PEU 455 Assignment 2

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1 8.4.1

(a)

$$\psi = 2\alpha^{\frac{3}{2}} x e^{-\alpha x}$$

$$\int_0^\infty \psi\psi * dx$$

$$= 4\alpha^3 \int_0^\infty x^2 e^{-2\alpha x} dx$$

$$\begin{bmatrix} x^2 & e^{-2\alpha x} \\ 2x & \frac{1}{-2\alpha} e^{-2\alpha x} \\ 2 & \frac{1}{4\alpha^2} e^{-2\alpha x} \\ 0 & \frac{1}{-8\alpha^3} e^{-2\alpha x} \end{bmatrix}$$

$$= 4\alpha^3 \left[-\frac{x^2}{2\alpha} e^{-2\alpha x} - \frac{x}{2\alpha^2} e^{-2\alpha x} - \frac{1}{4\alpha^3} e^{-2\alpha x} \right]_0^\infty = 1$$

ψ is normalized.

(b)

$$\int_0^\infty \psi x^{-1} \psi * dx$$

$$= 4\alpha^3 \int_0^\infty xe^{-2\alpha x}$$

$$= 4\alpha^3 \int_0^\infty xe^{-2\alpha x}$$

$$\begin{bmatrix} x & e^{-2\alpha x} \\ 1 & \frac{1}{-2\alpha} e^{-2\alpha x} \\ 0 & \frac{1}{4\alpha^2} e^{-2\alpha x} \end{bmatrix}$$

$$4\alpha^3 \left[x \frac{1}{-2\alpha} e^{-2\alpha x} - \frac{1}{4\alpha^2} e^{-2\alpha x} \right]_0^\infty = \alpha$$

(c)

$$\frac{d\psi}{dx} = 2\alpha^{\frac{3}{2}} \frac{d(xe^{-\alpha x})}{dx} = 2\alpha^{\frac{3}{2}} e^{-\alpha x}(1 - \alpha x)$$

$$\frac{d^2\psi}{dx^2} = 2\alpha^{\frac{3}{2}} \frac{d(e^{-\alpha x}(1 - \alpha x))}{dx} = -2\alpha^{\frac{3}{2}} (\alpha e^{-\alpha x} + \alpha e^{-\alpha x}(1 - \alpha x))$$

$$= -2\alpha^{\frac{5}{2}} e^{-\alpha x}(2 - \alpha x)$$

$$\int_0^\infty \psi * \frac{d^2\psi}{dx^2} dx$$

$$-4\alpha^4 \int_0^\infty xe^{-2\alpha x}(2 - \alpha x) dx$$

$$-8\alpha^4 \int_0^\infty xe^{-2\alpha x} dx + 4\alpha^5 \int_0^\infty x^2 e^{-2\alpha x} dx$$

$$\int_0^\infty xe^{-2\alpha x} dx = \frac{1}{4\alpha^2}, \quad \int_0^\infty x^2 e^{-2\alpha x} dx = \frac{1}{4\alpha^3}$$

$$= -\alpha^2$$

(d)

$$\left\langle \psi \middle| -\frac{1}{2} \frac{d^2}{dx^2} - \frac{1}{x} \middle| \psi \right\rangle$$

$$= -(\frac{1}{2}\left\langle \psi \left| \frac{d^2}{dx^2} \right| \psi \right\rangle + \left\langle \psi \left| x^{-1} \right| \psi \right\rangle)$$

$$= \frac{\alpha^2}{2} - \alpha$$

$$\frac{d(\frac{\alpha^2}{2} - \alpha)}{d\alpha} = 0$$

$$\alpha = 1$$

$$\min(\left\langle \psi \left| -\frac{1}{2}\frac{d^2}{dx^2} - \frac{1}{x} \right| \psi \right\rangle) = -\frac{1}{2}$$

2 P2

Let $\psi_{\text{trial}} = \psi_0(\beta)$ where ψ_0 is the old ground state of hydrogen atom. Where we will vary $a_0 \to \frac{a_0}{\beta}$.

$$\psi_{\text{trial}} = \sqrt{\frac{\beta^3}{\pi a_0^3}} e^{-\frac{r\beta}{a_0}}$$

$$H = -(\frac{\hbar^2}{2m}\nabla^2 + \frac{e^2}{4\pi\epsilon_0}\frac{e^{-\mu r}}{r})$$

