12 Klein-Gordon Equation:

12.1 Schrödinger Equation:

Nonrelativistic dispersion: $E = \frac{\vec{p}^2}{2m}$

Jordan rule: $\vec{p} \longrightarrow \hat{\vec{p}} = \frac{\hbar}{i}\vec{\nabla}$, $E \longrightarrow \hat{E} = i\hbar\frac{\partial}{\partial t}$

$$\left.\begin{aligned} i\hbar\frac{\partial\psi}{\partial t} &= -\frac{\hbar^2}{2m}\Delta\psi & \Big|\cdot\psi^* \\ -i\hbar\frac{\partial\psi^*}{\partial t} &= -\frac{\hbar^2}{2m}\Delta\psi^* & \Big|\cdot\psi \end{aligned}\right.$$

$$i\hbar\underbrace{\left\{\psi^*\frac{\partial\psi}{\partial t} + \psi\frac{\partial\psi^*}{\partial t}\right\}}_{=\frac{\partial}{\partial t}\{\psi^*\psi\}} = -\frac{\hbar^2}{2m}\underbrace{\left\{\psi^*\Delta\psi - \psi\Delta\psi^*\right\}}_{=\vec{\nabla}\{\psi^*\vec{\nabla}\psi - \psi\vec{\nabla}\psi^*\}}$$

Continuity equation:

$$\frac{\partial}{\partial t}\underbrace{(\psi^*\psi)}_{=\rho} + \mathrm{div}\underbrace{\frac{\hbar}{2mi}\left\{\psi^*\vec{\nabla}\psi - \psi\vec{\nabla}\psi^*\right\}}_{=\vec{j}} = 0$$

Note: $\psi = \psi^* \longrightarrow \vec{j} = \vec{0}$

Integration:

Dirichlet

$$\frac{\partial}{\partial t}\int d^3x\, \psi^*\psi = -\int d^3x\, \mathrm{div}\,\vec{j} \overset{\text{Gauß}}{=} -\oint_\infty \vec{j}\cdot d\vec{S} \equiv 0$$

$\Rightarrow \int d^3x\, \psi^*\psi = \text{const.}$ → normalization possible

Schrödinger for charged particle moving in electrodynamic field:

minimal coupling

$$\vec{p} \rightarrow \vec{p} - q\vec{A} \xrightarrow{\text{Jordan}} \hat{\vec{p}} \rightarrow \hat{\vec{p}} - q\vec{A} = \frac{\hbar}{i}\vec{\nabla} - q\vec{A}$$

$$E \rightarrow E - q\varphi \xrightarrow{\text{Jordan}} \hat{E} \rightarrow \hat{E} - q\varphi = i\hbar\frac{\partial}{\partial t} - q\varphi$$

Local gauge transformation:

$$\psi(\vec{x},t) = \psi'(\vec{x},t)\, e^{\frac{i}{\hbar} q \underbrace{\Lambda(\vec{x},t)}_{\text{gauge function}}}$$

covariant derivative

$$\boxed{\left(\frac{\hbar}{i}\vec{\nabla} - q\vec{A}(\vec{x},t)\right)}\psi(\vec{x},t) = e^{\frac{i}{\hbar}q\Lambda(\vec{x},t)}\left\{\boxed{\frac{\hbar}{i}\vec{\nabla} + \underbrace{q\vec{\nabla}\Lambda(\vec{x},t) - q\vec{A}(\vec{x},t)}}\right\}\psi'(\vec{x},t)$$

$$\vec{A}'(\vec{x},t) = \vec{A}(\vec{x},t) - \vec{\nabla}\Lambda(\vec{x},t) \quad \Leftarrow \quad = -q\vec{A}'(\vec{x},t)$$

$$\left(i\hbar\frac{\partial}{\partial t} - q\varphi(\vec{x},t)\right)\psi(\vec{x},t) = e^{\frac{i}{\hbar}q\Lambda(\vec{x},t)}\left\{i\hbar\frac{\partial}{\partial t}\underbrace{- q\frac{\partial\Lambda(\vec{x},t)}{\partial t} - q\varphi(\vec{x},t)}\right\}\psi'(\vec{x},t)$$

$$\varphi'(\vec{x},t) = \varphi(\vec{x},t) + \frac{\partial\Lambda(\vec{x},t)}{\partial t} \quad \Leftarrow \quad = -q\varphi'(\vec{x},t)$$

