VI. Relativistic wave equations for particles, Klein-Gordon eqs.

VI.1 General properties

To construct a wave equation for particles similar to the Schrödinger equation but which is invariant under Lorentz transformations we have to fulfill the following requirements

(i) equation should be linear (save superposition principle)

(ii) space and time coordinates should appear in the same way (Schrödinger eq. excluded!)

Furthermore

- localization of particle should never be stronger than

(319) $$\Delta x \geq \boxed{\lambda_c = \frac{\hbar}{m_0 c}}$$ Compton wavelength

since if $\Delta x < \lambda_c$

$$\Delta p \gtrsim \frac{\hbar}{\Delta x} > \frac{\hbar}{\lambda_c} = m_0 c$$

$$\Delta E \geq \sqrt{c^2 \Delta p^2 + m_0^2 c^4}$$

comparable $\Rightarrow$ pair creation of particles

- temporal resolution should not be better than

(320) $$\Delta t \gtrsim \boxed{\frac{\lambda_c}{c} = \frac{\hbar}{m_0 c^2}}$$ Compton time

relation between non-relativistic mechanics and non-relativistic quantum mechanics

class. mechanics		quantum mechanics
x	$\longrightarrow$	$\hat{x} = x$
p	$\longrightarrow$	$\hat{p} = \frac{\hbar}{i}\frac{\partial}{\partial x}$

- relativistic 4-momentum in spatial representation

(327) $$\boxed{\vec{p} \to p^\mu \qquad -i\hbar\vec{\nabla} \longrightarrow -i\hbar\partial^\mu}$$

- relativistic Hamilton function

$$H = \sqrt{c^2 p^2 + m_0^2 c^4} \tag{322}$$

from this we could guess a stationary wave equation

$$\sqrt{-\hbar^2 c^2 \Delta + m_0^2 c^4}\, \psi \overset{?}{=} E \psi \tag{323}$$

or by associating $H \to i\hbar \frac{\partial}{\partial t}$

$$i\hbar \frac{\partial}{\partial t} \psi = \sqrt{-\hbar^2 c^2 \Delta + m_0^2 c^4}\, \psi \tag{324}$$

problem: square root; expanding the square root into a power series in Δ yields derivatives of arbitrary order

$\lightning$

To avoid this problem we square (322)

$$H^2 = c^2 p^2 + m_0^2 c^4 \tag{325}$$

$$\Rightarrow \quad -\hbar^2 \frac{\partial^2}{\partial t^2} \psi = \left(-\hbar^2 c^2 \Delta + m_0^2 c^4 \right) \psi$$

which can be written in terms of the 4-gradient

$$\boxed{\left[\partial_\mu \partial^\mu + \left(\frac{m_0 c}{\hbar} \right)^2 \right] \psi = 0} \tag{326}$$

Klein Gordon equation

VI.2 Relativistic wave equation for spin-0 particles: Klein-Gordon equation

$$\left[\partial_\mu \partial^\mu + \left(\frac{m_0 c}{\hbar}\right)^2\right]\psi = \left[\Box + \left(\frac{m_0 c}{\hbar}\right)^2\right]\psi = 0 \tag{326}$$

(A) 4 current density and continuity equation

An important aspect of the Schrödinger equation was a continuity equation for the field density

$$\rho = |\psi|^2 \qquad\qquad \partial_t \rho + \vec{\nabla}\vec{j} = 0 \tag{327}$$

which followed from Schrödingers equation and was the basis for the interpretation of ρ as probability density. We will now see that a similar relation to (327) can be derived for the K-G field, a probability interpretation is however not possible.

(326) $\Rightarrow$

$$(\hat{p}_\mu \hat{p}^\mu - m_0^2 c^2)\psi = 0 \qquad (\hat{p}_\mu \hat{p}^\mu - m_0^2 c^2)\psi^* = 0$$

i.e.

$$\psi^*(\hat{p}_\mu \hat{p}^\mu - m_0^2 c^2)\psi - \psi(\hat{p}_\mu \hat{p}^\mu - m_0^2 c^2)\psi^* = 0$$

