Schrodinger for charged particle

This is the Schrodinger equation for a charged particle.

$$
\begin{aligned}
i\hbar\frac{\partial\psi}{\partial t} &= \frac{1}{2m}\left(\frac{\hbar}{i}\nabla - \frac{q}{c}\mathbf{A}\right)^2\psi + q\phi\psi \\
&= -\frac{\hbar^2}{2m}\nabla^2\psi + \frac{i\hbar q}{2mc}\nabla\cdot\mathbf{A}\psi + \frac{i\hbar q}{2mc}\mathbf{A}\cdot\nabla\psi + \frac{q^2}{2mc^2}\mathbf{A}^2\psi + q\phi\psi
\end{aligned}
$$

Derive the Schrodinger equation from the Lagrangian

$$
L(\mathbf{x},\dot{\mathbf{x}},t) = \frac{m\dot{\mathbf{x}}^2}{2} + \frac{q}{c}\dot{\mathbf{x}}\cdot\mathbf{A}(\mathbf{x},t) - q\phi(\mathbf{x},t)
$$

Note that

$$
\nabla\cdot\mathbf{A}\psi = (\nabla\cdot\mathbf{A})\psi + \mathbf{A}\cdot\nabla\psi
$$

Hence for the Coulomb gauge $\nabla\cdot\mathbf{A} = 0$ the Schrodinger equation is

$$
i\hbar\frac{\partial\psi}{\partial t} = -\frac{\hbar^2}{2m}\nabla^2\psi + \frac{i\hbar q}{mc}\mathbf{A}\cdot\nabla\psi + \frac{q^2}{2mc^2}\mathbf{A}^2\psi + q\phi\psi \tag{1}
$$

Start with the path integral for an action S.

$$
\psi(\mathbf{x}_b,t_b) = C\int_{\mathbb{R}^3}\exp\left(\frac{i}{\hbar}S(b,a)\right)\psi(\mathbf{x}_a,t_a)\,d\mathbf{x}_a,\qquad \int_{\mathbb{R}^3} \equiv \int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}
$$

For a small time interval $\epsilon = t_b - t_a$ we can use the approximation

$$
S = \epsilon L
$$

and write the path integral as

$$
\psi(\mathbf{x}_b,t+\epsilon) = C\int_{\mathbb{R}^3}\exp\left[\frac{i}{\hbar}\epsilon L\left(\frac{\mathbf{x}_b-\mathbf{x}_a}{\epsilon},\frac{\mathbf{x}_b+\mathbf{x}_a}{2},t\right)\right]\psi(\mathbf{x}_a,t)\,d\mathbf{x}_a
$$

Substitute for L.

$$
\begin{aligned}
\psi(\mathbf{x}_b,t+\epsilon) = C\int_{\mathbb{R}^3}\exp\Bigg[&\frac{im(\mathbf{x}_b-\mathbf{x}_a)^2}{2\hbar\epsilon} + \frac{iq}{\hbar c}(\mathbf{x}_b-\mathbf{x}_a)\cdot\mathbf{A}\left(\frac{\mathbf{x}_b+\mathbf{x}_a}{2},t\right) \\
&- \frac{iq\epsilon}{\hbar}\phi\left(\frac{\mathbf{x}_b+\mathbf{x}_a}{2},t\right)\Bigg]\psi(\mathbf{x}_a,t)\,d\mathbf{x}_a
\end{aligned}
$$

Let

$$
\mathbf{x}_a = \mathbf{x}_b + \boldsymbol{\eta},\quad d\mathbf{x}_a = d\boldsymbol{\eta}
$$

and write

$$
\psi(\mathbf{x}_b,t+\epsilon) = C\int_{\mathbb{R}^3}\exp\left[\frac{im\boldsymbol{\eta}^2}{2\hbar\epsilon} - \frac{iq}{\hbar c}\boldsymbol{\eta}\cdot\mathbf{A}\left(\mathbf{x}_b+\frac{\boldsymbol{\eta}}{2},t\right) - \frac{iq\epsilon}{\hbar}\phi\left(\mathbf{x}_b+\frac{\boldsymbol{\eta}}{2},t\right)\right]\psi(\mathbf{x}_b+\boldsymbol{\eta},t)\,d\boldsymbol{\eta}
$$

