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.

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

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

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

Let

$$y = x + \eta$$

Then

$$(\mathbf{x} - \mathbf{y})^2 = \boldsymbol{\eta}^2$$

and

$$\frac{\mathbf{x} + \mathbf{y}}{2} = \mathbf{x} + \frac{1}{2}\boldsymbol{\eta}$$

Hence

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

Factor the exponential.

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

Now we are going to use an approximation for the second exponential. 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 very 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

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

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

Expand the right-hand side.

$$\frac{\psi(\mathbf{x},t)}{A} \int_{\mathbb{R}^{3}} \exp\left(\frac{im}{2\hbar\epsilon} \boldsymbol{\eta}^{2}\right) d\eta_{1} d\eta_{2} d\eta_{3} 
+ \frac{1}{A} \int_{\mathbb{R}^{3}} \exp\left(\frac{im}{2\hbar\epsilon} \boldsymbol{\eta}^{2}\right) \boldsymbol{\eta} \cdot \nabla \psi d\eta_{1} d\eta_{2} d\eta_{3} 
+ \frac{1}{2A} \int_{\mathbb{R}^{3}} \exp\left(\frac{im}{2\hbar\epsilon} \boldsymbol{\eta}^{2}\right) \boldsymbol{\eta} \cdot \nabla (\boldsymbol{\eta} \cdot \nabla \psi) d\eta_{1} d\eta_{2} d\eta_{3} 
- \frac{i\epsilon}{A\hbar} V(\mathbf{x},t) \psi(\mathbf{x},t) \int_{\mathbb{R}^{3}} \exp\left(\frac{im}{2\hbar\epsilon} \boldsymbol{\eta}^{2}\right) d\eta_{1} d\eta_{2} d\eta_{3} 
- \frac{i\epsilon}{A\hbar} V(\mathbf{x},t) \int_{\mathbb{R}^{3}} \exp\left(\frac{im}{2\hbar\epsilon} \boldsymbol{\eta}^{2}\right) \boldsymbol{\eta} \cdot \nabla \psi d\eta_{1} d\eta_{2} d\eta_{3} 
- \frac{i\epsilon}{2A\hbar} V(\mathbf{x},t) \int_{\mathbb{R}^{3}} \exp\left(\frac{im}{2\hbar\epsilon} \boldsymbol{\eta}^{2}\right) \boldsymbol{\eta} \cdot \nabla \psi d\eta_{1} d\eta_{2} d\eta_{3}$$
(8)
$$- \frac{i\epsilon}{2A\hbar} V(\mathbf{x},t) \int_{\mathbb{R}^{3}} \exp\left(\frac{im}{2\hbar\epsilon} \boldsymbol{\eta}^{2}\right) \boldsymbol{\eta} \cdot \nabla (\boldsymbol{\eta} \cdot \nabla \psi) d\eta_{1} d\eta_{2} d\eta_{3}$$
(9)

We will use the following integrals provided by the authors.

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

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

$$\int_{-\infty}^{\infty} \exp\left(\frac{imx^2}{2\hbar\epsilon}\right) x^2 dx = \left(-\frac{2\pi i\hbar^3 \epsilon^3}{m^3}\right)^{1/2}$$
 (12)

Rewrite the integral in (6) and (8) in component notation.

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

Then by (11) 
$$\int_{\mathbb{R}^3} \exp\left(\frac{im}{2\hbar\epsilon} \eta^2\right) \eta \cdot \nabla \psi \, d\eta_1 \, d\eta_2 \, d\eta_3 = 0$$

Rewrite the integral in (7) and (9) in component notation.

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

By equation (10)

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