$\Rightarrow$

$$-\psi^*\left(\hbar^2\partial_\mu\partial^\mu+\cancel{m_0^2c^2}\right)\psi+\psi\left(\hbar^2\partial_\mu\partial^\mu+\cancel{m_0^2c^2}\right)\psi^*=0$$

$$\Rightarrow \quad \partial_\mu\left(\psi^*\partial^\mu\psi-\psi\partial^\mu\psi^*\right)\Rightarrow\partial_\mu j^\mu=0$$

4-current density of Klein-Gordon field

(328) $$\boxed{j_\mu=\frac{i\hbar}{2m_0}\left(\psi^*\partial_\mu\psi-\psi\partial_\mu\psi^*\right)}$$

conservation law

(329) $$\boxed{\partial^\mu j_\mu=\partial_\mu j^\mu=0}$$

written in time and space coordinates & components

(330) $$\frac{\partial}{\partial t}\left[\frac{i\hbar}{2m_0c^2}\left(\psi^*\partial_t\psi-\psi\partial_t\psi^*\right)\right]+\vec{\nabla}\cdot\left[-\frac{i\hbar}{2m_0}\left(\psi^*\vec{\nabla}\psi-\psi\vec{\nabla}\psi^*\right)\right]=0$$

this has the same form as the equation for the Schrödinger field

(331) $$\frac{\partial}{\partial t}\rho+\vec{\nabla}\cdot\vec{j}=0$$

i.e.

(332) $$\boxed{\frac{d}{dt}\int_{V_\infty}dV\,\rho=0}$$

global conservation law

i.e. can we interpret

(333) $$\boxed{\rho = \frac{i\hbar}{2m_0c^2}\left(\psi^*\frac{\partial\psi}{\partial t} - \psi\frac{\partial\psi^*}{\partial t}\right)}$$

as probability density and

(334) $$\boxed{\vec{j} = -\frac{i\hbar}{2m_0}\left(\psi^*\vec{\nabla}\psi - \psi\vec{\nabla}\psi^*\right)}$$

as probability current density ?: No!

ρ is not positive definite !!

$\rho \mathrel{\hat{=}}$ charge density

$\vec{j} \mathrel{\hat{=}}$ current density

KGE describes "charged" field

One recognizes

(335) $$\boxed{\psi \longleftrightarrow \psi^* \qquad \rho \longleftrightarrow -\rho}$$

▶ ψ^* describes field with opposite charge to ψ

if $\psi^* = \psi$ real Klein-Gordon field

(336) $\Rightarrow$ $\boxed{\rho \equiv 0}$ neutral particle

(B) The non-relativistic limit

In order for the KGE to be a sensible relativistic generalization of the Schrödinger equation it should agree with the latter in the non-relativistic limit

Since in the limit $\vec{p} \to 0$ the energy of a classical particle is not zero but the rest energy

$$\vec{p} \to 0 \quad E \to E_0 = m_0 c^2$$

we make the ansatz

(337) $$\psi(\vec{r},t) = \phi(\vec{r},t)\, e^{-i\frac{m_0 c^2}{\hbar}t}$$

this gives

$$\frac{\partial}{\partial t}\psi = \left(\frac{\partial \phi}{\partial t} - i\frac{m_0 c^2}{\hbar}\phi\right) e^{-i\frac{m_0c^2}{\hbar}t}$$

As we will see later

(338) $$\left| i\hbar \frac{\partial \phi}{\partial t} \right| \sim \underbrace{(E - m_0 c^2)}_{=E_{kin}} |\phi|$$

non-relativistic limit

(339) $$E_{kin} \ll m_0 c^2$$

i.e.

(340) $$\left|\frac{\partial \phi}{\partial t}\right| \ll \left|\frac{m_0 c^2}{\hbar}\phi\right|$$

$$\frac{\partial^2 \psi}{\partial t^2} = \left(\frac{\partial^2 \phi}{\partial t^2} - 2i\frac{m_0 c^2}{\hbar}\frac{\partial \phi}{\partial t} - \frac{m_0^2 c^4}{\hbar^2}\phi\right) e^{-\frac{i m_0 c^2 t}{\hbar}}$$

$\Rightarrow$ in KGE (326)

$$\frac{1}{c^2}\Big(\underbrace{\cancel{\frac{\partial^2 \phi}{\partial t^2}}}_{\approx 0} - \frac{2 i m_0 c^2}{\hbar}\frac{\partial \phi}{\partial t} - \cancel{\frac{m_0^2 c^4}{\hbar^2}\phi}\Big) - \Delta \phi + \cancel{\frac{m_0^2 c^2}{\hbar^2}\phi} = 0$$

