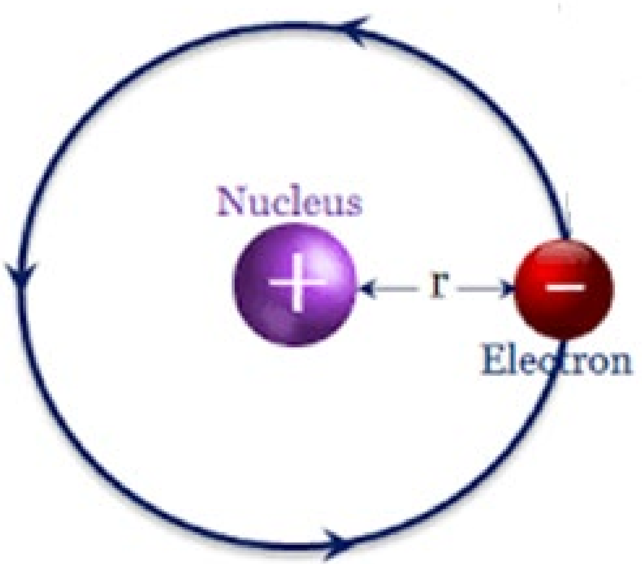
Day-1

- Brief overview of quantum mechanics
- Dipole approximation for light-matter interaction
- Schrodinger equation and Dirac equation
- Spin-orbit coupling

$$\boxed{\hat{H}_{SOC} = \frac{1}{2m^2c^2}\left(\frac{\hbar}{2}\vec{\sigma}\right)\cdot\left(\nabla V(\mathbf{r})\times\hat{\vec{p}}\right)}$$

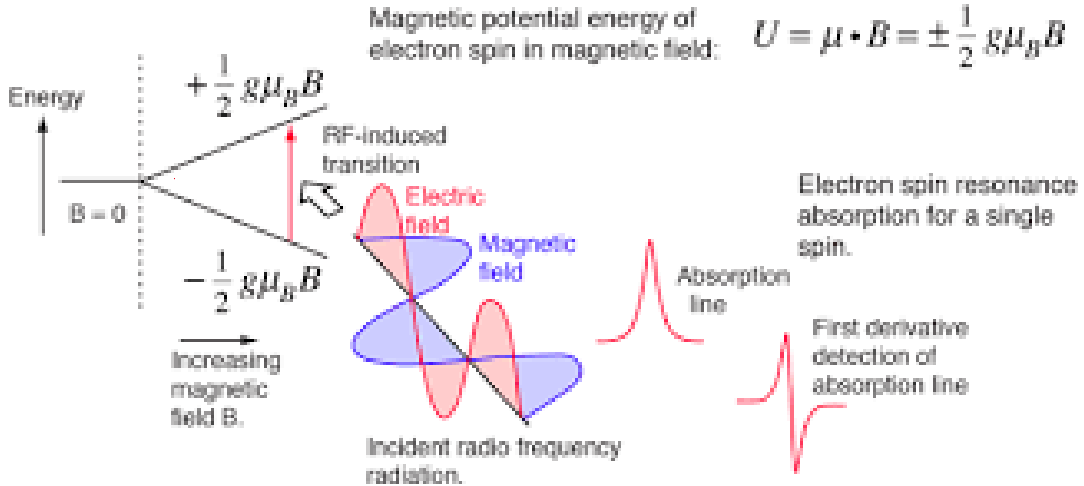
Pauli's recognition of the doublet

1. Besides the Rydberg series, Pauli and others well recognized that the level can be split, depending on the magnetic field



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

$$E_n=-\frac{me^4}{2\hbar^2}\frac{1}{n^2}$$

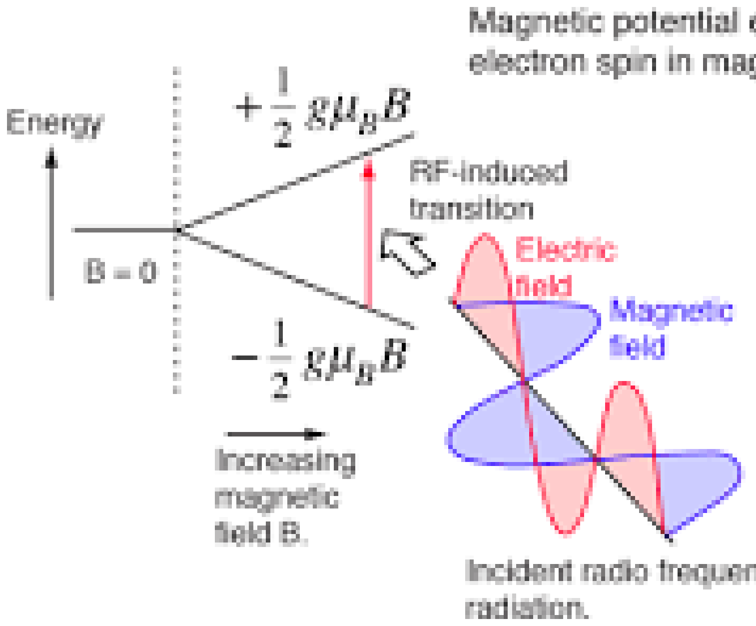


Early recognition of the electron's spin

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

It might be possible to postulate the equation in terms of an intrinsic magnetic dipole, which seems to be quantized by a two state (spin up, spin down)

$$\mu=\pm\frac{e\hbar}{2mc}=\frac{e}{mc}\left(\pm\frac{\hbar}{2}\right)$$



- Now let us consider the special relativity.

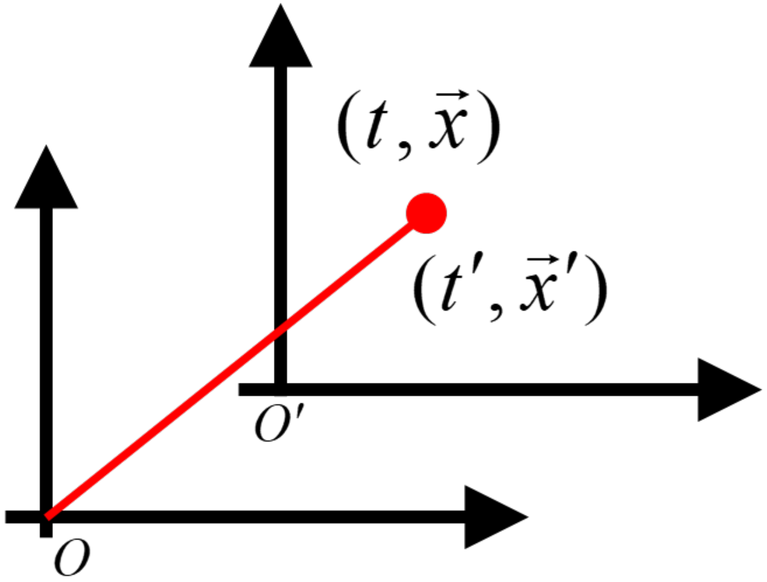
- The Lorentz-covariance of the matter wave equation ?

