Exam 2013: solutions

Section S18 ADVANCED QUANTUM MECHANICS

1. A non-relativistic quantum particle of mass m and wavenumber k is incident from the negative x direction on the one-dimensional potential well

$$U(x) = \begin{cases} -U_0, & |x| \le \frac{a}{2}\,, \\ 0, & |x| > \frac{a}{2}\,. \end{cases}$$

In the region $x > a/2$, the particle is described by the wave function $\psi(x) = S(E)e^{ik(x-a)}$, where $E = \hbar^2 k^2/2m$.

Show that the transmission amplitude $S(E)$ is given by

$$S(E) = \frac{k\kappa}{k\kappa\cos\kappa a - \frac{i}{2}\left(k^2+\kappa^2\right)\sin\kappa a}\,,$$

where $\kappa = \sqrt{2m(E+|U_0|)}/\hbar$. [6]

Find the transmission probability $T(E)$. [4]

Show that the transmission amplitude has singularities (zeros of the denominator of $S(E)$) in the complex k plane determined by the equations

$$\tan\frac{\kappa a}{2} = -\frac{ik}{\kappa}\,, \qquad \cot\frac{\kappa a}{2} = \frac{ik}{\kappa}\,.$$

[5]

Find the even and odd parity wave functions corresponding to the stationary states with $E < 0$ (bound states) in the potential well. [4]

Find equations determining the bound state energies in the potential well and show that these energies coincide with the singularities of the transmission amplitude. [4]

Find the energies E for which the transmission probability $T(E)$ reaches its maximum value. Sketch the function $T(E)$ for $E \ge 0$.

Treating E formally as a complex variable, sketch (qualitatively) the location of the poles of the transmission amplitude in the complex k plane and the complex E plane. [2]

2. A spinless relativistic particle of mass m in an external scalar field $\Phi(\mathbf{r},t)$ obeys the equation

$$\left[\frac{1}{c^2}\frac{\partial^2}{\partial t^2} - \Delta + \frac{m^2c^2}{\hbar^2} + \frac{2m}{\hbar^2}\Phi(\mathbf{r},t)\right]\psi = 0\,.$$

Show that in the non-relativistic limit $\Phi(\mathbf{r},t)$ has the meaning of the usual potential energy. [5]

Show that the wave function $R(r) = r\psi(r)$ of the s-wave spinless particle in the external field

$$\Phi(r) = \begin{cases} -U_0, & r \le a\,, \\ 0, & r > a \end{cases}$$

satisfying the boundary condition $R(0) = 0$ is

$$R(r) = \begin{cases} A\sin\left(r\sqrt{\frac{2mU_0}{\hbar^2} - \kappa^2}\right), & r \le a\,, \\ B\,e^{-\kappa r}, & r > a\,, \end{cases}$$

where $\kappa = \sqrt{m^2c^4 - \epsilon^2}/\hbar c > 0$. [Hint: You may use $\Delta\psi = \frac{1}{r}\frac{d^2(r\psi)}{dr^2}$.] [5]

Show that the discrete energy spectrum ϵ_n is determined by the equation

$$\tan\sqrt{\frac{2mU_0a^2}{\hbar^2} - \kappa_n^2a^2} = -\frac{1}{\kappa_n a}\sqrt{\frac{2mU_0a^2}{\hbar^2} - \kappa_n^2a^2}\,,$$

where $\kappa_n = \sqrt{m^2c^4 - \epsilon_n^2}/\hbar c$.

What is the spectrum of an antiparticle in this field? [6]

Find the algebraic equation determining the critical value $U_{0,crit}$ of the external field corresponding to $\epsilon_{n=0} = 0$. What physical processes one may expect to occur for external fields exceeding the critical value? Is the one-particle equation adequate in this case? Explain. [5]

A spinless relativistic particle of mass m and charge e in an external electrostatic field ϕ obeys the equation

$$\left(-\hbar^2c^2\Delta + m^2c^4\right)\psi = (\mathrm{i}\hbar\partial_t - e\phi)^2\,\psi\,.$$

For energies close to the rest energy, i.e. for $\epsilon = mc^2 + E$, where $|E| \ll mc^2$, show that in sufficiently strong fields, the force experienced by the particle is attractive irrespective of the sign of the particle's charge. [Hint: Reduce the equation to the Schrödinger equation with the appropriate effective potential.] [4]

3. The Dirac equation in an external electromagnetic field $A^\mu = (\Phi, \mathbf{A})$ is

$$\left[\gamma^\mu \left(p_\mu - \frac{e}{c} A_\mu\right) - mc\right]\psi = 0,$$

where $\psi = \begin{pmatrix} \varphi \\ \chi \end{pmatrix}$ is the four-component Dirac spinor. The Minkowski metric is given by $\eta_{\mu\nu} = \mathrm{diag}(+1, -1, -1, -1)$, $p_\mu = \mathrm{i}\hbar\partial_\mu$, and the Dirac matrices are

$$\gamma^0 = \begin{pmatrix} I & 0 \\ 0 & -I \end{pmatrix}, \qquad \gamma^k = \begin{pmatrix} 0 & \sigma^k \\ -\sigma^k & 0 \end{pmatrix},$$

where I is the identity matrix, and σ^k are the Pauli matrices obeying $\sigma_i\sigma_k = \delta_{ik} + \mathrm{i}\epsilon_{ikl}\sigma_l$.

