Day-1

I. Brief overview of quantum mechanics

II. Dipole approximation for light-matter interaction

III. Schrodinger equation and Dirac equation

IV. Spin-orbit coupling

Schrodinger equation for a single particle

$$i\hbar\frac{\partial\psi(\mathbf{r},t)}{\partial t}=\left[-\frac{\hbar^2}{2m}\nabla^2+V(\mathbf{r})\right]\psi(\mathbf{r},t)$$

1. The equation of motion for the matter wave for a Newtonian particle.

2. Instead of Newtonian trajectory every observable is now to be obtained from the information contained in the matter wave $\Psi(\vec{r},t)$

Newtonian

$$\frac{d}{dt}\begin{Bmatrix}\mathbf{r}(t)\\ \mathbf{p}(t)\end{Bmatrix}=\begin{Bmatrix}\dfrac{\partial H}{\partial \mathbf{p}}\\ -\dfrac{\partial H}{\partial \mathbf{p}}\end{Bmatrix}$$

Schrodinger equation for a single particle

$$i\hbar\frac{\partial\psi(\mathbf{r},t)}{\partial t}=\left[-\frac{\hbar^2}{2m}\nabla^2+V(\mathbf{r})\right]\psi(\mathbf{r},t)$$

$$V(\mathbf{r})=-\frac{e^2}{r}$$

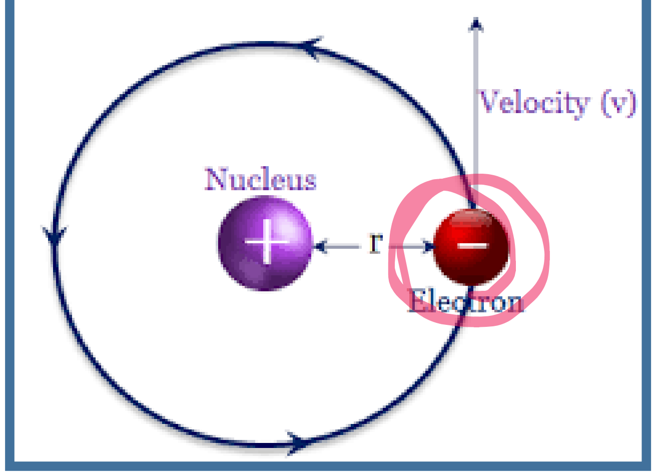
1. For the Bohr's stationary state,

$$\psi(\mathbf{r},t)=e^{-i(\text{Real Number})t}\psi(\mathbf{r})=e^{-i\frac{E}{\hbar}t}\psi(\mathbf{r})$$

2. We have time-independent eigenvalue equation

$$\left[-\frac{\hbar^2}{2m}\nabla^2+V(\mathbf{r})\right]\psi_n(\mathbf{r})=E_n\psi_n(\mathbf{r})$$

