Skammtafræði 2

Afstæðar jöfnur

Fjöleindakerfi

Rafsegulsvið

Hreyfijöfnur fyrir Lorentz-óbreytanleg kerfi

Jafna Schrödingers er ekki leidd út frá jöfnu Newtons

Tilrauna staðreyndir

⇣

Tilgáta um hreyfijöfnu

↕

Samanburður við tilraunir

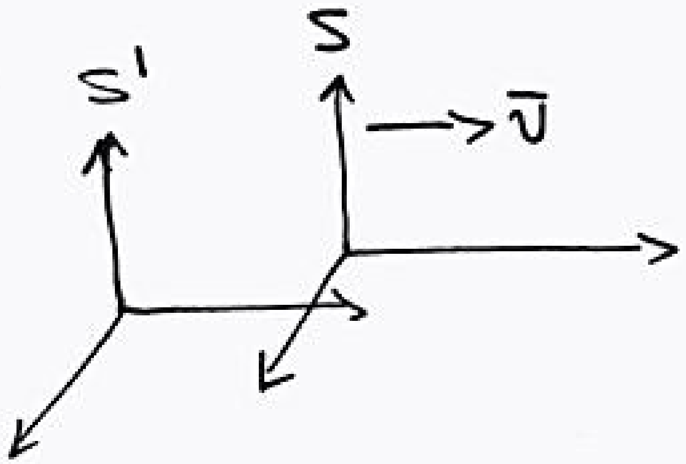
Hvers vegna viljum við skoða Lorentz-óbreytanl. framsetn.

* Viljum skilja hvað bætist við Schrödinger lýsinguna, hverjar eru takmarkanir hennar?

* Betri skilningur á skammtafr. og lýsingu Schrödingers

* Lorentz-óbreytanl. lýsing . . . hvað svo?

Galilei-óbreytanleiki — frjáls eind



$$\boxed{\begin{aligned}\bar{x}' &= \bar{x} + \bar{v}\cdot t \\ \bar{p}' &= \bar{p} + m\bar{v}\end{aligned}}$$

$$E = \frac{p^2}{2m}$$

$$E' = \frac{p^2}{2m} + \bar{p}\cdot\bar{v} + \frac{mv^2}{2} = \frac{(p')^2}{2m}$$

↑ orkan er óbreytanleg $E = E'$

$\boxed{\text{Gildir líka almennt}}$

$$H = H(x,p) \qquad \dot{x} = \frac{\partial H}{\partial p} \qquad \dot{p} = -\frac{\partial H}{\partial x} = 0$$

$$\Rightarrow H = H(p)$$

Tilraunaniðurstöður

t.d. $E = \hbar\omega$ . . . .

í gegnum skömmtunar-kröfur $[\hat{x},\hat{p}] = i\hbar$ leiða til hreyfijöfnu fyrir bylgjuföll í xt-rúmi

$$\boxed{i\hbar\partial_t \psi(\bar{x}t) = \frac{1}{2m}\left(-i\hbar\bar{\nabla}\right)^2\psi(\bar{x}t)}$$

frjálsa Schrödingerjafnan

$\boxed{\text{Sannreynd aftur í tilraunum}}$

Heildarorka Lorentz-óbreytanlegrar eindar er

$$\boxed{E = \sqrt{p^2c^2 + m^2c^4}}$$

því gætu okkur dottið í hug ýmsar aðferðir t.þ.a. finna samsvarandi hreyfijöfnu

Sumar gætu lýst einhverjum fyrirbærum í náttúrunni, en aðrar engum

1. tilraun

Notum eins og fyrir Schrödingerjöfnuna

$$E \to i\hbar\partial_t \,, \quad \bar{p} \to -i\hbar\bar{\nabla}$$

og $E = \sqrt{p^2c^2 + m^2c^4}$

Hvað þá með

$$\boxed{i\hbar\partial_t\psi = H\psi = \sqrt{m^2c^4 - \hbar^2c^2\nabla^2}\,\psi}$$

$\uparrow$

jafna af óendanlegri gráðu $\to$ óstaðbundin upphafsstilyrði erfið

Skoðum aðra útfærslu

Bylgjufall eða jöfnu má skoða í skriðþungarúminu

$$\boxed{\psi(\bar{x}t) = \frac{1}{(2\pi)^3}\int d\bar{p}\, e^{\frac{i\bar{p}\cdot\bar{x}}{\hbar}}\, \psi(\bar{p},t)}$$

Jafna Schrödingers væri þá

$$\boxed{i\hbar\partial_t \psi(\bar{p}t) = \frac{p^2}{2m}\psi(\bar{p}t)}$$

og því dytti okkur í hug að reyna

$$\boxed{i\hbar\partial_t \psi(\bar{p}t) = \sqrt{p^2c^2 + m^2c^4}\,\psi(\bar{p}t)}$$

Ef við ummyndum þessa jöfnu til baka í staðarrúmið fæst:

$$\boxed{\begin{aligned} i\hbar\partial_t \psi(\bar{x}t) &= \int d\bar{x}'\, K(\bar{x}-\bar{x}')\psi(\bar{x}'t) \\ K(\bar{x}-\bar{x}') &= \int \frac{d\bar{p}}{(2\pi\hbar)^3}\, e^{i\bar{p}\cdot(\bar{x}-\bar{x}')/\hbar}\, c\sqrt{p^2+m^2c^2} \end{aligned}}$$

Heildis afleiðujafna, óstaðbundin

↑

Ef $\bar{x}$ er innan $\frac{\hbar}{mc}$ frá $\bar{x}'$ er K ekki smátt

munur á meðhöndlun tíma- og rúm hnits

brýtur afst. orsaka samband

2. tilraun

notum $E \to i\hbar\partial_t$, $\bar{p} \to -i\hbar\bar{\nabla}$
en núna
$$E^2 = p^2c^2 + m^2c^4$$

Við munum greinilega purfa að fást við neikvæða orku!

$$\boxed{\left(\frac{i\hbar}{c}\partial_t\right)^2 \psi(\bar{x}t) = \left(\frac{\hbar}{i}\bar{\nabla}\right)^2 \psi(\bar{x}t) + m^2c^2\psi(\bar{x}t)}$$

Eða

$$\left\{\frac{1}{c^2}\frac{\partial^2}{\partial t^2} - \nabla^2 + \left(\frac{mc}{\hbar}\right)^2\right\}\psi(\bar{x}t) = 0$$

Klassísk bylgjujafna (skalar bylgja) með massalið

Strengur með massa

Klein-Gordon jafnan

Við munum að bylgjujafnan er
Lorentz-óbreytanleg

Eins er $(\bar{A}, \phi)$ fjórvigur og
Klein-Gordon jafnan fyrir
eind í rafsegulsviði er