This gauge transformation of $\vec{A}$, φ does not change electromagnetic field:

$$\vec{B} = \mathrm{rot}\,\vec{A},\quad \vec{B}' = \mathrm{rot}\,\vec{A}' = \mathrm{rot}\left(\vec{A} - \vec{\nabla}\Lambda\right) = \mathrm{rot}\,\vec{A} = \vec{B} \quad ✓$$

$$\vec{E} = -\vec{\nabla}\varphi - \frac{\partial\vec{A}}{\partial t},\quad \vec{E}' = -\vec{\nabla}\varphi' - \frac{\partial\vec{A}'}{\partial t} = -\vec{\nabla}\left(\varphi + \frac{\partial\Lambda}{\partial t}\right) - \frac{\partial}{\partial t}\left(\vec{A} - \vec{\nabla}\Lambda\right) \overset{\Uparrow}{=} \vec{E} \quad ✓$$

$$\vec{\nabla}\frac{\partial}{\partial t}\Lambda - \frac{\partial}{\partial t}\vec{\nabla}\Lambda = 0 \quad \Leftarrow \text{ theorem of Schwarz}$$

Schrödinger equation in presence of electromagnetic field:

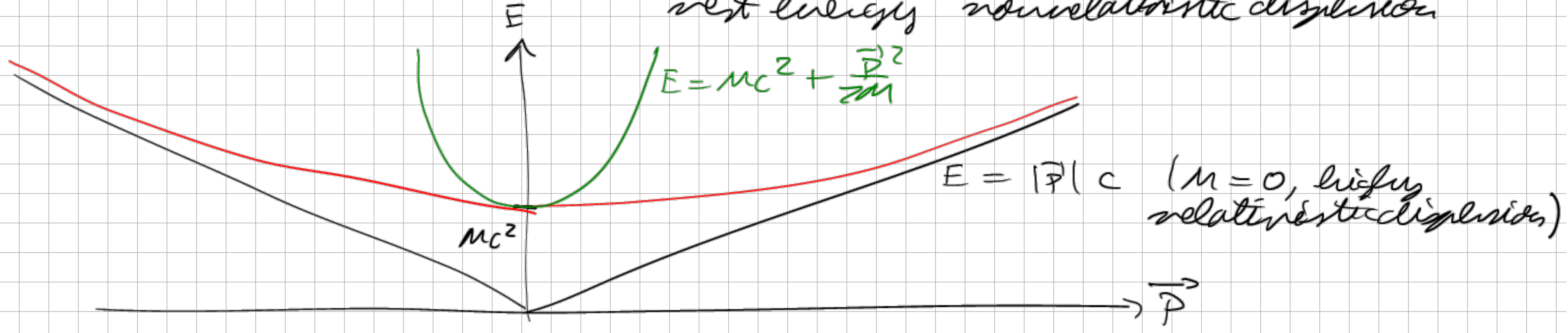
$$i\hbar\frac{\partial}{\partial t}\psi = \left\{-\frac{\hbar^2}{2m}\Delta + i\frac{q\hbar}{m}\vec{A}\cdot\vec{\nabla} + \frac{iq\hbar}{2m}\,\mathrm{div}\,\vec{A} + \frac{q^2\vec{A}^2}{2m} + q\varphi\right\}\psi$$

12.2 Derivation of Klein-Gordon Equation:

Relativistic dispersion: $E = \sqrt{\vec{p}^2 c^2 + m^2 c^4}$

nonrelativistic limit: $|\vec{p}| \ll mc$

$$E = mc^2\sqrt{1+\frac{\vec{p}^2}{m^2c^2}} = mc^2\left\{1+\frac{1}{2}\,\frac{\vec{p}^2}{2m^2c^2}+\dots\right\} = \underbrace{mc^2}_{\text{rest energy}} + \underbrace{\frac{\vec{p}^2}{2m}}_{\text{nonrelativistic dispersion}} + \dots$$



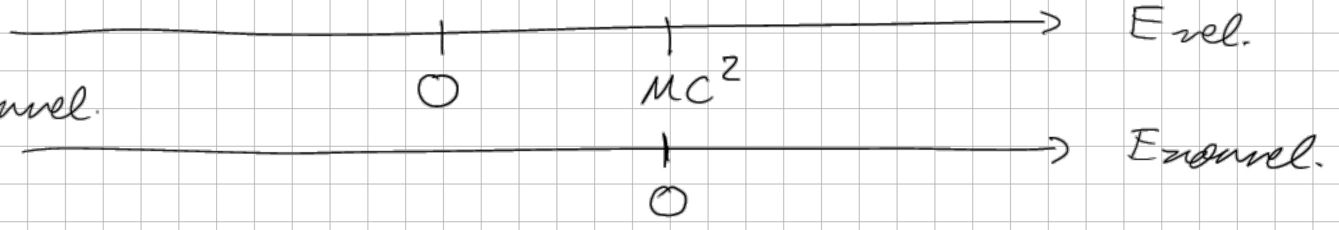
$E^2 = \vec{p}^2c^2 + m^2c^4$ + Jordan rule

