Advanced Quantum Mechanics

S18 Exam 2016

Solutions

Problem 1

The Schrödinger eq. can be written as

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} - E\psi = -U(x)\,\psi(x),$$

i.e. $\hat{L}(x)\,\psi(x) = f(x)$, where

1 $f(x) = -U(x)\,\psi(x)$. Then the solution can be written in the form

$$\psi(x) = \psi_0(x) + \int G(x,x')\,f(x')\,dx',$$

where $L\psi_0 = 0$ and G obeys

$$\hat{L}(x)\,G(x,x') = \delta(x,x')$$

In our case,

1 $$\psi(x) = Ae^{-\varkappa x} + Be^{\varkappa x} - \int_{-\infty}^{\infty} G(x,x')\,U(x')\,\psi(x')\,dx'$$

and $A, B = 0$ since our b. c. are $\psi(x) \to 0$ for $x \to \pm\infty$ $(E<0!)$

Using the explicit form of $G(x, x')$ given in the problem, we find

$$\psi(x) = -\frac{m}{\varkappa \hbar^2} \int_{-\infty}^{\infty} e^{-\varkappa |x-x'|} U(x') \psi(x') dx',$$

as required. (This method has been discussed in the lectures.)

Now, for $U(x) = -\alpha \left[\delta(x-a) + \delta(x) + \delta(x+a) \right]$, we find

$$\psi(x) = +\frac{m\alpha}{\varkappa \hbar^2} \left[e^{-\varkappa|x-a|} \psi(a) + e^{-\varkappa|x|} \psi(0) + e^{-\varkappa|x+a|} \psi(-a) \right]$$

In particular,

$$\psi(a) = \frac{m\alpha}{\varkappa \hbar^2} \left[\psi(a) + e^{-\varkappa a} \psi(0) + e^{-2\varkappa a} \psi(-a) \right]$$

$$\psi(0) = \frac{m\alpha}{\varkappa \hbar^2} \left[e^{-\varkappa a} \psi(a) + \psi(0) + e^{-\varkappa a} \psi(-a) \right]$$

$$\psi(-a) = \frac{m\alpha}{\varkappa \hbar^2} \left[e^{-2\varkappa a} \psi(a) + e^{-\varkappa a} \psi(0) + \psi(-a) \right]$$

We can introduce $y = \varkappa a$,
$\lambda = \hbar^2/ma\alpha$ and write these eqs
in the matrix form:

1
$$\begin{bmatrix} 1-\lambda y & e^{-y} & e^{-2y} \\ e^{-y} & 1-\lambda y & e^{-y} \\ e^{-2y} & e^{-y} & 1-\lambda y \end{bmatrix} \begin{pmatrix} \psi(a) \\ \psi(0) \\ \psi(-a) \end{pmatrix} = 0.$$

This system has a non-triv. solution
1 iff: $\det(\text{Matrix}) = 0 \Rightarrow$
2 $1 + X - 2e^{2X/\lambda}(1-X) + e^{4X/\lambda}(1-X)^3 = 0$

$X \equiv \lambda y$.

1) Small λ: the term with $e^{4X/\lambda}$
1 dominates in the limit $\lambda \to 0 \Rightarrow$
1
1 $X \approx 1$ i.e. $y \approx 1/\lambda$ (triple degen.)