$\longrightarrow$ $\boxed{\psi'(\bar{x}'t') = \psi(\bar{x}t)}$

$$\boxed{\frac{1}{c^2}\left\{i\hbar\partial_t - e\phi(\bar{x}t)\right\}^2\psi(\bar{x}t) = \left\{\left[\frac{\hbar}{i}\bar{\nabla} - \frac{e}{c}\bar{A}(\bar{x}t)\right]^2 + m^2c^2\right\}\psi(\bar{x},t)}$$

Annars stigs jafna

upphafsskilyrði $\underbrace{\psi(\bar{x}t) \text{ og } \partial_t\psi(\bar{x}t)}_{\text{tvöfalt magn m.v. Schröd..}}$

$$E = \pm c\sqrt{p^2 + m^2c^2}$$

$\longrightarrow$ $\boxed{\text{mun leiða til andeinda}}$

Straumur og hleðsla

Nú vill svo til að

$$\boxed{\partial_t \int d\bar{x}\, \psi^*(\bar{x}t)\,\psi(\bar{x}t) \neq 0}$$

því er $\psi^*\psi$ <u>ekki</u> túlkanlegt sem líkinda þéttleiki

<u>Athugum</u>

$$-\hbar^2 \partial_t^2 \psi = m^2c^4\psi - \hbar^2c^2\nabla^2\psi$$

$$-\hbar^2 \partial_t^2 \psi^* = m^2c^4\psi^* - \hbar^2c^2\nabla^2\psi$$

margföldum með ψ^* eða ψ og finnum mismuninn

þá fæst

$$-\hbar^2\partial_t\left\{\psi^*\partial_t\psi - \psi\partial_t\psi^*\right\}$$

$$= -\hbar^2c^2\,\bar{\nabla}\cdot\left\{\psi^*\bar{\nabla}\psi - \psi\bar{\nabla}\psi^*\right\}$$

Berum saman við samfellnijöfnuna

$$\boxed{\partial\rho(\bar{x}t) + \bar{\nabla}\cdot\bar{J}(\bar{x}t) = 0}$$

þá sést að

$$\boxed{\begin{aligned} \rho(\bar{x}t) &= \frac{i\hbar}{2mc^2}\left\{\psi^*\partial_t\psi - \psi\partial_t\psi^*\right\} \\ \bar{J}(\bar{x}t) &= \frac{\hbar}{2im}\left\{\psi^*\bar{\nabla}\psi - \psi\bar{\nabla}\psi^*\right\} \end{aligned}}$$

Eða með rafsegulsviði

(8)

$$\boxed{\bar{J}(\bar{x}t) = \frac{1}{2m}\left[\psi^*\left(\frac{\hbar}{i}\bar{\nabla} - \frac{e}{c}\bar{A}\right)\psi + \psi\left(-\frac{\hbar}{i}\bar{\nabla} - \frac{e}{c}\bar{A}\right)\psi^*\right]}$$

rétt eins og fyrir jöfnu Schrödingers, en nú er

$$\boxed{\rho(\bar{x}t) = \frac{1}{2mc^2}\left\{\psi^*\left(i\hbar\partial_t - e\phi\right)\psi + \psi\left(-i\hbar\partial_t - e\phi\right)\psi^*\right\}}$$

J er ekki líkindastraumþéttleiki og ρ er ekki líkindaþéttl.

$e\rho \leftarrow$ hleðsluþéttleiki

$e\bar{J} \leftarrow$ rafstraumþéttleiki

Frjáls ástönd með neikvæða og jákvæða orku

Í kerfi S: $p = 0$

$$\psi(\bar{x}t) = e^{-imc^2 t/\hbar}$$

ögn með massa mc^2

Athugið að normun er ekki kassanormun hér

Í S' sem hreyfist með $-\bar{v}$ m.v. S er

$$\boxed{\psi'(\bar{x}', t') = e^{i(\bar{p}\cdot\bar{x}' - E_p t')/\hbar} = \psi(\bar{x}t)}$$

fjórvigur

$$\bar{p}\cdot\bar{x}' - E_p t' = -mc^2 t$$

$$E_p = \frac{mc^2}{\sqrt{1-v^2/c^2}}$$

$$\bar{p} = \frac{m\bar{v}}{\sqrt{1-v^2/c^2}}$$

$$\rho(\bar{x}t) = 1, \quad \rho(\bar{x}'t') = \frac{E_p}{mc^2}$$

$$\bar{j}(\bar{x}'t') = \frac{\bar{p}}{m} = \frac{\bar{p}c^2}{E_p}\rho(\bar{x}'t') = \bar{v}\rho(\bar{x}'t')$$

rel. hraði

þéttleiki

Neikvæð orka

Í S með $\bar{p}=0$

$$\psi(\bar{x}t) = e^{imc^2t/\hbar}$$

$$\rightarrow \rho(\bar{x}t) = -1$$

$$\bar{J}(\bar{x}'t') = -\frac{\bar{p}}{m} = \frac{\bar{p}c^2}{E_p}\rho(\bar{x}'t')$$

Eind með orku $-mc^2$ er andeind með orku mc^2

Andeind með hraða $\bar{v}$ $\rightarrow$ straumur í hina áttina

Andeind er eind með orku $-E_p$ og skriðþunga $-\bar{p}$

Fyrir hlaðna eind er formerkið sett á hleðsluna

(Skilgreint þannig)

Með rafsegulsviði

$$\boxed{\frac{1}{c^2}\left\{i\hbar + e\phi\right\}^2 \psi^* = \left\{\left(\frac{\hbar}{i}\bar{\nabla} + e\bar{A}\right)^2 + m^2c^2\right\}\psi^*}$$

ψ^* er lausn KG-jöfnunar með $-e$ og sama m

$$\rho(\bar{x}t) = -\rho_c(\bar{x}t)$$

Charge-Conjugate solution
Hleðslu samoka lausn

$$j_c(\bar{x}t) = -j(\bar{x}t)$$

Lausnir má staðla með

$$\boxed{\int \rho(\bar{x}t)\, d\bar{x} = \pm 1}$$

tímaóháð

$$\int \rho(\bar{x}t)\, d\bar{x} = -\int \rho_c(\bar{x}t)\, d\bar{x}$$

fyrsta stigs KG-jafna

Skilgreinum $\boxed{\psi^0(\bar{r}t) = \left\{\partial_t + \frac{ie}{\hbar}\phi(\bar{r}t)\right\}\psi(\bar{r}t)}$ ①

þá verður KG ②

$$\boxed{\left\{\partial_t + \frac{ie}{\hbar}\phi\right\}\psi^0(\bar{r}t) = \left\{c^2\left(\bar{\nabla} - \frac{ie\bar{A}}{\hbar c}\right)^2 - \frac{m^2c^4}{\hbar^2}\right\}\psi(\bar{r}t)}$$

