

4-1. Show that for a single particle moving in three dimensions in a potential energy  $V(\mathbf{x}, t)$  the Schrodinger equation is

$$\frac{\partial \psi(\mathbf{x}, t)}{\partial t} = -\frac{i}{\hbar} \left( -\frac{\hbar^2}{2m} \nabla^2 \psi(\mathbf{x}, t) + V(\mathbf{x}, t) \psi(\mathbf{x}, t) \right)$$


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From equation (4.3) we have

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

where

$$\int_{\mathbb{R}^3} \equiv \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty}$$

From p. 77 the Lagrangian is

$$L(\dot{\mathbf{x}}, \mathbf{x}) = \frac{m}{2} \dot{\mathbf{x}}^2 - V(\mathbf{x}, t)$$

It follows that

$$L \left( \frac{\mathbf{x} - \mathbf{y}}{\epsilon}, \frac{\mathbf{x} + \mathbf{y}}{2} \right) = \frac{m}{2\epsilon^2} (\mathbf{x} - \mathbf{y})^2 - V \left( \frac{\mathbf{x} + \mathbf{y}}{2}, t \right)$$

Hence

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

Let

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

Then

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

Hence

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

Factor the exponential.

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

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

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

Then for small  $\epsilon$

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

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

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

Substitute (3) into (2) and obtain

$$\psi(\mathbf{x}, t + \epsilon) = \frac{1}{A} \left(1 - \frac{i\epsilon}{\hbar} V(\mathbf{x}, t)\right) \int_{\mathbb{R}^3} \exp\left(\frac{im}{2\hbar\epsilon} \boldsymbol{\eta}^2\right) \times \psi(\mathbf{x} + \boldsymbol{\eta}, t) d\eta_1 d\eta_2 d\eta_3 \quad (4)$$

Next we will use the following Taylor series approximations.

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

Note: In component notation

$$\nabla \psi \cdot \boldsymbol{\eta} = \eta_1 \frac{\partial \psi}{\partial x_1} + \eta_2 \frac{\partial \psi}{\partial x_2} + \eta_3 \frac{\partial \psi}{\partial x_3}$$

and

$$\begin{aligned}\nabla(\nabla\psi \cdot \boldsymbol{\eta}) \cdot \boldsymbol{\eta} &= \eta_1^2 \frac{\partial^2 \psi}{\partial x_1^2} + \eta_2^2 \frac{\partial^2 \psi}{\partial x_2^2} + \eta_3^2 \frac{\partial^2 \psi}{\partial x_3^2} \\ &\quad + 2\eta_1\eta_2 \frac{\partial^2 \psi}{\partial x_1 \partial x_2} + 2\eta_1\eta_3 \frac{\partial^2 \psi}{\partial x_1 \partial x_3} + 2\eta_2\eta_3 \frac{\partial^2 \psi}{\partial x_2 \partial x_3}\end{aligned}$$

Substitute the approximations (5) into (4).

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

Expand the integrand.

$$\begin{aligned}&\int_{\mathbb{R}^3} \exp\left(\frac{im}{2\hbar\epsilon} \boldsymbol{\eta}^2\right) \left( \psi(\mathbf{x}, t) + \nabla\psi \cdot \boldsymbol{\eta} + \frac{1}{2} \nabla(\nabla\psi \cdot \boldsymbol{\eta}) \cdot \boldsymbol{\eta} \right) d\eta_1 d\eta_2 d\eta_3 \\ &= \int_{\mathbb{R}^3} \exp\left(\frac{im}{2\hbar\epsilon} \boldsymbol{\eta}^2\right) \psi(\mathbf{x}, t) d\eta_1 d\eta_2 d\eta_3\end{aligned}\quad (7)$$

$$+ \int_{\mathbb{R}^3} \exp\left(\frac{im}{2\hbar\epsilon} \boldsymbol{\eta}^2\right) \nabla\psi \cdot \boldsymbol{\eta} d\eta_1 d\eta_2 d\eta_3 \quad (8)$$

$$+ \int_{\mathbb{R}^3} \exp\left(\frac{im}{2\hbar\epsilon} \boldsymbol{\eta}^2\right) \frac{1}{2} \nabla(\nabla\psi \cdot \boldsymbol{\eta}) \cdot \boldsymbol{\eta} d\eta_1 d\eta_2 d\eta_3 \quad (9)$$