For a non-varying function in θ and ϕ

$$\nabla^2 = \frac{1}{r^2}\frac{\partial}{\partial r}(r^2\frac{\partial}{\partial r})$$

$$H|\psi\rangle = -\sqrt{\frac{\beta^3}{\pi a_0^3}}\left(\frac{\hbar^2}{2mr^2}\frac{d}{dr}(r^2\frac{d}{dr}) + \frac{e^2}{4\pi\epsilon_0}\frac{e^{-\mu r}}{r}\right)e^{-\frac{r\beta}{a_0}}$$

$$= -\sqrt{\frac{\beta^3}{\pi a_0^3}}\left(\frac{\hbar^2}{2mr^2}\frac{d(r^2\frac{d(e^{-\frac{r\beta}{a_0}})}{dr})}{dr} + \frac{e^{2-r(\mu+\frac{\beta}{a_0})}}{4\pi\epsilon_0 r}\right)$$

$$= -\sqrt{\frac{\beta^3}{\pi a_0^3}}\left(-\frac{\hbar^2\beta}{2mr^2a_0}\frac{d(r^2e^{-\frac{r\beta}{a_0}})}{dr} + \frac{e^{2-r(\mu+\frac{\beta}{a_0})}}{4\pi\epsilon_0 r}\right)$$

$$= \sqrt{\frac{\beta^3}{\pi a_0^3}}e^{-\frac{r\beta}{a_0}}\left(\frac{\hbar^2\beta}{2mr^2a_0}(2r - \frac{\beta r^2}{a_0}) - \frac{e^{2-r\mu}}{4\pi\epsilon_0 r}\right)$$

$$= \sqrt{\frac{\beta^3}{\pi a_0^3}}e^{-\frac{r\beta}{a_0}}\left(\frac{\hbar^2\beta}{mra_0} - \frac{\hbar^2\beta^2}{2ma_0^2} - \frac{e^{2-r\mu}}{4\pi\epsilon_0 r}\right)$$

$$\langle\psi\,|H|\,\psi\rangle = \frac{\beta^3}{\pi a_0^3}\int_0^\infty re^{-\frac{2r\beta}{a_0}}\left(\frac{\hbar^2\beta}{ma_0} - \frac{e^2}{4\pi\epsilon_0}e^{-r\mu} - \frac{\hbar^2\beta^2}{2ma_0^2}r\right)dr$$

$$
\begin{aligned}
\langle \psi \left| H \right| \psi \rangle &= 4\pi \frac{\beta^3}{\pi a_0^3} \int_0^\infty e^{-\frac{2r\beta}{a_0}} \left(\frac{\hbar^2 \beta}{m r a_0} - \frac{e^2}{4\pi\epsilon_0 r} e^{-r\mu} - \frac{\hbar^2\beta^2}{2ma_0^2} \right) r^2 dr \\
&= \frac{4\beta^3}{a_0^3} \int_0^\infty \left(\frac{\hbar^2\beta}{ma_0} r e^{-\frac{2r\beta}{a_0}} - \frac{e^2}{4\pi\epsilon_0} r e^{-r(\mu + 2\frac{\beta}{a_0})} - \frac{\hbar^2\beta^2}{2ma_0^2} r^2 e^{-\frac{2r\beta}{a_0}} \right) dr \\
&= \frac{4\beta^3}{a_0^3} \left[\frac{\hbar^2\beta}{ma_0} \left(-r\frac{a_0}{2\beta} - \left(\frac{a_0}{2\beta}\right)^2 \right) e^{-\frac{2r\beta}{a_0}} \right]_0^\infty \\
&- \frac{4\beta^3}{a_0^3} \left[\frac{e^2}{4\pi\epsilon_0} \left(-r\frac{1}{\mu + 2\frac{\beta}{a_0}} - \left(\frac{1}{\mu + 2\frac{\beta}{a_0}} \right)^2 \right) e^{-r(\mu + 2\frac{\beta}{a_0})} \right]_0^\infty \\
&- \frac{\beta^3}{\pi a_0^3} \left[\frac{\hbar^2\beta^2}{2ma_0^2} \left(-r^2 \frac{a_0}{2\beta} - 2r\left(\frac{a_0}{2\beta}\right)^2 - 2\left(\frac{a_0}{2\beta}\right)^3 \right) e^{-\frac{2r\beta}{a_0}} \right]_0^\infty \\
&= \frac{4\beta^3}{a_0^3} \left[\frac{\hbar^2\beta}{ma_0} \left(\frac{a_0}{2\beta}\right)^2 - \frac{e^2}{4\pi\epsilon_0} \left(\frac{1}{\mu + 2\frac{\beta}{a_0}} \right)^2 - 2\frac{\hbar^2\beta^2}{2ma_0^2} \left(\frac{a_0}{2\beta}\right)^3 \right] \\
&= \frac{4\beta^3}{a_0^3} \left[\frac{\hbar^2 a_0}{4m\beta} - \frac{e^2}{4\pi\epsilon_0} \left(\frac{1}{\mu + 2\frac{\beta}{a_0}} \right)^2 - \frac{\hbar^2 a_0}{8m\beta} \right] \\
&= \frac{\beta^3}{a_0^3} \left[\frac{\hbar^2 a_0}{2m\beta} - \frac{e^2}{\pi\epsilon_0} \left(\frac{1}{\mu + 2\frac{\beta}{a_0}} \right)^2 \right]
\end{aligned}
$$