Assuming the external field is time-independent, consider stationary solutions of the Dirac equation with the time dependence of the form $\psi \sim \exp(-\mathrm{i}\epsilon t/\hbar)$.

Write down the system of coupled equations for the two-component spinors φ and χ. [6]

Consider the positive energy solution with $\epsilon = mc^2 + E$. Show that in the non-relativistic limit, where $|E| \ll mc^2$, $|e\Phi| \ll mc^2$, the spinor φ obeys the Pauli equation

$$\mathrm{i}\hbar\frac{\partial\varphi}{\partial t} = \left[\frac{(\mathbf{p} - \frac{e}{c}\mathbf{A})^2}{2m} + e\Phi - \mu\boldsymbol{\sigma}\cdot\mathbf{B}\right]\varphi$$

and find the value of the magnetic moment μ. [8]

Is the value of μ universal for all charged particles with spin 1/2?

Do you expect the theoretical prediction for μ following from the Dirac equation to be exact? Explain.

Is the value of the magnetic moment fixed uniquely by the Dirac equation? [Hint: Consider a non-minimal coupling to an electromagnetic field.] [3]

Consider further the case of $\mathbf{A} = 0$, and let $e\Phi = U(r)$. By expanding the Dirac equation to the next order in $|E|/mc^2 \ll 1$, $|U|/mc^2 \ll 1$, show that the spinor φ obeys the equation

$$\mathrm{i}\hbar\frac{\partial\varphi}{\partial t} = \left(\frac{\mathbf{p}^2}{2m} + U(r) + H_1\right)\varphi,$$

where the perturbation operator is given by

$$H_1 = -\frac{\mathbf{p}^4}{8m^3c^2} + \frac{1}{2m^2c^2}\frac{1}{r}\frac{dU(r)}{dr}\mathbf{L}\cdot\mathbf{S} - \frac{\hbar^2}{4m^2c^2}\frac{dU}{dr}\frac{d}{dr}.$$

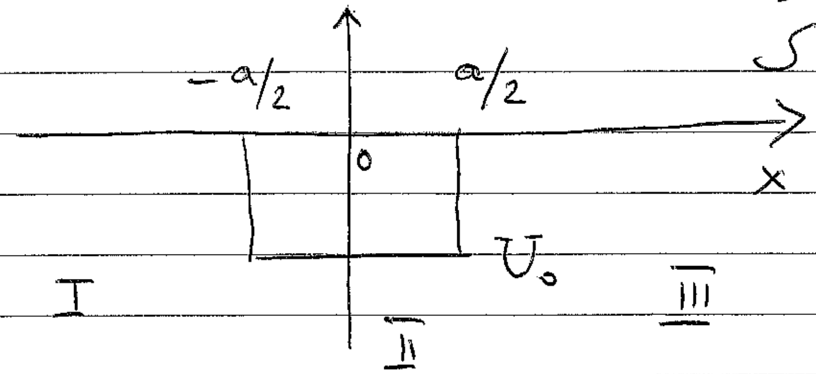
What is the physical meaning of terms in H_1? [8]

[You may use the following identity without proof:

$$(\boldsymbol{\sigma}\cdot\mathbf{p})f(\boldsymbol{\sigma}\cdot\mathbf{p}) = f\mathbf{p}^2 - \hbar^2(\partial_i f)\partial_i - \mathrm{i}\hbar^2\sigma^i\epsilon_{ijk}(\partial_j f)\partial_k\,. \;]$$

S18 Advanced Quantum Mechanics 2013 Solutions

1.



Solutions of the 1d-im Schrödinger eq in regions I, II, III are

$$\psi_{I} = e^{ikx} + Ae^{-ikx}, \quad x < -a/2$$

$$\psi_{II} = Be^{i\varkappa x} + Ce^{-i\varkappa x}, \quad -a/2 < x < \frac{a}{2} \quad [2]$$

$$\psi_{III} = Se^{ik(x-a)}, \quad x > a/2,$$

where $k^2 = 2mE/\hbar^2$, $\varkappa^2 = 2m(E+|U_0|)/\hbar^2$

Continuity conditions at $x = \pm a/2$ for ψ and ψ' lead to the following system of eqs:

$$e^{-ika/2} + Ae^{ika/2} = Be^{-i\varkappa a/2} + Ce^{i\varkappa \frac{a}{2}}$$

$$Be^{i\varkappa\frac{a}{2}} + Ce^{-i\varkappa\frac{a}{2}} = Se^{-ika/2} \quad [2]$$

$$ik\, e^{-ika/2} - ik\, Ae^{ika/2} = i\varkappa\, Be^{-i\varkappa a/2} - i\varkappa\, Ce^{i\varkappa a/2}$$

$$i\varkappa\, Be^{i\varkappa\frac{a}{2}} - i\varkappa\, Ce^{-i\varkappa\frac{a}{2}} = Se^{-ika/2} \cdot ik$$

This can be solved in a variety of ways.