$\Rightarrow$

(341) $$i\hbar \frac{\partial \phi}{\partial t} = -\frac{\hbar^2}{2m_0}\Delta \phi$$ free Schrödinger equation ✓

I.e. in the non relativistic limit the KG-wave-function is the Schrödinger wavefunction with an oscillatory phase term accounting for the rest energy

(342) $$\psi \xrightarrow[|\vec{v}| \ll c]{} \phi_{\text{Schrödinger}}\, e^{-\frac{i m_0 c^2 t}{\hbar}}$$

(C) The free Klein Gordon field

After we have convinced ourselves that the KGE is a sensible relativistic generalization of the SE let's study some simple problems starting with the free particle.

$$(\hat{p}^\mu \hat{p}_\mu - m_0^2 c^2)\psi = 0$$

ansatz

(343) $$\psi = A e^{-i p_\mu x^\mu / \hbar}$$

wave ansatz

$$\frac{p_\mu x^\mu}{\hbar} = -\omega t + \vec{k}\vec{r}$$ p_μ is a c-number!!!

using $\hat{p}_\mu = -i\hbar \partial_\mu$ $\quad \hat{p}^\mu = -i\hbar g^{\mu\nu}\partial_\nu$

$\Rightarrow$

(344) $$\hat{p}_\mu \hat{p}^\mu = -\hbar^2 g^{\mu\nu}\partial_\mu \partial_\nu$$

Substituting (343) and (344) into KGE yields

(345) $$(p_\mu p^\mu - m_0^2 c^2) A = 0$$

with $p_0 = E/c = \hbar\omega/c$, eq. (345) implies

$$\omega^2 = \frac{c^2}{\hbar^2}(\vec{p}^{\,2} + m_0^2 c^2)$$

or

(346) $$\boxed{\omega = \pm \omega_p = \pm \frac{c}{\hbar}\sqrt{\vec{p}^{\,2} + m_0^2 c^2}}$$

This expression looks as we would expect from the energy-momentum relation of a relativistic particle, eq. (317).

However, we notice that for a given momentum $\vec{p}$ there are two solutions!

$$(347) \quad \boxed{\psi_\pm = A_\pm \, e^{i\left(\frac{\vec{p}\cdot\vec{x}}{\hbar} \mp \omega_p t\right)}}$$

positive and negative energy solutions

If we calculate the charge density of the two solutions following eq. (333) we find

$$(348) \quad \boxed{\rho_\pm = \pm \frac{\hbar \omega_p}{m_0 c^2} \underbrace{\psi_\pm^* \psi_\pm}_{>0}}$$

$\Rightarrow$ positive- and negative energy solutions have opposite charge

ψ_+ particle with positive charge & energy

ψ_- — " — negative — " —

(D) Schrödinger representation of KGE

There is an interesting mapping between the KG field and its first time derivative to a two component field. As you will show in the problem course one can introduce the two fields:

$$\varphi \equiv \frac{1}{2}\left(\psi + \frac{i\hbar}{m_0c^2}\frac{\partial\psi}{\partial t}\right)$$

and (349)

$$\chi \equiv \frac{1}{2}\left(\psi - \frac{i\hbar}{m_0c^2}\frac{\partial\psi}{\partial t}\right)$$

which can be summarized in a two-component field

(350)
$$\boxed{\Psi \equiv \begin{pmatrix}\varphi\\ \chi\end{pmatrix}}$$

which then fulfills the equation

(351)
$$\boxed{i\hbar\frac{\partial}{\partial t}\Psi = \hat{H}\Psi}$$

Schrödinger representation of KGE

with

(352)
$$\boxed{\begin{aligned}\hat{H} &= (\sigma_z + i\sigma_y)\frac{\hat{\vec{P}}^2}{2m_0} + \sigma_z m_0c^2\\ &= \begin{pmatrix}1 & 1\\ -1 & -1\end{pmatrix}\frac{\hat{\vec{P}}^2}{2m_0} + \begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix}m_0c^2\end{aligned}}$$