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

$$\int_{-\infty}^{\infty} \exp\left(\frac{imx^2}{2\hbar\epsilon}\right) dx = \left(\frac{2\pi i\hbar\epsilon}{m}\right)^{1/2} \quad (10)$$

$$\int_{-\infty}^{\infty} x \exp\left(\frac{imx^2}{2\hbar\epsilon}\right) dx = 0 \quad (11)$$

$$\int_{-\infty}^{\infty} x^2 \exp\left(\frac{imx^2}{2\hbar\epsilon}\right) dx = \frac{i\hbar\epsilon}{m} \left(\frac{2\pi i\hbar\epsilon}{m}\right)^{1/2} \quad (12)$$

Rewrite the integral in (7) in component notation.

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

Then by equation (10)

$$\int_{\mathbb{R}^3} \exp\left(\frac{im}{2\hbar\epsilon}\boldsymbol{\eta}^2\right) \psi(\mathbf{x}, t) d\eta_1 d\eta_2 d\eta_3 = \left(\frac{2\pi i\hbar\epsilon}{m}\right)^{3/2} \psi(\mathbf{x}, t) \quad (13)$$

Rewrite the integral in (8) in component notation.

$$\begin{aligned} & \int_{\mathbb{R}^3} \exp\left(\frac{im}{2\hbar\epsilon}\boldsymbol{\eta}^2\right) \nabla\psi \cdot \boldsymbol{\eta} d\eta_1 d\eta_2 d\eta_3 \\ &= \int_{\mathbb{R}^3} \exp\left(\frac{im\eta_1^2}{2\hbar\epsilon}\right) \exp\left(\frac{im\eta_2^2}{2\hbar\epsilon}\right) \exp\left(\frac{im\eta_3^2}{2\hbar\epsilon}\right) \eta_1 \frac{\partial\psi}{\partial x_1} d\eta_1 d\eta_2 d\eta_3 \\ &+ \int_{\mathbb{R}^3} \exp\left(\frac{im\eta_1^2}{2\hbar\epsilon}\right) \exp\left(\frac{im\eta_2^2}{2\hbar\epsilon}\right) \exp\left(\frac{im\eta_3^2}{2\hbar\epsilon}\right) \eta_2 \frac{\partial\psi}{\partial x_2} d\eta_1 d\eta_2 d\eta_3 \\ &+ \int_{\mathbb{R}^3} \exp\left(\frac{im\eta_1^2}{2\hbar\epsilon}\right) \exp\left(\frac{im\eta_2^2}{2\hbar\epsilon}\right) \exp\left(\frac{im\eta_3^2}{2\hbar\epsilon}\right) \eta_3 \frac{\partial\psi}{\partial x_3} d\eta_1 d\eta_2 d\eta_3 \end{aligned}$$

Then by equation (11)

$$\int_{\mathbb{R}^3} \exp\left(\frac{im}{2\hbar\epsilon}\boldsymbol{\eta}^2\right) \nabla\psi \cdot \boldsymbol{\eta} d\eta_1 d\eta_2 d\eta_3 = 0 \quad (14)$$

Rewrite the integral in (9) in component notation.

