

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

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

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

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

Factor the exponential.

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

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

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

Then for small ϵ

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

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

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

Substitute (3) into (2).

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

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.

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

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.

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

Hence

$$\begin{aligned}\psi(\mathbf{x},t+\epsilon)&=\frac{1}{A}\left(1-\frac{ie\epsilon}{\hbar}\phi\right)\int_{\mathbb{R}^3}\exp\left(\frac{im}{2\hbar\epsilon}\boldsymbol{\eta}^2\right) \\ &\times\left(1-\frac{ie}{\hbar c}\boldsymbol{\eta}\cdot\mathbf{A}-\frac{ie}{2\hbar c}\boldsymbol{\eta}\cdot(\boldsymbol{\eta}\cdot\nabla\mathbf{A})+\frac{1}{2}\left(-\frac{ie}{\hbar c}\boldsymbol{\eta}\cdot\mathbf{A}\right)^2\right) \\ &\times\psi(\mathbf{x}+\boldsymbol{\eta},t)d\eta_1d\eta_2d\eta_3\end{aligned}\tag{4}$$

Next we will use the following Taylor series approximations.

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

Substitute the approximations (5) into (4).

$$\begin{aligned}\psi+\epsilon\frac{\partial\psi}{\partial t}&=\frac{1}{A}\left(1-\frac{ie\epsilon}{\hbar}\phi\right)\int_{\mathbb{R}^3}\exp\left(\frac{im}{2\hbar\epsilon}\boldsymbol{\eta}^2\right) \\ &\times\left(1-\frac{ie}{\hbar c}\boldsymbol{\eta}\cdot\mathbf{A}-\frac{ie}{2\hbar c}\boldsymbol{\eta}\cdot(\boldsymbol{\eta}\cdot\nabla\mathbf{A})+\frac{1}{2}\left(-\frac{ie}{\hbar c}\boldsymbol{\eta}\cdot\mathbf{A}\right)^2\right) \\ &\times\left(\psi+\boldsymbol{\eta}\cdot\nabla\psi+\frac{1}{2}\boldsymbol{\eta}\cdot\nabla(\boldsymbol{\eta}\cdot\nabla\psi)\right)d\eta_1d\eta_2d\eta_3\end{aligned}\tag{6}$$

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 ϵ^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

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

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 .

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

Expand the product and discard terms of order ϵ^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 ψ and divide through by ϵ .

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

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 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 $2m$.

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

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).

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