Substitute $\mathbf{x}$ for $\mathbf{x}_b$.

$$\psi(\mathbf{x}, t+\epsilon) = C \int_{\mathbb{R}^3} \exp\left[\frac{im\boldsymbol{\eta}^2}{2\hbar\epsilon} - \frac{iq}{\hbar c}\boldsymbol{\eta}\cdot\mathbf{A}\left(\mathbf{x}+\frac{\boldsymbol{\eta}}{2}, t\right) - \frac{iq\epsilon}{\hbar}\phi\left(\mathbf{x}+\frac{\boldsymbol{\eta}}{2}, t\right)\right]\psi(\mathbf{x}+\boldsymbol{\eta}, t)\, d\boldsymbol{\eta}$$

Because the exponential is highly oscillatory for large $|\boldsymbol{\eta}|$, most of the contribution to the integral is from small $|\boldsymbol{\eta}|$. Hence use the approximation $\mathbf{x} + \frac{1}{2}\boldsymbol{\eta} \approx \mathbf{x}$ for small $|\boldsymbol{\eta}|$.

$$\psi(\mathbf{x}, t+\epsilon) = C \int_{\mathbb{R}^3} \exp\left(\frac{im\boldsymbol{\eta}^2}{2\hbar\epsilon} - \frac{iq}{\hbar c}\boldsymbol{\eta}\cdot\mathbf{A}(\mathbf{x}, t) - \frac{iq\epsilon}{\hbar}\phi\left(\mathbf{x}, t\right)\right)\psi(\mathbf{x}+\boldsymbol{\eta}, t)\, d\boldsymbol{\eta}$$

Use the approximation $\exp(y) \approx 1 + y$ for the exponential of ϕ.

$$\psi(\mathbf{x}, t+\epsilon) = C \int_{\mathbb{R}^3} \exp\left(\frac{im\boldsymbol{\eta}^2}{2\hbar\epsilon} - \frac{iq}{\hbar c}\boldsymbol{\eta}\cdot\mathbf{A}\right)\psi(\mathbf{x}+\boldsymbol{\eta}, t)\, d\boldsymbol{\eta} \times \left(1 - \frac{iq\epsilon}{\hbar}\phi\right)$$

Expand $\psi(\mathbf{x}+\boldsymbol{\eta}, t)$ as the power series

$$\psi(\mathbf{x}+\boldsymbol{\eta}, t) \approx \psi + \boldsymbol{\eta}\cdot\nabla\psi + \tfrac{1}{2}\boldsymbol{\eta}^2\nabla^2\psi$$

to obtain

$$\psi(\mathbf{x}, t+\epsilon) = C \int_{\mathbb{R}^3} \exp\left(\frac{im\boldsymbol{\eta}^2}{2\hbar\epsilon} - \frac{iq}{\hbar c}\boldsymbol{\eta}\cdot\mathbf{A}\right)\left(\psi + \boldsymbol{\eta}\cdot\nabla\psi + \tfrac{1}{2}\boldsymbol{\eta}^2\nabla^2\psi\right)\, d\boldsymbol{\eta} \times \left(1 - \frac{iq\epsilon}{\hbar}\phi\right)$$

Rewrite as

$$\psi(\mathbf{x}, t+\epsilon) = C(I_1 + I_2 + I_3)\left(1 - \frac{iq\epsilon}{\hbar}\phi\right) \tag{2}$$