Note that

(353)
$$\hat{H}^{+} \neq \hat{H}$$

but

(354) $$\hat{H}^2 = c^2 \hat{\vec{p}}^2 + m_0^2 c^4$$

This is because $\sigma_j^2 = \mathbb{1}_2$ and $\{\sigma_\ell, \sigma_m\} = 2i\varepsilon_{\ell m k}\sigma_k + 2\delta_{\ell m}$

As you will show in the problem course for a free particle of momentum $\vec{p} = \hbar \vec{k}$

$$\hbar\omega = \pm \hbar\omega_p = \pm c\sqrt{p^2 + m_0^2 c^2}$$

$\boxed{\omega = +\omega_p}$

(355) $$\Psi^{(+)}(\vec{p}) = A_{(+)} \begin{pmatrix} m_0 c^2 + \hbar\omega_p \\ m_0 c^2 - \hbar\omega_p \end{pmatrix} e^{i(\vec{k}\cdot\vec{x} - \omega_p t)}$$

In the nonrelativistic limit $\frac{p^2}{2m_0} \ll m_0 c^2$

(356) $$\Psi^{(+)}(\vec{p}) \longrightarrow A_{(+)} \begin{pmatrix} 1 \\ 0 \end{pmatrix} e^{i(\vec{k}\cdot\vec{x} - \omega_p t)}$$

$\boxed{\omega = -\omega_p}$

(357) $$\Psi^{(-)}(\vec{p}) = A_{(-)} \begin{pmatrix} m_0 c^2 - \hbar\omega_p \\ m_0 c^2 + \hbar\omega_p \end{pmatrix} e^{i(\vec{k}\cdot\vec{x} + \omega_p t)}$$

In nonrelativistic limit $\frac{p^2}{2m_0} \ll m_0 c^2$

(358) $$\Psi^{(-)}(\vec{p}) \longrightarrow A_{(-)} \begin{pmatrix} 0 \\ 1 \end{pmatrix} e^{i(\vec{k}\cdot\vec{x} + \omega_p t)}$$

It is instructive to represent the charge density ρ (eq.(333)) in terms of ϕ and χ

$$\rho = \frac{i\hbar}{2m_0c^2}\left(\psi^*\frac{\partial\psi}{\partial t} - \psi\frac{\partial\psi^*}{\partial t}\right)$$

from (349)

(359) $\psi = \varphi + \chi \qquad i\hbar\frac{\partial}{\partial t}\psi = (\varphi - \chi)m_0c^2$

$$\Rightarrow \quad \rho = \frac{m_0c^2}{2m_0c^2}\left((\varphi^* + \chi^*)(\varphi-\chi) + (\varphi+\chi)(\varphi^*-\chi^*)\right)$$

i.e.

(360) $$\boxed{\rho = \underbrace{\varphi^*\varphi}_{\text{positive}} - \underbrace{\chi^*\chi}_{\text{negative}} = \Psi^+ \sigma_z \Psi}$$

charge

Away from the non-relativistic limit $\Psi^{(+)}$ will have also a small component χ and $\Psi^{(-)}$ a small component φ, so we require the

charge normalization

(361) $$\boxed{\int d^3x \; \Psi^+ \sigma_z \Psi = \pm 1}$$

(E) Charge conjugation

Comparing the two solutions of a free KG particle (355) and (357) we see

(362) $$\Psi^{(-)}(-\vec{p}) = \sigma_x \, \Psi^{(+)}(\vec{p})^*$$

i.e. if $\Psi = \begin{pmatrix} \varphi \\ \chi \end{pmatrix}$ corresponds to a positive charge, i.e.

$$\int d^3x \, \Psi^\dagger \sigma_z \Psi = +1$$

then

(363) $$\boxed{\Psi_c \equiv \sigma_x \Psi^* = \begin{pmatrix} \chi^* \\ \varphi^* \end{pmatrix}}$$

describes a state with negative charge! i.e.

