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 ϕ are the vector and scalar potentials. Show that the corresponding Schrodinger equation is

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

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

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

This is the Lagrangian with arguments from (1).

$$L\left(\frac{\mathbf{y} - \mathbf{x}}{\epsilon}, \frac{\mathbf{x} + \mathbf{y}}{2}\right)$$

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

Hence

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

Let

$$y = x + \eta$$

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

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

Factor the exponential.

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

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

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

Then for small ϵ

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

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

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

Substitute (3) into (2).

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

Approximate the exponential involving A with a Taylor series.

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

Expand the right-hand side as a power series.

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

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.

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

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

Hence

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

$$\times \left(1 - \frac{ie}{\hbar c} \boldsymbol{\eta} \cdot \mathbf{A} - \frac{ie}{2\hbar c} \boldsymbol{\eta} \cdot (\boldsymbol{\eta} \cdot \nabla \mathbf{A}) + \frac{1}{2} \left(-\frac{ie}{\hbar c} \boldsymbol{\eta} \cdot \mathbf{A} \right)^2 \right)$$

$$\times \psi(\mathbf{x} + \boldsymbol{\eta}, t) d\eta_1 d\eta_2 d\eta_3$$

$$(4)$$

Next we will use the following Taylor series approximations.

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

Substitute the approximations (5) into (4).

$$\psi + \epsilon \frac{\partial \psi}{\partial t} = \frac{1}{A} \left(1 - \frac{ie\epsilon}{\hbar} \phi \right) \int_{\mathbb{R}^3} \exp\left(\frac{im}{2\hbar\epsilon} \boldsymbol{\eta}^2 \right)$$

$$\times \left(1 - \frac{ie}{\hbar c} \boldsymbol{\eta} \cdot \mathbf{A} - \frac{ie}{2\hbar c} \boldsymbol{\eta} \cdot (\boldsymbol{\eta} \cdot \nabla \mathbf{A}) + \frac{1}{2} \left(-\frac{ie}{\hbar c} \boldsymbol{\eta} \cdot \mathbf{A} \right)^2 \right)$$

$$\times \left(\psi + \boldsymbol{\eta} \cdot \nabla \psi + \frac{1}{2} \boldsymbol{\eta} \cdot \nabla (\boldsymbol{\eta} \cdot \nabla \psi) \right) d\eta_1 d\eta_2 d\eta_3$$
(6)

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

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

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

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

The integrand in (6) has twelve terms. The following table summarizes the integrals $\int uv$ for each factor pair uv.

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

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

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

$$I_{5} = \frac{i\hbar\epsilon}{m} \left(\frac{2\pi i\hbar\epsilon}{m}\right)^{3/2} \frac{-ie}{\hbar c} \mathbf{A} \cdot \nabla \psi$$

$$I_{7} = \frac{i\hbar\epsilon}{m} \left(\frac{2\pi i\hbar\epsilon}{m}\right)^{3/2} \frac{-ie}{2\hbar c} \nabla \cdot \mathbf{A} \psi$$

$$I_{10} = \frac{i\hbar\epsilon}{m} \left(\frac{2\pi i\hbar\epsilon}{m}\right)^{3/2} \frac{1}{2} \left(\frac{-ie}{\hbar c}\right)^{2} \mathbf{A}^{2} \psi$$

Substitute the solved integrals into (6) to obtain

$$\psi + \epsilon \frac{\partial \psi}{\partial t} = \frac{1}{A} \left(1 - \frac{ie\epsilon}{\hbar} \phi \right) \left(\frac{2\pi i\hbar\epsilon}{m} \right)^{3/2}$$

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

In the limit as $\epsilon \to 0$ 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.

$$\psi + \epsilon \frac{\partial \psi}{\partial t} = \left(1 - \frac{ie\epsilon}{\hbar}\phi\right)$$

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

Expand the product and discard terms of order ϵ^2 .

$$\psi + \epsilon \frac{\partial \psi}{\partial t}$$

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

Cancel leading terms ψ and divide through by ϵ .

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

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

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

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

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

and because **A** is a vector and ψ 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.

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

Add the scalar potential.

$$\frac{1}{2m} \left(\frac{\hbar}{i} \nabla - \frac{e}{c} \mathbf{A} \right)^{2} \psi + e \phi \psi$$

$$= -\frac{\hbar^{2}}{2m} \nabla^{2} \psi + \frac{ie\hbar}{mc} \mathbf{A} \cdot \nabla \psi + \frac{ie\hbar}{2mc} \nabla \cdot \mathbf{A} \psi + \frac{e^{2}}{2mc^{2}} \mathbf{A}^{2} \psi + e \phi \psi$$

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

$$-\frac{i}{\hbar} \left(\frac{1}{2m} \left(\frac{\hbar}{i} \nabla - \frac{e}{c} \mathbf{A} \right)^2 \psi + e \phi \psi \right)$$

$$= \frac{i\hbar}{2m} \nabla^2 \psi + \frac{e}{mc} \mathbf{A} \cdot \nabla \psi + \frac{e}{2mc} \nabla \cdot \mathbf{A} \psi - \frac{ie^2}{2m\hbar c^2} \mathbf{A}^2 \psi - \frac{ie}{\hbar} \phi \psi$$

The result is identical to (7).

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