① og ② eru tengdar 1. afleiðujöfnur, jafngildar KG

Innleiðum

$$\left.\begin{aligned} \varphi &= \frac{1}{2}\left\{\psi + \frac{i\hbar}{mc^2}\psi^0\right\} \\ \chi &= \frac{1}{2}\left\{\psi - \frac{i\hbar}{mc^2}\psi^0\right\} \end{aligned}\right\} \Rightarrow \boxed{\begin{aligned} \left\{i\hbar\partial_t - e\phi\right\}\varphi &= \frac{1}{2m}\left\{\frac{\hbar}{i}\bar{\nabla} - \frac{e}{c}\bar{A}\right\}^2(\varphi+\chi) + mc^2\varphi \\ \left\{i\hbar\partial_t - e\phi\right\}\chi &= \frac{-1}{2m}\left\{\frac{\hbar}{i}\bar{\nabla} - \frac{e}{c}\bar{A}\right\}^2(\varphi+\chi) - mc^2\chi \end{aligned}}$$

þar má gera „samhverfari með"

$$\boxed{\Psi(\bar{r}t) \equiv \begin{pmatrix} \varphi(\bar{r}t) \\ \chi(\bar{r}t) \end{pmatrix}} \quad \text{og} \quad \boxed{\tau_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \ \tau_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \ \tau_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}}$$

Pauli τ ......

$$\boxed{i\hbar\partial_t \Psi(\bar{r}t) = \left\{\frac{1}{2m}\left(\frac{\hbar}{i}\bar{\nabla} - \frac{e}{c}\bar{A}\right)^2(\tau_3 + i\tau_2) + mc^2\tau_3 + e\phi\right\}\Psi(\bar{r}t)}$$

<u>Jafngild KG</u> <u>Ekki spunaþáttur</u> heldur <u>hleðsluþáttur</u>

því $\boxed{\rho(\bar{r}t) = |\varphi|^2 - |\chi|^2 = \Psi^+\tau_3\Psi}$

$$\rho = (\varphi^*, \chi^*)\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}\begin{pmatrix} \varphi \\ \chi \end{pmatrix} = |\varphi|^2 - |\chi|^2$$

Straumurinn verður

$$\boxed{\bar{J}(\bar{r}t) = \frac{\hbar}{2im}\left\{\Phi^{+}\tau_3(\tau_3+i\tau_2)\bar{\nabla}\Phi - (\bar{\nabla}\Phi^{+})\tau_3(\tau_3+i\tau_2)\Phi\right\} - \frac{e\bar{A}}{mc}\Phi^{+}\tau_3(\tau_3+i\tau_2)\Phi}$$

Lítur illilega út en

$$\tau_3 + i\tau_2 = \begin{pmatrix} 1 & 1 \\ -1 & -1 \end{pmatrix}$$

$$\tau_3(\tau_3+i\tau_2) = \begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix} = (\tau_1 + \mathbb{1})$$

$$\tau_3^{+} = \tau_3 \qquad \tau_2^{+} = -\tau_2$$

Stöðlunarkrafan er því

$$\int d\bar{r}\, \Phi^{+}\tau_3\Phi = \pm 1$$

sem skilgreinir innfeldi

$$\boxed{\langle\Phi|\Phi'\rangle \equiv \int d\bar{r}\, \Phi^{+}\tau_3\Phi'}$$

Hreyfijafnan er

$$\boxed{i\hbar\partial_t \Psi = H\Psi}$$

með

$$H = \frac{1}{2m}\left(\bar{p} - \frac{e}{c}\bar{A}\right)^2(\tau_3 + i\tau_2) + e\phi + mc^2\tau_3$$

$$H^+ = \frac{1}{2m}\left(\bar{p} - \frac{e}{c}\bar{A}\right)^2(\tau_3 - i\tau_2) + e\phi + mc^2\tau_3$$

Nú er $(\tau_3 + i\tau_2)^+ = \tau_3 - i\tau_2$

og $\tau_3(\tau_3 + i\tau_2)\tau_3 = \tau_3 + i\tau_3\tau_2\tau_3 = \tau_3 - i\tau_3\tau_3\tau_2$

$$= \tau_3 - i\tau_2$$

passar líka

þessvegna

$$\langle\Psi'|H|\Psi\rangle = \int d\bar{r}\, \Psi'^+\tau_3 H\Psi = \int d\bar{r}\, \Psi^{*+} H^+\tau_3^+ \Psi'$$

$$= \langle\Psi|H^+|\Psi'\rangle^* \qquad \text{eða} \qquad H = \tau_3 H^+\tau_3$$

$\bar{p}^{+} = \bar{p}$, en $\bar{p}^{*} = -\bar{p}$ pui sést ad

$$H^{*}(e) = \frac{1}{2m}\left(-\bar{p} - \frac{e}{c}\bar{A}\right)^{2}(\tau_3 + i\tau_2) + e\phi + mc^{2}\tau_3$$

Einnig $\boxed{\Psi_c = \tau_1 \Psi^{*}}$

pui mā finna ad

charge conjugation

$$\boxed{-i\hbar\partial_t \Psi_c = H^{*}(-e)\Psi_c}$$

frjáls ögn

Bylgjufall staðlað á „einingar" þéttleika

$$\psi = \sqrt{\frac{mc^2}{E_p}}\, e^{i(\bar{p}\cdot\bar{r} - E_p t)/\hbar}$$

jákvæð orka

Fyrir tveggja þátta KG-jöfnuna fæst

$$\boxed{\begin{aligned} \Psi^{(+)}(\bar{r}t) &= \frac{1}{2}\frac{1}{\sqrt{E_p mc^2}}\begin{pmatrix} mc^2 + E_p \\ mc^2 - E_p \end{pmatrix} e^{\frac{i}{\hbar}(\bar{p}\cdot\bar{r} - E_p t)} \\ \Psi^{(-)}(\bar{r}t) &= \frac{1}{2}\frac{1}{\sqrt{E_p mc^2}}\begin{pmatrix} mc^2 - E_p \\ mc^2 + E_p \end{pmatrix} e^{-\frac{i}{\hbar}(\bar{p}\cdot\bar{r} - E_p t)} \end{aligned}}$$

