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

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

From equation (4.3) we have

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

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

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

Let

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

Then

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

Hence

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

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

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

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

Note: In component notation

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

and

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

Substitute the approximations (5) into (4).

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

Expand the integrand.

$$\int_{\mathbb{R}^{3}} \exp\left(\frac{im}{2\hbar\epsilon}\boldsymbol{\eta}^{2}\right) \left(\psi(\mathbf{x},t) + \nabla\psi\cdot\boldsymbol{\eta} + \frac{1}{2}\nabla(\nabla\psi\cdot\boldsymbol{\eta})\cdot\boldsymbol{\eta}\right) d\eta_{1} d\eta_{2} d\eta_{3}$$

$$= \int_{\mathbb{R}^{3}} \exp\left(\frac{im}{2\hbar\epsilon}\boldsymbol{\eta}^{2}\right) \psi(\mathbf{x},t) d\eta_{1} d\eta_{2} d\eta_{3} \tag{7}$$

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

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

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

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

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

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

Rewrite the integral in (7) in component notation.

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

Then by equation (10)

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

Rewrite the integral in (8) in component notation.

$$\int_{\mathbb{R}^{3}} \exp\left(\frac{im}{2\hbar\epsilon}\boldsymbol{\eta}^{2}\right) \nabla\psi \cdot \boldsymbol{\eta} \, d\eta_{1} \, d\eta_{2} \, d\eta_{3}$$

$$= \int_{\mathbb{R}^{3}} \exp\left(\frac{im\eta_{1}^{2}}{2\hbar\epsilon}\right) \exp\left(\frac{im\eta_{2}^{2}}{2\hbar\epsilon}\right) \exp\left(\frac{im\eta_{3}^{2}}{2\hbar\epsilon}\right) \eta_{1} \frac{\partial\psi}{\partial x_{1}} \, d\eta_{1} \, d\eta_{2} \, d\eta_{3}$$

$$+ \int_{\mathbb{R}^{3}} \exp\left(\frac{im\eta_{1}^{2}}{2\hbar\epsilon}\right) \exp\left(\frac{im\eta_{2}^{2}}{2\hbar\epsilon}\right) \exp\left(\frac{im\eta_{3}^{2}}{2\hbar\epsilon}\right) \eta_{2} \frac{\partial\psi}{\partial x_{2}} \, d\eta_{1} \, d\eta_{2} \, d\eta_{3}$$

$$+ \int_{\mathbb{R}^{3}} \exp\left(\frac{im\eta_{1}^{2}}{2\hbar\epsilon}\right) \exp\left(\frac{im\eta_{2}^{2}}{2\hbar\epsilon}\right) \exp\left(\frac{im\eta_{3}^{2}}{2\hbar\epsilon}\right) \eta_{3} \frac{\partial\psi}{\partial x_{3}} \, d\eta_{1} \, d\eta_{2} \, d\eta_{3}$$

Then by equation (11)

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

Rewrite the integral in (9) in component notation.

$$\int_{\mathbb{R}^{3}} \exp\left(\frac{im}{2\hbar\epsilon}\boldsymbol{\eta}^{2}\right) \frac{1}{2}\nabla(\nabla\psi\cdot\boldsymbol{\eta})\cdot\boldsymbol{\eta} d\eta_{1} d\eta_{2} d\eta_{3}$$

$$= \frac{1}{2}\int_{\mathbb{R}^{3}} \exp\left(\frac{im\eta_{1}^{2}}{2\hbar\epsilon}\right) \exp\left(\frac{im\eta_{2}^{2}}{2\hbar\epsilon}\right) \exp\left(\frac{im\eta_{3}^{2}}{2\hbar\epsilon}\right) \eta_{1}^{2} \frac{\partial^{2}\psi}{\partial x_{1}^{2}} d\eta_{1} d\eta_{2} d\eta_{3}$$

$$+ \frac{1}{2}\int_{\mathbb{R}^{3}} \exp\left(\frac{im\eta_{1}^{2}}{2\hbar\epsilon}\right) \exp\left(\frac{im\eta_{2}^{2}}{2\hbar\epsilon}\right) \exp\left(\frac{im\eta_{3}^{2}}{2\hbar\epsilon}\right) \eta_{2}^{2} \frac{\partial^{2}\psi}{\partial x_{2}^{2}} d\eta_{1} d\eta_{2} d\eta_{3}$$