2) Shallow well: $\lambda \gg 1 \Rightarrow$ can
expand exponents $\Rightarrow$

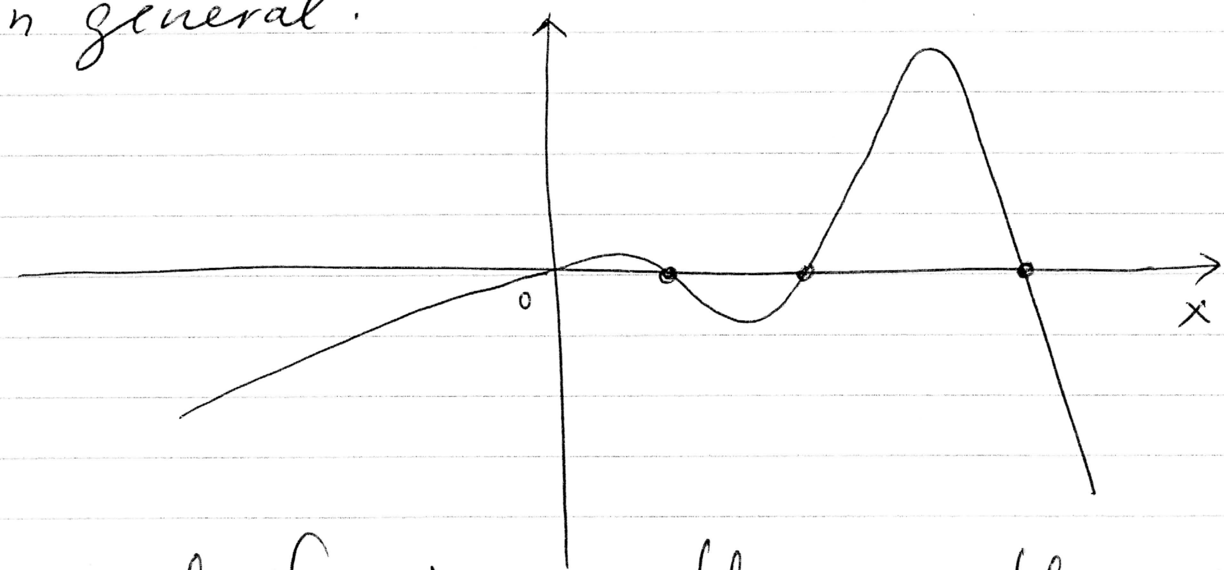
1 $\quad 1 + x - 2(1-x) + (1-x)^3 \approx 0$

$\Rightarrow \; -x^2(x-3) \approx 0$

$\Rightarrow \; x = 3$ non-triv. solution

1 $\quad \Rightarrow \; \eta \approx 3/\lambda$ (single root)

In general:



3 roots for $\lambda \ll 1$, then 2, then 1 for $\lambda \gg 1$.

Scattering states

$$\psi(x) = e^{ikx} - \int_{-\infty}^{\infty} G^+(x,x')\,U(x')\,\psi(x')\,dx'$$

$$G^+(x,x') = \frac{im}{k\hbar^2}\, e^{ik|x-x'|}$$

Subst. $U(x')$, get the solution

2 $$\psi(x) = e^{ikx} + \frac{i\alpha m}{k\hbar^2}\Big[e^{ik|x-a|}\psi(a) + e^{ik|x|}\psi(0) + e^{ik|x+a|}\psi(-a)\Big]$$

To extract $S(k)$, look at asympt. at $x \to +\infty$ $\left(\sim S(k)e^{ikx}\right)$:

$$\psi(x) \sim e^{ikx}\Big[1 + \frac{i\alpha m}{k\hbar^2}\left(\psi(a)e^{-ika} + \psi(0) + e^{ika}\psi(-a)\right)\Big]$$

2 $$\Rightarrow S(k) = 1 + \frac{i\alpha m}{k\hbar^2}\left(\psi(a)e^{-ika} + \psi(0) + e^{ika}\psi(-a)\right).$$

Now we need to find $\psi(a), \psi(0), \psi(-a)$.

Subst. in the solution for $\psi(x)$:

1 $$\psi(0) = 1 + \frac{i\alpha m}{k\hbar^2}\Big[e^{ika}\psi(a) + \psi(0) + e^{ika}\psi(-a)\Big]$$

$\psi(a) = \ldots$

$\psi(-a) = \ldots$

Introduce $\xi = ka$, $\lambda = \dfrac{\hbar^2}{\alpha m a}$; then

we can write the 3-eqs in matrix form

as

1 $$\begin{pmatrix} i e^{i\xi} & i - \lambda\xi & i e^{i\xi} \\ i - \lambda\xi & i e^{i\xi} & i e^{i2\xi} \\ i e^{i2\xi} & i e^{i\xi} & i - \lambda\xi \end{pmatrix} \begin{pmatrix} \psi(a) \\ \psi(0) \\ \psi(-a) \end{pmatrix} =$$

$$= \begin{pmatrix} -\lambda\xi \\ -\lambda\xi e^{i\xi} \\ -\lambda\xi e^{-i\xi} \end{pmatrix}$$

This is eq. of the form $AX = B$,

1 so the solution for $X = \begin{pmatrix} \psi(a) \\ \psi(0) \\ \psi(-a) \end{pmatrix}$

2 is $X = A^{-1}B$. Note that A^{-1} is

built as $A^{-1} = \dfrac{1}{\det A}(\cdots)$, so

the singularities of x (and thus
1 of $S(k)$) are the zeros of $\det A$.
Consider such zeros on the Im axis
of ξ by setting $\xi = i\eta$. The
$\det A = 0$ then gives

$$1+\eta\lambda - 2e^{2\eta}(1-\eta\lambda) + e^{4\eta}(1-\eta\lambda)^3 = 0$$

i.e. exactly the condition for bound
states found earlier.