Four-vector and Lorentz transformation

- Let's first think of the space-time coordinates and their transformation rules.

$$x^{\mu} = (ct, \vec{x}) \rightarrow x'^{\mu} = (ct', \vec{x}')$$

$$x'^{\mu} = \sum_{\nu}^{4} \Lambda^{\mu}{}_{\nu} x^{\nu} = \Lambda^{\mu}{}_{\nu} x^{\nu}$$



- The Einstein's assertion of *the invariance of speed of light* requires that the following quantity should be invariant (i.e. being the four scalar) over the transformation.

$$c^2 t^2 - \vec{x}^2 = c^2 t'^2 - \vec{x}'^2$$

Four-vector & Minkowskii metrics

1. Contravariant four vector

$$x^\mu = (ct, \mathbf{r}) \rightarrow x'^\mu = \Lambda^\mu{}_\lambda x^\lambda$$

2. Minkowskii metrics

$$g_{\mu\nu} = g^{\mu\nu} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix}$$

3. Covariant four vector

$$x_\mu = (ct, -\mathbf{r}) = g_{\mu\nu} x^\nu$$

Four-vector & Minkowskii metrics

4. The inner product of two four vector be invariant, being the four scalar, over the Lorentz transformation.

$$x \cdot y = x_\mu y^\mu = x_\mu g^{\mu\lambda} y_\lambda = x^\lambda y_\lambda$$

5. Invariance of the scalar over the Lorentz transformation

$$x'^\mu = \Lambda^\mu{}_\alpha x^\alpha , y'^\nu = \Lambda^\nu{}_\beta y^\beta$$

$$x'^\mu y'_\mu = x'^\mu y'^\nu g_{\mu\nu} = g_{\mu\nu} \Lambda^\mu{}_\alpha \Lambda^\nu{}_\beta x^\alpha y^\beta = x^\alpha y_\alpha = g_{\alpha\beta} x^\alpha y^\beta$$

Lorentz transformation

- The matrix should be of

$$\boxed{g_{\mu\nu}\Lambda^{\mu}{}_{\alpha}\Lambda^{\nu}{}_{\beta}=g_{\alpha\beta}}$$

Four vectors in E&M

- 4-momentum

$$p^\mu = \left(E/c\,, p_x, p_y, p_z\right) = \left(\gamma mc, \gamma m\vec{v}\right) \ .$$

Note that the Four-scalar $p^\mu p_\mu = \left(\gamma mc\right)^2 - \left(\gamma mv\right)^2 = m^2c^2$

- 4-current and 4-potential

$$A^\mu = \left(\phi/c\,, A_x, A_y, A_z\right) \qquad j^\mu = \left(\rho c, j_x, j_y, j_z\right)$$

4-gradient and 4-momentum

1. Four gradient

$$\frac{\partial}{\partial x^\mu} = \left(\frac{\partial}{c\partial t}, \vec{\nabla}\right) = \partial_\mu \quad , \quad \frac{\partial}{\partial x_\mu} = \left(\frac{\partial}{c\partial t}, -\vec{\nabla}\right) = \partial^\mu$$

The 4-gradient of the contravariant position transforms as a covariant 4-vector.

Four-momentum as a four vector

- Since the contravariant and covariant form of four-derivatives are available obviously, we may easily define the four-momenta.

$$\hat{p}^{\mu} = i\hbar \frac{\partial}{\partial x_{\mu}} = i\partial^{\mu} = (i\partial_t, -i\vec{\nabla}) = (\hat{H}, \hat{\vec{p}})$$

$$\hat{p}_{\mu} = i\hbar \frac{\partial}{\partial x^{\mu}} = i\partial_{\mu} = (i\partial_t, i\vec{\nabla}) = (\hat{H}, -\hat{\vec{p}})$$

Equations for the matter wave

- Schrodinger equation is the equation for the matter wave corresponding to Newtonian Energy-momentum relation. For example, for a free particle (the energy-momentum eigenstate)

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

$$\psi(\mathbf{r},t)=Ae^{i(\mathbf{k}\cdot\mathbf{r}-\omega t)}$$

$$E=\hbar\omega=\frac{\hbar^2\mathbf{k}^2}{2m}=\frac{1}{2m}\mathbf{p}^2$$

Equations for the matter wave

- Klein & Gordon suggested the following form of matter wave equation

$$-\hbar^2 \frac{\partial^2 \psi}{\partial t^2} = \left[-\hbar^2 c^2 \nabla^2 + m^2 c^4 \right] \psi$$

- To fit with the relativistic energy-momentum equation

For a free-particle energy momentum state $\psi(\mathbf{r}, t) = Ae^{i(\mathbf{k}\cdot\mathbf{r} - \omega t)}$

$$E = \hbar\omega = \mathbf{p}^2 c^2 + m^2 c^4$$

Equations for the matter wave

- To make a Lorentz-covariant matter wave equation, the equation must be linear in terms of four momentum, all linear in $\partial_\mu = \partial/\partial x^\mu$

- Dirac recognize that, to implement the relativistic energy-momentum relation ($E^2 = p^2c^2 + m^2c^4$) into the matter wave from, in accordance with the Plank's quantized radiation ($\omega = E/\hbar$) and de Broglie ($\lambda = 2\pi\hbar/p$) ,

- the vector wavefunction with multiple wavefunctions is inevitable.

The equation Dirac proposed

- Dirac intended to invent an equation with the first order in time by introducing four matrices and vector wave function.

$$(\gamma^{\mu}\hat{p}_{\mu} - mc)\psi = 0$$

Is this four vector ?, and then $\gamma^{\mu}\hat{p}_{\mu}$ is four-scalar ? :

NO !!, Don't be confused. It is just the name of 4x4 matrices.

- Later, we assign a transformation rule on ψ so that it successfully produces 4-vector current density with a positive-definite density

$$j^{\mu} = \bar{\psi}\gamma^{\mu}\psi \quad , \quad \partial_{\mu} j^{\mu} = 0$$

Lorentz-covariant equation of motion

- Let us search for general attributes that the γ matrices should have.

$$(\gamma^{\mu}\hat{p}_{\mu}+mc)(\gamma^{\lambda}\hat{p}_{\lambda}-mc)\psi=0\ ,\ \ \left(\gamma^{\mu}\gamma^{\lambda}\hat{p}_{\mu}\hat{p}_{\lambda}-m^{2}c^{2}\right)\psi=0$$

- Since the momentum operators are commuting, $[\hat{p}_{\mu},\hat{p}_{\nu}]=0$

$$\gamma^{\mu}\gamma^{\lambda}\hat{p}_{\mu}\hat{p}_{\lambda}=\gamma^{\lambda}\gamma^{\mu}\hat{p}_{\lambda}\hat{p}_{\mu}=\gamma^{\lambda}\gamma^{\mu}\hat{p}_{\mu}\hat{p}_{\lambda}$$

$$\left(\frac{1}{2}\left\{\gamma^{\mu},\gamma^{\lambda}\right\}\hat{p}_{\mu}\hat{p}_{\lambda}-m^{2}c^{2}\right)\psi=0$$

Clifford algebra

- Let's require to find

$$\left(\gamma^{\mu}\gamma^{\lambda}+\gamma^{\lambda}\gamma^{\mu}\right)=2g^{\mu\lambda}$$

$$\boxed{\begin{aligned}&\{\gamma^{\mu},\gamma^{\upsilon}\}=0 \ \text{ for } \ \mu\neq\upsilon\\&\left(\gamma^{0}\right)^{2}=1,\ \left(\gamma^{i}\right)^{2}=-1 \ \text{ for } \ i=1,2,3\end{aligned}}$$

- What are these four symbols ? $\gamma^0, \gamma^1, \gamma^2, \gamma^3$

- There are no representation of the Clifford algebra using 2x2 or 3x3 matrices.
- The simplest representation of the Clifford algebra is 4x4, but there are many representation with 4x4 matrices.