Neikvæð orka

$$\boxed{\Psi^{(+)} = \tau_1 \Psi^{(-)}}$$

Athugum hvað gerist þegar $v/c \to 0$

$$E_p = \sqrt{c^2p^2 + m^2c^4} = mc^2\sqrt{\frac{c^2p^2}{m^2c^4} + 1}$$

$$\simeq mc^2\left(1 + \frac{1}{2}\frac{p^2}{m^2c^2} + \cdots\right)$$

$$= mc^2 + \frac{1}{2}mv^2 + \cdots$$

$$\Psi^{(+)} \to \begin{pmatrix} 1 \\ -\frac{v^2}{4c^2} \end{pmatrix} \cdots$$

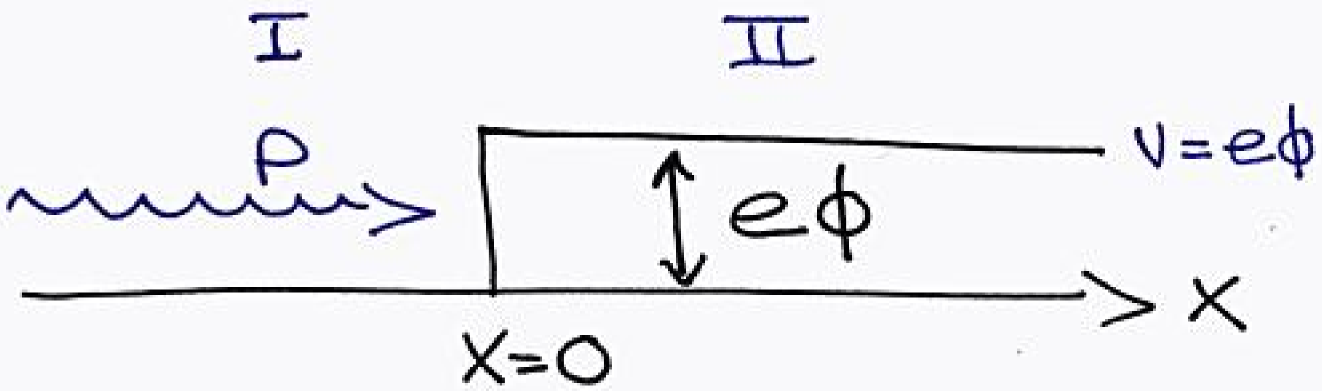
Bera saman við $\begin{pmatrix} \varphi \\ \chi \end{pmatrix}$
Hvertandi liðir með
andhverfa hleðslu

$$\Psi^{(-)} \to \begin{pmatrix} -\frac{v^2}{4c^2} \\ 1 \end{pmatrix} \cdots$$

fyrir φ og χ^* fæst
Schrödinger jöfnur fyrir
eind með e og $-e$

Mótsögn Kleins

Skoðum árekstur við þrep



KG-jafnan er þá

$$\boxed{(i\hbar\partial_t - V)^2\psi = m^2c^4\psi - c^2\hbar^2\partial^2_{x^2}\psi}$$

á svæði (I)

$$\psi_I = \left(a e^{i\frac{p}{\hbar}x} + b e^{-i\frac{p}{\hbar}x}\right) e^{-i\frac{E_p t}{\hbar}}$$

Innkoma frá vinstri

á svæði (II)

$$\psi_{II} = d e^{iKx} e^{-i\frac{E_p t}{\hbar}}$$

ψ og ψ' eru samfelld í $x=0$

eða

$$\left(\frac{\psi_I'}{\psi_I}\right)_{x=0} = \left(\frac{\psi_{II}'}{\psi_{II}}\right)_{=0}$$

Sem gefur

$$\frac{ia\frac{p}{\hbar} - ib\frac{p}{\hbar}}{a+b} = iK$$

$$\hbar(Ka+Kb) = pa - pb$$

$$(\hbar K + p)b = (p - \hbar K)a$$

einnig $a+b=d$ eða $\frac{d}{a} = \frac{b}{a} + 1$

$$\frac{b}{a} = \frac{p-\hbar K}{p+\hbar K} \qquad \frac{d}{a} = \frac{2p}{p+\hbar K}$$

Hreyfijafnan gefur

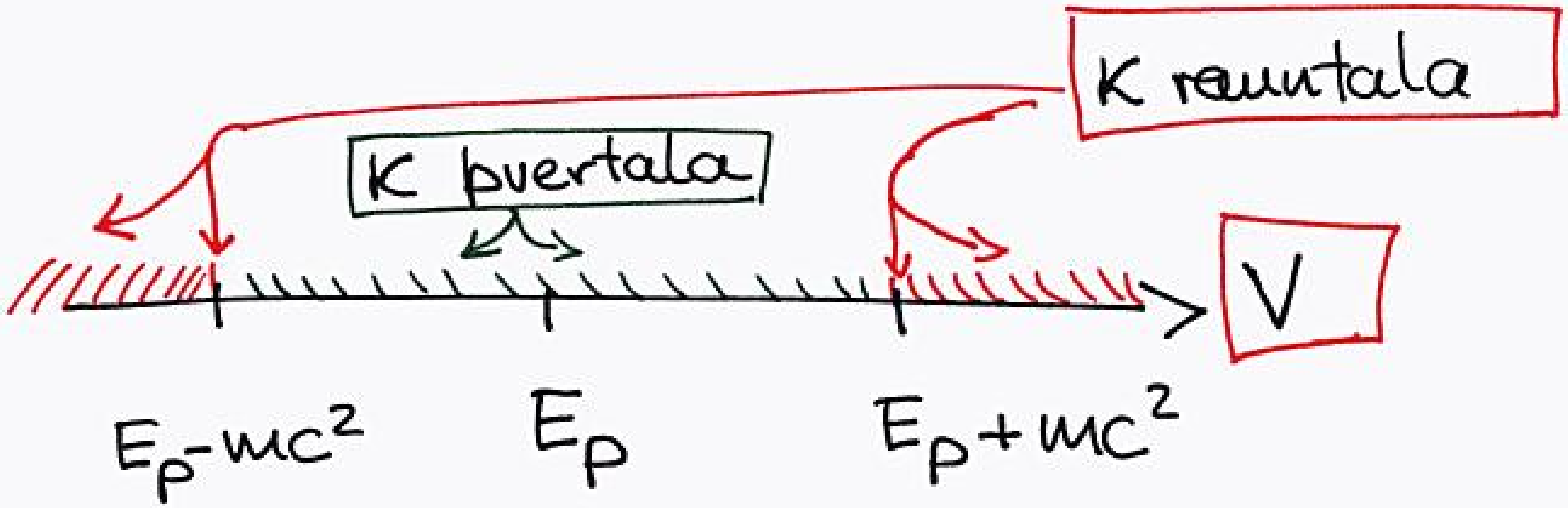
$$(E_p - V)^2\psi = (m^2c^4 + c^2\hbar^2K^2)\psi$$

eða

$$c^2\hbar^2K^2 = (E_p-V)^2 - m^2c^4$$

$$\boxed{K = \frac{\sqrt{(E_p-V)^2 - m^2c^4}}{c\hbar}}$$

Skoðum orkuskala



fyrir $E_p - V > mc^2$ eða $(V < E_p - mc^2)$

er K rauntala, hluti bylgju kemst áfram og hluti endurkastast

sama og fyrir Schrödinger jöfnuna

Ef $(E_p - V)^2 < m^2c^4$ þá $E_p - mc^2 < V < E_p + m c^2$

$$K = i\kappa = i\,\frac{\sqrt{m^2c^4 - (E_p - V)^2}}{\hbar c}$$

$$|\psi_{II}|^2 = |d|^2 e^{-2\kappa x}$$

$$\rho = \frac{1}{2mc^2}\left\{\psi^*(i\hbar\partial_t - V)\psi - \psi(-i\hbar\partial_t - V)\psi^*\right\}$$