$$\int d^3x \, \Psi_c^\dagger \sigma_z \Psi_c = -1$$

This operation (in (363)) is called

charge conjugation C

Obviously

(364) $$(\Psi_c)_c = \sigma_x (\sigma_x \Psi^*)^* = \sigma_x^2 \Psi = \Psi$$

interpretation

$$\boxed{\begin{array}{ll} \Psi & \text{particle} \\ \Psi_c & \text{antiparticle} \end{array}}$$

$$\varphi^{(+)} \xrightarrow{C} \chi^{(-)}$$

$$\chi^{(+)} \longrightarrow \varphi^{(-)}$$

$$\vec{p} \longrightarrow -\vec{p}$$

$$\omega = \omega_p \longrightarrow \omega = -\omega_p$$

In this sense neutral particles with real KG wavefunction are their own anti-particle

$$\psi = \varphi + \chi = \psi^*$$

then $\quad \Psi_c = \sigma_x \Psi^* = \alpha \Psi \qquad \alpha = \alpha^*$

(365)

Since $\quad (\Psi_c)_c = \Psi$

$$(\Psi_c)_c = (\alpha \Psi)_c = \sigma_x \alpha \Psi^* = \alpha \sigma_x \Psi^* = \alpha^2 \Psi$$

(366) $\quad \Longrightarrow \quad \alpha = \pm 1$

$\boxed{\alpha = +1}$ $\boxed{\alpha = -1}$

neutral particles with positive charge parity

$$\Psi_c = \Psi$$

neutral particles with negative charge parity

$$\Psi_c = -\Psi$$

- remark:

one can show that

$$[\hat{C}, \hat{H}_{\text{strong interaction}}] = 0$$

(367) $$[\hat{C}, \hat{H}_{\text{elm interaction}}] = 0$$

but $$[\hat{C}, \hat{H}_{\text{weak interaction}}] \neq 0$$

i.e. the weak interaction is not invariant under charge conjugation

(F) Klein Gordon field in an electromagnetic field

After we have discussed a free Klein Gordon field let us consider a slightly more involved situation of a KG field / particle in an external elm. field.

remember in non-relativistic quantum mechanics we had

minimal coupling

(368) $\hat{H} \longrightarrow i\hbar\frac{\partial}{\partial t} - eA_0 \qquad \vec{p} \longrightarrow -i\hbar\vec{\nabla} - \frac{e}{c}\vec{A}$

or in covariant formulation

$$\hat{p}^\mu \longrightarrow \hat{p}^\mu - \frac{e}{c}\hat{A}^\mu \qquad \hat{p}_\mu \longrightarrow \hat{p}_\mu - \frac{e}{c}\hat{A}_\mu$$

$\Rightarrow$ this yields

(369) $$\boxed{\left[\left(\hat{p}^\mu - \frac{e}{c}A^\mu\right)\left(\hat{p}_\mu - \frac{e}{c}A_\mu\right) - m_0^2c^2\right]\psi = 0}$$

Klein-Gordon equation in an elm. field

also in an external field the continuity eqs. holds

(370) $$\partial_\mu \tilde{j}^\mu = 0$$

however with an additional contribution to the current

(371) $$\boxed{\tilde{j}_\nu = \frac{i\hbar}{2m_0}\left(\psi^*\partial_\nu\psi - \psi\partial_\nu\psi^*\right) - \frac{eA_\nu}{m_0c}\psi^*\psi}$$

Gauge invariance

From Edyn we know that the gauge trafo

(372) $$A_\mu(x) \longrightarrow A'_\mu(x) = A_\mu(x) + \frac{\partial \lambda(x)}{\partial x^\mu}$$

leaves Maxwells equations invariant. We would like to preserve this property also for a KG particle coupled to the elm. field, i.e. we request that for the transformed elm. field also ψ transforms such that

(373) $$\left(i\hbar\partial^\mu - \frac{e}{c}A^{\mu\prime}\right)\left(i\hbar\partial_\mu - \frac{e}{c}A'_\mu\right)\psi' - m_0^2c^2\psi' \overset{!}{=} 0$$

i.e.

