EC574A1 Supporting Information V.2

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September 15, 2024

1 Introduction

In Section 4 this document we outline the proof of the Ehrenferst's Theorems and in Section 5 their ganaralization.

2 Some Useful Mathematical Tools

2.1 Schrödinger Equation and its Conjugate

It is useful to wrtite the Schrödinger equation and its conjugate.

$$\boxed{\imath\hbar\frac{\partial}{\partial t}\Psi(\vec{r},t) = \left[-\frac{\hbar^2}{2\,m}\nabla^2 + V(\vec{r},t)\right]\Psi(\vec{r},t)} \tag{1}$$

and it conjugate

$$\boxed{-\imath\hbar\frac{\partial}{\partial t}\Psi^*(\vec{r},t) = \left[-\frac{\hbar^2}{2\,m}\nabla^2 + V(\vec{r},t)\right]\Psi^*(\vec{r},t)} \tag{2}$$

Note that on the LHS of both equations we have the Hamiltonian operator in the time dpendent form and on the RHS the Hamiltonial in the spatial dependent form. These two equation ar usefult to exchange time derivatibe of the wavefunction with spatial derivative of the same wavefunction. For example we can write:

$$\boxed{\frac{\mathrm{d}}{\mathrm{d}t}\Psi(\vec{r},t) = \frac{1}{\imath\hbar}\mathrm{H}\Psi(\vec{r},t)} \tag{3}$$

and

$$\boxed{\frac{\mathrm{d}}{\mathrm{d}t}\Psi^*(\vec{r},t) = \frac{1}{-\imath\hbar}\mathrm{H}\Psi^*(\vec{r},t)} \tag{4}$$

2.2 Green's Identities

Consider two scalar functions $v(\vec{r}) = v(x,y,z)$ and $u(\vec{r}) = u(x,y,z)$ defined on a volume V with surface S. We also assume that $u, v \in C^2$ (note that for the first identity it can only be $u \in C^1$). The first Green's idendity is given by:

$$\boxed{\int_V \left[u\nabla^2 v + \overrightarrow{\nabla u} \cdot \overrightarrow{\nabla v}\right] d\vec{r} = \int_S u\overrightarrow{\nabla v} \cdot dS} \tag{5}$$

The integral on the LHS is a volume integral while on the RHS the integral is on the surface S of the volume V. Note that we can also write:

$$\int_V u\nabla^2 v d\vec{r} = \int_S u\overrightarrow{\nabla v} \cdot dS - \int_V \overrightarrow{\nabla u} \cdot \overrightarrow{\nabla v} d\vec{r}$$

and

$$\int_V \overrightarrow{\nabla u} \cdot \overrightarrow{\nabla v} d\vec{r} = \int_S u\overrightarrow{\nabla v} \cdot dS - \int_V u\nabla^2 v d\vec{r} \tag{6}$$

The second Green's idendity is given by:

$$\boxed{\int_V \left[u\nabla^2 v - v\nabla^2 u\right] d\vec{r} = \int_S \left[u\overrightarrow{\nabla v} + v\overrightarrow{\nabla u}\right] \cdot dS} \tag{7}$$

The integral on the RHS is a volume integral while on the LHS the integral is on the surface S of the volume V.

2.3 Differentiation under the Sign of Integral The Liebnitz Integral Rule

Let $f(x,t)$ be a function such that both $f(x,t)$ and its partial derivative $f_x(x,t)$ are continuous in t and x in some region of the xt-plane, including $a(x) \leq t \leq b(x)$ $x_0 \leq x \leq x_1$. Also suppose that the functions $a(x)$ and $b(x)$ are both continuous and both have continuous derivatives for $x_0 \leq x \leq x_1$. Then, for $x_0 \leq x \leq x_1$,

$$\begin{aligned}
&\frac{d}{dx}\left(\int_{a(x)}^{b(x)} f(x,t)\,dt\right) = \\
&= f\big(x,b(x)\big) \cdot \frac{d}{dx}b(x) - f\big(x,a(x)\big) \cdot \frac{d}{dx}a(x) + \int_{a(x)}^{b(x)} \frac{\partial}{\partial x} f(x,t)\,dt
\end{aligned} \tag{8}$$