$$+ \frac{1}{2}\int_{\mathbb{R}^{3}} \exp\left(\frac{im\eta_{1}^{2}}{2\hbar\epsilon}\right) \exp\left(\frac{im\eta_{2}^{2}}{2\hbar\epsilon}\right) \exp\left(\frac{im\eta_{3}^{2}}{2\hbar\epsilon}\right) \eta_{3}^{2} \frac{\partial^{2}\psi}{\partial x_{3}^{2}} d\eta_{1} d\eta_{2} d\eta_{3}$$

$$+ \int_{\mathbb{R}^{3}} \exp\left(\frac{im\eta_{1}^{2}}{2\hbar\epsilon}\right) \exp\left(\frac{im\eta_{2}^{2}}{2\hbar\epsilon}\right) \exp\left(\frac{im\eta_{3}^{2}}{2\hbar\epsilon}\right) \eta_{1}\eta_{2} \frac{\partial^{2}\psi}{\partial x_{1}\partial x_{2}} d\eta_{1} d\eta_{2} d\eta_{3}$$

$$+ \int_{\mathbb{R}^{3}} \exp\left(\frac{im\eta_{1}^{2}}{2\hbar\epsilon}\right) \exp\left(\frac{im\eta_{2}^{2}}{2\hbar\epsilon}\right) \exp\left(\frac{im\eta_{3}^{2}}{2\hbar\epsilon}\right) \eta_{1}\eta_{3} \frac{\partial^{2}\psi}{\partial x_{1}\partial x_{3}} d\eta_{1} d\eta_{2} d\eta_{3}$$

$$+ \int_{\mathbb{R}^{3}} \exp\left(\frac{im\eta_{1}^{2}}{2\hbar\epsilon}\right) \exp\left(\frac{im\eta_{2}^{2}}{2\hbar\epsilon}\right) \exp\left(\frac{im\eta_{3}^{2}}{2\hbar\epsilon}\right) \eta_{1}\eta_{3} \frac{\partial^{2}\psi}{\partial x_{1}\partial x_{3}} d\eta_{1} d\eta_{2} d\eta_{3}$$

$$+ \int_{\mathbb{R}^{3}} \exp\left(\frac{im\eta_{1}^{2}}{2\hbar\epsilon}\right) \exp\left(\frac{im\eta_{2}^{2}}{2\hbar\epsilon}\right) \exp\left(\frac{im\eta_{3}^{2}}{2\hbar\epsilon}\right) \eta_{2}\eta_{3} \frac{\partial^{2}\psi}{\partial x_{2}\partial x_{3}} d\eta_{1} d\eta_{2} d\eta_{3}$$

By equations (10) and (12)

$$\frac{1}{2} \int_{\mathbb{R}^{3}} \exp\left(\frac{im\eta_{1}^{2}}{2\hbar\epsilon}\right) \exp\left(\frac{im\eta_{2}^{2}}{2\hbar\epsilon}\right) \exp\left(\frac{im\eta_{3}^{2}}{2\hbar\epsilon}\right) \eta_{1}^{2} \frac{\partial^{2}\psi}{\partial x_{1}^{2}} d\eta_{1} d\eta_{2} d\eta_{3}$$

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

$$\frac{1}{2} \int_{\mathbb{R}^{3}} \exp\left(\frac{im\eta_{1}^{2}}{2\hbar\epsilon}\right) \exp\left(\frac{im\eta_{2}^{2}}{2\hbar\epsilon}\right) \exp\left(\frac{im\eta_{3}^{2}}{2\hbar\epsilon}\right) \eta_{2}^{2} \frac{\partial^{2}\psi}{\partial x_{2}^{2}} d\eta_{1} d\eta_{2} d\eta_{3}$$

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

$$\frac{1}{2} \int_{\mathbb{R}^{3}} \exp\left(\frac{im\eta_{1}^{2}}{2\hbar\epsilon}\right) \exp\left(\frac{im\eta_{2}^{2}}{2\hbar\epsilon}\right) \exp\left(\frac{im\eta_{3}^{2}}{2\hbar\epsilon}\right) \eta_{3}^{2} \frac{\partial^{2}\psi}{\partial x_{3}^{2}} d\eta_{1} d\eta_{2} d\eta_{3}$$

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

By equation (11)

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

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

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

Hence

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

$$= \frac{i\hbar\epsilon}{2m} \left(\frac{2\pi i\hbar\epsilon}{m}\right)^{3/2} \left(\frac{\partial^2}{\partial x_1^2} + \frac{\partial^2}{\partial x_2^2} + \frac{\partial^2}{\partial x_3^2}\right) \psi \quad (15)$$

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  $\epsilon \to 0$  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  $\epsilon$ .

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