Block off-diagonal matrix

- Block 2x2 operations

$$\begin{bmatrix} 0_{2\times2} & A_{2\times2} \\ B_{2\times2} & 0_{2\times2} \end{bmatrix} \begin{bmatrix} 0_{2\times2} & C_{2\times2} \\ D_{2\times2} & 0_{2\times2} \end{bmatrix} = \begin{bmatrix} AD & 0 \\ 0 & BC \end{bmatrix}$$

- Block transpose

$$\begin{bmatrix} 0_{2\times2} & A_{2\times2} \\ B_{2\times2} & 0_{2\times2} \end{bmatrix}^T = \begin{bmatrix} 0 & B^T \\ A^T & 0 \end{bmatrix}$$

Chiral-Weyl representation

- Four matrices and the fifths

$$\gamma^0 = \begin{pmatrix} 0 & 1_2 \\ 1_2 & 0 \end{pmatrix}, \quad \vec{\gamma} = \begin{pmatrix} 0 & \vec{\sigma} \\ -\vec{\sigma} & 0 \end{pmatrix}, \gamma^5 = -i\gamma^0\gamma^1\gamma^2\gamma^3 = \begin{pmatrix} 1_2 & 0 \\ 0 & -1_2 \end{pmatrix}$$

- Transpose-conjugate matrix

$$\gamma^0\gamma^\mu\gamma^0 = \left(\gamma^\mu\right)^+$$

- [Proof] it is obvious for $\mu = 0$

$$\gamma^0\gamma^i\gamma^0 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}\begin{pmatrix} 0 & \sigma_i \\ -\sigma_i & 0 \end{pmatrix}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} = \begin{pmatrix} 0 & -\sigma_i \\ \sigma_i & 0 \end{pmatrix}$$

Majorana representation

- To make every component complex number

$$\gamma^0 = \begin{pmatrix} 0 & \sigma_2 \\ \sigma_2 & 0 \end{pmatrix}, \ \gamma^1 = \begin{pmatrix} i\sigma_3 & 0 \\ 0 & i\sigma_3 \end{pmatrix}, \ \gamma^2 = \begin{pmatrix} 0 & -\sigma_2 \\ \sigma_2 & 0 \end{pmatrix}, \ \gamma^3 = \begin{pmatrix} -i\sigma_1 & 0 \\ 0 & -i\sigma_1 \end{pmatrix}$$

- Show that the fifth

$$\gamma^5 = i\gamma^0\gamma^1\gamma^2\gamma^3 = \begin{pmatrix} \sigma_2 & 0 \\ 0 & -\sigma_2 \end{pmatrix}$$

Dirac-Pauli representation

- The gamma 4-vector $\gamma^0, \gamma^1, \gamma^2, \gamma^3, \gamma^4$

$$\gamma^0 = \begin{pmatrix} I & 0 \\ 0 & -I \end{pmatrix}, \quad \vec{\gamma} = \begin{pmatrix} 0 & \vec{\sigma} \\ -\vec{\sigma} & 0 \end{pmatrix}, \gamma^5 = i\gamma^0\gamma^1\gamma^2\gamma^3 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$

- The Dirac equation

$$\gamma^0(\gamma^0 \hat{p}_0 - \vec{\gamma}\cdot\hat{\vec{p}} - mc)\psi = 0 \; , \; i\frac{\partial\psi}{c\partial t} = (\gamma^0\vec{\gamma}\cdot\hat{\vec{p}} + \gamma^0 mc)\psi$$

- Multiply γ^0 on both sides

$(\gamma^0 \hat{p}_0 - \vec{\gamma}\cdot\vec{p} - mc)\psi = 0$

$$\boxed{i\frac{\partial}{\partial t}\psi = \left[c\vec{\alpha}\bullet\hat{\vec{p}} + mc^2\beta\right]\psi = 0}$$

Dirac eq

$$\vec{\alpha} = \gamma^0\vec{\gamma}, \quad \vec{\gamma} = \gamma^0\vec{\alpha}, \quad \beta = \gamma^0$$

Pauli matrices

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix},\ \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix},\ \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

1. $\sigma_i \sigma_j = i \sum_k \varepsilon_{ijk} \sigma_k + \delta_{ij}$

2. $\left[\sigma_i, \sigma_j\right] = i \sum_k \varepsilon_{ijk} \sigma_k - i \sum_k \varepsilon_{jik} \sigma_k = 2i \varepsilon_{ijk} \sigma_k$

3. $\left\{\sigma_i, \sigma_j\right\} = 2\delta_{i,j}$

4. $\{\vec{A} \cdot \vec{\sigma}\}\{\vec{B} \cdot \vec{\sigma}\} = \sum_i A_i \sigma_i \sum_j B_j \sigma_j = \sum_{i,j} A_i B_j \sigma_i \sigma_j$

$$= \sum_{i,j} A_i B_j \left[\delta_{ij} + i \sum_k \varepsilon_{ijk} \sigma_k \right] = \sum_i A_i B_i + i \sum_k \sum_{i,j} \left(\varepsilon_{ijk} A_i B_j \right) \sigma_k$$

$$= \vec{A} \cdot \vec{B} + i \sum_k \left(\vec{A} \times \vec{B} \right)_k \sigma_k$$

$$= \vec{A} \cdot \vec{B} + i \vec{A} \times \vec{B} \cdot \vec{\sigma}$$

Dirac-Pauli representation

- The Dirac equation for a free particle

$$i\frac{\partial}{\partial t}\psi = \left[c\vec{\alpha}\bullet\hat{\vec{p}} + mc^2\beta \right]\psi = 0$$

$$\alpha^i = \gamma^0\gamma^i = \begin{pmatrix} 0 & \sigma^i \\ \sigma^i & 0 \end{pmatrix} \qquad \beta = \gamma^0 = \begin{pmatrix} 1_2 & 0 \\ 0 & -1_2 \end{pmatrix}$$

Dirac-Pauli representation

- For a particle with a charge of q under a E&M field

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

Dirac equation

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

$$\psi=\begin{pmatrix}\checkmark\\\checkmark\\\checkmark\\\checkmark\end{pmatrix}$$

I. The wavefunction is not a scalar, it has 4 components.

II. The equation is Lorentz covariant.

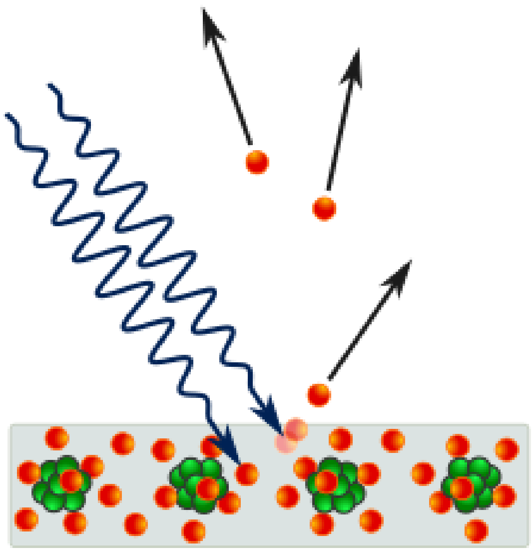
III. Very natural identification of spin.