(374) $$\left(i\hbar\partial^\mu - \frac{e}{c}A^\mu - \frac{e}{c}\partial^\mu\lambda(x)\right)\left(i\hbar\partial_\mu - \frac{e}{c}A_\mu - \frac{e}{c}\partial_\mu\lambda(x)\right)\psi' - m_0^2c^2\psi' = 0$$

this holds if

$$\psi' = \psi\, e^{-i\frac{e}{\hbar c}\lambda(x)}$$

gauge invariance of Klein-Gordon and elm field

(375) $$\boxed{\begin{aligned} A_\mu(x) &\longrightarrow A'_\mu(x) = A_\mu(x) + \partial_\mu\lambda(x) \\ \psi(x) &\longrightarrow \psi'(x) = \psi(x)\, e^{-\frac{ie}{\hbar c}\lambda(x)} \end{aligned}}$$

With this we can now consider a KG particle in a Coulomb potential (Hydrogen problem)

(376) $$eA_0 = V(r) = -\frac{Ze^2}{r} \qquad \vec{A} = 0$$

You will show in the problem courses that the stationary solution of the KGE in this elm. field

$$\left[\left(i\hbar\partial_t - V(r) \right)^2 - m_0^2 c^4 + \hbar^2 c^2 \Delta \right] \Psi(\vec{r},t) = 0$$

has the form

(377) $$\Psi(\vec{r},t) = \phi_\varepsilon(\vec{r}) e^{-\frac{i}{\hbar}\varepsilon t}$$

where the energy ε and eigenfunction $\phi_\varepsilon(\vec{r})$ follows from

(378) $$\left[\left(\varepsilon - V(r) \right)^2 - m_0^2 c^4 + \hbar^2 c^2 \Delta \right] \phi_\varepsilon(\vec{r}) = 0$$

Ansatz:

(379) $$\phi_\varepsilon(\vec{r}) = \frac{R_{\varepsilon l}(r)}{r} Y_{lm}(\vartheta, \varphi)$$

$\Rightarrow \cdots \Rightarrow$

$$\left(\frac{d^2}{dr^2} - \frac{l(l+1)}{r^2} + \frac{\left(\varepsilon - V(r) \right)^2}{\hbar^2 c^2} - \frac{m_0^2 c^2}{\hbar^2} \right) R_{\varepsilon l}(r) = 0$$

(380)

this can be written in the form

$$(381)\quad \left[\frac{d^2}{dr^2}-\frac{l(l+1)-(Z\alpha)^2}{r^2}+\frac{2\varepsilon Z\alpha}{\hbar c r}-\frac{m_0^2c^4-\varepsilon^2}{\hbar^2c^2}\right]R_{\varepsilon l}(r)=0$$

where we have introduced

$$(382)\quad \boxed{\alpha=\frac{e^2}{\hbar c}=\frac{1}{137.03602}}$$

fine-structure constant

We are interested in bound states with $\varepsilon^2 \leq (m_0c^2)^2$

abbreviations!

$$\beta = 2\frac{\sqrt{m_0^2c^4-\varepsilon^2}}{\hbar c}$$

$$\varrho = \beta r$$

$$\mu = \sqrt{\left(l+\frac{1}{2}\right)^2-(Z\alpha)^2}$$

$$\lambda = \frac{2Z\alpha\varepsilon}{\hbar c\beta}$$

then (381) simplifies to

$$(383)\quad \left[\frac{d^2}{d\varrho^2}-\frac{\mu^2-1/4}{\varrho^2}+\frac{\lambda}{\varrho}-\frac{1}{4}\right]R_{\varepsilon l}(r)=0$$

To solve this equation we use Sommerfeld's method as in non-relativistic quantum mechanics

So first consider limiting case:

$\underline{\rho \to \infty}$

$$\left(\frac{d^2}{d\rho^2} - 1\right) R_{\varepsilon\ell}(\rho) = 0$$

(384) $$\Rightarrow \quad R_{\varepsilon\ell}(\rho) \underset{\rho \sim \infty}{=} A e^{-\rho/2} + \cancel{B e^{\rho/2}}$$

cannot be normalized!

