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

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

Then

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

Hence

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

Factor the exponential.

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

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

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

For small ϵ we have the approximation

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

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

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

Substitute (3) into (2) and obtain

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

Next we will use the following Taylor series approximations.

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

Note: In component notation

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

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).

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

Expand the integrand.

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

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

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

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

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

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

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

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

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.

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

Then by equation (11)

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

Rewrite the integral in (9) in component notation.

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

By equations (10) and (12)

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

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

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

Substitute the solved integrals into (6) to obtain

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

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 and drop the order ϵ^2 term.

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

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

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

Divide through by ϵ.

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