IV. Presence of antiparticle ➔ Vacuum is NOT nothing. Creation and annihilation of particle and antiparticle➔ Quantum Field Theory

Dirac equation

IV. Presence of antiparticle ➔ Vacuum is NOT nothing. Creation and annihilation of particle and antiparticle➔ Quantum Field Theory

Photon $E = \hbar\omega$



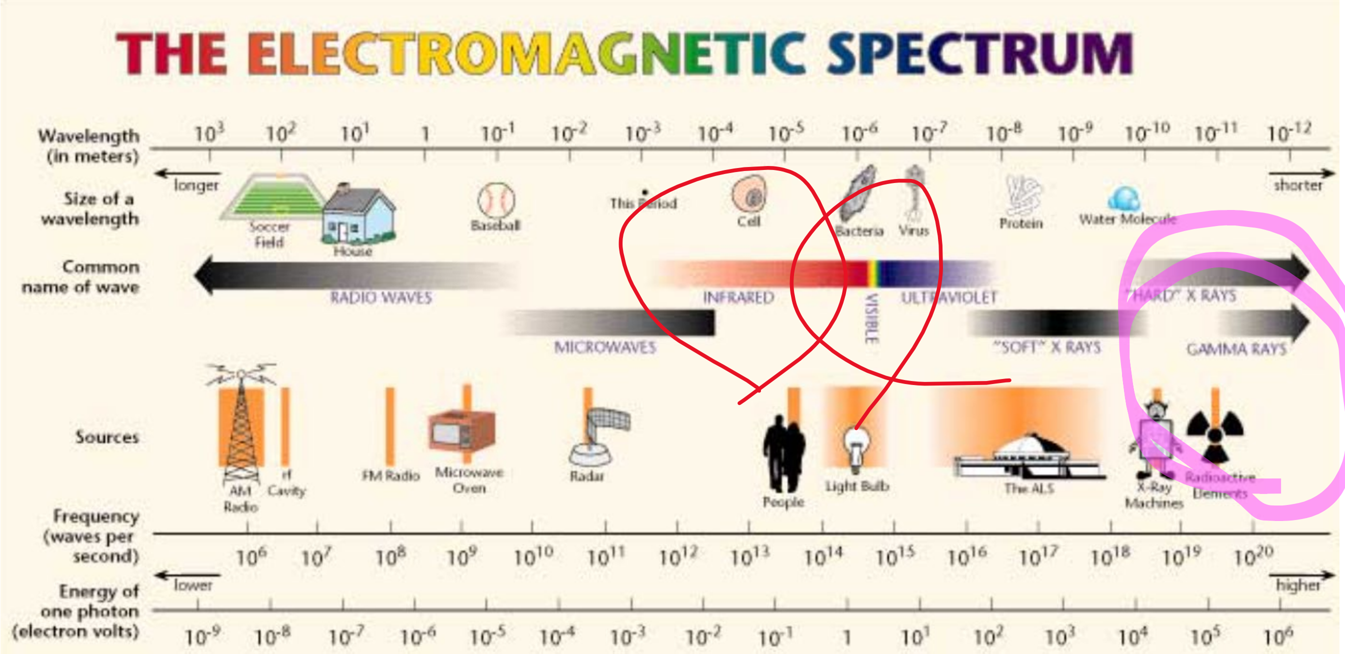
$E \ll mc^2$, particle numbers are conserved.

$E \approx 2mc^2$, the amplitude of the antiparticle cannot be ignored.

Number is not conserved.

Energy scale

IV. Presence of antiparticle ➔ Vacuum is NOT nothing. Creation and annihilation of particle and antiparticle➔ Quantum Field Theory



Electron mass

Constant	Values	Units
m_e	$9.109\,383\,7015(28) \times 10^{-31}$ [1]	kg
	$5.485\,799\,090\,65(16) \times 10^{-4}$	Da
	$8.187\,105\,7769(25) \times 10^{-14}$	J/c^2
	$0.510\,998\,950\,00(15)$	MeV/c^2
Energy of m_e	$8.187\,105\,7769(25) \times 10^{-14}$	J
	$0.510\,998\,950\,00(15)$	MeV

The photons near the visible range never create electron-positron pair.
Gamma ray with MeV energy can do the creation.

Time-independent equation for the stationary

$$i\hbar\frac{\partial}{\partial t}\psi(\mathbf{r},t)=\left[c\vec{\alpha}\cdot\left(\hat{\mathbf{p}}-\frac{q}{c}\mathbf{A}\right)+mc^2\beta+q\varphi(\mathbf{r})\right]\psi(\mathbf{r},t)\ \text{with}\ \underline{\psi(\mathbf{r},t)=\psi(\mathbf{r})e^{-i\omega t}}$$

$$\boxed{\left(E-q\varphi(\mathbf{r})\right)\psi(\mathbf{r})=\left[c\vec{\alpha}\cdot\left(\hat{\mathbf{p}}-\frac{q}{c}\mathbf{A}\right)+mc^2\beta\right]\psi(\mathbf{r})}$$

Time-independent Dirac equation

Time-independent equation for the stationary

$$i\hbar\frac{\partial}{\partial t}\psi(\mathbf{r},t)=\left[c\vec{\alpha}\cdot\left(\hat{\mathbf{p}}-\frac{q}{c}\mathbf{A}\right)+mc^2\beta+q\varphi(\mathbf{r})\right]\psi(\mathbf{r},t)\ \text{with}\ \psi(\mathbf{r},t)=\psi(\mathbf{r})e^{-i\omega t}$$

$$\big(E-q\varphi(\mathbf{r})\big)\psi(\mathbf{r})=\left[c\vec{\alpha}\cdot\left(\hat{\mathbf{p}}-\frac{q}{c}\mathbf{A}\right)+mc^2\beta\right]\psi(\mathbf{r})$$