Just like in the case of 2 δ-funct.
wells considered in detail in the lectures,
1 we expect other singularities (e.g.
resonances) in the complex plane of ξ
but not on $\mathrm{Im}\,\xi$ axis. For example, in
the limit of $\lambda \to 0$ (deep wells),
we expect the refl. coeff. $R \to 1$, $T \to 0$
except for resonance states $\Rightarrow$ expect
poles close to real axis + Breit-Wigner
behaviour.

Problem 2

Quantum theory subst. $E \to i\hbar \frac{\partial}{\partial t}$

$p_i \to -i\hbar \frac{\partial}{\partial x^i}$ convert the rel. disp. rel. $E^2 = p^2c^2 + m^2c^4$ into Klein-

1 Gordon eq. $\left(\frac{1}{c^2}\frac{\partial^2}{\partial t^2} - \frac{\partial^2}{\partial x_i^2} + \frac{m^2c^2}{\hbar^2}\right)\psi = 0$

Conversely, solutions of the eq. in the form of plane waves (a la

1 de Broglie) $\sim e^{-iEt/\hbar + ip_i x^i/\hbar}$

exist for $E^2 = p^2c^2 + m^2c^4$.

The associated dispers. rel. is

1 $E^2 = \hbar^2 c^2 \alpha U + \vec{p}^{\,2}c^2 + m^2c^4$

and we have

$$E = mc^2\left[1 + \frac{\vec{p}^{\,2}c^2}{m^2c^4} + \frac{\hbar^2c^2}{m^2c^4}\alpha U\right]^{1/2} \approx$$

$$\approx mc^2\left[1 + \frac{\vec{p}^{\,2}}{2m^2c^2} + \frac{\hbar^2}{2m^2c^2}\alpha U + \dots\right]$$

1

$$= mc^2 + \frac{\vec{p}^{\,2}}{2m} + \frac{\hbar^2}{2m}\alpha U + \dots$$

This gives the usual non-rel. energy for $E - mc^2$ if $\alpha = \frac{2m}{\hbar^2}$.

The eqs. satisfied by ψ and ψ^* are (let $c = 1$):

1 (a) $\left[\Box + ie\left(\partial_\mu A^\mu + 2A^\mu \partial_\mu + ieA_\mu A^\mu\right) + m^2\right]\psi = 0$

1 (b) $\left[\Box - ie\left(\partial_\mu A^\mu + 2A^\mu \partial_\mu - ieA_\mu A^\mu\right) + m^2\right]\psi^* = 0$

On the other hand,

1 $\partial_\mu j^\mu = -\frac{i}{2}\left(\partial_\mu \psi\, \partial^\mu \psi^* + \psi \Box \psi^* - \partial_\mu \psi\, \partial^\mu \psi^* - \psi^* \Box \psi\right) - e\left(\psi A^\mu \partial_\mu \psi^* + \psi \psi^* \partial_\mu A^\mu + \psi^* A^\mu \partial_\mu \psi\right)$. (c)

1 Multiplying eq (a) by ψ^* and (b) by ψ and subtracting we get:

$\psi \Box \psi^* - \psi^* \Box \psi - 2ie\left(\psi\psi^*\right)\partial_\mu A^\mu +$

1 $+ A^\mu \psi^* \partial_\mu \psi + A^\mu \psi \partial_\mu \psi^* \Big) = 0$

Now, subst. in (c) results in

1 $\partial_\mu j^\mu = 0.$

The time-indep. elm. field $\Rightarrow$ can consider $\psi(t, \vec{r}) = e^{-i\varepsilon t/\hbar} \varphi(\vec{r})$.