The right hand side may also be written using Lagrange's notation as:

$$f(x,b(x))\,b'(x) - f(x,a(x))\,a'(x) + \int_{a(x)}^{b(x)} f_x(x,t)\,dt \tag{9}$$

2.4 Review of Statistics and Random Variables

Consider an expriment **E** defined on a given space Ω. The elements, or points, in Ω, that we call ζ, are the random outcomes of the experiment **E**. To each ζ we assign a real number $X(\zeta)$, consequenlty we have established a correspondence between the elements ζ of Ω and the $\mathbb{R}$. This rule, under additional strict requirements (*) is calles a *random variable*. Notice that the random variable X in reality is a function X(.) that maps the space Ω into the real axis $\mathbb{R}$. Specifically the function $X(\zeta)$ associates a randon element ζ in Ω to a value in $\mathbb{R}$.

We conside now a specific experiment outcome such as: $\{\zeta : X(\zeta) \leq x\}$, or $\{X \leq x\}$, to which we want ot assign a probability.

> The probability $P[X \leq x] \triangleq F_X(x)$ is called the *probability distribution function* (or CDS *comulative probability distribution function*) of X

$F_X(x)$ has the following properties:

- $F_X(-\infty) = 0$ and $F_X(\infty) = 1$
- if $x_1 \leqslant x_2$ then $F_X(x_1) \leqslant F_X(x_2)$
- $F_X(x)$ is continous from the right: $\lim\limits_{\epsilon \to 0} F_X(x + \epsilon) = F_X(x)$, with $\epsilon > 0$

> If $F_X(x)$ is continous and differentiable, then:
>
> $$f_X(x) = \frac{\mathrm{d}F_X(x)}{\mathrm{d}x} \tag{10}$$
>
> it is the *probability density function* (PDF) of X

$f_X(x)$ has the following properties:

- $f_X(x) \geq 0$
- $\int_{-\infty}^{\infty} f_X(\gamma)\mathrm{d}\gamma = F_X(\infty) - F_X(-\infty) = 1$
- $F_X(x) = \int_{-\infty}^{x} f_X(\gamma)\mathrm{d}\gamma = P[X \leq x]$
- $F_X(x_2) - F_X(x_1) = \int_{-\infty}^{x_2} f_X(\gamma)\mathrm{d}\gamma - \int_{-\infty}^{x_1} f_X(\gamma)\mathrm{d}\gamma = \int_{x_1}^{x_2} f_X(\gamma)\mathrm{d}\gamma = P[x_1 \leq X \leq x]$

Consider a random variable X with a PDF of $f_X(x)$ then:

> The *expected* or *average* value of X with PDF $f_X(x)$ is given by:
>
> $$E[X] = \int_{-\infty}^{\infty} x f_X(x)\mathrm{d}x \tag{11}$$

Consider a second random variable Y function of X obtained as: $Y = g(X)$, then:

The *expected* or *average* value of Y is given by:

$$E[\mathrm{Y}] = \int_{-\infty}^{\infty} g(x) f_{\mathrm{X}}(x) \mathrm{d}x \tag{12}$$

For a random variable X with a PDF of $f_{\mathrm{X}}(x)$, we can generalize the definition of average values by introducing the nth *moment* and *central moment*, as follows:

The nth *moment* of X with PDF $f_{\mathrm{X}}(x)$ is given by:

$$E[\mathrm{X}^{\mathrm{n}}] = \int_{-\infty}^{\infty} x^n f_{\mathrm{X}}(x) \mathrm{d}x \tag{13}$$

Accordingly the *central moment* is defined as follows:

The nth *moment* of X with PDF $f_{\mathrm{X}}(x)$ is given by:

$$E[(\mathrm{X} - E[X])^n] = \int_{-\infty}^{\infty} (x - E[X])^n f_{\mathrm{X}}(x) \mathrm{d}x \tag{14}$$