Under a static E-field, $\vec{A} = 0$

$$\left(E - q\varphi(\mathbf{r})\right)\psi(\mathbf{r}) = \left[c\vec{\alpha}\cdot\hat{\mathbf{p}} + mc^2\beta\right]\psi(\mathbf{r}) \quad , \quad \text{with } \psi = \begin{pmatrix}\psi \\ \eta\end{pmatrix} \quad \text{we have}$$

$$\begin{pmatrix} E - q\varphi - mc^2 & 0 \\ 0 & E - q\varphi + mc^2 \end{pmatrix}\begin{pmatrix}\psi \\ \eta\end{pmatrix} = c\begin{pmatrix} 0 & \vec{\sigma}\cdot\hat{\vec{p}} \\ \vec{\sigma}\cdot\hat{\vec{p}} & 0 \end{pmatrix}\begin{pmatrix}\psi \\ \eta\end{pmatrix}$$

$$\left(E - q\varphi - mc^2\right)\psi = c\vec{\sigma}\cdot\hat{\vec{p}}\eta$$

$$\left(E - q\varphi + mc^2\right)\eta = c\vec{\sigma}\cdot\hat{\vec{p}}\psi$$

$$\psi = \begin{pmatrix}\checkmark \\ \checkmark \\ \checkmark \\ \checkmark\end{pmatrix} = \begin{pmatrix}\psi & \times \\ & \times \\ \eta & \times \\ & \times\end{pmatrix}$$

Under a static E-field, $\vec{A} = 0$

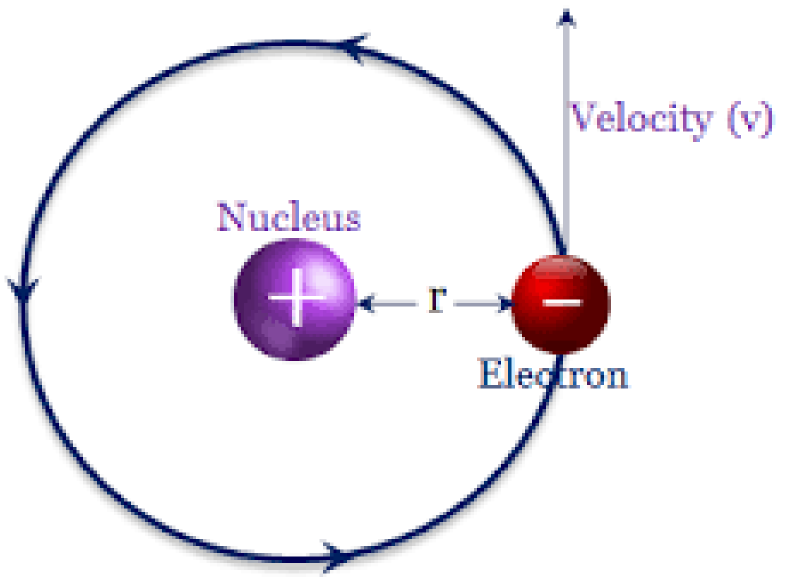
$$\left(E - q\varphi - mc^2\right)\psi = c\vec{\sigma}\cdot\hat{\vec{p}}\eta = c\vec{\sigma}\cdot\hat{\vec{p}}\frac{1}{\left(E - q\varphi + mc^2\right)}c\vec{\sigma}\cdot\hat{\vec{p}}\psi$$

With $E_s = E - mc^2$ we have

$$\left(E_s - q\varphi\right)\psi = \vec{\sigma}\cdot\hat{\vec{p}}\frac{c^2}{\left(E_s - q\varphi + 2mc^2\right)}\vec{\sigma}\cdot\hat{\vec{p}}\psi = \frac{\vec{\sigma}\cdot\hat{\vec{p}}}{2m}\frac{1}{1+\frac{E_s - q\varphi}{2mc^2}}\vec{\sigma}\cdot\hat{\vec{p}}\psi$$

$$\sim\left(\frac{v}{c}\right)^2$$

Note, for the electron



$$E = mc^2 + \frac{1}{2}mv^2 - \frac{e^2}{r},$$

$$\boxed{E_s - q\varphi} \sim \frac{1}{2}mv^2$$

Under a static E-field, $\vec{A} = 0$

$$(E_s - q\varphi)\psi = \frac{\vec{\sigma}\cdot\hat{\vec{p}}}{2m}\left(1 - \frac{E_s - q\varphi}{2mc^2}\right)\vec{\sigma}\cdot\hat{\vec{p}}\psi$$

In the limit $\frac{v}{c} \to 0$ we have

$$\left\{\vec{A}\cdot\vec{\sigma}\right\}\left\{\vec{B}\cdot\vec{\sigma}\right\} = \vec{A}\cdot\vec{B} + i\vec{A}\times\vec{B}\cdot\vec{\sigma}$$

$$E_s\psi = \left[\frac{1}{2m}\left(\vec{\sigma}\cdot\hat{\vec{p}}\right)^2 + q\varphi\right]\psi$$

$$\underbrace{E_s\psi = \left[\frac{1}{2m}\left(\hat{\vec{p}}\right)^2 + q\varphi\right]\psi}$$

This is the Schrodinger equation for a particle of charge q in an electrostatic potential

Normalization

$$\left(E_s - q\varphi\right)\psi = \frac{\vec{\sigma}\cdot\hat{\vec{p}}}{2m}\left(1 - \frac{E_s - q\varphi}{2mc^2}\right)\vec{\sigma}\cdot\hat{\vec{p}}\psi$$

$$\left[\frac{(\hat{\vec{p}})^2}{2m} - \frac{\vec{\sigma}\cdot\hat{\vec{p}}(E_s - q\varphi)\vec{\sigma}\cdot\hat{\vec{p}}}{4m^2c^2} + q\varphi\right]\psi = E\psi$$

At this point, we must be cautious in interpreting Ψ as a wavefunction of non-relativistic wavefunction with relativistic corrections. We must consider the normalization.

$$1 = \int \psi^+(\mathbf{r},t)\psi(\mathbf{r},t)d^3\mathbf{r} + \int \eta^+(\mathbf{r},t)\eta(\mathbf{r},t)d^3\mathbf{r}$$

$$1 = \int \psi^+(\mathbf{r},t)\psi(\mathbf{r},t)d^3\mathbf{r} + \int \psi^+(\mathbf{r},t)\left(\frac{\vec{\sigma}\cdot\hat{\mathbf{p}}}{2mc}\right)^2\psi(\mathbf{r},t)d^3\mathbf{r}$$

$$\text{Set } \psi(\mathbf{r},t) = \left(1 - \frac{\hat{\mathbf{p}}^2}{8m^2c^2}\right)\psi_s(\mathbf{r},t) \text{ with } \int \psi_s^+(\mathbf{r},t)\psi_s(\mathbf{r},t)d^3\mathbf{r} = 1$$

$$\left[\frac{(\hat{\vec{p}})^2}{2m}+q\varphi-\frac{\vec{\sigma}\cdot\hat{\vec{p}}(E_s-q\varphi)\vec{\sigma}\cdot\hat{\vec{p}}}{4m^2c^2}\right]\left(1-\frac{\hat{\mathbf{p}}^2}{8m^2c^2}\right)\psi_s(\mathbf{r})=E\left(1-\frac{\hat{\mathbf{p}}^2}{8m^2c^2}\right)\psi_s(\mathbf{r})$$