Newtonian Picture

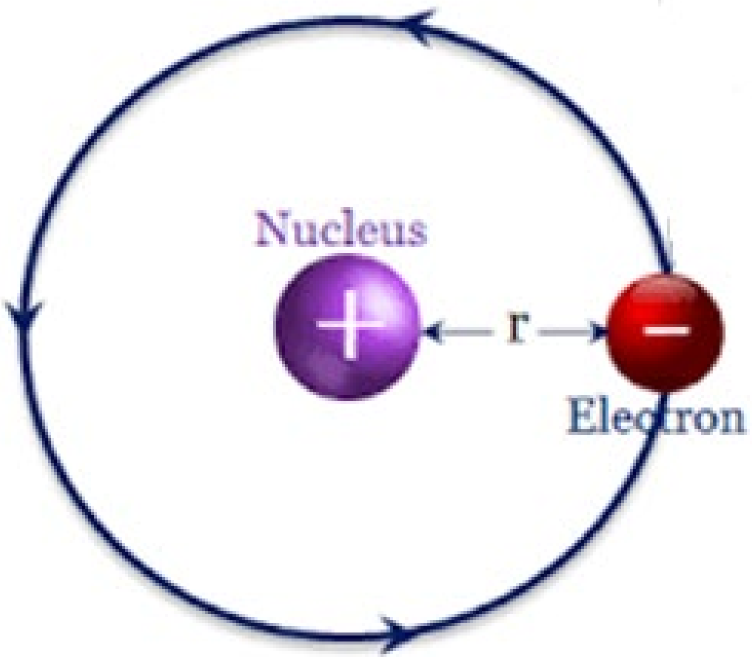


$$V(r)=-\frac{e^2}{r}$$

Schrodinger equation for a single particle

3. Rydberg series for hydrogen atom

$$E_n = -\frac{me^4}{2\hbar^2}\frac{1}{n^2} = -\frac{e^2}{2a_0} \text{, where } a_0 = \frac{\hbar^2}{me^2}$$

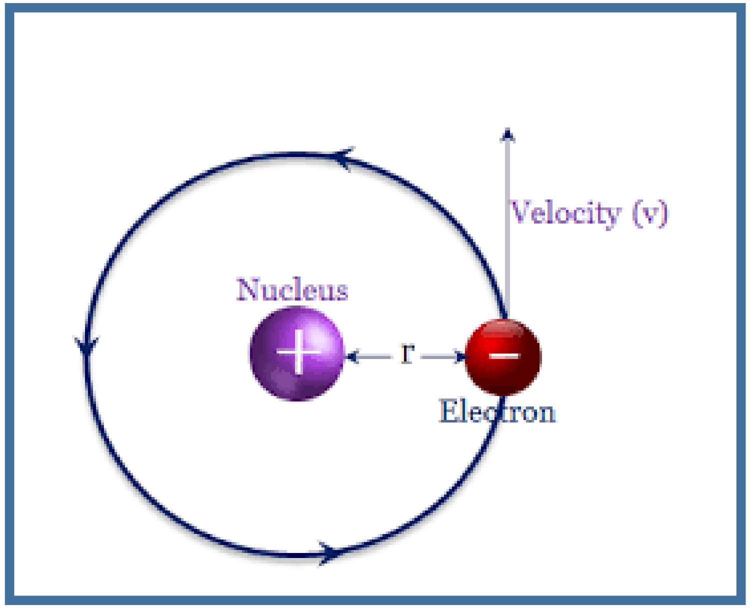


Schrodinger equation for a single particle

4. The quantities in atomic world

- Scales of quantity in atomic world
- Length : Bohr Radius $\boxed{a_0 = \frac{\hbar^2}{me^2}}$
- Energy $R = \frac{e^2}{2a_0} = \boxed{\frac{1}{2}\frac{me^4}{\hbar^2}}$ Hatree, $H_a = \frac{me^4}{\hbar^2}$
- Time $t_0 = \frac{\hbar}{\frac{e^2}{2a_0}} = \frac{2a_0\hbar}{e^2} = \boxed{\frac{2\hbar^3}{me^4}} = 1$ $\approx 48.4\,\mathrm{as}$
- 1/137 = [illegible] $\frac{1}{137} = \alpha = \frac{e^2}{\hbar c}$, $\boxed{c = \frac{e^2}{\hbar}\frac{1}{\alpha}}$

Schrodinger equation for a single particle



Potential energy

$$V(\mathbf{r}) = -\frac{e^2}{r} = -e\varphi(\mathbf{r})$$

Electrostatic potential

$$\varphi(\vec{r}) = \frac{e}{r}$$

Schrodinger equation for a particle

$$\boxed{i\hbar\frac{\partial\psi(\mathbf{r},t)}{\partial t}=\left[-\frac{\hbar^2}{2m}\nabla^2-e\varphi(\mathbf{r})\right]\psi(\mathbf{r},t)}$$

for an electron

electrostatic potential $\varphi(\vec{r})$

Maxwell's theories for E&M

1. The fields generated by the sources in the vacuum

$$\nabla \cdot \mathbf{E}(\mathbf{r},t) = 4\pi\rho(\mathbf{r}) \quad , \quad \nabla \cdot \mathbf{B}(\mathbf{r},t) = 0$$

$$\nabla \times \mathbf{B}(\mathbf{r},t) - \frac{1}{c}\frac{\partial}{\partial t}\mathbf{E}(\mathbf{r},t) = \frac{4\pi}{c}\mathbf{j}(\mathbf{r},t) \quad , \quad \nabla \times \mathbf{E}(\mathbf{r},t) + \frac{1}{c}\frac{\partial}{\partial t}\mathbf{B}(\mathbf{r},t) = 0$$