where

$$\begin{aligned}
I_1 &= \int_{\mathbb{R}^3} \exp\left(\frac{im\boldsymbol{\eta}^2}{2\hbar\epsilon} - \frac{iq}{\hbar c}\boldsymbol{\eta}\cdot\mathbf{A}\right)\psi\, d\boldsymbol{\eta} \\
I_2 &= \int_{\mathbb{R}^3} \exp\left(\frac{im\boldsymbol{\eta}^2}{2\hbar\epsilon} - \frac{iq}{\hbar c}\boldsymbol{\eta}\cdot\mathbf{A}\right)\boldsymbol{\eta}\cdot\nabla\psi\, d\boldsymbol{\eta} \\
I_3 &= \int_{\mathbb{R}^3} \exp\left(\frac{im\boldsymbol{\eta}^2}{2\hbar\epsilon} - \frac{iq}{\hbar c}\boldsymbol{\eta}\cdot\mathbf{A}\right)\tfrac{1}{2}\boldsymbol{\eta}^2\nabla^2\psi\, d\boldsymbol{\eta}
\end{aligned}$$

The solutions are

$$\begin{aligned}
I_1 &= \left(\frac{2\pi i\hbar\epsilon}{m}\right)^{\frac{3}{2}} \exp\left(-\frac{iq^2\epsilon}{2\hbar mc^2}\mathbf{A}^2\right)\psi \\
I_2 &= \left(\frac{2\pi i\hbar\epsilon}{m}\right)^{\frac{3}{2}} \exp\left(-\frac{iq^2\epsilon}{2\hbar mc^2}\mathbf{A}^2\right)\frac{q\epsilon}{mc}\mathbf{A}\cdot\nabla\psi \\
I_3 &= \left(\frac{2\pi i\hbar\epsilon}{m}\right)^{\frac{3}{2}} \exp\left(-\frac{iq^2\epsilon}{2\hbar mc^2}\mathbf{A}^2\right)\frac{i\hbar\epsilon}{2m}\nabla^2\psi
\end{aligned}$$

Use the approximation $\exp(y) \approx 1 + y$ to write the solutions this way.

$$
\begin{aligned}
I_1 &= \left(\frac{2\pi i\hbar\epsilon}{m}\right)^{\frac{3}{2}} \left(1 - \frac{iq^2\epsilon}{2\hbar mc^2}\mathbf{A}^2\right)\psi \\
I_2 &= \left(\frac{2\pi i\hbar\epsilon}{m}\right)^{\frac{3}{2}} \left(1 - \frac{iq^2\epsilon}{2\hbar mc^2}\mathbf{A}^2\right)\frac{q\epsilon}{mc}\mathbf{A}\cdot\nabla\psi \\
I_3 &= \left(\frac{2\pi i\hbar\epsilon}{m}\right)^{\frac{3}{2}} \left(1 - \frac{iq^2\epsilon}{2\hbar mc^2}\mathbf{A}^2\right)\frac{i\hbar\epsilon}{2m}\nabla^2\psi
\end{aligned}
$$

Discard terms of order ϵ^2.

$$
I_1 + I_2 + I_3 = \left(\frac{2\pi i\hbar\epsilon}{m}\right)^{\frac{3}{2}} \left(\psi + \frac{i\hbar\epsilon}{2m}\nabla^2\psi + \frac{q\epsilon}{mc}\mathbf{A}\cdot\nabla\psi - \frac{iq^2\epsilon}{2\hbar mc^2}\mathbf{A}^2\psi\right)
$$

Let

$$
C = \left(\frac{2\pi i\hbar\epsilon}{m}\right)^{-\frac{3}{2}}
$$

Substitute C and $I_1 + I_2 + I_3$ into equation (2) to obtain

$$
\psi(\mathbf{x}, t+\epsilon) = \left(\psi + \frac{i\hbar\epsilon}{2m}\nabla^2\psi + \frac{q\epsilon}{mc}\mathbf{A}\cdot\nabla\psi - \frac{iq^2\epsilon}{2\hbar mc^2}\mathbf{A}^2\psi\right)\left(1 - \frac{iq\epsilon}{\hbar}\phi\right)
$$

Discard terms of order ϵ^2.

$$
\psi(\mathbf{x}, t+\epsilon) = \psi + \frac{i\hbar\epsilon}{2m}\nabla^2\psi + \frac{q\epsilon}{mc}\mathbf{A}\cdot\nabla\psi - \frac{iq^2\epsilon}{2\hbar mc^2}\mathbf{A}^2\psi - \frac{iq\epsilon}{\hbar}\phi\psi
$$

