

4-2. For a particle of charge  $e$  in a magnetic field the Lagrangian is

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

where  $\dot{\mathbf{x}}$  is the velocity vector,  $c$  is the velocity of light, and  $\mathbf{A}$  and  $\phi$  are the vector and scalar potentials. Show that the corresponding Schrodinger equation is

$$\frac{\partial \psi}{\partial t} = -\frac{i}{\hbar} \left( \frac{1}{2m} \left( \frac{\hbar}{i} \nabla - \frac{e}{c} \mathbf{A} \right) \cdot \left( \frac{\hbar}{i} \nabla - \frac{e}{c} \mathbf{A} \right) \psi + e\phi \psi \right) \quad (4.18)$$

From equation (4.3) with a minor correction of  $y - x$  instead of  $x - y$ .

$$\psi(\mathbf{x}, t + \epsilon) = \frac{1}{A} \int_{\mathbb{R}^3} \exp \left( \frac{i\epsilon}{\hbar} L \left( \frac{\mathbf{y} - \mathbf{x}}{\epsilon}, \frac{\mathbf{x} + \mathbf{y}}{2} \right) \right) \psi(\mathbf{y}, t) dy_1 dy_2 dy_3 \quad (1)$$

This is the Lagrangian with arguments from (1).

$$\begin{aligned} L \left( \frac{\mathbf{y} - \mathbf{x}}{\epsilon}, \frac{\mathbf{x} + \mathbf{y}}{2} \right) \\ = \frac{m}{2\epsilon^2} (\mathbf{x} - \mathbf{y})^2 - \frac{e}{c\epsilon} (\mathbf{x} - \mathbf{y}) \cdot \mathbf{A} \left( \frac{\mathbf{x} + \mathbf{y}}{2}, t \right) - e\phi \left( \frac{\mathbf{x} + \mathbf{y}}{2}, t \right) \end{aligned}$$

Hence

$$\begin{aligned} \psi(\mathbf{x}, t + \epsilon) &= \frac{1}{A} \int_{\mathbb{R}^3} \\ &\exp \left( \frac{im}{2\hbar\epsilon} (\mathbf{x} - \mathbf{y})^2 - \frac{ie}{\hbar c} (\mathbf{x} - \mathbf{y}) \cdot \mathbf{A} \left( \frac{\mathbf{x} + \mathbf{y}}{2}, t \right) - \frac{ie\epsilon}{\hbar} \phi \left( \frac{\mathbf{x} + \mathbf{y}}{2}, t \right) \right) \\ &\times \psi(\mathbf{y}, t) dy_1 dy_2 dy_3 \end{aligned}$$

Let

$$\mathbf{y} = \mathbf{x} + \boldsymbol{\eta}$$

Then

$$\mathbf{x} - \mathbf{y} = \boldsymbol{\eta}, \quad \frac{\mathbf{x} + \mathbf{y}}{2} = \mathbf{x} + \frac{1}{2}\boldsymbol{\eta}, \quad dy_1 dy_2 dy_3 = d\eta_1 d\eta_2 d\eta_3$$

Hence

$$\begin{aligned} \psi(\mathbf{x}, t + \epsilon) &= \frac{1}{A} \int_{\mathbb{R}^3} \exp \left( \frac{im}{2\hbar\epsilon} \boldsymbol{\eta}^2 - \frac{ie}{\hbar c} \boldsymbol{\eta} \cdot \mathbf{A} \left( \mathbf{x} + \frac{1}{2}\boldsymbol{\eta}, t \right) - \frac{ie\epsilon}{\hbar} \phi \left( \mathbf{x} + \frac{1}{2}\boldsymbol{\eta}, t \right) \right) \\ &\times \psi(\mathbf{x} + \boldsymbol{\eta}, t) d\eta_1 d\eta_2 d\eta_3 \end{aligned}$$

Factor the exponential.

$$\begin{aligned} \psi(\mathbf{x}, t + \epsilon) &= \frac{1}{A} \int_{\mathbb{R}^3} \\ &\exp\left(\frac{im}{2\hbar\epsilon}\boldsymbol{\eta}^2\right) \exp\left(-\frac{ie}{\hbar c}\boldsymbol{\eta} \cdot \mathbf{A}\left(\mathbf{x} + \frac{1}{2}\boldsymbol{\eta}, t\right)\right) \exp\left(-\frac{ie\epsilon}{\hbar}\phi\left(\mathbf{x} + \frac{1}{2}\boldsymbol{\eta}, t\right)\right) \\ &\times \psi(\mathbf{x} + \boldsymbol{\eta}, t) d\eta_1 d\eta_2 d\eta_3 \end{aligned} \quad (2)$$