2 Direct subst. gives the stationary KG eq:

$$\left[c^2\left(\hat{p} - \frac{e}{c}A\right)^2 + m^2c^4\right]\varphi = (\varepsilon - e\Phi)^2\varphi$$

For $\vec{A} = 0$ and $e\Phi = -Ze^2/r$,

we get

1 $$\left(-c^2\hbar^2\nabla^2 + m^2c^4\right)\varphi = \left(\varepsilon + \frac{Ze^2}{r}\right)^2\varphi$$

Let $\varepsilon = mc^2 + E$, then the eq is

1 $$\nabla^2\varphi + \frac{1}{\hbar^2c^2}\left[\left(E + mc^2 + \frac{Ze^2}{r}\right)^2 - m^2c^4\right]\varphi = 0$$

With $\varphi = R(r)\, Y_{lm}(\theta, \varphi)$ and using $\nabla^2 = \nabla_r^2 + \frac{1}{r^2} \nabla_{\theta,\varphi}^2$

$$\nabla^2 \varphi = \frac{1}{r} \frac{d^2(rR)}{dr^2} Y_{\ell m} - \frac{\ell(\ell+1)}{r^2} R Y_{\ell m}$$

we find:

$$\frac{1}{r} \frac{d^2(rR)}{dr^2} - \frac{\ell(\ell+1)}{r^2} R +$$

$$+ \frac{1}{\hbar^2 c^2} \left[\left(E + mc^2 + \frac{Ze^2}{r} \right)^2 - m^2 c^4 \right] R = 0$$

This can be written in the form

$$\frac{1}{r} \frac{d^2(rR)}{dr^2} - V_{eff} R = A R(r),$$

where

$$A = \frac{m^2 c^2}{\hbar^2} - \frac{(E + mc^2)^2}{\hbar^2 c^2} =$$

$$= \frac{m^2 c^2}{\hbar^2} \left[1 - \left(1 + \frac{E}{mc^2} \right)^2 \right] \to -\frac{2mE}{\hbar^2}$$

in the non-rel. limit,

$$V_{eff} = \frac{l(l+1)}{r^2} - \frac{2}{\hbar^2 c^2}(E+mc^2)\frac{Ze^2}{r} - \frac{Z^2 e^4}{\hbar^2 c^2 r^2} = \frac{l(l+1) - Z^2\alpha_{em}^2}{r^2} - \frac{2B}{r},$$

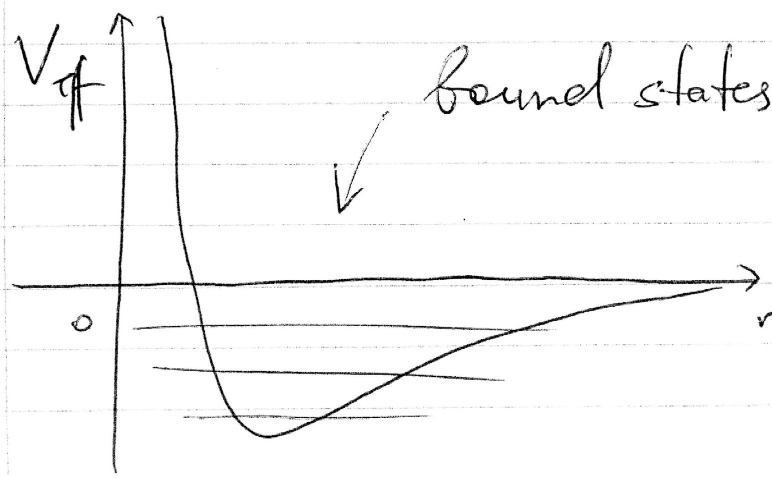
where $\alpha_{em} = e^2/\hbar c$,

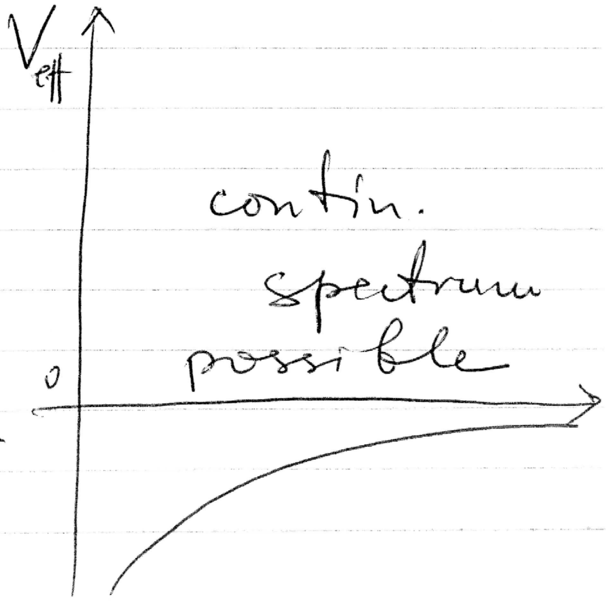
$$B = \frac{Ze^2}{\hbar^2 c^2}(E+mc^2) = \frac{Ze^2 m}{\hbar^2}\left(1+\frac{E}{mc^2}\right)$$