~ 1

$\sim \left(\frac{v}{c}\right)^2$

$$\left(1+\frac{\hat{\mathbf{p}}^2}{8m^2c^2}\right)\left[\frac{(\hat{\vec{p}})^2}{2m}+q\varphi-\frac{\vec{\sigma}\cdot\hat{\vec{p}}(E_s-q\varphi)\vec{\sigma}\cdot\hat{\vec{p}}}{4m^2c^2}\right]\left(1-\frac{\hat{\mathbf{p}}^2}{8m^2c^2}\right)\psi_s(\mathbf{r})=E\left(1-(\frac{\hat{\mathbf{p}}^2}{8m^2c^2})^2\right)\psi_s(\mathbf{r})$$

$$\left[\frac{(\hat{\vec{p}})^2}{2m}+q\varphi-\frac{\vec{\sigma}\cdot\hat{\vec{p}}(E_s-q\varphi)\vec{\sigma}\cdot\hat{\vec{p}}}{4m^2c^2}+q\frac{\hat{\mathbf{p}}^2\varphi-\varphi\hat{\mathbf{p}}^2}{8m^2c^2}\right]\psi_s(\mathbf{r})=E\psi_s(\mathbf{r})$$

Note that

$$\left[(E_s - q\varphi), \vec{\sigma}\cdot\hat{\vec{p}}\right] = \left[E_s, \vec{\sigma}\cdot\hat{\vec{p}}\right] - q\left[\varphi, \vec{\sigma}\cdot\hat{\vec{p}}\right] = -q\left[\varphi, \vec{\sigma}\cdot\hat{\vec{p}}\right] = -q\left[\varphi(\mathbf{r}), \vec{\sigma}\cdot\hat{\vec{p}}\right] = -q\vec{\sigma}\cdot\left[\varphi(\mathbf{r}), \hat{\vec{p}}\right]$$

$$(E_s - q\varphi)\vec{\sigma}\cdot\hat{\vec{p}} = \left[(E_s - q\varphi), \vec{\sigma}\cdot\hat{\vec{p}}\right] + \vec{\sigma}\cdot\hat{\vec{p}}(E_s - q\varphi)$$

$$\vec{\sigma}\cdot\hat{\vec{p}}(E_s - q\varphi)\vec{\sigma}\cdot\hat{\vec{p}} = -q(\vec{\sigma}\cdot\hat{\vec{p}})\vec{\sigma}\cdot\left[\varphi(\mathbf{r}), \hat{\vec{p}}\right] + (\vec{\sigma}\cdot\hat{\vec{p}})^2(E_s - q\varphi)$$

$$-\frac{\vec{\sigma}\cdot\hat{\vec{p}}(E_s - q\varphi)\vec{\sigma}\cdot\hat{\vec{p}}}{4m^2c^2} = \frac{1}{4m^2c^2}\left(q\hbar^2\nabla^2\varphi(\mathbf{r}) + q\hbar^2\nabla\varphi\cdot\nabla\right) - \frac{\hbar q}{4m^2c^2}\left(\hat{\vec{p}}\times\nabla\varphi(\mathbf{r})\cdot\vec{\sigma}\right) - \frac{(\vec{\sigma}\cdot\hat{\vec{p}})^2(E_s - q\varphi}{4m^2c^2}$$

$$-q(\vec{\sigma}\cdot\hat{\vec{p}})\vec{\sigma}\cdot\left[\varphi(\mathbf{r}), \hat{\vec{p}}\right] = -q\hat{\vec{p}}\cdot\left[\varphi(\mathbf{r}), \hat{\vec{p}}\right] - qi\hat{\vec{p}}\times\left[\varphi(\mathbf{r}), \hat{\vec{p}}\right]\cdot\vec{\sigma}$$

$$= -q\hbar^2\nabla^2\varphi(\mathbf{r}) - q\hbar^2\nabla\varphi\cdot\nabla + \hbar q\hat{\vec{p}}\times\nabla\varphi(\mathbf{r})\cdot\vec{\sigma}$$

$$\left\{\vec{A}\cdot\vec{\sigma}\right\}\left\{\vec{B}\cdot\vec{\sigma}\right\} = \vec{A}\cdot\vec{B} + i\vec{A}\times\vec{B}\cdot\vec{\sigma}$$

$$\left(E_s - q\varphi\right)\psi = \frac{\vec{\sigma}\cdot\hat{\vec{p}}}{2m}\left(1 - \frac{E_s - q\varphi}{2mc^2}\right)\vec{\sigma}\cdot\hat{\vec{p}}\psi$$

$$(\vec{\sigma}\cdot\hat{\vec{p}})^2(E_s - q\varphi)\psi \approx \frac{(\vec{\sigma}\cdot\hat{\vec{p}})^4}{2m}\psi = \frac{(\hat{\vec{p}})^4}{2m}\psi$$

$$q\frac{\hat{\mathbf{p}}^2\varphi - \varphi\hat{\mathbf{p}}^2}{8m^2c^2} = -q\hbar^2\frac{1}{8m^2c^2}\nabla^2\varphi - 2q\hbar^2\frac{1}{8m^2c^2}\nabla\varphi\cdot\nabla$$

Under a static E-field, $\vec{A} = 0$

$$\hat{H}_{rel-corr}\psi = E\psi$$

$$\hat{H}_{rel-corr} = \left(\frac{\hat{\mathbf{p}}^2}{2m} + q\varphi\right) + \frac{\hat{\mathbf{p}}^4}{8m^3c^2} + \frac{q\hbar^2\nabla^2\varphi(\mathbf{r})}{8m^2c^2} - \frac{\hbar q}{4m^2c^2}\left(\hat{\vec{p}} \times \nabla\varphi(\mathbf{r}) \cdot \vec{\sigma}\right)$$

$$\hat{H}_{SOC} = -\frac{\hbar q}{4m^2c^2}\left(\hat{\vec{p}} \times \nabla\varphi(\mathbf{r}) \cdot \vec{\sigma}\right) = -\frac{\hbar q}{4m^2c^2}\vec{\sigma} \cdot \left(\hat{\vec{p}} \times \nabla\varphi(\mathbf{r})\right) = -\frac{\hbar q}{4m^2c^2}\vec{\sigma} \cdot \left(\hat{\vec{p}} \times \nabla\varphi(\mathbf{r})\right)$$

Note that the operators

$$\hat{\vec{p}} \times \nabla \varphi(\mathbf{r}) = -i\hbar \nabla \times \nabla \varphi(\mathbf{r}) \cancel{= \nabla \varphi(\mathbf{r}) \times (-i\hbar \nabla)}$$

$$\boxed{\hat{\vec{p}} \times \nabla \varphi(\mathbf{r}) = -i\hbar \nabla \times \nabla \varphi(\mathbf{r}) = -\nabla \varphi(\mathbf{r}) \times (-i\hbar \nabla) = -\nabla \varphi(\mathbf{r}) \times \hat{\vec{p}}}$$