From the identity  $\exp(i\theta) = \cos(\theta) + i\sin(\theta)$  we have

$$\begin{aligned} \exp\left(-\frac{ie\epsilon}{\hbar}\phi\left(\mathbf{x} + \frac{1}{2}\boldsymbol{\eta}, t\right)\right) \\ = \cos\left(-\frac{e\epsilon}{\hbar}\phi\left(\mathbf{x} + \frac{1}{2}\boldsymbol{\eta}, t\right)\right) + i\sin\left(-\frac{e\epsilon}{\hbar}\phi\left(\mathbf{x} + \frac{1}{2}\boldsymbol{\eta}, t\right)\right) \end{aligned}$$

Then for small  $\epsilon$

$$\exp\left(-\frac{ie\epsilon}{\hbar}\phi\left(\mathbf{x} + \frac{1}{2}\boldsymbol{\eta}, t\right)\right) \approx 1 - \frac{ie\epsilon}{\hbar}\phi\left(\mathbf{x} + \frac{1}{2}\boldsymbol{\eta}, t\right)$$

The  $\boldsymbol{\eta}$  term can be discarded because the integral is Gaussian. (Contributions to the integral are small for  $\boldsymbol{\eta}^2 > 2\hbar\epsilon/m$ .)

$$\exp\left(-\frac{ie\epsilon}{\hbar}\phi\left(\mathbf{x} + \frac{1}{2}\boldsymbol{\eta}, t\right)\right) \approx 1 - \frac{ie\epsilon}{\hbar}\phi(\mathbf{x}, t) \quad (3)$$

Substitute (3) into (2).

$$\begin{aligned} \psi(\mathbf{x}, t + \epsilon) &= \frac{1}{A} \left(1 - \frac{ie\epsilon}{\hbar}\phi\right) \int_{\mathbb{R}^3} \\ &\exp\left(\frac{im}{2\hbar\epsilon}\boldsymbol{\eta}^2\right) \exp\left(-\frac{ie}{\hbar c}\boldsymbol{\eta} \cdot \mathbf{A}\left(\mathbf{x} + \frac{1}{2}\boldsymbol{\eta}, t\right)\right) \psi(\mathbf{x} + \boldsymbol{\eta}, t) d\eta_1 d\eta_2 d\eta_3 \end{aligned}$$

Approximate the exponential involving  $\mathbf{A}$  with a Taylor series.

$$\exp\left(-\frac{ie}{\hbar c}\boldsymbol{\eta} \cdot \mathbf{A}\left(\mathbf{x} + \frac{1}{2}\boldsymbol{\eta}, t\right)\right) \approx \exp\left(-\frac{ie}{\hbar c}\boldsymbol{\eta} \cdot \mathbf{A}(\mathbf{x}) - \frac{ie}{2\hbar c}\boldsymbol{\eta} \cdot (\boldsymbol{\eta} \cdot \nabla \mathbf{A}(\mathbf{x}))\right)$$

Expand the right-hand side as a power series.

$$\exp\left(-\frac{ie}{\hbar c}\boldsymbol{\eta} \cdot \mathbf{A}\left(\mathbf{x} + \frac{1}{2}\boldsymbol{\eta}, t\right)\right) \approx (1 + T + \frac{1}{2}T^2)$$

where

$$T = -\frac{ie}{\hbar c} \boldsymbol{\eta} \cdot \mathbf{A}(\mathbf{x}) - \frac{ie}{2\hbar c} \boldsymbol{\eta} \cdot (\boldsymbol{\eta} \cdot \nabla \mathbf{A}(\mathbf{x}))$$

Discard high order terms.

$$\begin{aligned} & \exp \left( -\frac{ie}{\hbar c} \boldsymbol{\eta} \cdot \mathbf{A} \left( \mathbf{x} + \frac{1}{2} \boldsymbol{\eta}, t \right) \right) \\ & \approx 1 - \frac{ie}{\hbar c} \boldsymbol{\eta} \cdot \mathbf{A}(\mathbf{x}) - \frac{ie}{2\hbar c} \boldsymbol{\eta} \cdot (\boldsymbol{\eta} \cdot \nabla \mathbf{A}(\mathbf{x})) + \frac{1}{2} \left( -\frac{ie}{\hbar c} \boldsymbol{\eta} \cdot \mathbf{A}(\mathbf{x}) \right)^2 \end{aligned}$$

Hence

$$\begin{aligned} \psi(\mathbf{x}, t + \epsilon) &= \frac{1}{A} \left( 1 - \frac{ie\epsilon}{\hbar} \phi \right) \int_{\mathbb{R}^3} \exp \left( \frac{im}{2\hbar\epsilon} \boldsymbol{\eta}^2 \right) \\ &\times \left( 1 - \frac{ie}{\hbar c} \boldsymbol{\eta} \cdot \mathbf{A} - \frac{ie}{2\hbar c} \boldsymbol{\eta} \cdot (\boldsymbol{\eta} \cdot \nabla \mathbf{A}) + \frac{1}{2} \left( -\frac{ie}{\hbar c} \boldsymbol{\eta} \cdot \mathbf{A} \right)^2 \right) \\ &\times \psi(\mathbf{x} + \boldsymbol{\eta}, t) d\eta_1 d\eta_2 d\eta_3 \end{aligned} \quad (4)$$