$$\begin{aligned} & \int_{\mathbb{R}^3} \exp\left(\frac{im}{2\hbar\epsilon}\boldsymbol{\eta}^2\right) \frac{1}{2} \nabla(\nabla\psi \cdot \boldsymbol{\eta}) \cdot \boldsymbol{\eta} d\eta_1 d\eta_2 d\eta_3 \\ &= \frac{1}{2} \int_{\mathbb{R}^3} \exp\left(\frac{im\eta_1^2}{2\hbar\epsilon}\right) \exp\left(\frac{im\eta_2^2}{2\hbar\epsilon}\right) \exp\left(\frac{im\eta_3^2}{2\hbar\epsilon}\right) \eta_1^2 \frac{\partial^2\psi}{\partial x_1^2} d\eta_1 d\eta_2 d\eta_3 \\ &+ \frac{1}{2} \int_{\mathbb{R}^3} \exp\left(\frac{im\eta_1^2}{2\hbar\epsilon}\right) \exp\left(\frac{im\eta_2^2}{2\hbar\epsilon}\right) \exp\left(\frac{im\eta_3^2}{2\hbar\epsilon}\right) \eta_2^2 \frac{\partial^2\psi}{\partial x_2^2} d\eta_1 d\eta_2 d\eta_3 \\ &+ \frac{1}{2} \int_{\mathbb{R}^3} \exp\left(\frac{im\eta_1^2}{2\hbar\epsilon}\right) \exp\left(\frac{im\eta_2^2}{2\hbar\epsilon}\right) \exp\left(\frac{im\eta_3^2}{2\hbar\epsilon}\right) \eta_3^2 \frac{\partial^2\psi}{\partial x_3^2} d\eta_1 d\eta_2 d\eta_3 \\ &+ \int_{\mathbb{R}^3} \exp\left(\frac{im\eta_1^2}{2\hbar\epsilon}\right) \exp\left(\frac{im\eta_2^2}{2\hbar\epsilon}\right) \exp\left(\frac{im\eta_3^2}{2\hbar\epsilon}\right) \eta_1 \eta_2 \frac{\partial^2\psi}{\partial x_1 \partial x_2} d\eta_1 d\eta_2 d\eta_3 \\ &+ \int_{\mathbb{R}^3} \exp\left(\frac{im\eta_1^2}{2\hbar\epsilon}\right) \exp\left(\frac{im\eta_2^2}{2\hbar\epsilon}\right) \exp\left(\frac{im\eta_3^2}{2\hbar\epsilon}\right) \eta_1 \eta_3 \frac{\partial^2\psi}{\partial x_1 \partial x_3} d\eta_1 d\eta_2 d\eta_3 \\ &+ \int_{\mathbb{R}^3} \exp\left(\frac{im\eta_1^2}{2\hbar\epsilon}\right) \exp\left(\frac{im\eta_2^2}{2\hbar\epsilon}\right) \exp\left(\frac{im\eta_3^2}{2\hbar\epsilon}\right) \eta_2 \eta_3 \frac{\partial^2\psi}{\partial x_2 \partial x_3} d\eta_1 d\eta_2 d\eta_3 \end{aligned}$$

By equations (10) and (12)

$$\begin{aligned}
& \frac{1}{2} \int_{\mathbb{R}^3} \exp\left(\frac{im\eta_1^2}{2\hbar\epsilon}\right) \exp\left(\frac{im\eta_2^2}{2\hbar\epsilon}\right) \exp\left(\frac{im\eta_3^2}{2\hbar\epsilon}\right) \eta_1^2 \frac{\partial^2 \psi}{\partial x_1^2} d\eta_1 d\eta_2 d\eta_3 \\
&= \frac{i\hbar\epsilon}{2m} \left(\frac{2\pi i\hbar\epsilon}{m}\right)^{3/2} \frac{\partial^2 \psi}{\partial x_1^2} \\
& \frac{1}{2} \int_{\mathbb{R}^3} \exp\left(\frac{im\eta_1^2}{2\hbar\epsilon}\right) \exp\left(\frac{im\eta_2^2}{2\hbar\epsilon}\right) \exp\left(\frac{im\eta_3^2}{2\hbar\epsilon}\right) \eta_2^2 \frac{\partial^2 \psi}{\partial x_2^2} d\eta_1 d\eta_2 d\eta_3 \\
&= \frac{i\hbar\epsilon}{2m} \left(\frac{2\pi i\hbar\epsilon}{m}\right)^{3/2} \frac{\partial^2 \psi}{\partial x_2^2} \\
& \frac{1}{2} \int_{\mathbb{R}^3} \exp\left(\frac{im\eta_1^2}{2\hbar\epsilon}\right) \exp\left(\frac{im\eta_2^2}{2\hbar\epsilon}\right) \exp\left(\frac{im\eta_3^2}{2\hbar\epsilon}\right) \eta_3^2 \frac{\partial^2 \psi}{\partial x_3^2} d\eta_1 d\eta_2 d\eta_3 \\
&= \frac{i\hbar\epsilon}{2m} \left(\frac{2\pi i\hbar\epsilon}{m}\right)^{3/2} \frac{\partial^2 \psi}{\partial x_3^2}
\end{aligned}$$