Spin-Orbit Coupling

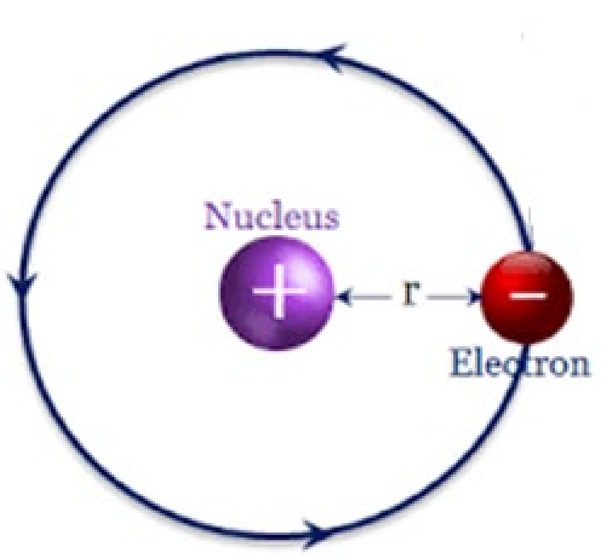
$$\hat{H}_{SOC} = -\frac{\hbar q}{4m^2c^2}\vec{\sigma}\cdot\left(\hat{\vec{p}}\times\nabla\varphi(\mathbf{r})\right) = -\frac{\hbar q}{4m^2c^2}\vec{\sigma}\cdot\left(\hat{\vec{p}}\times\nabla\varphi(\mathbf{r})\right) = \frac{q}{2m^2c^2}\left(\frac{\hbar}{2}\vec{\sigma}\right)\cdot\left(\nabla\varphi(\mathbf{r})\times\hat{\vec{p}}\right)$$

With the potential energy for the particle $V(\mathbf{r})$

$$\boxed{\hat{H}_{SOC} = \frac{1}{2m^2c^2}\left(\frac{\hbar}{2}\vec{\sigma}\right)\cdot\left(\nabla V(\mathbf{r})\times\hat{\vec{p}}\right)}$$

$\vec{S}$

Spin-orbit coupling



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

$$\hat{H}_{SOC}=\frac{1}{2m^2c^2}\left(\frac{\hbar}{2}\vec{\sigma}\right)\cdot\left(\nabla V(\mathbf{r})\times\hat{\vec{p}}\right)$$

For a spherical symmetric potential $\nabla V(\mathbf{r})=\nabla V(r)=\frac{dV}{dr}\frac{\mathbf{r}}{r}$

$$\hat{H}_{SOC}=\frac{1}{2m^2c^2}\left(\frac{\hbar}{2}\vec{\sigma}\right)\cdot\left(\frac{1}{r}\frac{dV}{dr}\right)\mathbf{r}\times\hat{\vec{p}}=\frac{1}{2m^2c^2}\left(\frac{1}{r}\frac{dV}{dr}\right)\hat{\vec{S}}\cdot\hat{\vec{L}}$$

Again, for the zero-th order

$$\left(E_s - q\varphi\right)\psi = \frac{\vec{\sigma}\cdot\hat{\vec{p}}}{2m}\left(1 - \frac{E_s - q\varphi}{2mc^2}\right)\vec{\sigma}\cdot\hat{\vec{p}}\psi$$

In the limit $\frac{v}{c} \to 0$ we have the non-relativistic Schrodinger

$$E_s\psi = \left[\frac{1}{2m}\left(\vec{\sigma}\cdot\hat{\vec{p}}\right)^2 + q\varphi\right]\psi$$

$$E_s\psi = \left[\frac{1}{2m}\left(\hat{\vec{p}}\right)^2 + q\varphi\right]\psi$$

Are these two identical equation ?

Yes or No

$$\left\{\vec{A}\cdot\vec{\sigma}\right\}\left\{\vec{B}\cdot\vec{\sigma}\right\} = \vec{A}\cdot\vec{B} + i\vec{A}\times\vec{B}\cdot\vec{\sigma}$$

With the vector potential

$$\big(E - q\varphi(\mathbf{r})\big)\psi(\mathbf{r}) = \left[c\vec{\alpha}\cdot(\hat{\mathbf{p}} - \frac{q}{c}\mathbf{A}) + mc^2\beta \right]\psi(\mathbf{r}) \quad , \text{ with } \psi = \begin{pmatrix} \psi \\ \eta \end{pmatrix} \text{ we have}$$

$$\begin{pmatrix} E - q\varphi - mc^2 & 0 \\ 0 & E - q\varphi + mc^2 \end{pmatrix} \begin{pmatrix} \psi \\ \eta \end{pmatrix} = c \begin{pmatrix} 0 & \vec{\sigma}\cdot\hat{\vec{p}} - \frac{q}{c}\mathbf{A} \\ \vec{\sigma}\cdot\hat{\vec{p}} - \frac{q}{c}\mathbf{A} & 0 \end{pmatrix} \begin{pmatrix} \psi \\ \eta \end{pmatrix}$$

$$\left(E - q\varphi - mc^2\right)\psi = c\vec{\sigma}\cdot(\hat{\vec{p}} - \frac{q}{c}\mathbf{A})\eta$$

$$\left(E - q\varphi + mc^2\right)\eta = c\vec{\sigma}\cdot(\hat{\vec{p}} - \frac{q}{c}\mathbf{A})\psi$$

The zero-th order in the limit $v/c \to 0$

Exactly the same way through which we derived the non-relativistic Schrodinger

$$\left[\frac{1}{2m}\left(\vec{\sigma}\cdot\hat{\vec{p}}\right)^2 + V(\mathbf{r})\right]\psi = E_s\psi$$

We can derive the zero-th order equation, the non-relativistic limit,

$$\left[\frac{1}{2m}\left(\vec{\sigma}\cdot(\hat{\mathbf{p}}-\frac{q}{c}\mathbf{A})\right)^2 + V(\mathbf{r})\right]\psi = E_s\psi$$

$$\left\{\vec{A}\cdot\vec{\sigma}\right\}\left\{\vec{B}\cdot\vec{\sigma}\right\} = \vec{A}\cdot\vec{B} + i\vec{A}\times\vec{B}\cdot\vec{\sigma}$$

The zero-th order, for the particle in magnetic field

Note that $\{\vec{A}\cdot\vec{\sigma}\}\{\vec{B}\cdot\vec{\sigma}\} = \vec{A}\cdot\vec{B} + i\vec{A}\times\vec{B}\cdot\vec{\sigma}$