2. The potential

$$\mathbf{E}(\mathbf{r},t) = -\nabla\varphi(\mathbf{r},t) - \frac{1}{c}\frac{\partial}{\partial t}\mathbf{A}(\mathbf{r},t) \quad , \quad \mathbf{B}(\mathbf{r},t) = \nabla \times \mathbf{A}(\mathbf{r},t)$$

Maxwell’s theory for E&M

3. The potential functions are not unique➔ Gauge degree of freedom. Note that the scalar and vector potential provide the same E&M field.

$$\mathbf{A} \to \mathbf{A}' = \mathbf{A} + \nabla \lambda(\mathbf{r}, t)$$

$$\varphi \to \varphi' = \varphi - \frac{1}{c}\frac{\partial}{\partial t}\lambda(\mathbf{r}, t)$$

Example : Spatially uniform E-field

- Show that the following two sets of potential fields produces the same electric field $\vec{E}(t)$?

$$\mathbf{A}(\mathbf{r},t) = -c\int^{t} \mathbf{E}(t')dt'$$

$$\varphi(\mathbf{r},t) = 0$$

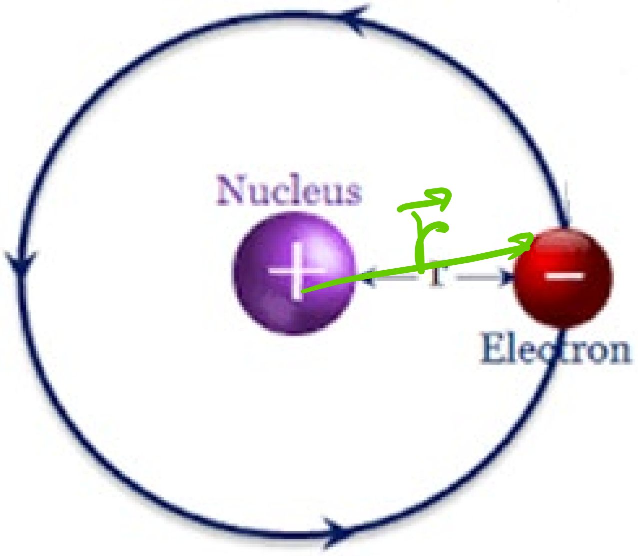
$$\mathbf{A}(\mathbf{r},t) = 0$$

$$\varphi(\mathbf{r},t) = -\mathbf{r}\cdot\mathbf{E}(t)$$

Example :

- The Schrodinger equation for the electron in H atom

$$i\hbar\frac{\partial\psi(\mathbf{r},t)}{\partial t}=\left[\frac{\hat{\mathbf{p}}^2}{2m}+(-e)\varphi(\mathbf{r})\right]\psi(\mathbf{r},t)\text{ , where }\varphi(\mathbf{r})=\frac{e}{r}.$$

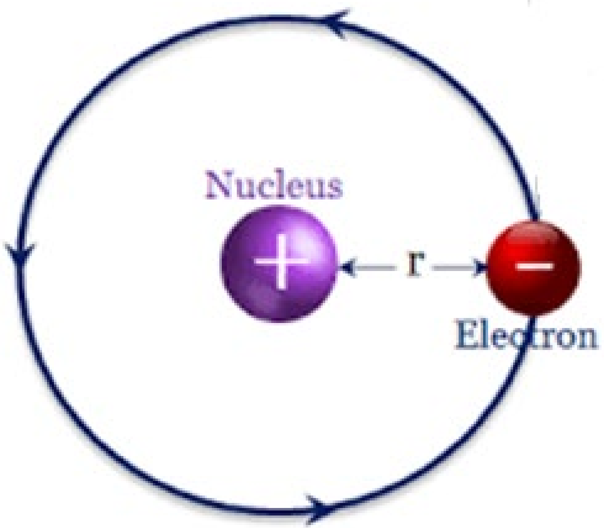


See !!! the potential is NOT unique ?