$$\left(i\hbar\frac{\partial}{\partial t}\right)^2\Psi = \left\{c^2\left(\frac{\hbar}{i}\vec{\nabla}\right)^2 + m^2c^4\right\}\Psi \Rightarrow \left(\frac{1}{c^2}\frac{\partial^2}{\partial t^2} - \Delta + + \underbrace{\frac{m^2c^2}{\hbar^2}}\right)\Psi(\vec{x},t) = 0$$

$\pi^+ \hat{=}\ m = 140\,\text{MeV} \Rightarrow \lambda_c = 9\,\text{fm}$ $\quad \lambda_c = \frac{h}{mc} = 2\pi\frac{\hbar}{mc}$ "mass term" corresponds to Compton wave length

Nonrelativistic limit of Klein-Gordon equation:

$E_{rel} = mc^2 + E_{nonrel}$



$$\Psi(\vec{x},t) = \psi(\vec{x},t)\, e^{-\frac{i}{\hbar}mc^2 t}$$

$$\frac{\partial \Psi}{\partial t} = \left(-\frac{i}{\hbar}mc^2\psi + \frac{\partial\psi}{\partial t}\right) e^{-\frac{i}{\hbar}mc^2 t}$$

$$\underbrace{\frac{1}{c^2}\cancel{\Big\{}\frac{\partial^2\psi}{\partial t^2}}_{\to\ 0,\ c\to\infty} - 2\frac{i}{\hbar}m\cancel{c^2}\frac{\partial\psi}{\partial t} - \cancel{\frac{m^2c^4}{\hbar^2}\psi}\cancel{\Big\}} e^{-\frac{i}{\hbar}mc^2 t} - \Delta\psi e^{-\frac{i}{\hbar}mc^2 t} + \cancel{\frac{m^2c^2}{\hbar^2}\psi\, e^{-\frac{i}{\hbar}mc^2 t}} = 0 \quad \Big/ \cdot \frac{-\hbar^2}{2m}$$

$$\Rightarrow \quad i\hbar\frac{\partial}{\partial t}\psi = -\frac{\hbar^2}{2m}\Delta\psi \quad ✓$$

12.3 Continuity Equation for Klein-Gordon Equation:

$$\left(\frac{1}{c^2}\frac{\partial^2}{\partial t^2} - \Delta + \frac{m^2c^2}{\hbar^2}\right)\Psi = 0 \qquad \Big|\, \Psi^*$$

$$\left(\frac{1}{c^2}\frac{\partial^2}{\partial t^2} - \Delta + \frac{m^2c^2}{\hbar^2}\right)\Psi^* = 0 \qquad \Big|\, \Psi$$

$$\frac{1}{c^2}\underbrace{\left\{\Psi^*\frac{\partial^2\Psi}{\partial t^2} - \Psi\frac{\partial^2\Psi^*}{\partial t^2}\right\}}_{\frac{\partial}{\partial t}\left\{\Psi^*\frac{\partial\Psi}{\partial t} - \Psi\frac{\partial\Psi^*}{\partial t}\right\}} + \underbrace{\Psi\Delta\Psi^* - \Psi^*\Delta\Psi}_{\vec{\nabla}\left\{\Psi\vec{\nabla}\Psi^* - \Psi^*\vec{\nabla}\Psi\right\}} = 0 \qquad \Big|\, K$$

$$\Rightarrow \qquad \frac{\partial}{\partial t}\rho + \operatorname{div}\vec{j} = 0$$

$$\rho = \frac{K}{c^2}\left\{\Psi^*\frac{\partial\Psi}{\partial t} - \Psi\frac{\partial\Psi^*}{\partial t}\right\}, \qquad \vec{j} = K\left\{\Psi\vec{\nabla}\Psi^* - \Psi^*\vec{\nabla}\Psi\right\}$$