Expand $\psi(\mathbf{x}, t+\epsilon)$ as the power series

$$
\psi(\mathbf{x}, t+\epsilon) \approx \psi + \epsilon\frac{\partial\psi}{\partial t}
$$

to obtain

$$
\psi + \epsilon\frac{\partial\psi}{\partial t} = \psi + \frac{i\hbar\epsilon}{2m}\nabla^2\psi + \frac{q\epsilon}{mc}\mathbf{A}\cdot\nabla\psi - \frac{iq^2\epsilon}{2\hbar mc^2}\mathbf{A}^2\psi - \frac{iq\epsilon}{\hbar}\phi\psi
$$

Cancel leading ψ.

$$
\epsilon\frac{\partial\psi}{\partial t} = \frac{i\hbar\epsilon}{2m}\nabla^2\psi + \frac{q\epsilon}{mc}\mathbf{A}\cdot\nabla\psi - \frac{iq^2\epsilon}{2\hbar mc^2}\mathbf{A}^2\psi - \frac{iq\epsilon}{\hbar}\phi\psi
$$

Multiply both sides by $i\hbar/\epsilon$.

$$
i\hbar\frac{\partial\psi}{\partial t} = -\frac{\hbar^2}{2m}\nabla^2\psi + \frac{i\hbar q}{mc}\mathbf{A}\cdot\nabla\psi + \frac{q^2}{2mc^2}\mathbf{A}^2\psi + q\phi\psi
$$

Eigenmath code

Integrals for ay^2 either negative or imaginary.

$$\int_{-\infty}^{\infty} \exp(ay^2 + by)\,dy = \left(-\frac{\pi}{a}\right)^{\frac{1}{2}} \exp\left(-\frac{b^2}{4a}\right)$$
$$\int_{-\infty}^{\infty} y\exp(ay^2 + by)\,dy = \left(-\frac{\pi}{a}\right)^{\frac{1}{2}} \left(-\frac{b}{2a}\right) \exp\left(-\frac{b^2}{4a}\right)$$
$$\int_{-\infty}^{\infty} y^2\exp(ay^2 + by)\,dy = \left(-\frac{\pi}{a}\right)^{\frac{1}{2}} \left(-\frac{1}{2a}\right)\left(1-\frac{b^2}{2a}\right) \exp\left(-\frac{b^2}{4a}\right)$$

```
G0(a,b) = sqrt(-pi / a) exp(-b^2 / (4 a))
G1(a,b) = sqrt(-pi / a) (-b / (2 a)) exp(-b^2 / (4 a))
G2(a,b) = sqrt(-pi / a) (-1 / (2 a)) (1 - b^2 / (2 a)) exp(-b^2 / (4 a))
```

$$a = \frac{im}{2\hbar\epsilon}, \quad b = -\frac{iq}{\hbar c}$$

$$\begin{aligned}
I_1 &= \int_{\mathbb{R}^3} \exp\left(\frac{im\boldsymbol{\eta}^2}{2\hbar\epsilon} - \frac{iq}{\hbar c}\boldsymbol{\eta}\cdot\mathbf{A}(\mathbf{x},t)\right)\psi\,d\boldsymbol{\eta} \\
&= \int_{\mathbb{R}^3} \exp\left(a\eta_x^2 + b\eta_x A_x\right)\exp\left(a\eta_y^2 + b\eta_y A_y\right)\exp\left(a\eta_z^2 + b\eta_z A_z\right)\psi\,d\eta_x\,d\eta_y\,d\eta_z
\end{aligned}$$

```
a = i m / (2 hbar epsilon)
b = -i q / (hbar c)
I1 = G0(a, b Ax) G0(a, b Ay) G0(a, b Az) psi
```