$\varphi(\vec{r})$ $\quad U=-e\varphi(\vec{r})$

Disaster !!! : the potential is NOT unique !!!

$$\vec{E} = \frac{\vec{r}}{r^3} e$$



Gauge-1

$$\mathbf{A}(\mathbf{r},t) = -ce\frac{\mathbf{r}}{r^3}t \quad , \; \varphi = 0$$

Gauge-2

$$\varphi = -\frac{e}{r} \quad , \; \mathbf{A} = 0$$

U(1) gauge symmetry

- For a particle with the charge q in a given E&M field, the Schrodinger equation must be

$$\boxed{i\hbar\frac{\partial\psi(\mathbf{r},t)}{\partial t}=\left[\frac{1}{2m}(\hat{\mathbf{p}}-\frac{q}{c}\mathbf{A})^2+q\varphi(\mathbf{r})\right]\psi(\mathbf{r},t)} \quad (O)$$

$$i\hbar\frac{\partial\psi(\mathbf{r},t)}{\partial t}=\left[\frac{1}{2m}(\hat{\mathbf{p}})^2+q\varphi(\mathbf{r})\right]\psi(\mathbf{r},t) \quad (\times)$$

Hamiltonian of a charged particle in E&M

Since classical Lagrangian (which brings Lorentz force Law) for a particle in EM field is

$$L = \frac{1}{2}mv^2 - q\phi + \frac{q}{c}\vec{A}\cdot\vec{v}$$

Canoniacal momentum of the particle is defined as

$$\vec{p} = \frac{\partial L}{\partial \dot{q}} = m\vec{v} + \frac{q}{c}\vec{A}$$

So hamiltonian is

$$H = \vec{p}v - L = \frac{\vec{p}}{m}\left(\vec{p} - \frac{q}{c}\vec{A}\right) - \frac{1}{2}mv^2 + q\phi - \frac{q}{c}\vec{A}\cdot\vec{v}$$

$$= \frac{\vec{p}}{m}\left(\vec{p} - \frac{q}{c}\vec{A}\right) - \frac{1}{2m}\left(\vec{p} - \frac{q}{c}\vec{A}\right)^2 - \frac{q}{m}\vec{A}\cdot\left(\vec{p} - \frac{q}{c}\vec{A}\right) + q\phi = \frac{1}{2m}\left(\vec{p} - \frac{q}{c}\vec{A}\right)\left(2\vec{p} - \vec{p} + \frac{q}{c}\vec{A} - 2\frac{q}{c}\vec{A}\right) + q\phi$$

$$\boxed{= \frac{1}{2m}\left(\vec{p} - \frac{q}{c}\vec{A}\right)^2 + q\phi = \frac{1}{2}mv^2 + q\phi}$$

This means that what needs for magnetic field contribution is just changing classical momentum to canonical momentum.

U(1) gauge symmetry

- Let us think of the Schrodinger equation for a particle with a charge q.
- Every physical observables are invariant over the change $\Psi \rightarrow e^{i\theta}\Psi$ for a real constant θ. This is called global phase symmetry.
- Actually, the Schrodinger field is invariant over the local phase change $\Psi \rightarrow e^{i\theta(\vec{r},t)}\Psi$, owing to the presence of gauge field.

U(1) gauge symmetry

$$\mathbf{A} \to \mathbf{A}' = \mathbf{A} + \nabla\lambda(\mathbf{r},t)$$

$$\varphi \to \varphi' = \varphi - \frac{1}{c}\frac{\partial}{\partial t}\lambda(\mathbf{r},t)$$

$$i\hbar\frac{\partial\psi(\mathbf{r},t)}{\partial t} = \left[\frac{1}{2m}\left(\hat{\mathbf{p}} - \frac{q}{c}\mathbf{A}\right)^2 + q\varphi(\mathbf{r})\right]\psi(\mathbf{r},t)$$

$$\cancel{i\hbar\frac{\partial}{\partial t}\psi = \left[\frac{p^2}{2m} + (-e)\varphi\right]\psi}$$

$$i\hbar\frac{\partial\psi'(\mathbf{r},t)}{\partial t} = \left[\frac{1}{2m}\left(\hat{\mathbf{p}} - \frac{q}{c}\mathbf{A}'\right)^2 + q\varphi'(\mathbf{r})\right]\psi'(\mathbf{r},t)$$

Show that $\psi'(\mathbf{r},t) = e^{i\frac{q\lambda(\mathbf{r},t)}{\hbar c}}\psi(\mathbf{r},t)$

Example.