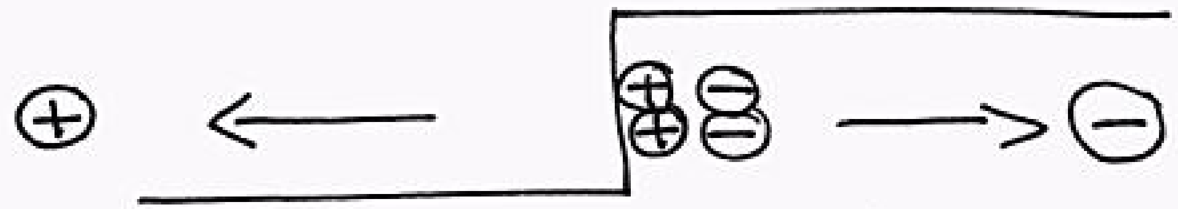
$$= \frac{(E_p - V)}{mc^2}|d|^2 e^{-2\kappa x} \leftarrow$$ dofnunarlausn í þrepi

En hleðslan er neikvæð eða jákvæð eftir því hvort $E_p > V$ eða $E_p < V$

Sterkt mótti $V > E_p + mc^2$

Búunst við dotunarlausn,

en k er rauntala



Grúpuhraði bylgjuna á II

$$v_g = \frac{\partial E_p}{\partial(\hbar k)} \quad \text{og} \quad (E_p - V)^2 = m^2c^4 + \hbar^2c^2k^2$$

$$\rightarrow \quad v_g = \frac{c^2\hbar k}{E_p - V}$$

$E_p < V \rightarrow \underline{k<0}$ til þess að hafa straum til hogri

Líkur á endurkasti til vinstri $|b|^2$

og $\frac{b}{a} > 1$

meira endurkastast enn kemur inn

$$\rho_{II} = \frac{1}{2mc^2}\left(\psi_{II}^*(i\hbar\partial_t - V)\psi_{II} - \psi_{II}(-i\hbar\partial_t - V)\psi_{II}^*\right)$$

$$= \frac{(E_p - V)}{mc^2} < 0 \qquad \text{en} \qquad \rho_I > 0$$

Við þröskuldinn myndast eindar-andeindarpör

Andeindirnar dragast að háa mættinu!
vegna $-e\phi$ stöðuorku þeirra

Í raun má sjá að hvert lítið mætti blandar andeindaþætti inn í ástöndin

Bundin ástönd í Coulomb-mætti $(\pi^- p)$

Bundind eind með jákvæða orku

$$\to \quad \psi(\bar{r}t) = e^{-iEt/\hbar}\,\psi(\bar{r})$$

$$\left(i\hbar\partial_t + \frac{ze^2}{r}\right)^2 \psi(\bar{r}t) = \left(m^2c^4 - \hbar^2c^2\nabla^2\right)\psi(\bar{r}t)$$

verður

$$\left(E + \frac{ze^2}{r}\right)^2 \psi(\bar{r}) = \left(m^2c^4 - \hbar^2c^2\nabla^2\right)\psi(\bar{r})$$

Gerum ráð fyrir

$$\psi(\bar{r}) = \sum_{\ell} R_\ell(r)\, Y_{\ell m}(\Omega)$$

Hleðslan

$$e\rho(\vec{r}) = \frac{e(E - e\phi(r))}{mc^2} |\psi(\vec{r})|^2$$

Nærri kjarnanum þ.s. $E < e\phi(r)$
er hleðslu þéttleikinn með andhverfa
hleðslu

Mottið skautar rúmið!

er ekki heldur
Lorentz óbreytileg
framsetning mættis
⋮
seinkun . . . . . .

$\frac{Ze^2}{r}$ er ekki virka mættið
fyrir eina eind →
fjöleindafræði

Berum saman við
jöfnu Schrödingers

$$\boxed{E' R_{l'} = -\frac{\hbar^2}{2m'}\frac{1}{r^2}\frac{d}{dr}\left(r^2 \frac{d}{dr} R_{l'}\right) + \frac{\hbar^2}{2m'}\frac{l'(l'+1)}{r^2} R_{l'} + \frac{ze^2}{r} R_{l'}}$$

Jöfnurnar hafa sömu gerð ef við margföldum Schrödinger með $2m'$ og KG með -1
og samsömum

$$2m' = \frac{2E}{c^2} \qquad 2m'E' = \frac{E^2}{c^2} - m^2c^2$$

$$l'(l'+1) = l(l+1) - \left(\frac{ze^2}{\hbar c}\right)^2$$

$$2\frac{EE'}{c^2} = \frac{E^2}{c^2} - m^2c^2 \qquad (*)$$

Höfum

$$\left(E + \frac{Ze^2}{r}\right)^2 \psi(\bar{r}) = (m^2c^4 - \hbar^2 c^2 \nabla^2)\psi(\bar{r})$$

gerum ráð fyrir

$$\psi(\bar{r}) = \sum_{\ell} R_{\ell}(r)\, Y_{\ell m}(\Omega)$$

þá fæst

$$\nabla^2 \psi = \sum_{\ell} \left\{ \frac{1}{r^2}\frac{d}{dr}\left(r^2 \frac{d}{dr} R_{\ell}\right) - \frac{\ell(\ell+1)}{r^2} R_{\ell} \right\} Y_{\ell m}(\Omega)$$

og því fyrir KG-jöfnuna (útþáttun)

$$\boxed{\left(E + \frac{Ze^2}{r}\right)^2 R_{\ell} - m^2c^4 R_{\ell} + \hbar^2 c^2 \frac{1}{r}\frac{d}{dr}\left(r^2 \frac{d}{dr} R_{\ell}\right) - \frac{\hbar^2 c^2\, \ell(\ell+1)}{r^2} R_{\ell} = 0}$$

$$\rightarrow \frac{\hbar^2}{r^2}\frac{d}{dr}\left(r^2\frac{d}{dr}R_{\ell}\right) - \left(\frac{\hbar^2 \ell(\ell+1)}{r^2} - \frac{Z^2 e^4}{r^2}\right)R_{\ell} + \frac{2EZe^2}{c^2 r} R_{\ell} + \left(\frac{E^2}{c^2} - m^2c^2\right)R_{\ell} = 0$$

eða

$$E' = \frac{E}{2} - \frac{m^2c^4}{2E}$$

Við þekkjum lausnir Schrödingerjöfnunnar og vitum að

$$E' = -\frac{Z^2e^4m'}{2\hbar^2(n')^2} = -\frac{Z^2e^4}{2\hbar^2(n')^2}\frac{E}{c^2}$$