K identified by nonrelativistic limit:

$$\Psi = \psi\, e^{-\frac{i}{\hbar}mc^2 t}, \qquad \Psi^* = \psi^*\, e^{+\frac{i}{\hbar}mc^2 t}$$

$$\rho = \frac{K}{c^2}\left\{ \psi^* \cancel{e^{\frac{i}{\hbar}mc^2t}}\left[-\frac{i}{\hbar}mc^2\psi + \frac{\partial\psi}{\partial t}\right]\cancel{e^{-\frac{i}{\hbar}mc^2t}} - \psi\, \cancel{e^{-\frac{i}{\hbar}mc^2t}}\left[+\frac{i}{\hbar}mc^2\psi^* + \frac{\partial\psi^*}{\partial t}\right]\cancel{e^{\frac{i}{\hbar}mc^2t}}\right\}$$

$$= K\left\{-\frac{2i}{\hbar}m\psi^*\psi + \underbrace{\frac{1}{c^2}\left[\psi^*\frac{\partial\psi}{\partial t} - \psi\frac{\partial\psi^*}{\partial t}\right]}_{\to 0\ ,\ c\to\infty}\right\} = \underbrace{-\frac{2i}{\hbar}mK}_{\overset{!}{=}1}\psi^*\psi \quad \Rightarrow K = -\frac{\hbar}{2im}$$

$$\rho = \frac{i\hbar}{2mc^2}\left\{\Psi^*\frac{\partial\Psi}{\partial t} - \Psi\frac{\partial\Psi^*}{\partial t}\right\}, \quad \vec{j} = \frac{\hbar}{2im}\left\{\Psi^*\vec{\nabla}\Psi - \Psi\vec{\nabla}\Psi^*\right\}$$

different from Schrödinger theory   identical to Schrödinger current

but $Q = \int d^3x\, \rho(\vec{x},t) = \text{const.}$

$$\Psi(\vec{x},t) = \psi(\vec{x})e^{\mp\frac{i}{\hbar}mc^2t} \Rightarrow Q = \underbrace{\int d^3x\, |\psi(\vec{x})|^2}_{=1} = \frac{i\hbar}{2mc^2}\left(\mp\frac{2i}{\hbar}mc^2\right) = \underset{-mc^2}{\overset{mc^2}{\pm}} 1$$

no probability density possible

$$\rho = \frac{i\hbar e}{2mc^2}\left\{\Psi^*\frac{\partial\Psi}{\partial t} - \Psi\frac{\partial\Psi^*}{\partial t}\right\} \Rightarrow \text{charge density}$$

⇒ Klein-Gordon equation describes particles and antiparticles at the same time.

$Q = +e \Rightarrow E \geq mc^2$, $\quad Q = -e \Rightarrow E \leq -mc^2$

12.4 Pionic Atom: Klein-Gordon Equation

- add minimal coupling: covariant derivatives like in Schrödinger theory

$$\left(i\hbar\frac{\partial}{\partial t} - q\varphi\right)^2\Psi = c^2\left(\frac{\hbar}{i}\vec{\nabla} - q\vec{A}\right)^2\Psi + \frac{m^2c^4}{\hbar^2}\Psi$$

- Specialize: $\vec{A} = \vec{0}$, $q = -e$, $\varphi(\vec{r}) = \frac{e}{4\pi\varepsilon_0 r}$

$$\left(i\hbar\frac{\partial}{\partial t}+\underbrace{\frac{e^2}{4\pi\varepsilon_0}}_{=\alpha\hbar c}\frac{1}{r}\right)^2\Psi=-\hbar^2c^2\Delta\Psi+(Mc^2)^2\Psi$$

$\alpha=\frac{e^2}{4\pi\varepsilon_0\hbar c}$ Sommerfeld finestructure constant

separation of space and time: $\Psi(\vec{x},t)=\Psi(\vec{x})\,e^{-\frac{i}{\hbar}Et}$ (stationary state)

$$\left(E+\frac{\alpha\hbar c}{r}\right)^2\Psi(r,\vartheta,\varphi)=-\hbar c^2\underbrace{\left\{\frac{\partial^2}{\partial r^2}+\frac{2}{r}\frac{\partial}{\partial r}-\frac{\hat{L}^2}{\hbar^2r^2}\right\}}_{=\Delta}\Psi(r,\vartheta,\varphi)+M^2c^4\,\Psi(r,\vartheta,\varphi)$$

another separation ansatz: $\Psi(r,\vartheta,\varphi)=f(r)\;Y_{\ell m}(\vartheta,\varphi)$