For example, excluding A gives

$$2e^{-ika/2} = Be^{-i\varkappa a/2} + Ce^{i\varkappa a/2} +$$

$$+ \frac{\varkappa}{k} B e^{-i\varkappa a/2} - \frac{\varkappa}{k} C e^{i\frac{\varkappa a}{2}}$$

Then the second and third eqs give

$$\frac{Be^{i\varkappa a/2} - Ce^{-i\varkappa a/2}}{Be^{i\varkappa a/2} + Ce^{-i\varkappa a/2}} = \frac{k}{\varkappa}$$

$$\Rightarrow B = e^{-i\varkappa a} \frac{\left(1+\frac{k}{\varkappa}\right)}{\left(1-\frac{k}{\varkappa}\right)} C \quad \text{and}$$ [1]

$$C = \frac{2\left(1-\frac{k}{\varkappa}\right) e^{-\frac{ika}{2} + \frac{i\varkappa a}{2}}}{\left(1+\frac{\varkappa}{k}\right)\left(1+\frac{k}{\varkappa}\right)e^{-i\varkappa a} + \left(1-\frac{\varkappa}{k}\right)\left(1-\frac{k}{\varkappa}\right)e^{i\varkappa a}}$$

So for $S(k)$ we find:

$$S = \frac{4}{\frac{(k+\varkappa)^2}{k\varkappa} e^{-i\varkappa a} + \frac{(k-\varkappa)(\varkappa-k)}{k\varkappa} e^{i\varkappa a}}$$

$\Rightarrow$

$$S(E) = \frac{k\varkappa}{k\varkappa \cos\varkappa a - \frac{i}{2}(k^2+\varkappa^2)\sin\varkappa a}$$ [1]

The transmission probability is $T = |S|^2$ [1]

$$T = \left[\cos^2 \varkappa a + \frac{(k^2+\varkappa^2)^2}{4k^2\varkappa^2} \sin^2 \varkappa a\right]^{-1} =$$ [1]

$$= \left[1 + \frac{(k^2-\varkappa^2)^2}{4k^2\varkappa^2} \sin^2 \varkappa a\right]^{-1}.$$ [2]

The poles (zeros of denominator) of $S(E)$ are determined by the eq

$$\tan(\varkappa a) = -i \frac{2k\varkappa}{k^2+\varkappa^2}.$$ [1]

One can show by direct substitution (using the identities such as

$$\tan 2x = \frac{\sin 2x}{\cos 2x} = \frac{2\sin x \cos x}{\cos^2 x - \sin^2 x} = \frac{2\tan x}{1-\tan^2 x}$$) [2]

that the eq. is satisfied by the solutions to [2]

$$\tan \frac{\varkappa a}{2} = -\frac{ik}{\varkappa}, \quad \cot \frac{\varkappa a}{2} = \frac{ik}{\varkappa}.$$

Alternatively, one can use the identity $\tan 2x = \dfrac{2}{\cot x - \tan x}$ to rewrite the eq.

as

$$\cot\frac{\varkappa a}{2} - \tan\frac{\varkappa a}{2} = \frac{ik}{\varkappa} - \frac{\varkappa}{ik}.$$

This is a quadratic eq. for $X \equiv \cot\frac{\varkappa a}{2}$:

$$X - \frac{1}{X} = Y - \frac{1}{Y}, \text{ where}$$

$Y = ik/\varkappa$, with solutions $X = Y$, $X = -\frac{1}{Y}$,

i.e.

$$\cot\frac{\varkappa a}{2} = \frac{ik}{\varkappa}, \quad \tan\frac{\varkappa a}{2} = -\frac{ik}{\varkappa}$$

as before.

Now compare with bound state energies in the pot. well (as discussed in lectures extensively).

Since $k = \sqrt{2mE}/\hbar$ and E treated formally as a complex variable can be written as $E = |E|\, e^{i\varphi + i2\pi n}$,

where $n = 0, \pm 1, \pm 2, \ldots$,

$$E^{1/2} = |E|^{1/2} e^{i\varphi/2 + in\pi}$$

For $E < 0$: $\varphi = \pi \Rightarrow E^{1/2} = i\,|E|^{1/2}$ on the physical sheet of complex E.