Next we will use the following Taylor series approximations.

$$\begin{aligned} \psi(\mathbf{x}, t + \epsilon) &\approx \psi + \epsilon \frac{\partial \psi}{\partial t} \\ \psi(\mathbf{x} + \boldsymbol{\eta}, t) &\approx \psi + \boldsymbol{\eta} \cdot \nabla \psi + \frac{1}{2} \boldsymbol{\eta} \cdot \nabla (\boldsymbol{\eta} \cdot \nabla \psi) \end{aligned} \quad (5)$$

Substitute the approximations (5) into (4).

$$\begin{aligned} \psi + \epsilon \frac{\partial \psi}{\partial t} &= \frac{1}{A} \left( 1 - \frac{ie\epsilon}{\hbar} \phi \right) \int_{\mathbb{R}^3} \exp \left( \frac{im}{2\hbar\epsilon} \boldsymbol{\eta}^2 \right) \\ &\times \left( 1 - \frac{ie}{\hbar c} \boldsymbol{\eta} \cdot \mathbf{A} - \frac{ie}{2\hbar c} \boldsymbol{\eta} \cdot (\boldsymbol{\eta} \cdot \nabla \mathbf{A}) + \frac{1}{2} \left( -\frac{ie}{\hbar c} \boldsymbol{\eta} \cdot \mathbf{A} \right)^2 \right) \\ &\times \left( \psi + \boldsymbol{\eta} \cdot \nabla \psi + \frac{1}{2} \boldsymbol{\eta} \cdot \nabla (\boldsymbol{\eta} \cdot \nabla \psi) \right) d\eta_1 d\eta_2 d\eta_3 \end{aligned} \quad (6)$$

To solve the above integral, we will use the following formulas provided by the authors.

$$\int_{-\infty}^{\infty} \exp \left( \frac{im\eta_k^2}{2\hbar\epsilon} \right) d\eta_k = \left( \frac{2\pi i\hbar\epsilon}{m} \right)^{1/2} \quad (4.7)$$

$$\int_{-\infty}^{\infty} \eta_k \exp \left( \frac{im\eta_k^2}{2\hbar\epsilon} \right) d\eta_k = 0 \quad (4.9)$$

$$\int_{-\infty}^{\infty} \eta_k^2 \exp \left( \frac{im\eta_k^2}{2\hbar\epsilon} \right) d\eta_k = \frac{i\hbar\epsilon}{m} \left( \frac{2\pi i\hbar\epsilon}{m} \right)^{1/2} \quad (4.10)$$

The following table summarizes the solutions to

$$I = \int_{\mathbb{R}^3} \exp\left(\frac{im}{2\hbar\epsilon}\boldsymbol{\eta}^2\right) uv \, d\eta_1 \, d\eta_2 \, d\eta_3$$

for each factor pair  $uv$  in (6). Integrals  $I_9$  and  $I_{12}$  are proportional to  $\epsilon^2$  due to (4.10) and are discarded.

	$v = \psi$	$v = \boldsymbol{\eta} \cdot \nabla \psi$	$v = \frac{1}{2}\boldsymbol{\eta} \cdot \nabla(\boldsymbol{\eta} \cdot \nabla \psi)$
$u = 1$	$I_1$	0	$I_3$
$u = -\frac{ie}{\hbar c}\boldsymbol{\eta} \cdot \mathbf{A}$	0	$I_5$	0
$u = -\frac{ie}{2\hbar c}\boldsymbol{\eta} \cdot (\boldsymbol{\eta} \cdot \nabla \mathbf{A})$	$I_7$	0	$I_9 \propto \epsilon^2$
$u = \frac{1}{2}\left(-\frac{ie}{\hbar c}\boldsymbol{\eta} \cdot \mathbf{A}\right)^2$	$I_{10}$	0	$I_{12} \propto \epsilon^2$

$$\begin{aligned}
I_1 &= \left(\frac{2\pi i\hbar\epsilon}{m}\right)^{3/2} \psi \\
I_3 &= \frac{i\hbar\epsilon}{2m} \left(\frac{2\pi i\hbar\epsilon}{m}\right)^{3/2} \nabla^2 \psi \\
I_5 &= \frac{i\hbar\epsilon}{m} \left(\frac{2\pi i\hbar\epsilon}{m}\right)^{3/2} \frac{-ie}{\hbar c} \mathbf{A} \cdot \nabla \psi \\
I_7 &= \frac{i\hbar\epsilon}{m} \left(\frac{2\pi i\hbar\epsilon}{m}\right)^{3/2} \frac{-ie}{2\hbar c} \nabla \cdot \mathbf{A} \psi \\
I_{10} &= \frac{i\hbar\epsilon}{m} \left(\frac{2\pi i\hbar\epsilon}{m}\right)^{3/2} \frac{1}{2} \left(\frac{-ie}{\hbar c}\right)^2 \mathbf{A}^2 \psi
\end{aligned}$$