$B \to \dfrac{Ze^2 m}{\hbar^2}$ in the non-rel. limit.

So, $V_{eff}(r) = \dfrac{\alpha}{r^2} - \dfrac{\beta}{r}$, where

$\beta > 0$ but α can change sign dep. on Z, l.





The KG equation takes into account rel. effects but ignores spin.

2 Thus, the energy spectrum will not be in agreement with experiment (a priori and in reality), as discussed in detail in the lectures.

Problem 3.

$$i\hbar \frac{\partial \psi}{\partial t} = \frac{\hbar c}{i}\left(\alpha_1 \frac{\partial \psi}{\partial x^1} + \alpha_2 \frac{\partial \psi}{\partial x^2} + \alpha_3 \frac{\partial \psi}{\partial x^3}\right)$$

$$+ \beta m c^2 \psi \equiv H_D \psi$$

α_i and β cannot be numbers if

1 we want the eq. to be Lor-covar.

e.g. even rotations in $x^1 - x^2$ plane

would lead to a different eq.

in x' coordinates.

1 Square the eq: $-\hbar^2 \partial^2_{tt} \psi = i\hbar \hat{H}_D \frac{\partial \psi}{\partial t}$

$= \hat{H}_D^2 \psi$.

$$\Rightarrow \quad -\hbar^2 \frac{\partial^2 \psi}{\partial t^2} = -\hbar^2 c^2 \sum_{i,j=1}^{3} \frac{1}{2}(\alpha_j \alpha_i + \alpha_i \alpha_j) \frac{\partial^2 \psi}{\partial x^i \partial x^j}$$

2

$$+ \frac{\hbar m c^3}{i} \sum_{i=1}^{3} (\alpha_i \beta + \beta \alpha_i) \frac{\partial \psi}{\partial x^i} + \beta^2 m^2 c^4 \psi$$

$\Rightarrow$ this gives KG-eq. for each component ψ_α if

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

$\alpha_i\alpha_k + \alpha_k\alpha_i = 2\delta_{ik}$

Eigenvalues ~~of~~ α_i, β:

$$\alpha_i\varphi = \lambda\varphi$$

1 $$\alpha_i^2\varphi = \lambda\alpha_i\varphi = \lambda^2\varphi$$

But $\alpha_i^2 = \mathbb{1} \Rightarrow \lambda^2 = 1$ +

1 α_i - Hermitian $\Rightarrow$ eigenvalues real $\Rightarrow$ $\lambda = \pm 1$.

Same argument for β.

1 Now, $\operatorname{tr}\alpha_i = 0$, $\operatorname{tr}\beta = 0$:

Use $\alpha_i = -\beta\alpha_i\beta \Rightarrow$

1 $$\operatorname{tr}\alpha_i = -\operatorname{tr}\beta\alpha_i\beta = -\operatorname{tr}\alpha_i$$

$\Rightarrow \operatorname{tr}\alpha_i = 0$. Same for β.

1 Since $\operatorname{tr}\alpha_i = \sum_{k=1}^{N}\lambda_k = +1+1+\ldots-1-1$

$= 0 \Rightarrow$

$\Rightarrow N$ is even. $N = 2$ gives Pauli matrices $\Rightarrow$ 3 of them is NOT enough ($\alpha_{1,2,3}$ <u>and</u> β = 4).

$\Rightarrow N \geq 4$.