Thus, $k = i\sqrt{2m|E|}/\hbar$ and the eqs become:

$$\tan\left[\frac{\sqrt{2m}\,a}{2\hbar}\sqrt{|U_0|-|E|}\right] = \frac{\sqrt{|E|}}{\sqrt{|U_0|-|E|}}$$

$$\cot\left[\frac{\sqrt{2m}\,a}{2\hbar}\sqrt{|U_0|-|E|}\right] = -\frac{\sqrt{|E|}}{\sqrt{|U_0|-|E|}}.$$

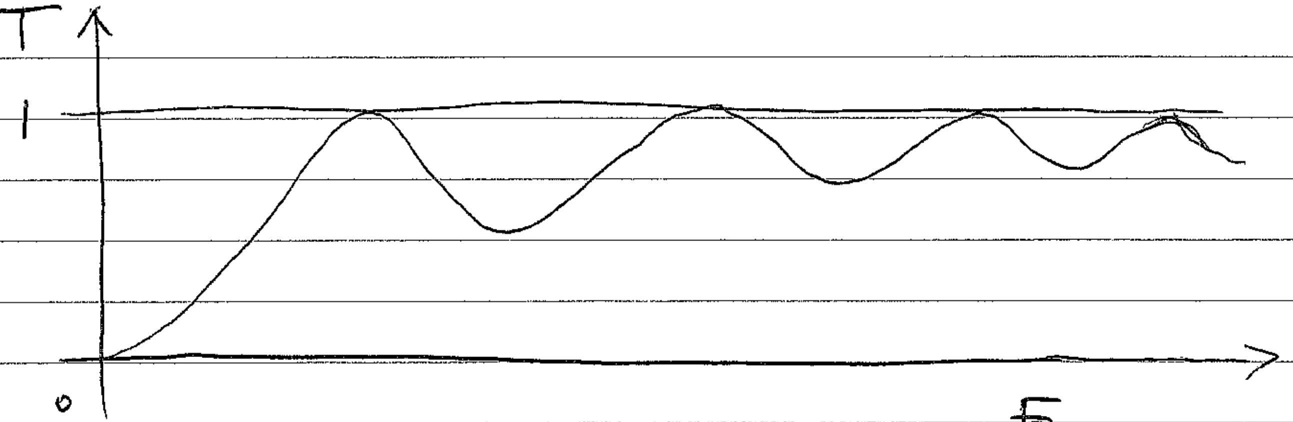
These eqs. determine energies of bound states in the pot. well. Indeed, for $E < 0$ the even stationary states are described by the wave function

$$\psi(x) = \begin{cases} A\cos\left(\frac{1}{\hbar}\sqrt{2m\left(|U_0|-|E|\right)}\,x\right), & |x| \le \frac{a}{2} \quad [2] \\ B\exp\left[-\frac{\sqrt{2m|E|}}{\hbar}x\right], & |x| > a/2 \quad [2] \end{cases}$$

The continuity condition for ψ, ψ' at $x = a/2$ (or $x = -a/2$) leads precisely to the first eq. above. Similarly, for odd parity states [4]
(with $\cos(\ldots) \to \sin(\ldots)$ in the wave function we obtain the second eq.

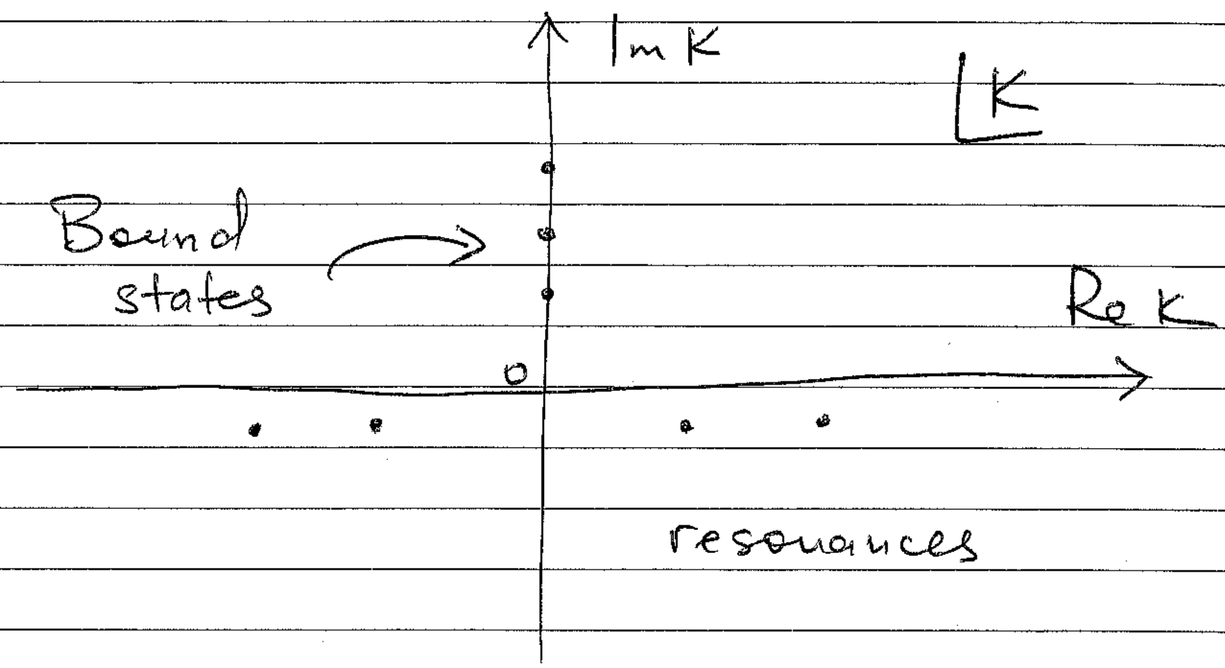
The max value of $T(E)$ is 1. From the explicit expression for $T(E)$ above one can see that this is [1]
achieved for $\sin \varkappa a = 0$, i.e. for