því $2m' = \frac{2E}{c^2}$

Notum nú (*) til að fá

$$-2\frac{Z^2e^4}{2\hbar^2(n')^2}\frac{E^2}{c^2} = E^2 - m^2c^4$$

$$\hookrightarrow \quad E = \frac{mc^2}{\left\{1 + \frac{Z^2e^4}{\hbar^2(n')^2c^2}\right\}^{1/2}}$$

Við höfðum líka $n' = \ell' + \nu + 1$, $\nu = 0, 1, 2, \dots$

en núna var

$$\ell'(\ell'+1) = \ell(\ell+1) - \left(\frac{Ze^2}{\hbar c}\right)^2 = \ell(\ell+1) - Z^2\alpha^2$$

þar sem $\alpha = \frac{e^2}{\hbar c}$ og

$$\ell' = -\frac{1}{2} \pm \sqrt{\left\{(\ell + 1/2)^2 - (Z\alpha)^2\right\}}$$

ℓ' er því ekki endilega heiltala, Lenz-vigur er ekki varðveittur, Coulomb-brautirnar lokast ekki. Slysamargfeldni Schrödinger lýsingunnar á Coulomb kerfinu er horfin

$$n' = \underbrace{l+\nu+1}_{n} + (l'-l) = n - \frac{1}{2} + \sqrt{(l+\tfrac{1}{2}) - (Z\alpha)^2} - l$$ (30)

Orkan er bæði háð nogl $E = E(n,l)$

$$\boxed{E = mc^2 \left\{ 1 + \frac{Z^2 e^4}{\hbar^2 c^2 \left[n - l + \sqrt{(l+\tfrac{1}{2}) - (Z\alpha)^2} \right]^2} \right\}^{-1/2}}$$

ef $Z\alpha << 1$

$$E(nl) \simeq mc^2 - \frac{mZ^2 e^4}{2\hbar^2 n^2} \left\{ 1 + \frac{Z^2 \alpha^2}{n^2} \left(\frac{n}{l+1/2} - \frac{3}{4} \right) + \cdots \right\}$$

ef $Z\alpha < l + \frac{1}{2}$

Ef $Z\alpha > \frac{1}{2}$ $\quad$ $\boxed{\text{þ.e.} \quad Z\frac{1}{137} > \frac{1}{2}}$

skiptir $\dfrac{l(l+1)-(Z\alpha)^2}{r^2}$ um formerki

eindin hrapa inn í miðjuna ......

> Vantar endanlega stærð kjarna og áhrif tómarúmsskautunar

leσið sjálf um margfeldið á KG
þegar $v/c \to 0$ og um skalar
víxlverkanir

π-miðeinda atóm sýna afstæð hrif um $\boxed{1\%}$
fínuna ranum stantum $\sim$ $\boxed{0{,}5\%}$

$$i\hbar \partial_t \phi(\bar{r}t) = \int d\bar{r}' K(\bar{r}-\bar{r}')\phi(\bar{r}'t)$$

með Coulomb mætti var enn einnar
mótmæla - - - - -

Jafna Diracs

$$E_{KG} = E(n,\ell)$$

$$\Delta E = E(n,\ell^{max}) - E(n,\ell^{min})$$

$$\sim \frac{1}{n^3}\,\frac{n-\frac{1}{2}}{n-1}$$

Stærra en í tilraunum fyrir H-atóm

Skoðum þá aftur

$$H \text{"="} \sqrt{c^2p^2+m^2c^4} \qquad \text{með} \qquad H\Phi = -i\hbar\partial_t\Phi$$

Er hægt að krefjast $H = c\,\bar{\alpha}\cdot\bar{p} + \beta mc^2$

þ.a. $H^2 = c^2p^2 + m^2c^4$ og $\bar{\alpha}$, β eru virkjar

Ef $H^2 = c^2p^2 + m^2c^4$

Gerum þá ráð fyrir að

$$H = c\,\bar{\alpha}\cdot\bar{p} + \beta mc^2$$

þar sem $\bar{\alpha}$ og β eru virkjar þá fast

$$H^2 = (c\alpha_x p_x + c\alpha_y p_y + c\alpha_z p_z + \beta mc^2)$$
$$\cdot\,(c\alpha_x p_x + c\alpha_y p_y + c\alpha_z p_z + \beta mc^2)$$

Hér er notað að $p_x p_y = p_y p_x$

$$= c^2(\alpha_x^2 p_x^2 + \alpha_y^2 p_y^2 + \alpha_z^2 p_z) + \beta^2 m^2 c^4$$
$$+ c^2(\alpha_x\alpha_y + \alpha_y\alpha_x)p_x p_y + c^2(\alpha_x\alpha_z + \alpha_z\alpha_x)p_x p_z$$
$$+ c^2(\alpha_y\alpha_z + \alpha_z\alpha_y)p_y p_z + mc^3\left\{(\beta\alpha_x + \alpha_x\beta) + (\beta\alpha_y + \alpha_y\beta) + (\beta\alpha_z + \alpha_z\beta)\right\}$$

Til þess að fá $H^2 = c^2p^2 + m^2c^4$ verður að gilda

$$\boxed{\begin{gathered} \alpha_x^2 = \alpha_y^2 = \alpha_z^2 = \beta^2 = 1 \\ \alpha_i\alpha_j + \alpha_j\alpha_i = 0 \qquad i \neq j \\ \beta\alpha_i + \alpha_i\beta = 0 \end{gathered}}$$

óháð hnitum → virkjarnir geta verið fylki

Nú eru fleiri en ein leið að velja $\overline{\alpha}$ og β, en við reynum hér

Pauli fylki

$$\boxed{\alpha_i = \begin{pmatrix} 0 & \sigma_i \\ \sigma_i & 0 \end{pmatrix} \qquad \beta = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}}$$