Substitute the solved integrals into (6) to obtain

$$\begin{aligned} \psi + \epsilon \frac{\partial \psi}{\partial t} &= \frac{1}{A} \left( 1 - \frac{ie\epsilon}{\hbar} \phi \right) \left( \frac{2\pi i \hbar \epsilon}{m} \right)^{3/2} \\ &\times \left( \psi + \frac{i\hbar\epsilon}{2m} \nabla^2 \psi + \frac{e\epsilon}{mc} \mathbf{A} \cdot \nabla \psi + \frac{e\epsilon}{2mc} \nabla \cdot \mathbf{A} \psi - \frac{ie^2\epsilon}{2m\hbar c^2} \mathbf{A}^2 \psi \right) \end{aligned}$$

In the limit as  $\epsilon \rightarrow 0$  we have

$$\psi = \frac{1}{A} \left( \frac{2\pi i \hbar \epsilon}{m} \right)^{3/2} \psi$$

hence

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

Cancel A.

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

Expand the product and discard terms of order  $\epsilon^2$ .

$$\begin{aligned} \psi + \epsilon \frac{\partial \psi}{\partial t} &= \psi + \frac{i\hbar\epsilon}{2m} \nabla^2 \psi + \frac{e\epsilon}{mc} \mathbf{A} \cdot \nabla \psi + \frac{e\epsilon}{2mc} \nabla \cdot \mathbf{A} \psi - \frac{ie^2\epsilon}{2m\hbar c^2} \mathbf{A}^2 \psi - \frac{ie\epsilon}{\hbar} \phi \psi \end{aligned}$$

Cancel leading terms  $\psi$  and divide through by  $\epsilon$ .

$$\frac{\partial \psi}{\partial t} = \frac{i\hbar}{2m} \nabla^2 \psi + \frac{e}{mc} \mathbf{A} \cdot \nabla \psi + \frac{e}{2mc} \nabla \cdot \mathbf{A} \psi - \frac{ie^2}{2m\hbar c^2} \mathbf{A}^2 \psi - \frac{ie}{\hbar} \phi \psi \quad (7)$$

To show that (7) is the same as (4.18), expand (4.18) step by step. First we have

$$\left( \frac{\hbar}{i} \nabla - \frac{e}{c} \mathbf{A} \right) \psi = -i\hbar \nabla \psi - \frac{e}{c} \mathbf{A} \psi$$

Next

$$\begin{aligned} \left( \frac{\hbar}{i} \nabla - \frac{e}{c} \mathbf{A} \right)^2 \psi &= \left( -i\hbar \nabla - \frac{e}{c} \mathbf{A} \right) \left( -i\hbar \nabla \psi - \frac{e}{c} \mathbf{A} \psi \right) \\ &= -\hbar^2 \nabla(\nabla \psi) + \frac{ie\hbar}{c} \nabla(\mathbf{A} \psi) + \frac{ie\hbar}{c} \mathbf{A} \cdot \nabla \psi + \frac{e^2}{c^2} \mathbf{A} \cdot \mathbf{A} \psi \end{aligned}$$

Because  $\nabla \psi$  is a vector we have

$$\nabla(\nabla \psi) = \nabla \cdot \nabla \psi = \nabla^2 \psi$$

and because  $\mathbf{A}$  is a vector and  $\psi$  is a scalar we have

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

Hence

$$\left( \frac{\hbar}{i} \nabla - \frac{e}{c} \mathbf{A} \right)^2 \psi = -\hbar^2 \nabla^2 \psi + \frac{2ie\hbar}{c} \mathbf{A} \cdot \nabla \psi + \frac{ie\hbar}{c} \nabla \cdot \mathbf{A} \psi + \frac{e^2}{c^2} \mathbf{A}^2 \psi$$

Divide through by  $2m$ .

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

Add the scalar potential.

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

Finally, multiply by  $-i/\hbar$ .

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

The result is identical to (7).

$$\frac{\partial \psi}{\partial t} = \frac{i\hbar}{2m} \nabla^2 \psi + \frac{e}{mc} \mathbf{A} \cdot \nabla \psi + \frac{e}{2mc} \nabla \cdot \mathbf{A} \psi - \frac{ie^2}{2m\hbar c^2} \mathbf{A}^2 \psi - \frac{ie}{\hbar} \phi \psi \quad (7)$$