

# 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

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

Start with the path integral for an action  $S$ .

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

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  $L$ .

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

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  $|\boldsymbol{\eta}|$ .

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

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

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

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

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

to obtain

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

Rewrite as

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

where

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

The solutions are

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

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  $\epsilon^2$ .

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

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  $\epsilon^2$ .

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

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  $\psi$ .

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

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.

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

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

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

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

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

$$\begin{aligned}
I3 &= G2(a, b \, Ax) \, G0(a, b \, Ay) \, G0(a, b \, Az) \, 1/2 \, d(\psi(),x,x) + \\
&\quad G0(a, b \, Ax) \, G2(a, b \, Ay) \, G0(a, b \, Az) \, 1/2 \, d(\psi(),y,y) + \\
&\quad G0(a, b \, Ax) \, G0(a, b \, Ay) \, G2(a, b \, Az) \, 1/2 \, d(\psi(),z,z)
\end{aligned}$$

-- discard terms of order C epsilon^2

$$I3 = \text{eval}(I3, \epsilon^{7/2}, 0)$$