4×4 fylki

Hreyfijafnan er því

$$\boxed{i\hbar\partial_t\psi = -ic\hbar\,\overline{\alpha}\cdot\overline{\nabla}\psi + \beta mc^2\psi}$$

með ψ sem 4×1 fylki

Jafna Dirac's

þá verður

$$\boxed{-i\hbar\partial_t\psi^{+} = i c\hbar\,\bar{\nabla}\psi^{+}\cdot\bar{\alpha}^{+} + mc^2\psi^{+}\beta^{+}}$$

en $\alpha^{+} = \alpha$ og $\beta^{+} = \beta$

þá getum við strax ~~skoðað~~ samfelldnijöfnuna

$$i\hbar\partial_t(\psi^{+}\psi) = -ic\hbar\left\{\psi^{+}\bar{\alpha}\cdot\bar{\nabla}\psi + \bar{\nabla}\psi^{+}\cdot\bar{\alpha}\psi\right\}$$

$$+ mc^2\underbrace{\left\{\psi^{+}\beta\psi - \psi^{+}\beta\psi\right\}}_{=0}$$

eða

$$i\hbar\partial_t\rho(\bar{r}t) = -ic\hbar\bar{\nabla}\cdot\left(\psi^{+}\bar{\alpha}\psi\right)$$

Berum saman við

$$\partial_t \rho + \overline{\nabla} \cdot \overline{j} = 0$$

til þess að fá

$$\boxed{\overline{j} = c\psi^{+}\overline{\alpha}\psi, \quad \rho = \psi^{+}\psi \geq 0}$$

fyrir Lorentz-óbreytanlega framsetningu er oft skrifað

$$\beta = \gamma^0 \qquad x^0 = ct$$

$$\beta\alpha^i = \gamma^i, \quad \beta^2 = 1$$

$$i\hbar\gamma^0 c \frac{\partial}{\partial x_0}\psi = -i\hbar c \sum_{i=1}^{3} \gamma^i \frac{\partial}{\partial x_i}\psi + mc^2\psi$$

eða

$$\boxed{i\hbar c \sum_{\mu=0}^{3} \gamma^{\mu} \frac{\partial}{\partial x_{\mu}}\psi - mc^2\psi = 0}$$

$$i\hbar\gamma^\mu \frac{\partial}{\partial x_\mu}\psi - mc\psi = 0$$

$$\boxed{i\hbar\gamma^\mu\partial_\mu\psi - mc\psi = 0}$$

$$\gamma^\mu p_\mu \psi + mc\psi = 0 \qquad \{\gamma^\mu p_\mu + mc\}\psi = 0$$

$$\gamma^\mu p_\mu = \not{p} \qquad \{\not{p} + mc\}\psi = 0$$

$$\alpha_i\alpha_j + \alpha_j\alpha_i = 2\delta_{ij}$$

$$\beta^2 = 1\,, \quad \beta\alpha_i + \alpha_i\beta = 0$$

$$\gamma_0^2 = 1$$

og

$$\gamma^i\gamma^j + \gamma^j\gamma^i = \beta\alpha^i\beta\alpha^j + \beta\alpha^j\beta\alpha^i$$

$$= -\alpha^i\beta^2\alpha^j - \alpha^j\beta^2\alpha^i = -(\alpha^i\alpha^j + \alpha^j\alpha^i) = -2\delta_{ij}$$

$$\gamma^i\gamma^0 + \gamma^0\gamma^i = -2\delta_{0i}$$

og þuī $\quad \gamma^\mu\gamma^\nu + \gamma^\nu\gamma^\mu = 2g^{\mu\nu}$

med

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

frjálseind — hraði

$$i\hbar \dot{\vec{r}} = [\vec{r}, H]$$

eitt hnit

$$i\hbar \dot{x} = [x, H] = [x, -i\hbar c\{\alpha_x \partial_x + \alpha_y \partial_y + \alpha_z \partial_z + \beta m c^2\}]$$

$$= i\hbar c \alpha_x \quad , \quad \dot{y} = c\alpha_y \, , \quad \dot{z} = c\alpha_z$$

því sést að

$$|\dot{x}| = c \cdot (\text{eigingildi } \alpha_x)$$

$$|\alpha_x - \lambda I| = 0 \longrightarrow \lambda = \pm 1 \quad \text{og því} \quad \dot{x} = \pm c$$

Athugum nú

$$\frac{1}{c} i\hbar \dot{\alpha}_x = \frac{1}{c}[\alpha_x, H] = \frac{2\alpha_x}{c}(H - \alpha_x c p_x)$$

eða

$$i\hbar \dot{\alpha}_x = 2\alpha_x H - 2p_x c$$

Einnig höfum við fyrir frjálsa eind

$$i\hbar \dot{H} = [H, H] = 0, \quad i\hbar \dot{p}_x = [p_x, H] = 0$$

og því fæst

$$i\hbar \ddot{\alpha}_x = 2\dot{\alpha}_x H$$

Sem gefur

$$\dot{\alpha}_x(t) = \dot{\alpha}_x(0) e^{-\frac{2iHt}{\hbar}}$$

Notum

$$i\hbar \dot{\alpha}_x = \dot{\alpha}_x(0) e^{-\frac{2iHt}{\hbar}} = 2\alpha_x H - 2p_x c$$

sem við snúum við til að fá

$$\alpha_x = p_x c H^{-1} + \frac{1}{2} i\hbar \dot{\alpha}_x(0) e^{-\frac{2iHt}{\hbar}} H^{-1}$$

Áður höfðum við $i\hbar \dot{x} = i\hbar c \alpha_x$ því fæst

$$\dot{x} = c^2 p_x H^{-1} + \frac{c}{2} i\hbar \dot{\alpha}_x(0) e^{-\frac{2iHt}{\hbar}} H^{-1}$$

og heildað

$$\boxed{x(t) = c^2 p_x H^{-1} t - \frac{\hbar^2 \dot{\alpha}_x(0) c}{4} e^{-\frac{2iHt}{\hbar}} H^{-2} + \text{fastar}}$$

hreyfing rafeindar

flökt vegna mc^2 getur hraðann c

Zitter-bewegung

Rafsegulsvið + Dirac

Með venjulegum tengslum við rafsegulsvið er Dirac jafnan

$$\left\{ i\hbar\partial_t - e\phi \right\}\Psi = \left\{ c\bar{\alpha}\cdot\left(\frac{\hbar}{i}\bar{\nabla} - \frac{e}{c}\bar{A}\right) + \beta mc^2 \right\}\Psi$$