The equation

$$\left(\vec{\sigma}\cdot(\hat{\mathbf{p}}-\frac{q}{c}\mathbf{A})\right)^2 = \vec{\sigma}\cdot(\hat{\mathbf{p}}-\frac{q}{c}\mathbf{A})\vec{\sigma}\cdot(\hat{\mathbf{p}}-\frac{q}{c}\mathbf{A})$$

$$= (\hat{\mathbf{p}}-\frac{q}{c}\mathbf{A})^2 + i(-i\hbar\nabla - \frac{q}{c}\mathbf{A})\times(-i\hbar\nabla - \frac{q}{c}\mathbf{A})\cdot\vec{\sigma}$$

$$= (\hat{\mathbf{p}}-\frac{q}{c}\mathbf{A})^2 + i(-i\hbar\nabla)\times(-\frac{q}{c}\mathbf{A})\cdot\vec{\sigma} + i(-\frac{q}{c}\mathbf{A})\times(-i\hbar\nabla)\cdot\vec{\sigma}$$

$$= (\hat{\mathbf{p}}-\frac{q}{c}\mathbf{A})^2 - \frac{q\hbar}{c}(\nabla\times\mathbf{A})\cdot\vec{\sigma} = (\hat{\mathbf{p}}-\frac{q}{c}\mathbf{A})^2 - \frac{q\hbar}{c}\mathbf{B}\cdot\vec{\sigma}$$

The zero-th order, for the particle in magnetic field

$$\left[\frac{1}{2m}\left(\vec{\sigma}\cdot(\hat{\mathbf{p}}-\frac{q}{c}\mathbf{A})\right)^2+V(\mathbf{r})\right]\psi=E_s\psi$$

$$\left[\frac{1}{2m}(\hat{\mathbf{p}}-\frac{q}{c}\mathbf{A})^2-\frac{q\hbar}{2mc}\mathbf{B}\cdot\vec{\sigma}+V(\mathbf{r})\right]\psi=E_s\psi$$

The equation very naturally produces the doublet term, that might have been recognized empirically by Pauli

$$\hat{H}_{Zeeman}=-\frac{q\hbar}{2mc}\mathbf{B}\cdot\vec{\sigma}=-\frac{q}{mc}\mathbf{B}\cdot\left(\frac{\hbar}{2}\vec{\sigma}\right)$$

Lorentz covariance

- Think of two reference frames

$$(\gamma^\mu \hat{p}_\mu - mc)\psi(x) = 0$$

$$(\gamma^\mu \hat{p}'_\mu - mc)\psi'(x') = 0$$

Is this four vector ?, and then $\gamma^\mu \hat{p}_\mu$ is four-scalar ? :
NO !!, Don't be confused. It is just the name of 4x4 matrices.

- Using the Lorentz transformation

$$x'^\mu = \Lambda^\mu{}_\alpha x^\alpha \ , \hat{p}'_\mu = \Lambda_\mu{}^\beta \hat{p}_\beta$$

Lorentz covariance

$$(\gamma^{\mu}\hat{p}'_{\mu} - mc)\psi'(x') = 0$$

$$(\gamma^{\mu}\Lambda_{\mu}{}^{\beta}\hat{p}_{\beta} - mc)\psi'(x') = 0 \text{ , Introducing } \boxed{\psi' = S\psi}$$

$$(S^{-1}\gamma^{\mu}\Lambda_{\mu}{}^{\beta}\hat{p}_{\beta}S - mc)\psi(\Lambda^{-1}x) = 0$$

$$(\gamma^{\beta}\hat{p}_{\beta} - mc)\psi(\Lambda^{-1}x) = 0$$

We can find the matrix such that $S^{-1}\gamma^{\mu}\Lambda_{\mu}{}^{\beta}S = \gamma^{\beta}$

$$S\gamma^{\beta}S^{-1} = \gamma^{\mu}\Lambda_{\mu}{}^{\beta} = \gamma^{\mu}\left(\Lambda^{-1}\right)^{\beta}{}_{\mu}$$

Lorentz covariance, transformation rule

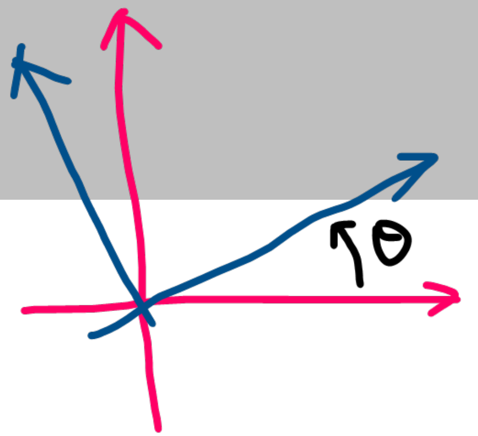
$$x^\mu \rightarrow \Lambda^\mu{}_\alpha x^\alpha$$

$$\hat{p}^\mu \rightarrow \Lambda^\mu{}_\alpha \hat{p}^\alpha$$

$$\psi \rightarrow S\psi$$

4x4 matrix

Rotation generator



- Find the rotation generator of an infinitesimal rotation

$$\psi \to S\psi = \left(1 - i\theta\frac{1}{\hbar}\hat{n}\cdot(\mathbf{r}\times\hat{\mathbf{p}} + \frac{\hbar}{2}\vec{\sigma})....\right)\psi$$

- For the 4-component wave, we have the rotation generator. We have the spin. It is a sort of angular momentum, because it is rotation generator.

$$\hat{\mathbf{J}} = \mathbf{r}\times\hat{\mathbf{p}} + \hat{\mathbf{S}}$$

Summary

I. In Dirac's relativistic theory for a particle, the spin is very naturally identified. It is spin 1/2.

II. In high-energy situation, there is no physics of isolated single particle. It automatically includes the presence of antiparticle, and we have a quantum theory for many particles.

III. In usual the condensed-matter situations, the presence of antiparticle can be ignored. However, the relativistic effect is still very important.

$$\boxed{\hat{H}_{SOC} = \frac{1}{2m^2c^2}\left(\frac{\hbar}{2}\vec{\sigma}\right)\cdot\left(\nabla V(\mathbf{r})\times\hat{\vec{p}}\right)}$$

Homework & Discussion : The zero-th order in the limit $v/c \to 0$

In the limit $\boldsymbol{v/c \to 0}$, Dirac equation converges into

$$\left[\frac{1}{2m}\left(\vec{\sigma}\cdot(\hat{\mathbf{p}}-\frac{q}{c}\mathbf{A})\right)^2+V(\mathbf{r})\right]\psi = E_s\psi$$

Using the identity $\{\vec{A}\cdot\vec{\sigma}\}\{\vec{B}\cdot\vec{\sigma}\}=\vec{A}\cdot\vec{B}+i\vec{A}\times\vec{B}\cdot\vec{\sigma}$

Show that the equation is identical to the following.

$$\left[\frac{1}{2m}(\hat{\mathbf{p}}-\frac{q}{c}\mathbf{A})^2-\frac{q\hbar}{2mc}\mathbf{B}\cdot\vec{\sigma}+V(\mathbf{r})\right]\psi = E_s\psi$$

Tomorrow 5 PM, let us have 10 minute discussion time on this. Uiseok may present this page.

Homework & Discussion

1. We derived the light-matter Hamiltonian in the long wave length limit.

$$\hat{H}' = \frac{e}{mc}\mathbf{A}\cdot\hat{\mathbf{p}} = \frac{e}{m\omega}\mathbf{E}(t)\cdot\hat{\mathbf{p}}$$

2. Can you suggest a next-order term for a near field, that can take into account the wave length dependence of the field ?