Feynman and Hibbs problem 4-1

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

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

This is the Lagrangian.

$$L(\dot{\mathbf{x}}, \mathbf{x}) = \frac{m}{2}\dot{\mathbf{x}}^2 - V(\mathbf{x}, t) \tag{1}$$

Extend equation (4.3) from one dimension to three dimensions.

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

where

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

From (1) we have

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

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

$$y = x + \eta$$

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.

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

Now we are going to use an approximation for the exponential of V. From the identity  $\exp(i\theta) = \cos(\theta) + i\sin(\theta)$  we have

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

For small  $\epsilon$  we have the approximation

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

The authors write that the  $\frac{1}{2}\eta$  term can be dropped "because the error is of higher order than  $\epsilon$ ." Hence

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

Substituting (3) into (2) yields

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

Next we will use the following Taylor series approximations.

$$\psi(\mathbf{x}, t + \epsilon) \approx \psi(\mathbf{x}, t) + \epsilon \frac{\partial \psi}{\partial t}$$

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

Note: In component notation

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

and

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

Substitute the approximations (5) into (4).

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

Expand the right-hand side.

$$\psi(\mathbf{x},t) + \epsilon \frac{\partial \psi}{\partial t} = \frac{\psi(\mathbf{x},t)}{A} \int_{\mathbb{R}^3} \exp\left(\frac{im}{2\hbar\epsilon} \boldsymbol{\eta}^2\right) d\eta_1 d\eta_2 d\eta_3$$
 (7)

$$+\frac{1}{A}\int_{\mathbb{R}^3} \exp\left(\frac{im}{2\hbar\epsilon}\boldsymbol{\eta}^2\right)\boldsymbol{\eta}\cdot\nabla\psi\,d\eta_1\,d\eta_2\,d\eta_3\tag{8}$$

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

$$-\frac{i\epsilon}{A\hbar}V(\mathbf{x},t)\,\psi(\mathbf{x},t)\int_{\mathbb{R}^3}\exp\left(\frac{im}{2\hbar\epsilon}\boldsymbol{\eta}^2\right)\,d\eta_1\,d\eta_2\,d\eta_3\tag{10}$$

$$-\frac{i\epsilon}{A\hbar}V(\mathbf{x},t)\int_{\mathbb{R}^3} \exp\left(\frac{im}{2\hbar\epsilon}\boldsymbol{\eta}^2\right)\boldsymbol{\eta}\cdot\nabla\psi\,d\eta_1\,d\eta_2\,d\eta_3\tag{11}$$

$$-\frac{i\epsilon}{2A\hbar}V(\mathbf{x},t)\int_{\mathbb{R}^3} \exp\left(\frac{im}{2\hbar\epsilon}\boldsymbol{\eta}^2\right)\boldsymbol{\eta}\cdot\nabla(\boldsymbol{\eta}\cdot\nabla\psi)\,d\eta_1\,d\eta_2\,d\eta_3 \qquad (12)$$

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

$$\int_{-\infty}^{\infty} \exp\left(\frac{imx^2}{2\hbar\epsilon}\right) dx = \left(\frac{2\pi i\hbar\epsilon}{m}\right)^{1/2} \tag{13}$$

$$\int_{-\infty}^{\infty} \exp\left(\frac{imx^2}{2\hbar\epsilon}\right) x \, dx = 0 \tag{14}$$

$$\int_{-\infty}^{\infty} \exp\left(\frac{imx^2}{2\hbar\epsilon}\right) x^2 dx = \left(-\frac{2\pi i\hbar^3 \epsilon^3}{m^3}\right)^{1/2}$$
 (15)

Rewrite the integral in (7) and (10) in component notation.

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

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

Then by equation (13)

$$\int_{\mathbb{R}^3} \exp\left(\frac{im}{2\hbar\epsilon} \boldsymbol{\eta}^2\right) d\eta_1 d\eta_2 d\eta_3 = \left(\frac{2\pi i\hbar\epsilon}{m}\right)^{3/2} \tag{16}$$

Rewrite the integral in (8) and (11) in component notation.

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

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

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

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

Then by equation (14)

$$\int_{\mathbb{R}^3} \exp\left(\frac{im}{2\hbar\epsilon} \boldsymbol{\eta}^2\right) \boldsymbol{\eta} \cdot \nabla \psi \, d\eta_1 \, d\eta_2 \, d\eta_3 = 0 \tag{17}$$

Rewrite the integral in (9) and (12) in component notation.