$\underline{\rho \to 0}$

$$\left(\frac{d^2}{d\rho^2} - \frac{\mu^2 - 1/4}{\rho^2}\right) R_{\varepsilon\ell}(\rho) = 0$$

(385) $$R_{\varepsilon\ell}(\rho) \sim \rho^{\nu} \Rightarrow \nu(\nu-1)\rho^{\nu-2} - \left(\mu^2 - \tfrac{1}{4}\right)\rho^{\nu-2} = 0$$

$$\Rightarrow \quad \nu^2 - \nu - \left(\mu^2 - \tfrac{1}{4}\right) = 0$$

$$\nu_{\pm} = \frac{1}{2} \pm \left[\frac{1}{4} + \mu^2 - \frac{1}{4}\right]^{1/2} = \frac{1}{2} \pm \mu$$

to have convergence for $\rho \to 0$ only

(386) $$\nu = \frac{1}{2} + \mu$$

<u>Sommerfeld ansatz</u>

(387) $$R_{\varepsilon\ell}(\rho) = A \rho^{\mu + \frac{1}{2}} e^{-\rho/2} f(\rho)$$

$$\Rightarrow \quad \frac{d^2 f}{d\rho^2} + \left(\frac{2\mu+1}{\rho} - 1\right)\frac{df}{d\rho} + \frac{\mu + \frac{1}{2} - \lambda}{\rho} f = 0$$

polynomial ansatz

$$f(\xi) = \sum_{m=0}^{\infty} a_m \xi^m \qquad (388)$$

$$\Rightarrow \sum_{m=2}^{\infty} a_m m(m-1) \xi^{m-2} + c \sum_{m=1}^{\infty} m a_m \xi^{m-2} - \sum_{m=2}^{\infty} (m-1) a_{m-1} \xi^{m-2} - a \sum_{m=1}^{\infty} a_{m-1} \xi^{m-2} = 0$$

where $c \equiv 2\mu + 1$ and $a \equiv \mu + \frac{1}{2} - \lambda$

comparison of coefficients yields

$$a_1 = a_0 \frac{a}{c} \qquad a_2 = \frac{a_1}{2} \frac{a+1}{c+1} \qquad (389)$$

and

$$a_{m+1} = \frac{a_m}{m+1} \frac{a+m}{c+m} \qquad (390)$$

(390) is a recursion. In order to get normalizable solutions we have to require that the recursion truncates at some index $m = n' \in \mathbb{N}$

i.e. $\qquad a + n' \stackrel{!}{=} 0 \qquad (391)$

since then $\qquad a_{n'+1} = a_{n'+2} = a_{n'+3} = \cdots = 0$

For (391) to hold we have to specify the energy

(392) $$\lambda = \frac{Z\alpha \mathcal{E}_n}{(m_0^2c^4 - \mathcal{E}_n^2)^{1/2}} \overset{!}{=} \mu + \frac{1}{2} + n'$$

This then gives (remember $\mu \leftrightarrow \ell$ see abbreviations)

(393) $$\mathcal{E}_{n'\ell}^{\,2} = \frac{m_0^2c^4}{1 + \frac{(Z\alpha)^2}{\left\{n' + \frac{1}{2} + \left[(\ell+\frac{1}{2}) - (Z\alpha)^2\right]^{1/2}\right\}^2}}$$

As in the non-relativistic Hydrogen problem we introduce the principle quantum number

(394) $$n = n' + \ell + 1$$

$$n = 1, 2, 3, \ldots \qquad \ell = 0, 1, 2, \ldots (n-1)$$

(395) $$\boxed{\mathcal{E}_{n\ell} = \frac{m_0c^2}{\left[1 + \frac{(Z\alpha)^2}{\left(n - \ell - \frac{1}{2} + \left[(\ell+\frac{1}{2})^2 - (Z\alpha)^2\right]^{1/2}\right)^2}\right]^{1/2}}}$$

Klein-Gordon Hydrogen energies depend on ℓ!

expansion in powers of $(Z\alpha)^2$ which should be good for light nuclei, i.e. Z small

$$E_{n\ell} \simeq m_0 c^2 \left[1 - \frac{Z^2\alpha^2}{2n^2} - \frac{Z^4\alpha^4}{2n^4}\left(\frac{n}{\ell+\frac{1}{2}} - \frac{3}{4}\right) + \dots \right] \tag{396}$$

rest energy

Schrödinger

relativistic correction

lifts the ℓ degeneracy of the non-relativistic Hydrogen problem

remark:

- For heavy nuclei where $Z\alpha > (\ell + \frac{1}{2})$ $E_{n\ell}$ becomes imaginary

$\Rightarrow$ there is no 1s state for $Z\alpha > \frac{1}{2}$

so $Z_{1s}^{crit} \simeq \frac{1}{2\alpha} \approx 68$