The second order moment, often denoted as σ^2, is the variance and given by:

$$\sigma^2 = E[(\mathrm{X} - E[X])^2] = \int_{-\infty}^{\infty} (x - E[X])^2 f_{\mathrm{X}}(x) \mathrm{d}x = E[\mathrm{X}^2] - E[\mathrm{X}]^2 \tag{15}$$

or, the second moment minus the square of the average. The *root means square* (RMS) value, denoted by σ is given by:

$$\sigma = \sqrt{E[(\mathrm{X} - E[X])^2]} = \sqrt{E[\mathrm{X}^2] - E[\mathrm{X}]^2} \tag{16}$$

3 First Ehrerferst Theorem

Consider a QM system described by a wavefunction $\Psi(\vec{r},t)$, defined on a volume V with surface S. We also know that:

$$\int |\Psi(\vec{r},t)|^2 \mathrm{d}\vec{r} = 1$$

which implies that $\lim_{|\vec{r}|\to\infty} \Psi(\vec{r},t) = 0$, the first Ehrerferst Theorem states that:

$$\boxed{\frac{\mathrm{d}}{\mathrm{d}t} < x > = \frac{1}{m} < p_x >}$$

Consider first the expression:

$$\frac{\mathrm{d}}{\mathrm{d}t} < x > = \frac{\mathrm{d}}{\mathrm{d}\,t} \int \Psi^*(\vec{r},t) \mathrm{x} \Psi(\vec{r},t) \mathrm{d}\vec{r}$$

Using the the Liebnitz Integral Rule, and remebersing that x is an operator and it is time-indepenedet we can write:

$$\frac{\mathrm{d}}{\mathrm{d}t} < x > = \int_V \left[\frac{\mathrm{d}}{\mathrm{d}\,t} \Psi^*(\vec{r},t) \mathrm{x} \Psi(\vec{r},t) \; + \; \Psi^*(\vec{r},t) \mathrm{x} \frac{\mathrm{d}}{\mathrm{d}\,t} \Psi(\vec{r},t) \right] \mathrm{d}\vec{r}$$

Using Eq. 3 and Eq. 4 we have can write:

$$\frac{\mathrm{d}}{\mathrm{d}t} < x > = \int_V \left[\frac{1}{-\imath\hbar} \mathrm{H} \Psi^*(\vec{r},t) \mathrm{x} \Psi(\vec{r},t) \; + \; \Psi^*(\vec{r},t) \mathrm{x} \frac{1}{\imath\hbar} \mathrm{H} \Psi(\vec{r},t) \right] \mathrm{d}\vec{r}$$

expanding the Hamiltonian operator we have:

$$\begin{aligned} \frac{\mathrm{d}}{\mathrm{d}t} < x > = \frac{1}{\imath\hbar} \Bigg[& \int_V \Psi^*(\vec{r},t) \mathrm{x} \left(-\frac{\hbar^2}{2\,m} \nabla^2 \Psi(\vec{r},t) \; + \; V(\vec{r},t) \Psi(\vec{r},t) \right) \mathrm{d}\vec{r} \; + \\ & - \int_V \left(-\frac{\hbar^2}{2\,m} \nabla^2 \Psi^*(\vec{r},t) \; + \; V(\vec{r},t) \Psi^*(\vec{r},t) \right) \mathrm{x} \Psi(\vec{r},t) \mathrm{d}\vec{r} \Bigg] \end{aligned}$$

or

$$\begin{aligned} \frac{\mathrm{d}}{\mathrm{d}t} < x > = \frac{1}{\imath\hbar} \Bigg[& \int_V \left[\Psi^*(\vec{r},t) \mathrm{x} V(\vec{r},t) \Psi(\vec{r},t) \mathrm{d}\vec{r} \; - \; V(\vec{r},t) \Psi^*(\vec{r},t) \mathrm{x} \Psi(\vec{r},t) \right] \mathrm{d}\vec{r} \\ & + \int_V \Psi^*(\vec{r},t) \mathrm{x} \left(-\frac{\hbar^2}{2\,m} \nabla^2 \Psi(\vec{r},t) \right) \; - \; \left(-\frac{\hbar^2}{2\,m} \nabla^2 \Psi^*(\vec{r},t) \right) \mathrm{x} \Psi(\vec{r},t) \mathrm{d}\vec{r} \Bigg] \end{aligned} \tag{17}$$

the first integral vanishes, and we have:

$$\frac{\mathrm{d}}{\mathrm{d}t} < x > = \frac{1}{\imath\hbar}\frac{\hbar^2}{2\,m}\left[\int_V -\Psi^*(\vec{r},t)\mathrm{x}\nabla^2\Psi(\vec{r},t) \;+\; \nabla^2\Psi^*(\vec{r},t)\mathrm{x}\Psi(\vec{r},t)\mathrm{d}\vec{r}\right]$$

we then use Eq. 5 with $u = \mathrm{x}\Psi$ and $v = \Psi^*$, then:

$$\int_V \nabla^2\Psi^*(\vec{r},t)\mathrm{x}\Psi(\vec{r},t)\mathrm{d}\vec{r} = \int_V \mathrm{x}\Psi(\vec{r},t)\nabla^2\Psi^*(\vec{r},t)\mathrm{d}\vec{r} =$$
$$\int_S \mathrm{x}\Psi(\vec{r},t)\overrightarrow{\nabla\Psi^*(\vec{r},t)}\cdot\mathrm{d}\vec{S} - \int_V \overrightarrow{\nabla\Psi^*(\vec{r},t)}\cdot\overrightarrow{\nabla(\mathrm{x}\Psi(\vec{r},t))}\mathrm{d}\vec{r}$$

Since we know that $\lim_{|\vec{r}|\to\infty}\Psi(\vec{r},t) = 0$, then the surface integral (first term on the RHS) is zero, and we have:

$$\frac{\mathrm{d}}{\mathrm{d}t} < x > = \frac{1}{\imath\hbar}\frac{\hbar^2}{2\,m}\left[\int_V -\Psi^*(\vec{r},t)\mathrm{x}\nabla^2\Psi(\vec{r},t) \;-\; \overrightarrow{\nabla\Psi^*(\vec{r},t)}\cdot\overrightarrow{\nabla(\mathrm{x}\Psi(\vec{r},t))}\mathrm{d}\vec{r}\right]$$

$$\frac{\mathrm{d}}{\mathrm{d}t} < x > = -\frac{1}{\imath\hbar}\frac{\hbar^2}{2\,m}\left[\int_V \Psi^*(\vec{r},t)\mathrm{x}\nabla^2\Psi(\vec{r},t) \;+\; \overrightarrow{\nabla\Psi^*(\vec{r},t)}\cdot\overrightarrow{\nabla(\mathrm{x}\Psi(\vec{r},t))}\mathrm{d}\vec{r}\right]$$

using again Eq. 6 on the second term in the intrgal on the RHS, we have:

$$\int_V \overrightarrow{\nabla\Psi^*(\vec{r},t)}\cdot\overrightarrow{\nabla(\mathrm{x}\Psi(\vec{r},t))}\mathrm{d}\vec{r} = \int_S \Psi^*(\vec{r},t)\overrightarrow{\nabla(\mathrm{x}\Psi(\vec{r},t))}\cdot\mathrm{d}\vec{S} - \int_V \Psi^*(\vec{r},t)\nabla^2(\mathrm{x}\Psi(\vec{r},t))\mathrm{d}\vec{r}$$

Once again, since we know that $\lim_{|\vec{r}|\to\infty}\Psi(\vec{r},t) = 0$, then the surface integral (first term on the RHS) is zero, and we have:

$$\int_V \overrightarrow{\nabla\Psi^*(\vec{r},t)}\cdot\overrightarrow{\nabla(\mathrm{x}\Psi(\vec{r},t))}\mathrm{d}\vec{r} = -\int_V \Psi^*(\vec{r},t)\nabla^2(\mathrm{x}\Psi(\vec{r},t))\mathrm{d}\vec{r}$$

and

$$\frac{\mathrm{d}}{\mathrm{d}t} < x > = -\frac{1}{\imath\hbar}\frac{\hbar^2}{2\,m}\left[\int_V \Psi^*(\vec{r},t)\mathrm{x}\nabla^2\Psi(\vec{r},t) \;-\; \int_V \Psi^*(\vec{r},t)\nabla^2(\mathrm{x}\Psi(\vec{r},t))\mathrm{d}\vec{r}\right]$$