vigursviðið tengist beint
innri frelsisgráðum
$\rightarrow$ $g = 2$ má leiða út

Óafstæð aðfella

Ef við tökum með

$$\psi = \begin{pmatrix} \varphi \\ \chi \end{pmatrix}$$ þ.s. φ og χ

eru tveggja þátta spinorar

fæst

$$\boxed{i\hbar\partial_t \begin{pmatrix} \varphi \\ \chi \end{pmatrix} = c\left(\frac{\hbar}{i}\bar{\nabla} - \frac{e}{c}\bar{A}\right)\cdot\begin{pmatrix} 0 & \tau \\ \tau & 0 \end{pmatrix}\begin{pmatrix} \varphi \\ \chi \end{pmatrix} + \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} mc^2 \begin{pmatrix} \varphi \\ \chi \end{pmatrix} + e\phi\begin{pmatrix} \varphi \\ \chi \end{pmatrix}}$$

eða fyrir tvo þættina

$$\boxed{\begin{aligned} i\hbar\partial_t \varphi &= c\left\{\frac{\hbar}{i}\bar{\nabla} - \frac{e}{c}\bar{A}\right\}\cdot\bar{\tau}\chi + (e\phi + mc^2)\varphi \\ i\hbar\partial_t \chi &= c\left\{\frac{\hbar}{i}\bar{\nabla} - \frac{e}{c}\bar{A}\right\}\cdot\bar{\tau}\varphi + (e\phi - mc^2)\chi \end{aligned}}$$

Við búumst við $\phi \sim e^{-imc^2t/\hbar}$. þættir með miklu lægri tíðni en $mc^2/\hbar$

$$\longrightarrow \quad i\hbar\partial_t \chi \approx mc^2\chi + \cdots\cdots$$

og því býður seinni jafnan

$$mc^2\chi = c\left\{\frac{\hbar}{i}\bar{\nabla} - \frac{e}{c}\bar{A}\right\}\cdot\bar{\tau}\varphi - mc^2\chi$$

Beitum henni í þeirri fyrri $\longrightarrow$

$$i\hbar\partial_t\varphi = \frac{1}{2m}\left\{\left(\frac{\hbar}{i}\bar{\nabla} - \frac{e}{c}\bar{A}\right)\cdot\bar{\tau}\right\}^2\varphi + (e\phi + mc^2)\varphi$$

Nú gildir einnig að

$$(\bar{A}\cdot\bar{\tau})(\bar{B}\cdot\bar{\tau}) = (\bar{A}\cdot\bar{B}) + i\bar{\tau}(\bar{A}\times\bar{B})$$

því fæst

$$\left\{\left(\frac{\hbar}{i}\bar{\nabla}-\frac{e}{c}\bar{A}\right)\cdot\bar{\tau}\right\}^2 = \left(\frac{\hbar}{i}\bar{\nabla}-\frac{e}{c}\bar{A}\right)^2\varphi - \frac{e\hbar}{c}\bar{\tau}\cdot\left(\bar{\nabla}\times\bar{A}+\bar{A}\times\bar{\nabla}\right)\varphi$$

en $$\bar{\nabla}\times(\bar{A}\varphi)+\bar{A}\times(\bar{\nabla}\varphi) = \varphi(\bar{\nabla}\times\bar{A}) + \underbrace{(\bar{\nabla}\varphi)\times\bar{A}+\bar{A}\times(\bar{\nabla}\varphi)}_{=0}$$
$$= \bar{B}\varphi$$

og þess vegna

$$\boxed{i\hbar\partial_t\varphi = \frac{1}{2m}\left\{\frac{\hbar}{i}\bar{\nabla}-\frac{e}{c}\bar{A}\right\}^2\varphi - \frac{e\hbar}{2mc}\bar{\tau}\cdot\bar{B}\varphi+(e\phi+mc^2)\varphi}$$

Sem er jafna Paulis fyrir ½-spuna, nema

$$\frac{1}{2}g\mu_B\bar{\tau}\cdot\bar{B} \qquad \mu_B=\frac{e\hbar}{2mc} \quad \longrightarrow \quad \boxed{g=2}$$

í tómarúmi án rúm-skautunar

$\bar{S}=\frac{\hbar}{2}\bar{\tau}$

þegar óaflstöðu aðfellan er athuguð bætur
fæst $+ o(v^2/c^2)$

$$i\hbar\partial_t\Phi = \left\{mc^2 + \frac{1}{2m}\left(\bar{p} - \frac{e}{c}\bar{A}\right)^2 - \frac{p^4}{8m^3c^2}\right\}\Phi$$

$$- \left\{\frac{e\hbar}{2mc}\bar{\sigma}\cdot\bar{B} + \frac{e\hbar}{4m^2c^2}\bar{\sigma}\cdot(\bar{E}\times\bar{p})\right\}\Phi$$

Zeeman

spuna-brautar

$$+ \left\{e\phi + \frac{\hbar^2}{8m^2c^2}\left(\nabla^2 e\phi\right)\right\}\Phi$$

liður Darwins

$$e\phi(\bar{r}+\delta\bar{r}) \simeq e\phi(\bar{r}) + \frac{1}{6}(\delta r)^2\nabla^2 e\phi(\bar{r}) \simeq e\phi(\bar{r}) + \frac{1}{6}\frac{\hbar^2}{m^2c^2}\nabla^2 e\phi(\bar{r})$$

„smyrja út“ . . . . . . !

lesa gālf un vetuis atōmid, par fost

$$E = mc^2 \left\{ 1 + \frac{(Ze^2/\hbar c)^2}{\left\{ n - j - \frac{1}{2} - \sqrt{(j+\frac{1}{2})^2 - \left(\frac{Ze^2}{\hbar c}\right)^2} \right\}^2} \right\}^{-1/2}$$

meet $\quad j = \frac{1}{2}, \frac{3}{2}, \frac{5}{2}, \dots \qquad n = 1, 2, \dots$

$$E_D = mc^2 \left\{ 1 - \frac{\alpha^2}{2n^2} - \frac{\alpha^4}{2n^4}\left(\frac{n}{|K|} - \frac{3}{4}\right) + O(\alpha^6) \right\}$$

$$E_{KG} = mc^2 \left\{ 1 - \frac{\alpha^2}{2n^2} - \frac{\alpha^4}{2n^4}\left(\frac{n}{l+\frac{1}{2}} - \frac{3}{4}\right) + \dots \right\}$$

$n = s - 1 + |K| \qquad K = \mp 1, \pm 2, \dots \qquad j = |K| - \frac{1}{2}$

$s = 1, 2, \dots \qquad \min(K) = 1 \qquad \max(K) = n$

$$\Delta E_{KG} = E(n, \max(l)) - E(n, \min(l)) = \frac{mc^2\alpha^4}{n^3} \frac{n-1}{n-1/2}$$

$$\Delta E_{Sch} = 0$$

$$\Delta E_{D} = E(n, \max(k)) - E(n, \min(k)) = \frac{mc^2\alpha^4}{2n^3} \frac{n-1}{n}$$