$$E_n = \frac{n^2 \pi^2 \hbar^2}{2ma^2} - |U_0| > 0, \quad n = 1, 2, \ldots$$



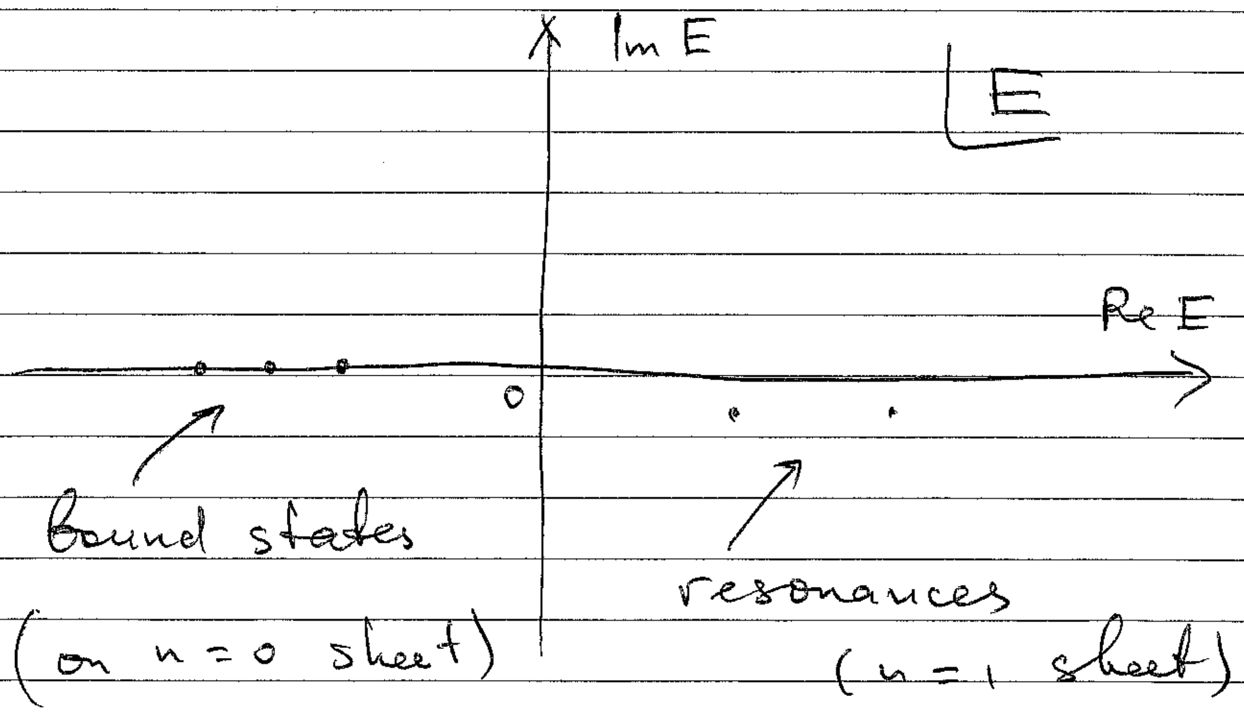
For $E = E_n$ the potential is transparent.

In the complex k-plane:



[1]

In the complex E-plane:



Only qualitative sketch is expected, as discussed in lectures.

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2 With the usual correspondence

$$\frac{E}{c} \to \frac{i\hbar}{c}\frac{\partial}{\partial t}, \quad \vec{p} \to -i\hbar\vec{\nabla}$$

the eq. gives $E^2 = p^2c^2 + m^2c^4 + 2mc^2\Phi$ [3]

$$\Rightarrow E = mc^2\left(1 + \frac{p^2}{m^2c^2} + \frac{2\Phi}{mc^2}\right)^{1/2} \approx$$

$\approx mc^2 + \frac{p^2}{2m} + \Phi + \ldots$ in the non-rel. limit. [2]

For spinless particles, the charge conjugation $\hat{C}$ acts as $\psi_c = \hat{C}\psi = \psi^*$. This [1] allows to interpret the negative energy solutions $\psi^{(-)}$ as antiparticles $\psi_c^{(+)} = \hat{C}\psi^{(-)}$. For real $\Phi(\vec{r},t)$, ψ_c obviously obeys the same eq. as ψ $\Rightarrow$ particles and antiparticles behave identically in an external scalar field. [1]

Stationary states of the discrete spectrum are determined by writing $\psi = e^{-i\varepsilon t/\hbar}\tilde{\psi}(r)$ and recasting the eq. as [1]

$$\left(-\frac{\hbar^2}{2m}\Delta + \Phi(r)\right)\tilde{\psi} = \frac{\varepsilon^2 - m^2c^4}{2mc^2}\tilde{\psi}$$

This is just a Schrödinger-type eq. [1]