➢A particle in a uniform electric field

$$\mathbf{A}(\mathbf{r},t) = -c\int^{t} \mathbf{E}(t')dt'$$

$$\varphi(\mathbf{r},t) = 0$$

$$\mathbf{A}(\mathbf{r},t) = 0$$

$$\varphi(\mathbf{r},t) = -\mathbf{r}\cdot\mathbf{E}(t)$$

➢For example, a uniform constant electric field in $\hat{z}$ direction.

$$\mathbf{A} = (0,0,-cEt)$$

$$\varphi = 0$$

$$\boxed{\mathbf{A} = (0,0,0)}$$

$$\boxed{\varphi = -Ez}$$

Maxwell's theory for E&M

4. The potential functions are not unique→ Gauge degree of freedom. Note that the scalar and vector potential provide the same E&M field.

5. Show that the coupled equation of motions for the potential fields :

axwell ⇒

$$\left(\nabla^2 - \frac{1}{c^2}\frac{\partial^2}{\partial t^2}\right)\mathbf{A} - \nabla\left(\nabla\cdot\mathbf{A} + \frac{1}{c}\frac{\partial\varphi}{\partial t}\right) = -\frac{4\pi}{c}\mathbf{j}$$

$$\nabla^2\varphi + \frac{1}{c}\frac{\partial}{\partial t}\nabla\cdot\mathbf{A} = -4\pi\rho$$

Maxwell's theory for E&M

6. In the Lorentz gauge, we choose

$$\nabla \cdot \mathbf{A} + \frac{1}{c}\frac{\partial \varphi}{\partial t} = 0$$

Now we have two un-coupled wave equations

$$\left(\nabla^2 - \frac{1}{c^2}\frac{\partial^2}{\partial t^2}\right)\mathbf{A} = -\frac{4\pi}{c}\mathbf{j}\ , \quad \left(\nabla^2 - \frac{1}{c^2}\frac{\partial^2}{\partial t^2}\right)\varphi = -4\pi\rho$$

Maxwell's theory for E&M

7. In the Coulomb gauge we choose

transverse Radiation

$$\boxed{\nabla \cdot \mathbf{A} = 0} \Rightarrow$$

And we have one wave-like equation and the Poisson's equation for the scalar field.

$$\left(\nabla^2 - \frac{1}{c^2}\frac{\partial^2}{\partial t^2}\right)\mathbf{A} = \nabla\left(\frac{1}{c}\frac{\partial \varphi}{\partial t}\right) - \frac{4\pi}{c}\mathbf{j}$$

$$\boxed{\nabla^2 \varphi = -4\pi\rho} \leftarrow \text{Poisson eq}$$

Maxwell's theory for E&M

7. The solution of the Poisson's equation

$$\nabla^2 \varphi = -4\pi\rho \quad \Leftrightarrow \quad \boxed{\varphi(\mathbf{r},t) = \int \frac{\rho(\mathbf{r}',t)}{|\mathbf{r}-\mathbf{r}'|} d^3\mathbf{r}'}$$

Can you guess why it is called Coulomb gauge ? Note that the scalar potential is just the instantaneous Coulomb potential ?

Then, it might violate the special Relativity causality condition ?

No !!!, we cannot say that way. The E&M fields to satisfy the Lorentz transformation.

The scalar potential decays as $1/r$ from the source.

