1-z}}\sqrt{1-z} + \gamma\sqrt{z}|^2 = 0
\end{aligned}
$$

etc.