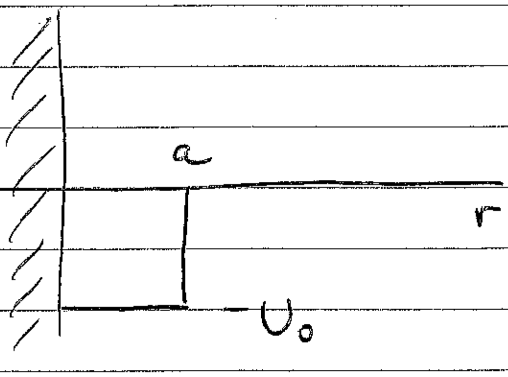
with $E \equiv \dfrac{\varepsilon^2 - m^2c^4}{2mc^2}$.

$$\Delta\tilde{\psi} = \frac{1}{r^2}\frac{d}{dr}\left(r^2\frac{d\tilde{\psi}}{dr}\right) = \frac{1}{r}\frac{d^2}{dr^2}\left(r\tilde{\psi}\right).$$

With $R = r\tilde{\psi}$, the eq. becomes

<u>1-dimensional</u>: $\dfrac{\hbar^2}{2m}R'' - \Phi(r)R = -ER$

$E<0$ corresp. to bound ~~states~~:



$$\begin{cases} R'' + \dfrac{2m}{\hbar^2}(E+U_0)R = 0, & r<a \\ R'' + \dfrac{2m}{\hbar^2}ER = 0, & r>a \end{cases}$$ [1]

$r>a$: $R'' - \varkappa^2 R = 0$, $\varkappa^2 = \dfrac{m^2c^4 - \varepsilon^2}{\hbar^2c^2} > 0$ [1]

$R(r) = Be^{-\varkappa r} \to 0$, $r \to \infty$.

$r<a$: $R'' + \dfrac{2m}{\hbar^2}(E+U_0)R = 0$

$R(0) = 0 \Rightarrow R = A\sin\left[\sqrt{\dfrac{2mU_0}{\hbar^2} - \varkappa^2}\; r\right]$. [1]

Conditions at $r=a$: R and R' should be cont. functions (as follows from the eq) $\Rightarrow$ [2]

$$\left.\begin{aligned} Be^{-\varkappa a} &= A\sin\left[\sqrt{}\,a\right] \\ -\varkappa B e^{-\varkappa a} &= A\cos\left[\sqrt{}\,a\right]\cdot\sqrt{} \end{aligned}\right\}$$ [1]

or $$\tan\sqrt{\frac{2mU_0a^2}{\hbar^2}-\varkappa^2a^2} = -\frac{\sqrt{\frac{2mU_0a^2}{\hbar^2}-\varkappa^2a^2}}{\varkappa a}$$ [1]

This eq. determines the spectrum ε_n.
The spectrum of antiparticles is the same in view of what was said about ψ_c above.

Substituting $\varepsilon_n^2=0$, we get eq. for the critical values of the field

$$\tan\left[\frac{mca}{\hbar}\sqrt{\frac{2U_{0,cr}}{mc^2}-1}\right] = -\sqrt{\frac{2U_{0,cr}}{mc^2}-1}$$ [1]

This can be further analysed for $a \gg \frac{\hbar}{mc}$ and $a \ll \frac{\hbar}{mc}$.

For external fields exceeding the critical value $U_{0,cr}$, $\varepsilon_n^2 < 0$ formally, [1] which indicates instability.

At $U = U_{0,cr}$, both particles and antiparticles have $\varepsilon_n^2 = 0$ => pairs of [2] particle-antiparticle can be spontaneously created by the external field.

In this situation, one-particle rel. [1] equation is inadequate and methods of quantum field theory should be used instead.

The eq. $\left(-\hbar^2 c^2 \Delta + m^2 c^4\right)\psi = \left(i\hbar\partial_t - e\phi\right)^2\psi$ can be written (for stationary solutions with $\psi \sim e^{-i\varepsilon t/\hbar}$) as

$$\left(-\hbar^2 c^2 \Delta + m^2 c^4\right)\tilde{\psi} = (\varepsilon - e\phi)^2 \tilde{\psi} \qquad [1]$$

With $\varepsilon = mc^2 + E$, $|E| \ll mc^2$, this can be written as

$$-\frac{\hbar^2}{2m}\Delta\tilde{\psi} = \left(\frac{(E - e\phi + mc^2)^2}{2mc^2} - \frac{mc^2}{2}\right)\tilde{\psi} \qquad [1]$$

$\Rightarrow$ for $|E| \ll mc^2$ this becomes

$$\left(-\frac{\hbar^2}{2m}\Delta + e\phi - \frac{(e\phi)^2}{2mc^2}\right)\tilde{\psi} = E\tilde{\psi} \qquad [1]$$

which is just the Schrödinger eq. with $U_{eff} = e\phi - \frac{(e\phi)^2}{2mc^2}$

For strong fields $|e\phi| > 2mc^2$

$U_{eff} < 0 \Rightarrow$ the potential is attractive for any sign of e. [1]

3 $$\left[\gamma^\mu\left(p_\mu - \frac{e}{c}A_\mu\right) - mc\right]\begin{pmatrix}\varphi \\ \chi\end{pmatrix} = 0$$

