Think of coordinate rescaling

$$\vec{x} = \alpha\vec{\mu}$$

$$\vec{x} = (x_1, x_2, x_3) \quad , \quad \vec{\mu} = (\mu_1, \mu_2, \mu_3)$$

$$\vec{\nabla}_x^2 = \frac{\partial}{\partial x_1^2} + \frac{\partial}{\partial x_2^2} + \frac{\partial}{\partial x_3^2} \quad , \vec{\nabla}_\mu^2 = \frac{\partial}{\partial \mu_1^2} + \frac{\partial}{\partial \mu_2^2} + \frac{\partial}{\partial \mu_3^2} = \alpha^2 \left(\frac{\partial}{\partial x_1^2} + \frac{\partial}{\partial x_2^2} + \frac{\partial}{\partial x_3^2} \right)$$

$$\vec{x} = \alpha\vec{\mu} \quad , \quad \partial_x^2 = \frac{\partial^2}{\partial \vec{x}^2} = \frac{1}{\alpha^2}\partial_\mu^2 = \frac{1}{\alpha^2}\frac{\partial^2}{\partial \vec{\mu}^2}$$

For example, the Schrodinger of H atom

$$\left(-\frac{\hbar^2}{2m}\nabla^2-\frac{e^2}{r}\right)\psi_n(\vec{r})=\varepsilon_n\psi_n(\vec{r})$$

Introduce a dimension-less length $\vec{y}$

$\vec{r}=\alpha\vec{y}$ and then we have $\dfrac{\partial}{\partial\vec{r}}=\dfrac{1}{\alpha}\dfrac{\partial}{\partial\vec{y}}$, $\vec{\nabla}^2=\dfrac{\partial^2}{\partial\vec{r}^2}=\dfrac{1}{\alpha^2}\dfrac{\partial^2}{\partial\vec{y}^2}$

$$\left(-\frac{\hbar^2}{2m}\frac{1}{\alpha^2}\nabla_y^2 - \frac{e^2}{\alpha y}\right)\psi_n(\alpha\vec{y}) = \varepsilon_n\psi_n(\alpha\vec{y})$$

$$\left(-\frac{1}{2}\nabla_y^2 - \left(\frac{m}{\hbar^2}\alpha e^2\right)\frac{1}{y}\right)\varphi_n(\vec{y}) = \frac{\varepsilon_n}{\left(\frac{\hbar^2}{m\alpha^2}\right)}\varphi_n(\vec{y})$$

Let us take $\alpha = \frac{\hbar^2}{me^2} = a_0$: Bohr radius.

And then we have $\frac{\hbar^2}{m\alpha^2} = \frac{me^4}{\hbar^2} = \frac{e^2}{a_0} = H_a$

Now we have the equation in dimension-less number

$$\left(-\frac{1}{2}\nabla^2 - \frac{1}{y}\right)\psi_n(\vec{y}) = E_n\psi_n(\vec{y})$$

- In this equation, the length is in the unit of a_0.
- Note that $a_0 = 0.52946541$Å.
- The energy is in unit of H_a. Note that $H_a = 4.35974e^{-18}$ Joule.
- Note that $Ry = \frac{e^2}{2a_0} = \frac{1}{2}H_a = 13.6eV$

Atomic-Hatree systems of unit

The equation, Kohn-Sham DFT equation

$$\left(-\frac{\hbar^2}{2m}\nabla^2 + U_{atom}(\vec{r}) + \int \frac{e^2\rho\left(\vec{r}'\right)}{\left|\vec{r}-\vec{r}'\right|} d^3\vec{r}' + v_{xc}[\rho(\vec{r})]\right)\psi_n(\vec{r}) = \varepsilon_n \psi_n(\vec{r})$$

By setting $m = 1, e = 1, \hbar = 1$, we have the atomic-Hatree systems of unit.