By equation (11)

$$\begin{aligned}
& \int_{\mathbb{R}^3} \exp\left(\frac{im\eta_1^2}{2\hbar\epsilon}\right) \exp\left(\frac{im\eta_2^2}{2\hbar\epsilon}\right) \exp\left(\frac{im\eta_3^2}{2\hbar\epsilon}\right) \eta_1 \eta_2 \frac{\partial^2 \psi}{\partial x_1 \partial x_2} d\eta_1 d\eta_2 d\eta_3 = 0 \\
& \int_{\mathbb{R}^3} \exp\left(\frac{im\eta_1^2}{2\hbar\epsilon}\right) \exp\left(\frac{im\eta_2^2}{2\hbar\epsilon}\right) \exp\left(\frac{im\eta_3^2}{2\hbar\epsilon}\right) \eta_1 \eta_3 \frac{\partial^2 \psi}{\partial x_1 \partial x_3} d\eta_1 d\eta_2 d\eta_3 = 0 \\
& \int_{\mathbb{R}^3} \exp\left(\frac{im\eta_1^2}{2\hbar\epsilon}\right) \exp\left(\frac{im\eta_2^2}{2\hbar\epsilon}\right) \exp\left(\frac{im\eta_3^2}{2\hbar\epsilon}\right) \eta_2 \eta_3 \frac{\partial^2 \psi}{\partial x_2 \partial x_3} d\eta_1 d\eta_2 d\eta_3 = 0
\end{aligned}$$

Hence

$$\begin{aligned}
& \int_{\mathbb{R}^3} \exp\left(\frac{im}{2\hbar\epsilon} \boldsymbol{\eta}^2\right) \frac{1}{2} \nabla(\nabla\psi \cdot \boldsymbol{\eta}) \cdot \boldsymbol{\eta} d\eta_1 d\eta_2 d\eta_3 \\
&= \frac{i\hbar\epsilon}{2m} \left(\frac{2\pi i\hbar\epsilon}{m}\right)^{3/2} \left(\frac{\partial^2}{\partial x_1^2} + \frac{\partial^2}{\partial x_2^2} + \frac{\partial^2}{\partial x_3^2}\right) \psi \quad (15)
\end{aligned}$$

Substitute the solved integrals into (6) to obtain

$$\psi(\mathbf{x}, t) + \epsilon \frac{\partial \psi}{\partial t} = \frac{1}{A} \left(1 - \frac{i\epsilon}{\hbar} V(\mathbf{x}, t)\right) \left(\frac{2\pi i\hbar\epsilon}{m}\right)^{3/2} \left(\psi(\mathbf{x}, t) + \frac{i\hbar\epsilon}{2m} \nabla^2 \psi\right)$$

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

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

Hence

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

Cancel  $A$ , expand the product and discard the  $\epsilon^2$  term.

$$\psi(\mathbf{x}, t) + \epsilon \frac{\partial \psi}{\partial t} = \psi(\mathbf{x}, t) + \frac{i \hbar \epsilon}{2m} \nabla^2 \psi - \frac{i \epsilon}{\hbar} V(\mathbf{x}, t) \psi$$

Cancel the  $\psi(\mathbf{x}, t)$  terms.

$$\epsilon \frac{\partial \psi}{\partial t} = \frac{i \hbar \epsilon}{2m} \nabla^2 \psi - \frac{i \epsilon}{\hbar} V(\mathbf{x}, t) \psi$$

Divide through by  $\epsilon$ .

$$\frac{\partial \psi}{\partial t} = \frac{i \hbar}{2m} \nabla^2 \psi - \frac{i}{\hbar} V(\mathbf{x}, t) \psi \tag{16}$$