Here $p_\mu = i\hbar\partial_\mu = \left(\frac{i\hbar}{c}\frac{\partial}{\partial t}, i\hbar\frac{\partial}{\partial x^i}\right) =$

$= \left(\frac{i\hbar}{c}\frac{\partial}{\partial t}, -\hat{p}\right)$, where $\hat{p} = -i\hbar\frac{\partial}{\partial x^i}$. [1]

$$p^\mu = i\hbar\frac{\partial}{\partial x_\mu} = \left(\frac{i\hbar}{c}\frac{\partial}{\partial t}, -i\hbar\frac{\partial}{\partial x^i}\right)$$

$A^\mu = (\Phi, \vec{A}) \Rightarrow \gamma^\mu\left(p_\mu - \frac{e}{c}A_\mu\right) - mc =$

$$= \left[\begin{pmatrix} I & 0 \\ 0 & -I\end{pmatrix}\left(p^0 - \frac{e}{c}\Phi\right) - \begin{pmatrix} 0 & \vec{\sigma} \\ -\vec{\sigma} & 0\end{pmatrix}\left(\vec{p} - \frac{e}{c}\vec{A}\right) - \begin{pmatrix} mc & 0 \\ 0 & mc\end{pmatrix}\right]$$ [1]

With $\psi \sim e^{-i\varepsilon t/\hbar}$ eq. becomes [1]

$$\begin{pmatrix} \frac{\varepsilon}{c} - \frac{e}{c}\Phi - mc & -\vec{\sigma}\left(\vec{p} - \frac{e}{c}\vec{A}\right) \\ \vec{\sigma}\left(\vec{p} - \frac{e}{c}\vec{A}\right) & -\frac{\varepsilon}{c} + \frac{e}{c}\Phi - mc \end{pmatrix}\begin{pmatrix}\varphi \\ \chi\end{pmatrix} = 0$$ [1]

or

$$\left(\varepsilon - e\Phi - mc^2\right)\varphi = c\vec{\sigma}\left(\vec{p} - \frac{e}{c}\vec{A}\right)\chi$$ [1]

$$\left(\varepsilon - e\Phi + mc^2\right)\chi = c\vec{\sigma}\left(\vec{p} - \frac{e}{c}\vec{A}\right)\varphi$$

With $\varepsilon = mc^2 + E$:

$$(E - e\Phi)\varphi = c\vec{\sigma}\left(\vec{p} - \frac{e}{c}\vec{A}\right)\chi$$

$$(E - e\Phi + 2mc^2)\chi = c\vec{\sigma}\left(\vec{p} - \frac{e}{c}\vec{A}\right)\varphi \quad [1]$$

For $|E| \ll mc^2$, $|e\Phi| \ll mc^2$ the second eq. can be expanded as

$$\chi = \frac{\vec{\sigma}\left(\vec{p} - \frac{e}{c}\vec{A}\right)}{2mc}\varphi + \dots \quad \text{and subst.} \quad [1]$$

into the first one:

$$(E - e\Phi)\varphi = \frac{1}{2m}\left[\vec{\sigma}\left(\vec{p} - \frac{e}{c}\vec{A}\right)\right]\left[\vec{\sigma}\left(\vec{p} - \frac{e}{c}\vec{A}\right)\right]\varphi \quad [1]$$

Need to simplify $(\vec{\sigma}\vec{A})(\vec{\sigma}\vec{B})$, where $\vec{A}, \vec{B}$ are vectors; using $\sigma_i\sigma_k = \delta_{ik} + i\varepsilon_{ikl}\sigma_l$ we get $\left(\vec{\underline{P}} = \vec{p} - \frac{e}{c}\vec{A}\right)$:

$$\left[\vec{\sigma}\left(\vec{p} - \frac{e}{c}\vec{A}\right)\right]\left[\vec{\sigma}\left(\vec{p} - \frac{e}{c}\vec{A}\right)\right]\varphi = \vec{\underline{P}}^2\varphi -$$

$$- i\hbar^2\sigma^i\varepsilon_{ijk}\left(\partial_j - \frac{ie}{\hbar c}A_j\right)\left(\partial_k\varphi - \frac{ie}{\hbar c}A_k\varphi\right) =$$

$$= \vec{\underline{P}}^2\varphi - i\hbar^2\sigma^i\varepsilon_{ijk}\left(\partial_j\partial_k\varphi - \frac{ie}{\hbar c}\partial_j A_k\varphi -\right.$$

$$\left. - \frac{ie}{\hbar c}A_k\partial_j\varphi - \frac{ie}{\hbar c}A_j\partial_k\varphi\right) =$$

$$= \vec{P}^2\varphi - \frac{e\hbar}{c}\sigma^i \varepsilon_{ijk}\partial_j A_k \varphi =$$

$$= \vec{p}^2\varphi - \frac{e\hbar}{c}\vec{\sigma}\cdot\vec{B}\varphi, \quad \vec{B} = \mathrm{curl}\,\vec{A}.$$ [3]

Thus the eq is:

$$\left(E - e\Phi\right)\varphi = \left[\frac{\left(\vec{p} - \frac{e}{c}\vec{A}\right)^2}{2m} - \frac{e\hbar}{2mc}\vec{\sigma}\cdot\vec{B}\right]\varphi$$ [1]

For non-rel. spinor $\varphi \sim e^{-iEt/\hbar}$:

$$i\hbar\frac{\partial\varphi}{\partial t} = \left[\frac{\left(\vec{p} - \frac{e}{c}\vec{A}\right)^2}{2m} + e\Phi - \mu_0\vec{\sigma}\cdot\vec{B}\right]\varphi,$$ [1]

where $\mu_0 = \frac{e\hbar}{2mc}$. (This is Pauli eq).