Maxwell's theory for E&M

$$\varphi(\vec{r},t) = \int \frac{\rho(\vec{r}\,')}{|\vec{r}-\vec{r}\,'|} d^3\vec{r}\,'$$

$$\vec{\nabla}\bullet\vec{A} = 0,$$

$$\left(\nabla^2 - \frac{1}{c^2}\frac{\partial^2}{\partial t^2}\right)\vec{A} = 0$$

$$\vec{A}(\vec{r},t) = e^{i(\vec{k}\cdot\vec{r}-\omega t)}$$

Wave in the vacuum.

Maxwell’s theory for E&M

8. At an infinitely separated field points $r \to \infty$

$$\Phi = \int \cancel{\frac{\rho(\vec{r}\,')}{|\vec{r}-\vec{r}\,'|}} d^3\vec{r}\,' \to 0$$

$$\vec{\nabla}\bullet\vec{A} = 0, \quad \boxed{\left(\nabla^2 - \frac{1}{c^2}\frac{\partial^2}{\partial t^2}\right)\vec{A} = 0}$$

The vector potential provides propagating transverse radiation field.

The contribution of the Coulomb potential is only to the near field.

Maxwell's theory for E&M

9. Propagating transverse radiation field (light)

$$\Phi = \int \frac{\rho(\vec{r}\,')}{|\vec{r}-\vec{r}\,'|} d^3\vec{r}\,' \to 0\ ,\quad \vec{\nabla}\bullet\mathbf{A} = 0\ ,\quad \left(\nabla^2 - \frac{1}{c^2}\frac{\partial^2}{\partial t^2}\right)\mathbf{A} = 0\ ,$$

$$\mathbf{A}(\mathbf{r},t) = \sum_{\mathbf{k}}\sum_{\hat{\varepsilon}}\left(\alpha(\mathbf{k})\hat{\varepsilon}e^{i(\mathbf{k}\cdot\mathbf{r}-\omega t)} + cc\right)$$

10. It is transversely oscillating plane-waves

$$\vec{\nabla}\bullet\mathbf{A} = \sum_{\mathbf{k}}\sum_{\hat{\varepsilon}}\left(\alpha(\mathbf{k})i\mathbf{k}\cdot\hat{\varepsilon}e^{i(\mathbf{k}\cdot\mathbf{r}-\omega t)} + cc\right) = 0$$

we have $\boxed{\mathbf{k}\cdot\hat{\varepsilon} = 0}$ light polarity $\perp \vec{k}$

Light field

1. Propagating transverse radiation field (light)

$$\Phi = \int \frac{\rho(\vec{r}')}{|\vec{r}-\vec{r}'|} d^3\vec{r}' \to 0 \;, \quad \vec{\nabla}\bullet\mathbf{A} = 0 \;, \quad \left(\nabla^2 - \frac{1}{c^2}\frac{\partial^2}{\partial t^2}\right)\mathbf{A} = 0 \;,$$

$$\mathbf{A}(\mathbf{r},t) = \sum_{\mathbf{k}}\sum_{\hat{\varepsilon}}\left(\alpha(\mathbf{k})\hat{\varepsilon}e^{i(\mathbf{k}\cdot\mathbf{r}-\omega t)} + cc\right)$$

2. It is transversely oscillating plane-waves

$$\vec{\nabla}\bullet\mathbf{A} = \sum_{\mathbf{k}}\sum_{\hat{\varepsilon}}\left(\alpha(\mathbf{k})i\mathbf{k}\cdot\hat{\varepsilon}e^{i(\mathbf{k}\cdot\mathbf{r}-\omega t)} + cc\right) = 0$$

