Tutorial 5: Solutions

1. Electric field in infinite square well

$$\psi_n^{(0)}(x) = \sqrt{\frac{2}{a}}\sin\left(\frac{n\pi x}{a}\right) \quad 0 \le x \le a$$

(a)

$$\begin{aligned}
\tilde{V} &= -eE\left(x - \frac{a}{2}\right) \\
E_n^{(1)} &= \langle n|\tilde{V}|n\rangle \\
&= \frac{2}{a}\int_0^a (-eE)\left(x - \frac{a}{2}\right)\sin^2\left(\frac{n\pi x}{a}\right)dx \\
f(x) &= \sin^2\left(\frac{n\pi x}{a}\right)\ ,\ 0 \le x \le a \\
&\quad \text{is even about } x = \frac{a}{2} \ \text{ for all } n \\
g(x) &= \left(x - \frac{a}{2}\right) \text{ is odd about } x = \frac{a}{2}
\end{aligned}$$

Thus $f(x)g(x)$ is odd about $x = \frac{a}{2}$ and

$$\begin{aligned}
\int_0^a f(x)g(x)dx = 0 \\
\Rightarrow E_n^{(1)} = 0 \ \text{ for all } n.
\end{aligned}$$

(Comment: In the above, it is important to mention that the functions are odd/even about $x = \frac{a}{2}$. Note that we are integrating only from $x = 0$ to $x = a$.)

(b)

$$\begin{aligned}
V &= -eEx \\
E_n^{(1)} &= \langle n|V|n\rangle \\
&= \langle n|\tilde{V}|n\rangle - \frac{1}{2}aeE\langle n|n\rangle \\
&= -\frac{1}{2}aeE \ \text{ for all } n.
\end{aligned}$$

2. Feynman-Hellmann theorem

$$E_n(\lambda) = \langle \psi_n(\lambda)|H(\lambda)|\psi_n(\lambda)\rangle$$

(a)

$$\begin{aligned}
\frac{\partial E_n(\lambda)}{\partial \lambda} &= \langle \frac{\partial \psi_n(\lambda)}{\partial \lambda}|H(\lambda)|\psi_n(\lambda)\rangle \\
&\quad + \langle \psi_n(\lambda)|\frac{\partial H(\lambda)}{\partial \lambda}|\psi_n(\lambda)\rangle \\
&\quad + \langle \psi_n(\lambda)|H(\lambda)|\frac{\partial \psi_n(\lambda)}{\partial \lambda}\rangle \\
&= E_n(\lambda)\Big(\langle \frac{\partial \psi_n}{\partial \lambda}|\psi_n\rangle + \langle \psi_n|\frac{\partial \psi_n}{\partial \lambda}\rangle\Big) + \langle \psi_n(\lambda)|\frac{\partial H(\lambda)}{\partial \lambda}|\psi_n(\lambda)\rangle \\
&= E_n(\lambda)\Big(\frac{\partial}{\partial \lambda}\langle \psi_n|\psi_n\rangle\Big) + \langle \psi_n(\lambda)|\frac{\partial H(\lambda)}{\partial \lambda}|\psi_n(\lambda)\rangle \\
&= \langle \psi_n(\lambda)|\frac{\partial H(\lambda)}{\partial \lambda}|\psi_n(\lambda)\rangle \qquad (1)
\end{aligned}$$

where $\frac{\partial}{\partial \lambda}\langle \psi_n|\psi_n\rangle = 0$ because $\langle \psi_n|\psi_n\rangle = 1$ for all λ.

(b)

$$\begin{aligned}
H &= H_0 + \lambda V \\
E_n(\lambda) &= E_n(0) + \lambda \frac{\partial E_n(\lambda)}{\partial \lambda}\Big|_{\lambda=0} + O(\lambda^2) \\
\frac{\partial E_n(\lambda)}{\partial \lambda}\Big|_{\lambda=0} &= \langle \psi_n(\lambda)|\frac{\partial H(\lambda)}{\partial \lambda}|\psi_n(\lambda)\rangle\Big|_{\lambda=0} \text{ from the Feynman} - \text{Hellmann theorem} \\
&= \langle \psi_n(0)|V|\psi_n(0)\rangle \text{ as in perturbation theory.}
\end{aligned}$$

(c)

$$\begin{aligned}
H &= -\frac{\hbar^2}{2m_e}\frac{d^2}{dr^2} + \frac{\hbar^2}{2m_e}\frac{\ell(\ell+1)}{r^2} - \frac{e^2}{4\pi\epsilon_0}\frac{1}{r} \quad \text{(SI units)} \\
E_n &= -\frac{m_e e^4}{32\pi^2\epsilon_0^2\hbar^2(j_{max}+\ell+1)^2}
\end{aligned}$$

Using $\lambda = e$,

$$\text{LHS of (1)}: \ \frac{\partial E_n}{\partial \lambda} = -\frac{4m_e e^3}{32\pi^2\epsilon_0^2\hbar^2(j_{max}+\ell+1)^2}$$

For RHS of (1):

$$\begin{aligned}
\frac{\partial H}{\partial \lambda} &= -\frac{2e}{4\pi\epsilon_0}\frac{1}{r} \\
\langle n\ell m|\frac{\partial H}{\partial \lambda}|n\ell m\rangle &= -\frac{2e}{4\pi\epsilon_0}\left\langle\frac{1}{r}\right\rangle \\
\therefore \left\langle\frac{1}{r}\right\rangle &= \frac{4\pi\epsilon_0}{2e}\frac{4m_e e^3}{32\pi^2\epsilon_0^2\hbar^2 n^2}\ , \ n = j_{max}+\ell+1 \\
&= \frac{m_e e^2}{4\pi\epsilon_0\hbar^2}\frac{1}{n^2} \\
&= \frac{1}{a_0 n^2}
\end{aligned}$$

(d) Using $\lambda = \ell$, and $E_n = -\frac{\hbar^2}{2m_e a_0^2}\frac{1}{n^2}$, $n = j_{max}+\ell+1$,

$$\begin{aligned}
&\text{LHS of (1)}: \ \frac{\partial E_n}{\partial \lambda} = \frac{\hbar^2}{m_e a_0^2}\frac{1}{n^3} \\
&\text{RHS of (1)}: \langle n\ell m|\frac{\partial H}{\partial \lambda}|n\ell m\rangle = \frac{\hbar^2}{2m_e}(2\ell+1)\left\langle\frac{1}{r^2}\right\rangle \\
&\Rightarrow \left\langle\frac{1}{r^2}\right\rangle = \frac{1}{(\ell+1/2)a_0^2 n^3}
\end{aligned}$$