$$\begin{split} \int_{\mathbb{R}^{3}} \exp\left(\frac{im}{2\hbar\epsilon}\boldsymbol{\eta}^{2}\right) \boldsymbol{\eta} \cdot \nabla(\boldsymbol{\eta} \cdot \nabla\psi) \, d\eta_{1} \, d\eta_{2} \, d\eta_{3} \\ &= \int_{\mathbb{R}^{3}} \exp\left(\frac{im\eta_{1}^{2}}{2\hbar\epsilon}\right) \exp\left(\frac{im\eta_{2}^{2}}{2\hbar\epsilon}\right) \exp\left(\frac{im\eta_{3}^{2}}{2\hbar\epsilon}\right) \eta_{1}^{2} \frac{\partial^{2}\psi}{\partial x_{1}^{2}} \, d\eta_{1} \, d\eta_{2} \, d\eta_{3} \\ &+ \int_{\mathbb{R}^{3}} \exp\left(\frac{im\eta_{1}^{2}}{2\hbar\epsilon}\right) \exp\left(\frac{im\eta_{2}^{2}}{2\hbar\epsilon}\right) \exp\left(\frac{im\eta_{3}^{2}}{2\hbar\epsilon}\right) \eta_{2}^{2} \frac{\partial^{2}\psi}{\partial x_{2}^{2}} \, d\eta_{1} \, d\eta_{2} \, d\eta_{3} \\ &+ \int_{\mathbb{R}^{3}} \exp\left(\frac{im\eta_{1}^{2}}{2\hbar\epsilon}\right) \exp\left(\frac{im\eta_{2}^{2}}{2\hbar\epsilon}\right) \exp\left(\frac{im\eta_{3}^{2}}{2\hbar\epsilon}\right) \eta_{3}^{2} \frac{\partial^{2}\psi}{\partial x_{3}^{2}} \, d\eta_{1} \, d\eta_{2} \, d\eta_{3} \\ &+ \int_{\mathbb{R}^{3}} \exp\left(\frac{im\eta_{1}^{2}}{2\hbar\epsilon}\right) \exp\left(\frac{im\eta_{2}^{2}}{2\hbar\epsilon}\right) \exp\left(\frac{im\eta_{3}^{2}}{2\hbar\epsilon}\right) 2\eta_{1}\eta_{2} \frac{\partial^{2}\psi}{\partial x_{1}\partial x_{2}} \, d\eta_{1} \, d\eta_{2} \, d\eta_{3} \\ &+ \int_{\mathbb{R}^{3}} \exp\left(\frac{im\eta_{1}^{2}}{2\hbar\epsilon}\right) \exp\left(\frac{im\eta_{2}^{2}}{2\hbar\epsilon}\right) \exp\left(\frac{im\eta_{3}^{2}}{2\hbar\epsilon}\right) 2\eta_{1}\eta_{3} \frac{\partial^{2}\psi}{\partial x_{1}\partial x_{3}} \, d\eta_{1} \, d\eta_{2} \, d\eta_{3} \\ &+ \int_{\mathbb{R}^{3}} \exp\left(\frac{im\eta_{1}^{2}}{2\hbar\epsilon}\right) \exp\left(\frac{im\eta_{2}^{2}}{2\hbar\epsilon}\right) \exp\left(\frac{im\eta_{3}^{2}}{2\hbar\epsilon}\right) 2\eta_{2}\eta_{3} \frac{\partial^{2}\psi}{\partial x_{2}\partial x_{3}} \, d\eta_{1} \, d\eta_{2} \, d\eta_{3} \end{split}$$

By equations (13) and (15)

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

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

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

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

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

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

By equation (14)

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

Hence

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

$$= \frac{i\hbar\epsilon}{m} \left(\frac{2\pi i\hbar\epsilon}{m}\right)^{3/2} \left(\frac{\partial^2}{\partial x_1^2} + \frac{\partial^2}{\partial x_2^2} + \frac{\partial^2}{\partial x_3^2}\right) \psi(\mathbf{x}, t) \quad (18)$$

Substitute the solved integrals into (6) to obtain

$$\psi(\mathbf{x},t) + \epsilon \frac{\partial \psi}{\partial t}$$

$$= \frac{1}{A} \left( \frac{2\pi i \hbar \epsilon}{m} \right)^{3/2} \psi(\mathbf{x},t) \qquad \text{from (7) and (16)}$$

$$+ \frac{i \hbar \epsilon}{2Am} \left( \frac{2\pi i \hbar \epsilon}{m} \right)^{3/2} \nabla^2 \psi(\mathbf{x},t) \qquad \text{from (9) and (18)}$$

$$- \frac{i \epsilon}{A\hbar} \left( \frac{2\pi i \hbar \epsilon}{m} \right)^{3/2} V(\mathbf{x},t) \psi(\mathbf{x},t) \qquad \text{from (10) and (16)}$$

$$+ \frac{\epsilon^2}{2Am} \left( \frac{2\pi i \hbar \epsilon}{m} \right)^{3/2} V(\mathbf{x},t) \nabla^2 \psi(\mathbf{x},t) \qquad \text{from (12) and (18)}$$

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 and drop the order  $\epsilon^2$  term.

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

The  $\psi(\mathbf{x},t)$  terms cancel.

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

Divide through by  $\epsilon$ .

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