we have $\mathbf{k}\cdot\hat{\varepsilon} = 0$

Light field

3. For example, a monochromatic field

$\varphi = 0.$

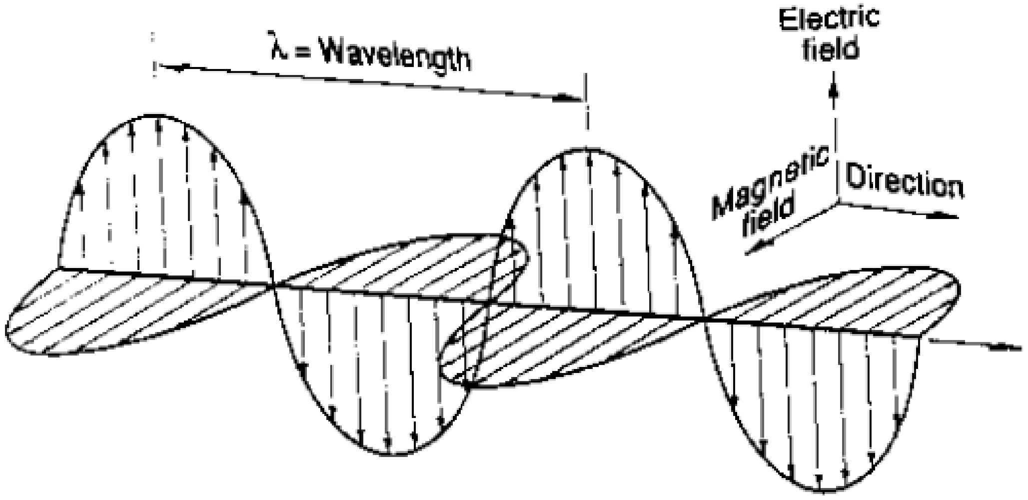
$$\vec{A} = A_0 \hat{\varepsilon} e^{i(\vec{k}\bullet\vec{r}-\omega t)} + cc. \qquad \text{Note} \quad \vec{\nabla}\bullet\vec{A} = 0, \quad \vec{k}\bullet\hat{\varepsilon} = 0$$

$$\vec{E} = -\frac{1}{c}\frac{\partial}{\partial t}\vec{A} = \frac{i\omega}{c} A_0 \hat{\varepsilon} e^{i(\vec{k}\bullet\vec{r}-\omega t)} + cc. = E_0 \hat{\varepsilon} e^{i(\vec{k}\bullet\vec{r}-\omega t)} + cc.$$

$$\vec{B} = \vec{\nabla}\times\vec{A} = -i\vec{k}\times(A_0 \hat{\varepsilon} e^{i(\vec{k}\bullet\vec{r}-\omega t)} + cc.)$$

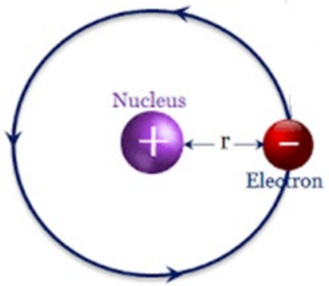
$e^{i(\vec{k}\cdot\vec{r}-\omega t)}$

$$A_0 = -i\frac{c}{\omega}E_0$$



Light-matter interaction

1. For example, a material (atom, molecule, solid) under a light field,



Material size is typically ~ 1 Angstrom

Wave length of light ~ 500 nm

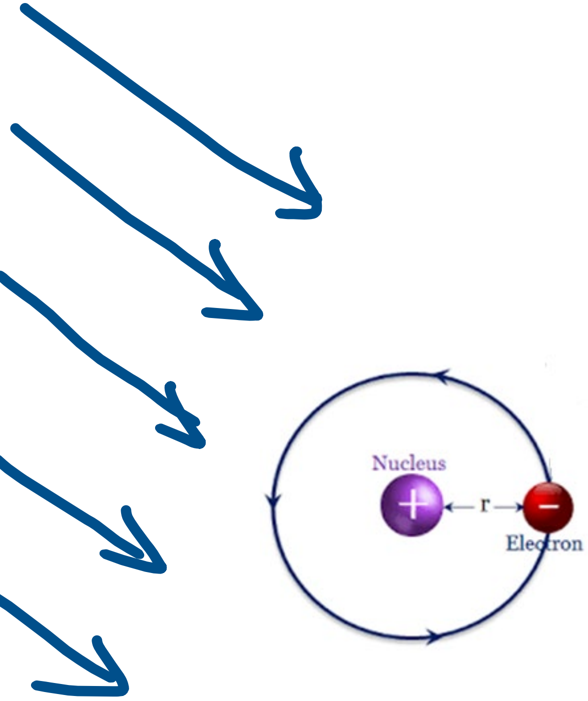
$$\vec{A} = A_0 \hat{\varepsilon} e^{i(\vec{k} \cdot \vec{r} - \omega t)} + cc. \approx \boxed{A_0 \hat{\varepsilon} e^{-i\omega t} + cc.}$$

In other word, in the long wave-length limit, the material experience the light field as a spatially uniform electric field.

