

## Atomic units

	conventional basic dimensions (mass, length, time)	unconventional basic dimensions (mass, length, energy = $ML^2/T^2$ )
$\hbar$	$[ML^2/T]$	$[M^{1/2}LE^{1/2}]$
$m$	$[M]$	$[M]$
$e^2/4\pi\epsilon_0$	$[ML^3/T^2]$	$[LE]$

### a. Characteristic energy:

Using unconventional basic dimensions, first combine quantities  $\hbar$  and  $e^2/4\pi\epsilon_0$  to get rid of [L]. (This is the *only* way to cancel out the [L]s.) This division results in

$$\text{quantity } \frac{\hbar}{e^2/4\pi\epsilon_0} \text{ with dimensions } [M^{1/2}/E^{1/2}].$$

Square both sides to get

$$\text{quantity } \frac{\hbar^2}{(e^2/4\pi\epsilon_0)^2} \text{ with dimensions } [M/E].$$

Invert and multiply by  $m$  (the *only* way to get rid of the [M]s) to find the *only* characteristic energy,

$$\text{quantity } \frac{m(e^2/4\pi\epsilon_0)^2}{\hbar^2} \text{ with dimensions } [E].$$

This energy is equal to two Rydberg units (2 Ry).

### b. Characteristic time:

Using conventional basic dimensions, first combine quantities  $\hbar$  and  $e^2/4\pi\epsilon_0$  to get rid of [L]:

$$\text{quantity } \frac{\hbar^3}{(e^2/4\pi\epsilon_0)^2} \text{ with dimensions } \frac{[M^3L^6/T^3]}{[M^2L^6/T^4]} = [MT].$$

Divide by  $m$  to get the only quantity with the dimensions of time:

$$\frac{\hbar^3}{m(e^2/4\pi\epsilon_0)^2} \equiv \tau_0.$$

I remember this as

$$\tau_0 = \frac{\hbar}{2\text{Ry}} = 2.4 \times 10^{-17} \text{ sec} = 0.024 \text{ fsec}.$$

### c. Bonus — Bohr model:

For classical circular orbits,

$$\frac{mv^2}{r} = \frac{1}{4\pi\epsilon_0} \frac{e^2}{r^2}.$$

To this Bohr adds the quantization condition for angular momentum, namely that for the  $n$ th Bohr orbit,

$$n\hbar = mv_n r_n.$$

Thus the radius of the  $n$ th Bohr orbit comes through

$$\frac{m}{r_n} v_n^2 = \frac{m}{r_n} \left( \frac{n\hbar}{mr_n} \right)^2 = \frac{1}{4\pi\epsilon_0} \frac{e^2}{r_n^2}$$

or

$$\frac{n^2 \hbar^2}{mr_n} = e^2 / 4\pi\epsilon_0$$

whence

$$r_n = n^2 \frac{\hbar^2}{m(e^2/4\pi\epsilon_0)} \equiv n^2 a_0.$$

Then the period of the  $n$ th Bohr orbit is

$$\begin{aligned} \text{period}_n &= \frac{\text{circumference}_n}{v_n} \\ &= \frac{2\pi r_n}{n\hbar/mr_n} \\ &= \frac{2\pi m r_n^2}{n\hbar} \\ &= \frac{2\pi m n^4 a_0^2}{n\hbar} \\ &= n^3 \frac{2\pi m a_0^2}{\hbar} \\ &= 2\pi n^3 \frac{m}{\hbar} \frac{\hbar^4}{m^2 (e^2/4\pi\epsilon_0)^2} \\ &= 2\pi n^3 \frac{\hbar^3}{m (e^2/4\pi\epsilon_0)^2} \\ &= 2\pi n^3 \tau_0 \end{aligned}$$

**d. Heartbeats to orbits:**

The average person lives about 80 years. The average heartbeat lasts about one second. The number of seconds in a year is surprisingly close to  $\pi \times 10^7$ . Thus the average heart beats about  $3 \times 10^9$  times. (This three billion beats represents spectacular performance: the fuel pump in a car can't do nearly as well.)

How long does it take an innermost electron to execute one Bohr orbit?

The orbital time is  $2\pi\tau_0$  or about  $1.5 \times 10^{-16}$  sec.

How long does it take this electron to execute three billion orbits (a "lifetime's worth")?

About  $5 \times 10^{-7}$  sec.

So how many "atom lifetimes" pass in one second?

About  $1/(5 \times 10^{-7})$  or two million.

**e. The time-dependent Schrödinger equation in scaled variables:**

For any function  $f(x)$  we have

$$\begin{aligned} \frac{\partial f(x)}{\partial x} &= \frac{\partial f(\tilde{x})}{\partial \tilde{x}} \frac{\partial \tilde{x}}{\partial x} = \frac{\partial f(\tilde{x})}{\partial \tilde{x}} \frac{1}{a_0} \\ \frac{\partial^2 f(x)}{\partial x^2} &= \frac{\partial}{\partial \tilde{x}} \left[ \frac{\partial f(\tilde{x})}{\partial \tilde{x}} \frac{1}{a_0} \right] \frac{\partial \tilde{x}}{\partial x} = \frac{\partial^2 f(\tilde{x})}{\partial \tilde{x}^2} \frac{1}{a_0^2}. \end{aligned}$$

Apply this to the time-dependent Schrödinger equation:

$$\begin{aligned}
 i\hbar \frac{\partial \Psi}{\partial t} &= -\frac{\hbar^2}{2m} \nabla^2 \Psi - \frac{e^2}{4\pi\epsilon_0} \frac{1}{r} \Psi \\
 i\hbar \frac{1}{\tau_0} \frac{\partial \Psi}{\partial \tilde{t}} &= -\frac{\hbar^2}{2m} \frac{1}{a_0^2} \tilde{\nabla}^2 \Psi - \frac{e^2}{4\pi\epsilon_0} \frac{1}{a_0 \tilde{r}} \Psi \\
 i \frac{\partial \Psi}{\partial \tilde{t}} &= -\frac{1}{2} \left[ \frac{\hbar}{m} \frac{\tau_0}{a_0^2} \right] \tilde{\nabla}^2 \Psi - \left[ \frac{\tau_0}{\hbar} \frac{e^2}{4\pi\epsilon_0} \frac{1}{a_0} \right] \frac{1}{\tilde{r}} \Psi.
 \end{aligned}$$

However, quick perusal of the definitions of  $a_0$  and  $\tau_0$  will convince you that both of the expressions in square brackets are equal to 1! Thus

$$i \frac{\partial \Psi}{\partial \tilde{t}} = -\frac{1}{2} \tilde{\nabla}^2 \Psi - \frac{1}{\tilde{r}} \Psi.$$

Multiply both sides by  $a_0^{3/2}$ , because  $\tilde{\Psi} = a_0^{3/2} \Psi$ , to get

$$i \frac{\partial \tilde{\Psi}}{\partial \tilde{t}} = -\frac{1}{2} \tilde{\nabla}^2 \tilde{\Psi} - \frac{1}{\tilde{r}} \tilde{\Psi}.$$

*Grading:*

- 2 points for part **a**
- 2 points for part **b**
- 2 points extra for part **c**
- 3 points for part **d**
- 3 points for part **e**