

Schrodinger for charged particle

Derive the Schrodinger equation for a charged particle

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

from the Lagrangian

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

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 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

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

to obtain

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

Rewrite as

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

where

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

The solutions are

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

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

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

Discarding terms of order ϵ^2 we have

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

Rearrange terms.

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

Note that

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

Hence taking $\nabla \cdot \mathbf{A} = 0$ we can write

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

Substitute

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

and the solved integrals into equation (1) to obtain

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

Discard terms of order ϵ^2 .

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

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

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

Cancel leading ψ .

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

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

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

Eigenmath code

Gaussian integrals where ay^2 is either negative or imaginary.

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

```
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))
```

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

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

```
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
```

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

$$\begin{aligned}
I_2 = & G_1(a, b, A_x) G_0(a, b, A_y) G_0(a, b, A_z) d(\psi(), x) + \\
& G_0(a, b, A_x) G_1(a, b, A_y) G_0(a, b, A_z) d(\psi(), y) + \\
& G_0(a, b, A_x) G_0(a, b, A_y) G_1(a, b, A_z) d(\psi(), z)
\end{aligned}$$

$$I_3 = \int_{\mathbb{R}^3} \exp\left(\frac{im\boldsymbol{\eta}^2}{2\hbar\epsilon} - \frac{iq}{\hbar c}\boldsymbol{\eta} \cdot \mathbf{A}(\mathbf{x}, t)\right) \frac{1}{2}\boldsymbol{\eta} \cdot \nabla(\boldsymbol{\eta} \cdot \nabla\psi) d\boldsymbol{\eta}$$

$$\begin{aligned}
\frac{1}{2}\boldsymbol{\eta} \cdot \nabla(\boldsymbol{\eta} \cdot \nabla\psi) = & \frac{1}{2} \left(\eta_x^2 \frac{\partial^2 \psi}{\partial x^2} + \eta_y^2 \frac{\partial^2 \psi}{\partial y^2} + \eta_z^2 \frac{\partial^2 \psi}{\partial z^2} \right) + \frac{1}{2} \left(\eta_x \frac{\partial \psi}{\partial x} + \eta_y \frac{\partial \psi}{\partial y} + \eta_z \frac{\partial \psi}{\partial z} \right) \\
& + \eta_x \eta_y \frac{\partial^2 \psi}{\partial x \partial y} + \eta_x \eta_z \frac{\partial^2 \psi}{\partial x \partial z} + \eta_y \eta_z \frac{\partial^2 \psi}{\partial y \partial z}
\end{aligned}$$

$$\begin{aligned}
I_3 = & 1/2 G_2(a, b, A_x) G_0(a, b, A_y) G_0(a, b, A_z) d(\psi(), x, x) + \\
& 1/2 G_0(a, b, A_x) G_2(a, b, A_y) G_0(a, b, A_z) d(\psi(), y, y) + \\
& 1/2 G_0(a, b, A_x) G_0(a, b, A_y) G_2(a, b, A_z) d(\psi(), z, z) +
\end{aligned}$$

$$\begin{aligned}
& 1/2 G_1(a, b, A_x) G_0(a, b, A_y) G_0(a, b, A_z) d(\psi(), x) + \\
& 1/2 G_0(a, b, A_x) G_1(a, b, A_y) G_0(a, b, A_z) d(\psi(), y) + \\
& 1/2 G_0(a, b, A_x) G_0(a, b, A_y) G_1(a, b, A_z) d(\psi(), z) +
\end{aligned}$$

$$\begin{aligned}
& G_1(a, b, A_x) G_1(a, b, A_y) G_0(a, b, A_z) d(\psi(), x, y) + \\
& G_1(a, b, A_x) G_0(a, b, A_y) G_1(a, b, A_z) d(\psi(), x, z) + \\
& G_0(a, b, A_x) G_1(a, b, A_y) G_1(a, b, A_z) d(\psi(), y, z)
\end{aligned}$$