Long wave length limit   Dipole Approx

Light-matter interaction

1. For example, a material (atom, molecule, solid) under a light field,



$$i\hbar\frac{\partial\psi(\mathbf{r},t)}{\partial t}=\left[\frac{1}{2m}(-i\hbar\nabla-\frac{q}{c}\mathbf{A})^2+V(\mathbf{r})\right]\psi(\mathbf{r},t)$$

$$(-i\hbar\nabla-\frac{q}{c}\mathbf{A})^2=(-i\hbar\nabla+\frac{e}{c}\mathbf{A})\cdot(-i\hbar\nabla+\frac{e}{c}\mathbf{A})^2$$

$$=-i\hbar\nabla\cdot(-i\hbar\nabla+\frac{e}{c}\mathbf{A})+\frac{e}{c}\mathbf{A}\cdot(-i\hbar\nabla+\frac{e}{c}\mathbf{A})$$

$$=(-i\hbar\nabla)^2-i\hbar\frac{e}{c}\nabla\cdot\mathbf{A}-i\hbar\frac{e}{c}\mathbf{A}\cdot\nabla+(\frac{e}{c}\mathbf{A})^2$$

$$=(-i\hbar\nabla)^2-i\hbar\frac{e}{c}\cancel{(\nabla\cdot\mathbf{A})}-2i\hbar\frac{e}{c}\mathbf{A}\cdot\nabla+(\frac{e}{c}\mathbf{A})^2$$

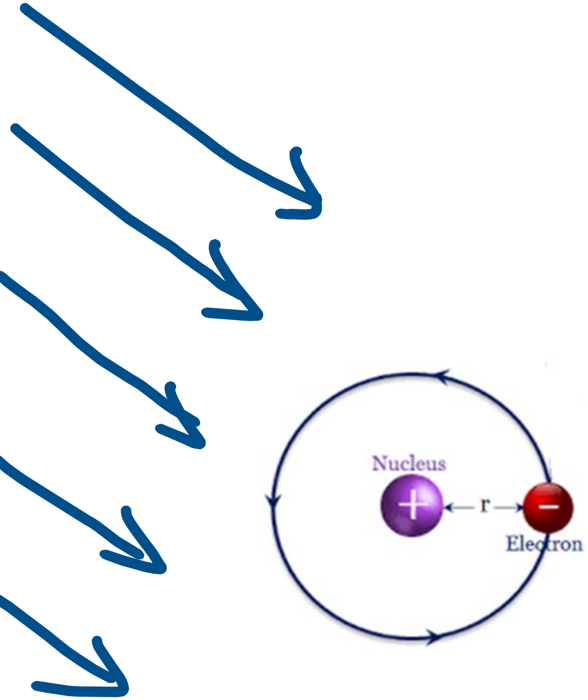
0

$=2\frac{e}{c}\vec{A}\cdot\hat{\vec{p}}$

Coulomb gauge : $\vec{\nabla}\cdot\vec{A}=0$

Light-matter interaction, up to first order

1. For example, a material (atom, molecule, solid) under a light field,



$$i\hbar\frac{\partial\psi(\mathbf{r},t)}{\partial t}=\left(\hat{H}_0+\hat{H}'\right)\psi(\mathbf{r},t)$$

$$\hat{H}_0=-\frac{\hbar^2}{2m}\nabla^2+V(\mathbf{r}) \quad \text{and} \quad \hat{H}'=\frac{e}{mc}\mathbf{A}\cdot\hat{\mathbf{p}}$$

$$\boxed{\hat{H}'=\frac{e}{m\omega}\mathbf{E}(t)\cdot\hat{\mathbf{p}}}=\frac{e}{m\omega}\left(\mathbf{E}(\omega)e^{i\omega t}+\mathbf{E}(-\omega)e^{-i\omega t}\right)\cdot\hat{\mathbf{p}}$$