$$
\begin{aligned}
\frac{d \langle \psi \left| H \right| \psi \rangle}{d\beta} &= 3\frac{\beta^2}{a_0^3} \left[\frac{\hbar^2 a_0}{2m\beta} - \frac{e^2}{\pi\epsilon_0} \left(\frac{1}{\mu + 2\frac{\beta}{a_0}} \right)^2 \right] + \frac{\beta^3}{a_0^3} \left[-\frac{\hbar^2 a_0}{2m\beta^2} + 4\frac{e^2}{\pi\epsilon_0 a_0} \left(\frac{1}{\mu + 2\frac{\beta}{a_0}} \right)^3 \right] \\
&= \frac{3\hbar^2\beta}{2ma_0^2} - 3\frac{\beta^2}{a_0^3}\frac{e^2}{\pi\epsilon_0} \left(\frac{1}{\mu + 2\frac{\beta}{a_0}} \right)^2 - \frac{\hbar^2\beta}{2ma_0^2} + 4\frac{\beta^3}{a_0^4}\frac{e^2}{\pi\epsilon_0} \left(\frac{1}{\mu + 2\frac{\beta}{a_0}} \right)^3 \\
&= \frac{\hbar^2\beta}{ma_0^2} - 3\frac{\beta^2}{a_0^3}\frac{e^2}{\pi\epsilon_0} \left(\frac{1}{\mu + 2\frac{\beta}{a_0}} \right)^2 + 4\frac{\beta^3}{a_0^4}\frac{e^2}{\pi\epsilon_0} \left(\frac{1}{\mu + 2\frac{\beta}{a_0}} \right)^3
\end{aligned}
$$

$$
\because \frac{e^2}{\pi\epsilon_0} = \frac{4\hbar^2}{ma_0}
$$

$$
\begin{aligned}
\frac{d\left\langle\psi\left|H\right|\psi\right\rangle}{d\beta} &= \frac{\hbar^2\beta}{ma_0^2} - 3\frac{\beta^2}{a_0^3}\frac{4\hbar^2}{ma_0}\left(\frac{1}{\mu+2\frac{\beta}{a_0}}\right)^2 + 4\frac{\beta^3}{a_0^4}\frac{4\hbar^2}{ma_0}\left(\frac{1}{\mu+2\frac{\beta}{a_0}}\right)^3 \\
&= \frac{\hbar^2\beta}{ma_0^2} - 12\frac{\beta^2}{a_0^4}\frac{\hbar^2}{m}\left(\frac{1}{\mu+2\frac{\beta}{a_0}}\right)^2 + 16\frac{\beta^3}{a_0^5}\frac{\hbar^2}{m}\left(\frac{1}{\mu+2\frac{\beta}{a_0}}\right)^3 \\
&= \frac{\hbar^2}{ma_0^2}\left[\beta - 12\frac{\beta^2}{a_0^2}\left(\frac{1}{\mu+2\frac{\beta}{a_0}}\right)^2 + 16\frac{\beta^3}{a_0^3}\left(\frac{1}{\mu+2\frac{\beta}{a_0}}\right)^3\right] \\
&= \frac{\hbar^2}{ma_0^2}\left[\beta - 12\frac{\beta^2}{a_0^2(\mu+2\frac{\beta}{a_0})^2} + 16\frac{\beta^3}{a_0^3(\mu+2\frac{\beta}{a_0})^3}\right] \\
&= 0
\end{aligned}
$$