The value of μ_0 is (almost) correct for an electron but for other charged [1] particles with spin $1/2$ deviations are significant and are due to interactions with other fields and rad. corrections.

The value of μ_0 predicted by the [1] (min. coupled) Dirac eq. cannot be exact due to QED corrections such as self-interaction, Lamb shift etc.

The prediction for μ_0 can be altered by including the „Pauli term"

$\alpha\,[\gamma^\mu\gamma^\nu]F_{\mu\nu}\,\psi$ with arbitrary α [2]

in the non-minimal coupling scheme (such term is Lor. and gauge-invar and in principle should be kept in the Dirac eq.) This is further clarified in QED.

Now let $\vec{A} = 0, \quad e\Phi = U(r)$.

Then:

$$(E-U)\varphi = c\,\vec{\sigma}\vec{p}\,\chi$$ [1]

$$(E-U+2mc^2)\chi = c\,\vec{\sigma}\cdot\vec{p}\,\varphi$$

$$\Rightarrow \chi = \left(1 - \frac{E-U}{2mc^2}\right)\frac{\vec{\sigma}\vec{p}}{2mc}\varphi + \dots$$ [2]

(keeping 2 terms now)

The eq. becomes

$$(E-U)\varphi = \frac{1}{2m}(\vec{\sigma}\vec{p})(\vec{\sigma}\vec{p}) - \frac{\vec{\sigma}\vec{p}}{2m}\frac{E-U}{2mc^2}\vec{\sigma}\vec{p}\varphi \quad [1]$$

Since $[\vec{\sigma}\vec{p}, f\vec{\sigma}\vec{p}] = -i\hbar(\partial_i f)\sigma^i(\vec{\sigma}\vec{p})$

and $(\vec{\sigma}\vec{p})(\vec{\sigma}\vec{p}) = \vec{p}^{\,2}$, one has

$$(\vec{\sigma}\vec{p})f(\vec{\sigma}\vec{p}) = f\vec{p}^{\,2} - \hbar^2(\partial_k f)\partial_k - i\hbar^2\sigma^l\varepsilon_{lki}\partial_k f\partial_i$$

(this formula is provided).

We find

$$(E-U)\varphi = \frac{\vec{p}^{\,2}}{2m}\varphi - \frac{(E-U)}{4m^2c^2}\vec{p}^{\,2}\varphi + \quad [1]$$

$$+ \frac{\hbar^2}{4m^2c^2}(\partial_k U)\partial_k\varphi - \frac{1}{4m^2c^2}i\hbar^2\sigma^l\varepsilon_{lki}\partial_k U\partial_i\varphi$$

To leading order, $E - U = \frac{\vec{p}^{\,2}}{2m}$ [1]

$$\Rightarrow (E-U)\varphi = \frac{\vec{p}^{\,2}}{2m}\varphi - \frac{\vec{p}^{\,4}}{8m^3c^2}\varphi + \frac{\hbar^2}{4m^2c^2}(\partial_k U)\partial_k\varphi$$

$$+ \frac{1}{r}\frac{dU}{dr}\frac{\vec{L}\vec{S}}{2m^2c^2}\varphi.$$

Again, for non-rel. spinor $\varphi \sim e^{-iEt/\hbar}$

$$i\hbar\frac{\partial\varphi}{\partial t}=\left(\frac{\hat{p}^2}{2m}+U+H_1\right)\varphi,$$

where

$$H_1\varphi=-\frac{\vec{p}^{\,4}}{8m^3c^2}\varphi+\frac{1}{2m^2c^2}\frac{1}{r}\frac{dU}{dr}\vec{L}\cdot\vec{S}\varphi+$$

$$+\frac{\hbar^2}{4m^2c^2}(\partial_k U)\,\partial_k\varphi,$$ [1]

where $\vec{S}=\hbar\frac{\vec{\sigma}}{2}$, $\vec{L}=\vec{r}\times\vec{p}$.

The first term in H_1 is the contribution to the expansion of $E=\varepsilon-mc^2=$

$$=mc^2\left(1+\frac{p^2}{m^2c^2}\right)^{1/2}-mc^2=\frac{p^2}{2m}-\frac{p^4}{8m^3c^2}+\ldots,$$ [1]

the second term is the spin-orbit coupling (incl. Thomas-Frenkel factor of $1/2$), the last term has no classical analogue.