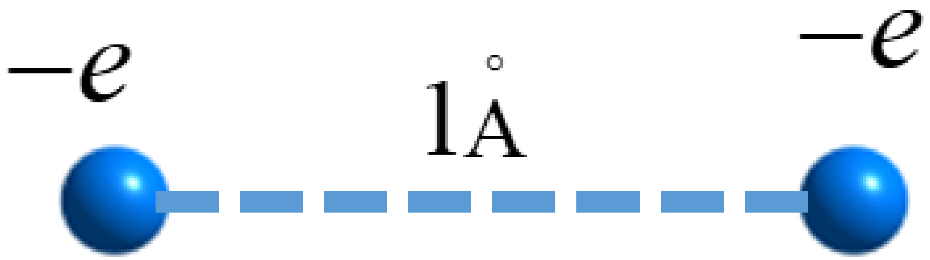
$$a_0 = \frac{\hbar^2}{me^2} = 1,\ \ R = \frac{e^2}{2a_0} = \frac{me^4}{2\hbar^2} = \frac{1}{2},\ \ H_a = \frac{e^2}{a_0} = \frac{me^4}{\hbar^2} = 1$$

[Example] Atomic-Hatree systems of unit

Calculate the potential energy between two point charges with the charge $-e$, separated by 1 Å

$$\text{Distance} = (1 \text{ angstrom}) = 1/0.529$$

$$E = \frac{q_1 q_2}{r} = \frac{1}{(1/0.529)} = 0.529$$



[Example] Atomic-Hatree systems of unit

Calculate the potential energy between two point charges with the charge $-e$, separated by 1 Å

Calculate the potential energy between two point charges with the charge $-e$, separated by 1 Å

$$E = \frac{1}{4\pi\varepsilon_0}\frac{q_1 q_2}{r} = 8.998\times 10^9 [\frac{Nm^2}{C^2}]\times\frac{(1.6\times 10^{-19})^2[C]^2}{10^{-10}[m]} \simeq 2.3035\times 10^{-18}[J]$$

$$0.529[H_a] = 2.3035\times 10^{-18}[J] \ , \ 1[H_a] \simeq 4.3544\times 10^{-18}[J]$$

Atomic-Hatree systems of unit

The equation, Kohn-Sham DFT equation

$$\left(-\frac{1}{2}\nabla^2 + U_{atom}(\vec{r}) + \int \frac{\rho(\vec{r}')}{|\vec{r}-\vec{r}'|} d^3\vec{r}' + v_{xc}[\rho(\vec{r})]\right)\psi_n(\vec{r}) = \varepsilon_n \psi_n(\vec{r})$$

By setting $m = 1, e = 1, \hbar = 1$, we have the atomic-Hatree systems of unit.

Atomic-Rydberg systems of unit

1. Atomic Rydberg systems of unit can be derived by setting

$$a_0 = \frac{\hbar^2}{me^2} = 1, \quad R = \frac{e^2}{2a_0} = \frac{me^4}{2\hbar^2} = \frac{1}{2}$$

2. In this systems of unit

$$\hbar = 1\ , \ e^2 = 2\ , \ m = \frac{1}{2}$$

3. For spin-orbit coupling or anything else, we need to have numbers for c.

$$\frac{e^2}{\hbar c} \approx \frac{1}{137} \quad , c \approx 274$$

Atomic-Rydberg systems of unit

$$\left(-\nabla^2 + U_{atom}(\vec{r}) + \int \frac{2\rho(\vec{r}')}{|\vec{r} - \vec{r}'|} d^3\vec{r}' + v_{xc}[\rho(\vec{r})] \right) \psi_n(\vec{r}) = \varepsilon_n \psi_n(\vec{r})$$

Atomic-Hatree systems of unit

1. Atomic Rydberg systems of unit can be derived by setting

$$a_0 = \frac{\hbar^2}{me^2} = 1, \quad R = \frac{e^2}{2a_0} = \frac{me^4}{2\hbar^2} = 1$$

2. In this systems of unit

$$\hbar = 1 \ , \ e^2 = 1 \ , \ m = 1$$

3. For spin-orbit coupling or anything else, we need to have numbers for c.

$$\frac{e^2}{\hbar c} \approx \frac{1}{137} \quad , c \approx 137$$