# PHY 472 - 2020

# Problem Set 10

1. The Hamiltonian is $H = -\frac{\hbar^2}{2m}\nabla^2 - \frac{e^2}{4\pi\varepsilon_0 r}$

It is spherically symmetric, and in the ground state the wave function should be maximally symmetric.

Choose $\Psi = Ce^{-\alpha r}$; Normalization:

$$\int |\Psi|^2 d\vec{r} = |C|^2 \int e^{-2\alpha r} r^2 dr\, d\Omega = 4\pi |C|^2 \cdot \frac{2}{(2\alpha)^3} = \frac{\pi |C|^2}{\alpha^3},$$

$$|C|^2 = \alpha^3/\pi$$

Since the wave function is independent of $\theta$ and $\varphi$, we can use only the radial part of the Laplacian when calculating the kinetic energy

$$\langle T\rangle = -\frac{\hbar^2}{2m}\int d\vec{r}\, \Psi(\vec{r})\nabla^2\Psi(\vec{r}) = -\frac{\hbar^2}{2m}\int r^2 dr\, d\Omega\, |C^2| e^{-\alpha r}$$

$$\times \frac{1}{r^2}\frac{d}{dr} r^2 \frac{d}{dr} e^{-\alpha r}$$

$$= -\frac{2\pi\hbar^2}{m}|C|^2 \int_0^\infty dr\, e^{-\alpha r}\frac{d}{dr} r^2(-\alpha e^{-\alpha r}) = -\frac{2\pi\hbar^2}{m}|C|^2\int_0^\infty dr\, e^{-\alpha r}(\alpha^2 r^2 - 2\alpha r)e^{-\alpha r}$$

$$= -\frac{2\pi\hbar^2}{m}|C|^2\left(\frac{2\alpha^2}{(2\alpha)^3} - \frac{2\alpha}{(2\alpha)^2}\right) = \frac{\pi\hbar^2}{m}|C|^2\frac{1}{2\alpha}$$

The potential energy is

$$\langle U\rangle = -\frac{e^2}{4\pi\varepsilon_0}|C|^2 \cdot 4\pi\int_0^\infty \frac{r^2 dr}{r} e^{-2\alpha r} = -\frac{e^2}{4\pi\varepsilon_0}\frac{\pi |C|^2}{\alpha^2}$$

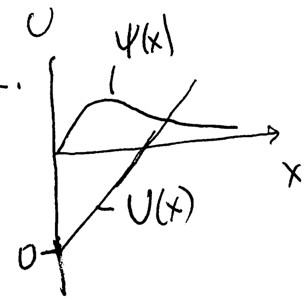
$$\langle E\rangle = \frac{\hbar^2}{2m}\alpha^2 - \frac{e^2}{4\pi\varepsilon_0}\alpha; \quad \frac{d\langle E\rangle}{d\alpha} = 0 \Rightarrow \alpha = \frac{1}{a} = \frac{me^2}{\hbar^2 \cdot 4\pi\varepsilon_0}$$

We took the right function and got the right answer,

$$\langle E\rangle = -\frac{\hbar^2}{2ma^2} = -\left(\frac{e^2}{4\pi\varepsilon_0}\right)^2\frac{m}{2\hbar^2}$$

PHY 472 - 2020

Problem Set 10

2. 

The wave function must be zero for $x=0$ from continuity. Then seek

$$\psi(x) = C x e^{-\alpha x}, \quad \int \psi^2(x)dx = C^2 \int x^2 e^{-2\alpha x} dx$$

$$= \frac{2C^2}{(2\alpha)^3} = \frac{C^2}{4\alpha^3} = 1 \Rightarrow C = 2\alpha^{3/2}.$$

Potential energy

$$\langle U \rangle = A \int_0^\infty x\, \psi^2(x)dx = A C^2 \int_0^\infty x^3 e^{-2\alpha x} dx = \frac{6AC^2}{(2\alpha)^4} = \frac{3A}{2\alpha}$$

Kinetic energy:

$$-\frac{\hbar^2}{2m}\int_0^\infty dx\, \psi(x)\left(-\frac{d^2\psi}{dx^2}\right) = \frac{\hbar^2}{2m}\int_0^\infty dx \left(\frac{d\psi}{dx}\right)^2 = \frac{\hbar^2}{2m} C^2 \int_0^\infty dx\, e^{-2\alpha x}(1-\alpha x)^2$$

$$= \frac{\hbar^2}{2m} C^2 \left[\frac{1}{2\alpha} - \frac{2\alpha}{(2\alpha)^2} + \frac{2\alpha^2}{(2\alpha)^3}\right] = \frac{\hbar^2}{2m}\frac{C^2}{4\alpha} = \frac{\hbar^2\alpha^2}{2m}$$

$$\langle E \rangle = \frac{\hbar^2\alpha^2}{2m} + \frac{3A}{2\alpha}; \quad \frac{d\langle E \rangle}{d\alpha} = 0 \Rightarrow \alpha = \left(\frac{3Am}{2\hbar^2}\right)^{1/3}$$

$$\langle E \rangle = \frac{3}{2}\left(\frac{3A\hbar}{2}\right)^{2/3}\frac{1}{m^{1/3}}$$

