

PEU 455 Assignment 2

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Contents

| | | |
|---|-------|----|
| 1 | 8.4.1 | 1 |
| 2 | P2 | 4 |
| 3 | P3 | 8 |
| 4 | P4 | 10 |

1 8.4.1

(a)

$$\begin{aligned}\psi &= 2\alpha^{\frac{3}{2}}x e^{-\alpha x} \\ \int_0^\infty \psi \psi^* dx \\ &= 4\alpha^3 \int_0^\infty x^2 e^{-2\alpha x} dx \\ &\quad \begin{bmatrix} x^2 & e^{-2\alpha x} \\ 2x & \frac{1}{-2\alpha} e^{-2\alpha x} \\ 2 & \frac{1}{4\alpha^2} e^{-2\alpha x} \\ 0 & \frac{1}{-8\alpha^3} e^{-2\alpha x} \end{bmatrix} \\ &= 4\alpha^3 \left[-\frac{x^2}{2\alpha} e^{-2\alpha x} - \frac{x}{2\alpha^2} e^{-2\alpha x} - \frac{1}{4\alpha^3} e^{-2\alpha x} \right]_0^\infty = 1\end{aligned}$$

ψ is normalized.

(b)

$$\begin{aligned}
& \int_0^\infty \psi x^{-1} \psi * dx \\
&= 4\alpha^3 \int_0^\infty x e^{-2\alpha x} \\
&= 4\alpha^3 \int_0^\infty x e^{-2\alpha x} \\
& \quad \begin{bmatrix} x & e^{-2\alpha x} \\ 1 & \frac{1}{-2\alpha} e^{-2\alpha x} \\ 0 & \frac{1}{4\alpha^2} e^{-2\alpha x} \end{bmatrix} \\
& 4\alpha^3 \left[x \frac{1}{-2\alpha} e^{-2\alpha x} - \frac{1}{4\alpha^2} e^{-2\alpha x} \right]_0^\infty = \alpha
\end{aligned}$$

(c)

$$\begin{aligned}
\frac{d\psi}{dx} &= 2\alpha^{\frac{3}{2}} \frac{d(xe^{-\alpha x})}{dx} = 2\alpha^{\frac{3}{2}} e^{-\alpha x} (1 - \alpha x) \\
\frac{d^2\psi}{dx^2} &= 2\alpha^{\frac{3}{2}} \frac{d(e^{-\alpha x}(1 - \alpha x))}{dx} = -2\alpha^{\frac{3}{2}} (\alpha e^{-\alpha x} + \alpha e^{-\alpha x}(1 - \alpha x)) \\
&= -2\alpha^{\frac{5}{2}} e^{-\alpha x} (2 - \alpha x) \\
& \int_0^\infty \psi * \frac{d^2\psi}{dx^2} dx \\
& -4\alpha^4 \int_0^\infty x e^{-2\alpha x} (2 - \alpha x) dx \\
& -8\alpha^4 \int_0^\infty x e^{-2\alpha x} dx + 4\alpha^5 \int_0^\infty x^2 e^{-2\alpha x} dx \\
& \int_0^\infty x e^{-2\alpha x} dx = \frac{1}{4\alpha^2}, \quad \int_0^\infty x^2 e^{-2\alpha x} dx = \frac{1}{4\alpha^3} \\
& = -\alpha^2
\end{aligned}$$

(d)

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

$$\begin{aligned}
&= -(\frac{1}{2} \left\langle \psi \left| \frac{d^2}{dx^2} \right| \psi \right\rangle + \langle \psi | x^{-1} | \psi \rangle) \\
&= \frac{\alpha^2}{2} - \alpha \\
&\frac{d(\frac{\alpha^2}{2} - \alpha)}{d\alpha} = 0 \\
&\alpha = 1 \\
\min(\left\langle \psi \left| -\frac{1}{2} \frac{d^2}{dx^2} - \frac{1}{x} \right| \psi \right\rangle) &= -\frac{1}{2}
\end{aligned}$$

2 P2

Let $\psi_{\text{trial}} = \psi_0(\beta)$ where ψ_0 is the old ground state of hydrogen atom.

Where we will vary $a_0 \rightarrow \frac{a_0}{\beta}$.

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

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

For a non-varying function in θ and ϕ

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

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

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

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

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

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

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

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

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

$$\therefore \frac{e^2}{\pi \epsilon_0} = \frac{4\hbar^2}{m a_0}$$

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

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

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

Using mathematica we get one real solution and two imaginaries:

The real solution:

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

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

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

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,

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

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

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

$$\begin{aligned}
df &= \frac{du + dv}{2} \left(\frac{\partial f}{\partial u} + \frac{\partial f}{\partial v} \right) + \frac{du - dv}{2} \left(\frac{\partial f}{\partial u} - \frac{\partial f}{\partial v} \right) \\
&= du \frac{\partial f}{\partial u} + dv \frac{\partial f}{\partial v}
\end{aligned}$$

(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

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

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

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

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

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

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

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

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

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

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

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](#).