$$
\begin{aligned}
&\left[\beta - 12\frac{\beta^2}{a_0^2(\mu+2\frac{\beta}{a_0})^2} + 16\frac{\beta^3}{a_0^3(\mu+2\frac{\beta}{a_0})^3}\right] \\
&= \left[\beta - \frac{3}{(\frac{a_0\mu}{2\beta}+1)^2} + \frac{2}{(\frac{a_0\mu}{2\beta}+1)^3}\right] \\
&= \left[\beta - 3\left(1 - \frac{a_0\mu}{\beta} + 3(\frac{a_0\mu}{\beta})^2 + \cdots\right) + \left(2 - 3\frac{a_0\mu}{\beta} + 12(\frac{a_0\mu}{\beta})^2 + \cdots\right)\right] \\
&= \left[\beta - 1 + 3(\frac{a_0\mu}{\beta})^2\right]
\end{aligned}
$$

$$\beta^3 - \beta^2 + 3(a_0\mu)^2 = 0$$

Using mathematica we get one real solution and two imaginaries:

The real solution:

$$\beta = \frac{\left(-81a_0^2\mu^2 + \sqrt{\left(2-81a_0^2\mu^2\right)^2 - 4} + 2\right)^{\frac{1}{3}}}{3\cdot 2^{\frac{1}{3}}} + \frac{2^{\frac{1}{3}}}{3\left(-81a_0^2\mu^2 + \sqrt{\left(2-81a_0^2\mu^2\right)^2 - 4} + 2\right)^{\frac{1}{3}}} + \frac{1}{3}$$

$$\beta \approx 1 - 3(a_0\mu)^2$$

$$\begin{aligned}
\langle \psi \left| H \right| \psi \rangle_{\min} &= \frac{\beta^3}{a_0^3}\left[\frac{\hbar^2 a_0}{2m\beta} - \frac{e^2}{\pi\epsilon_0}\left(\frac{1}{\mu + 2\frac{\beta}{a_0}}\right)^2\right] \\
&= \frac{(1-3(a_0\mu)^2)^3}{a_0^3}\left[\frac{\hbar^2 a_0}{2m(1-3(a_0\mu)^2)} - \frac{4\hbar^2}{ma_0}\left(\frac{1}{\mu + 2\frac{(1-3(a_0\mu)^2)}{a_0}}\right)^2\right] \\
&= \frac{(1-3(a_0\mu)^2)^3}{a_0^3}\left[\frac{\hbar^2 a_0}{2m(1-3(a_0\mu)^2)} - \frac{4\hbar^2 a_0}{m}\left(\frac{1}{\mu a_0 + 2(1-3(a_0\mu)^2)}\right)^2\right] \\
&= \frac{\hbar^2}{2ma_0^2}(1-3(a_0\mu)^2)^2 - \frac{4\hbar^2}{ma_0^2}(1-3(a_0\mu)^2)^3(\mu a_0 + 2(1-3(a_0\mu)^2))^{-2} \\
&= \frac{\hbar^2}{ma_0^2}\left[\frac{1}{2}(1-3(a_0\mu)^2)^2 - 4(1-3(a_0\mu)^2)^3(\mu a_0 + 2(1-3(a_0\mu)^2))^{-2}\right] \\
&\approx \frac{\hbar^2}{\mu a_0^2}\left[\frac{1}{2}(1-6(a_0\mu)^2) - 4(1-9(a_0\mu)^2)(\frac{1}{4} - \frac{\mu a_0}{4} + \frac{27(\mu a_0)^2}{16})\right] \\
&\approx \frac{\hbar^2}{\mu a_0^2}\left[\frac{1}{2}(1-6(a_0\mu)^2) - 4(\frac{1}{4} - \frac{\mu a_0}{4} + \frac{27(\mu a_0)^2}{16} - \frac{9}{4}(a_0\mu)^2)\right] \\
&= \frac{\hbar^2}{\mu a_0^2}\left[-\frac{1}{2} + \mu a_0 - \frac{3}{4}(\mu a_0)^2\right]
\end{aligned}$$

3 P3

$$u = x + t, \quad v = x - t$$

$$s' = \sqrt{2}s$$

(i)

$$\Lambda = \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix} = \underbrace{\sqrt{2}\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}}_{\text{scale}} \underbrace{\frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}}_{\text{reflection}}$$