PHY 472 - 2020

Problem Set 10

3. This is the problem of a turned-on perturbation. We have the transition frequency $\omega_{\uparrow\downarrow} = \frac{E_\uparrow - E_\downarrow}{\hbar} = \omega$.

$$P_\uparrow(t) = \frac{|V_{\uparrow\downarrow}|^2}{\hbar^2 \omega_{\uparrow\downarrow}^2} 4 \sin^2 \frac{\omega_{\uparrow\downarrow} t}{2} \; ; \qquad V_{\uparrow\downarrow} = \langle \uparrow | \tfrac{1}{2}\sigma_x V | \downarrow \rangle = \tfrac{1}{2} V$$

$$P_\uparrow(t) = \frac{|V|^2}{\hbar^2 \omega^2} \sin^2 \frac{\omega t}{2}$$

# PHY 472- 2020
# Problem Set 10

4. You are expected to consider the theory, not to solve a problem. Choose the wave function in the form

$$\psi(t) = a(t)\chi_+ e^{-i\omega t/2} + b(t)\chi_- e^{i\omega t/2}$$

Take into account that $\sigma_z \psi(t) = a(t)\chi_+ e^{-i\omega t/2} - b(t)\chi_- e^{i\omega t/2}$

and $\sigma_x \psi(t) = a(t)\chi_- e^{-i\omega t/2} + b(t)\chi_+ e^{i\omega t/2}$,

Substitute into the Schrödinger equation $i\hbar\dot{\psi} = H\psi$, multiply from the left by $\langle\chi_+|$ and then $\langle\chi_-|$ to obtain:

$$i\hbar\dot{a} = \frac{1}{2} V b \cos\omega t\, e^{i\omega t}, \qquad i\hbar\dot{b} = \frac{1}{2} V a \cos\omega t\, e^{-i\omega t}$$

Interestingly, $\cos\omega t\, e^{\pm i\omega t} = \frac{1}{2} + \frac{1}{2} e^{\pm 2i\omega t}$ ← fast oscillating

↑ this accumulates in time

In contrast to the perturbation theory we studied before, there are time-independent coefficients in the right-hand sides $\Rightarrow$ the perturbation theory breaks down for $|V|t/\hbar \gtrsim 1$.

To see this we take $a(0)=0$, $b(0)=1$. Then by perturbation theory

$$a(t) = \frac{1}{4}\frac{V}{i\hbar}t - \frac{1}{8\hbar\omega}V\left[e^{2i\omega t} - 1\right],$$

$|a(t)| \sim 1$ for $|Vt/\hbar| \sim 1$, but this simple perturbation theory assumes that $|a(t)| \ll 1$

PHY 472 - 2020

Problem Set 10

5. We sought $\psi(t) = a(t)\chi_+ e^{-i\omega t/2} + b(t)\chi_- e^{i\omega t/2}$

and obtained equations

$$i\hbar\dot{a} = \frac{1}{4}Vb\left(1+e^{2i\omega t}\right), \quad i\hbar\dot{b} = \frac{1}{4}Va\left(1+e^{-2i\omega t}\right)$$

The "dangerous" terms are the ones that do not oscillate.

If we keep these terms, we obtain

$$i\hbar\dot{a} \approx \frac{1}{4}Vb, \quad i\hbar\dot{b} = \frac{1}{4}Va$$

or $\ddot{a} = -\frac{i}{4}\frac{V}{\hbar}\dot{b} = -\left(\frac{V}{4\hbar}\right)^2 a \,;\quad a(t) = A_0\cos\left(\frac{V}{4\hbar}t+\varphi_0\right)$

$$b(t) = \frac{4i\hbar}{V}\dot{a} = -iA_0\sin\left(\frac{V}{4\hbar}t+\varphi_0\right)$$

Since $|a|^2+|b|^2=1$, we have $A_0=1$, or more generally, $A_0 = e^{i\alpha}$ with an arbitrary real $\alpha$.

As you see, the state populations $|a(t)|^2$ and $|b(t)|^2$ oscillate in time. This will be discussed in class