With $\psi^+ = (\psi_1^*, \ldots \psi_4^*)$ get

1 $$i\hbar \psi^+ \frac{\partial \psi}{\partial t} = \frac{\hbar c}{i} \sum_{k=1}^{3} \psi^+ \alpha_k \frac{\partial \psi}{\partial x^k} + mc^2 \psi^+ \beta \psi$$

and

1 $$-i\hbar \frac{\partial \psi^+}{\partial t} \psi = -\frac{\hbar c}{i} \sum_{k=1}^{3} \frac{\partial \psi^+}{\partial x^k} \alpha_k \psi + mc^2 \psi^+ \beta \psi.$$

Subtracting $\Rightarrow$

1 $$i\hbar \frac{\partial}{\partial t}(\psi^+ \psi) + i\hbar c \sum_{k=1}^{3} \frac{\partial}{\partial x^k}(\psi^+ \alpha_k \psi) = 0$$

2 i.e. $\frac{\partial \rho}{\partial t} + \operatorname{div} \vec{j} = 0$ with

$\rho = \psi^+ \psi$, $j_k = c \psi^+ \alpha_k \psi$.

The Dirac eq. is written as: Operator

$$\gamma^{\mu}\left(p_{\mu} - \frac{e}{c}A_{\mu}\right) - mc =$$

$$= \begin{pmatrix} \mathbb{1} & 0 \\ 0 & \mathbb{1} \end{pmatrix}\left(p^{0} - \frac{e}{c}\phi\right) - \begin{pmatrix} 0 & \vec{\sigma} \\ -\vec{\sigma} & 0 \end{pmatrix}\left(\vec{p} - \frac{e}{c}\vec{A}\right) -$$

$$- \begin{pmatrix} mc & 0 \\ 0 & mc \end{pmatrix} \Rightarrow \text{ acting on } \begin{pmatrix} \varphi \\ \chi \end{pmatrix}$$

$$\begin{pmatrix} \frac{E+mc^2}{c} - \frac{e}{c}\phi - mc & -\bar{\sigma}\left(\bar{p} - \frac{e}{c}\bar{A}\right) \\ \bar{\sigma}\left(\bar{p} - \frac{e}{c}\bar{A}\right) & -\frac{E+mc^2}{c} + \frac{e}{c}\phi - mc \end{pmatrix}$$

$$\times \begin{pmatrix} \varphi \\ \chi \end{pmatrix} = 0$$

$$\Rightarrow \left(E + mc^2 - e\phi - mc^2\right)\varphi =$$

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

and

$$\left(E + mc^2 - e\phi + mc^2\right)\chi = c\bar{\sigma}\left(\bar{p} - \frac{e}{c}\bar{A}\right)\varphi$$

So,

$$1 \quad \begin{cases} (E - e\Phi)\,\varphi = c\bar{\sigma}\left(\bar{p} - \frac{e}{c}\bar{A}\right)\chi \\ \left(E - e\Phi + 2mc^2\right)\chi = c\bar{\sigma}\left(\bar{p} - \frac{e}{c}\bar{A}\right)\varphi \end{cases}$$

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

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

subst. into the first one:

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

Simplify $(\bar{\sigma}\bar{A})(\bar{\sigma}\bar{B})$ by using

$\sigma_i\sigma_k = \delta_{ik} + i\,\varepsilon_{ikl}\sigma_l \quad \left(\bar{P} = \bar{p} - \frac{e}{c}\bar{A}\right)$;

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

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

$$= \vec{p}^{\,2}\varphi - i\hbar^2\sigma^i\varepsilon_{ijk}\Big(\partial_j\partial_k\varphi - \frac{ie}{\hbar c}\partial_j A_k\varphi$$

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

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

2 $$= \vec{p}^{\,2}\varphi - \frac{e\hbar}{c}\vec{\sigma}\cdot\vec{B}\varphi\,, \quad \text{where}$$

$\vec{B} = \text{curl}\,\vec{A}$. $\Big((\bar{\sigma}\cdot\bar{A})(\bar{\sigma}\bar{B}) = \bar{A}\bar{B} + i\bar{\sigma}\cdot\bar{A}\times\bar{B}\Big)$

The eq. becomes:

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

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

it can be written as

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

where $\mu_0 = e\hbar/2mc$. (Pauli eq)

The Dirac eq. predicts $\mu_0 = e\hbar/2mc$

but recall that we used minimal coupling to elm. field but can in principle include terms such as $\alpha [\gamma^\mu \gamma^\nu] F_{\mu\nu} \psi$ with arbitrary $\alpha \Rightarrow$ can alter value of μ_0.

This is further clarified in QED.