(ii) Since Λ is just reflection and scaling therefore u is still perpendicular (Λ is orthogonal)

(iii)

$$df = dx\frac{\partial f}{\partial x} + dt\frac{\partial f}{\partial t}$$

$$x = \frac{u+v}{2}, \quad t = \frac{u-v}{2}$$

$$dx = du\frac{\partial x}{\partial u} + dv\frac{\partial x}{\partial v}$$

$$dx = \frac{du + dv}{2}$$

And similarly,

$$dt = \frac{du - dv}{2}$$

$$\frac{\partial f}{\partial x} = \frac{\partial f}{\partial u}\frac{\partial u}{\partial x} + \frac{\partial f}{\partial v}\frac{\partial v}{\partial x} = \frac{\partial f}{\partial u} + \frac{\partial f}{\partial v}$$

$$\frac{\partial f}{\partial t} = \frac{\partial f}{\partial u}\frac{\partial u}{\partial t} + \frac{\partial f}{\partial v}\frac{\partial v}{\partial t} = \frac{\partial f}{\partial u} - \frac{\partial f}{\partial v}$$

$$df = \frac{du + dv}{2}(\frac{\partial f}{\partial u} + \frac{\partial f}{\partial v}) + \frac{du - dv}{2}(\frac{\partial f}{\partial u} - \frac{\partial f}{\partial v})$$

$$= du\frac{\partial f}{\partial u} + dv\frac{\partial f}{\partial v}$$

(iv)

$$u = x + iy = z, \quad v = x - iy = \bar{z}$$

$$df = dz\frac{\partial f}{\partial z} + d\bar{z}\frac{\partial f}{\partial \bar{z}}$$

4 P4

$$\nabla^2\phi = \frac{\partial^2\phi}{\partial x^2} + \frac{\partial^2\phi}{\partial y^2} = 0$$

$$\frac{\partial\phi}{\partial x} = \frac{\partial\phi}{\partial z}\frac{\partial z}{\partial x} + \frac{\partial\phi}{\partial\bar{z}}\frac{\partial\bar{z}}{\partial x} = \frac{\partial\phi}{\partial z} + \frac{\partial\phi}{\partial\bar{z}}$$

$$\frac{\partial^2\phi}{\partial x^2} = \frac{\partial(\frac{\partial\phi}{\partial z} + \frac{\partial\phi}{\partial\bar{z}})}{\partial z} + \frac{\partial(\frac{\partial\phi}{\partial z} + \frac{\partial\phi}{\partial\bar{z}})}{\partial\bar{z}} = \frac{\partial^2\phi}{\partial z^2} + 2\frac{\partial^2\phi}{\partial z\partial\bar{z}} + \frac{\partial^2\phi}{\partial\bar{z}^2}$$

$$\frac{\partial\phi}{\partial y} = \frac{\partial\phi}{\partial z}\frac{\partial z}{\partial y} + \frac{\partial\phi}{\partial\bar{z}}\frac{\partial\bar{z}}{\partial y} = i(\frac{\partial\phi}{\partial z} - \frac{\partial\phi}{\partial\bar{z}})$$

$$\frac{\partial^2\phi}{\partial y^2} = \frac{\partial(\frac{\partial\phi}{\partial z} - \frac{\partial\phi}{\partial\bar{z}})}{\partial\bar{z}} + \frac{\partial(\frac{\partial\phi}{\partial\bar{z}} - \frac{\partial\phi}{\partial z})}{\partial z} = -\frac{\partial^2\phi}{\partial z^2} + 2\frac{\partial^2\phi}{\partial z\partial\bar{z}} - \frac{\partial^2\phi}{\partial\bar{z}^2}$$

$$\nabla^2\phi = 4\frac{\partial^2\phi}{\partial z\partial\bar{z}}$$

$$\nabla^2\phi = 0 \to \frac{\partial^2\phi}{\partial z\partial\bar{z}} = 0$$

$$\frac{\partial\phi}{\partial z} = f'(z)$$

$$\phi = \int f'(z)dz$$

$$\phi = f(z) + g(\bar{z})$$

References

[1] G.B. Arfken, H.J. Weber, and F.E. Harris. *Mathematical Methods for Physicists: A Comprehensive Guide*. Elsevier Science, 2013.

[2] M.H. El-Deeb. PEU-455 Assignments.