$$\begin{aligned}
I_2 &= \int_{\mathbb{R}^3} \exp\left(\frac{im\boldsymbol{\eta}^2}{2\hbar\epsilon} - \frac{iq}{\hbar c}\boldsymbol{\eta}\cdot\mathbf{A}(\mathbf{x},t)\right)\boldsymbol{\eta}\cdot\nabla\psi\,d\boldsymbol{\eta} \\
&= \int_{\mathbb{R}^3} \exp\left(a\eta_x^2 + b\eta_x A_x\right)\exp\left(a\eta_y^2 + b\eta_y A_y\right)\exp\left(a\eta_z^2 + b\eta_z A_z\right)\eta_x\frac{\partial\psi}{\partial x}\,d\eta_x\,d\eta_y\,d\eta_z \\
&\quad + \int_{\mathbb{R}^3} \exp\left(a\eta_x^2 + b\eta_x A_x\right)\exp\left(a\eta_y^2 + b\eta_y A_y\right)\exp\left(a\eta_z^2 + b\eta_z A_z\right)\eta_y\frac{\partial\psi}{\partial y}\,d\eta_x\,d\eta_y\,d\eta_z \\
&\quad + \int_{\mathbb{R}^3} \exp\left(a\eta_x^2 + b\eta_x A_x\right)\exp\left(a\eta_y^2 + b\eta_y A_y\right)\exp\left(a\eta_z^2 + b\eta_z A_z\right)\eta_z\frac{\partial\psi}{\partial z}\,d\eta_x\,d\eta_y\,d\eta_z
\end{aligned}$$

```
I2 = G1(a, b Ax) G0(a, b Ay) G0(a, b Az) d(psi(),x) +
     G0(a, b Ax) G1(a, b Ay) G0(a, b Az) d(psi(),y) +
     G0(a, b Ax) G0(a, b Ay) G1(a, b Az) d(psi(),z)
```

$$
\begin{aligned}
I_3 &= \int_{\mathbb{R}^3} \exp\left(\frac{im\boldsymbol{\eta}^2}{2\hbar\epsilon} - \frac{iq}{\hbar c}\boldsymbol{\eta}\cdot\mathbf{A}(\mathbf{x},t)\right) \tfrac{1}{2}\boldsymbol{\eta}^2\nabla^2\psi\, d\boldsymbol{\eta} \\
&= \int_{\mathbb{R}^3} \exp\left(a\eta_x^2 + b\eta_x A_x\right) \exp\left(a\eta_y^2 + b\eta_y A_y\right) \exp\left(a\eta_z^2 + b\eta_z A_z\right) \tfrac{1}{2}\eta_x^2 \frac{\partial^2\psi}{\partial x^2}\, d\eta_x\, d\eta_y\, d\eta_z \\
&\quad + \int_{\mathbb{R}^3} \exp\left(a\eta_x^2 + b\eta_x A_x\right) \exp\left(a\eta_y^2 + b\eta_y A_y\right) \exp\left(a\eta_z^2 + b\eta_z A_z\right) \tfrac{1}{2}\eta_y^2 \frac{\partial^2\psi}{\partial y^2}\, d\eta_x\, d\eta_y\, d\eta_z \\
&\quad\quad + \int_{\mathbb{R}^3} \exp\left(a\eta_x^2 + b\eta_x A_x\right) \exp\left(a\eta_y^2 + b\eta_y A_y\right) \exp\left(a\eta_z^2 + b\eta_z A_z\right) \tfrac{1}{2}\eta_z^2 \frac{\partial^2\psi}{\partial z^2}\, d\eta_x\, d\eta_y\, d\eta_z
\end{aligned}
$$

```
I3 = G2(a, b Ax) G0(a, b Ay) G0(a, b Az) 1/2 d(psi(),x,x) +
     G0(a, b Ax) G2(a, b Ay) G0(a, b Az) 1/2 d(psi(),y,y) +
     G0(a, b Ax) G0(a, b Ay) G2(a, b Az) 1/2 d(psi(),z,z)

-- discard terms of order epsilon^(7/2)

I3 = eval(I3,epsilon^(7/2),0)
```