$$\left(E^2+\frac{2\alpha\hbar cE}{r}+\frac{\alpha^2\hbar^2c^2}{r^2}\right)\underset{u(r)}{\cancel{f(r)}}=-\hbar^2c^2\left(\frac{\partial^2}{\partial r^2}+\underline{\cancel{\frac{2}{r}\frac{\partial}{\partial r}}}-\frac{\ell(\ell+1)}{r^2}\right)\underset{u(r)}{\cancel{f(r)}}+M^2c^4\,\underset{u(r)}{\cancel{f(r)}}\;\Big|\cdot\frac{1}{2Mc^2}$$

ansatz: $f(r)=\frac{u(r)}{r}$

$$\left\{-\frac{\hbar^2}{2M}\frac{\partial^2}{\partial r^2}+\boxed{\hbar^2\,\frac{\ell(\ell+1)-\alpha^2}{2Mr^2}-\frac{\alpha\hbar cE}{Mc^2}\;\frac{1}{r}}\right\}u(r)=\frac{E^2-M^2c^4}{2Mc^2}\,u(r)$$

radial Klein-Gordon equation for hydrogen atom

$$\left\{-\frac{\hbar^2}{2M}\frac{\partial^2}{\partial r^2}+\boxed{\underbrace{\hbar^2\,\frac{\ell'(\ell'+1)}{2Mr^2}}_{\text{centrifugal barrier}}-\underbrace{\frac{\hbar c\alpha'}{r}}_{\text{coulomb potential}}}\right\}u(r)=E'\,u(r)$$

	Schrödinger	Klein-Gordon
r^0	E'	$\frac{E^2-M^2c^4}{2Mc^2}$
r^{-1}	α'	$\alpha\,\frac{E}{Mc^2}$
r^{-2}	$\ell'(\ell'+1)$	$\ell(\ell+1)-\alpha^2$

Solution of Schrödinger problem: $E' = -\frac{1}{2} mc^2 \alpha'^2 \frac{1}{n'^2}$; $\underbrace{n'}_{\text{main quantum number}} = \underbrace{n'_r}_{\text{radial quantum number}} + l' + 1$

$n'_r = 0, 1, 2, \ldots$

n'	n'_r	l'
1	0	0
2	1	0
2	0	1
3	2	0
3	1	1
3	0	2

for a given n we have that l' varies from 0 to $n'-1$

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1) $l'(l'+1) = l(l+1) - \alpha^2 \Rightarrow l'^2 + l' - l(l+1) + \alpha^2 = 0$

$l' = -\frac{1}{2} + \sqrt{(l+\frac{1}{2})^2 - \alpha^2}$ not integer

$\Rightarrow n' = n_r + l' + 1 = n_r + \frac{1}{2} + \sqrt{(l+\frac{1}{2})^2 - \alpha^2}$

$n_r = 0, 1, 2, \ldots$ integer but n' is not integer

2) $E' = -\frac{1}{2} mc^2 \alpha'^2 \frac{1}{n'^2} \Rightarrow \frac{E^2 - m^2c^4}{2mc^2} = -\frac{1}{2} mc^2 \alpha^2 \frac{E^2}{m^2c^4} \frac{1}{[n_r + \frac{1}{2} + \sqrt{(l+\frac{1}{2})^2 - \alpha^2}]^2}$

$$\Rightarrow E = \frac{mc^2}{\sqrt{1 + \frac{\alpha^2}{[n_r + \frac{1}{2} + \sqrt{(l+\frac{1}{2})^2 - \alpha^2}]^2}}} \quad ; \quad \left(\begin{aligned} n' &= n_r + \frac{1}{2} + \sqrt{(l+\frac{1}{2})^2 - \alpha^2} \\ &\approx n_r + \frac{1}{2} + (l + \frac{1}{2}) - \frac{\alpha^2}{2(l+\frac{1}{2})} + \ldots \end{aligned} \right.$$

Nonrelativistic limit: $\alpha \approx \frac{1}{137} \ll 1$) $n' = \underbrace{n_r + l + 1}_{= n} - \frac{\alpha^2}{2(l+\frac{1}{2})} + \dots$

$$E \approx mc^2 \Big\{ 1 - \frac{\alpha^2}{2n^2} - \frac{\alpha^4}{2n^4} \Big[\frac{n}{l + \frac{1}{2}} - \frac{3}{4} \Big] + \dots \Big)$$

$$E_{Dirac} \approx mc^2 \Big\{ 1 - \frac{\alpha^2}{2n^2} - \frac{\alpha^4}{2n^4} \Big[\frac{n}{j + \frac{1}{2}} - \frac{3}{4} \Big] + \dots \Big\}$$

Wrong prediction of finestructure due to missing spin 1/2 in Klein-Gordon theory