or

$$\frac{\mathrm{d}}{\mathrm{d}t} < x > = -\frac{1}{\imath\hbar}\frac{\hbar^2}{2\,m}\int_V \Psi^*(\vec{r},t)\left[\mathrm{x}\nabla^2\Psi(\vec{r},t) \;-\; \nabla^2(\mathrm{x}\Psi(\vec{r},t))\right]\mathrm{d}\vec{r}$$

now note that:

$$\frac{\partial^2}{\partial x^2}\left[\mathrm{x}\Psi(\vec{r},t)\right] \,=\, \frac{\partial}{\partial x}\left[\frac{\partial}{\partial x}(\mathrm{x}\Psi(\vec{r},t))\right] \,=\, \frac{\partial}{\partial x}\left[\Psi(\vec{r},t) \,+\, \mathrm{x}\frac{\partial}{\partial x}\Psi(\vec{r},t)\right] \,=$$

$$\frac{\partial}{\partial x}\Psi(\vec{r},t) \,+\, \mathrm{x}\frac{\partial^2}{\partial x^2}\Psi(\vec{r},t) \,+\, \frac{\partial}{\partial x}\Psi(\vec{r},t) \,=\, 2\frac{\partial}{\partial x}\Psi(\vec{r},t) \,+\, \mathrm{x}\frac{\partial^2}{\partial x^2}\Psi(\vec{r},t)$$

note also that:

$$\frac{\partial^2}{\partial y^2}\left[\mathrm{x}\Psi(\vec{r},t)\right] \,=\, \mathrm{x}\frac{\partial^2}{\partial y^2}\Psi(\vec{r},t)$$

$$\frac{\partial^2}{\partial z^2}\left[\mathrm{x}\Psi(\vec{r},t)\right] \,=\, \mathrm{x}\frac{\partial^2}{\partial z^2}\Psi(\vec{r},t)$$

it follows that:

$$\nabla^2(\mathrm{x}\Psi(\vec{r},t)) \,=\, 2\frac{\partial}{\partial x}\Psi(\vec{r},t) \,+\, \mathrm{x}\nabla^2\Psi(\vec{r},t)$$

consequently:

$$\frac{\mathrm{d}}{\mathrm{d}t} < x >= -\frac{1}{\imath\hbar}\frac{\hbar^2}{2\,m}\int_V \Psi^*(\vec{r},t)\left[\mathrm{x}\nabla^2\Psi(\vec{r},t) \,-\, 2\frac{\partial}{\partial x}\Psi(\vec{r},t) \,-\, \mathrm{x}\nabla^2(\Psi(\vec{r},t))\right]\mathrm{d}\vec{r}$$

it follows that:

$$\frac{\mathrm{d}}{\mathrm{d}t} < x >= -\frac{1}{\imath\hbar}\frac{\hbar^2}{2\,m}\int_V -\Psi^*(\vec{r},t)2\frac{\partial}{\partial x}\Psi(\vec{r},t)\mathrm{d}\vec{r}$$

rearranging:

$$\frac{\mathrm{d}}{\mathrm{d}t} < x >= \frac{-\imath\hbar}{m}\int_V \Psi^*(\vec{r},t)\frac{\partial}{\partial x}\Psi(\vec{r},t)\mathrm{d}\vec{r}$$

or:

$$\frac{\mathrm{d}}{\mathrm{d}t} < x >= \frac{1}{m}\int_V \Psi^*(\vec{r},t)(-\imath\hbar)\frac{\partial}{\partial x}\Psi(\vec{r},t)\mathrm{d}\vec{r}$$

$$\frac{\mathrm{d}}{\mathrm{d}t} < x >= \frac{1}{m}\int_V \Psi^*(\vec{r},t)p_x\Psi(\vec{r},t)\mathrm{d}\vec{r} \,=\, \frac{1}{m} < p_x >$$

That is first Ehrenferst theorem.

4 Second Ehrerferst Theorem

Consdier a QM system described by a wavefunction $\Psi(\vec{r},t)$, defined on a volume V with surface S. We also know that:

$$\int |\Psi(\vec{r},t)|^2 \mathrm{d}\vec{r} = 1$$

which implies that $\lim_{|\vec{r}|\to\infty} \Psi(\vec{r},t) = 0$, the second Ehrerferst Theorem states that:

$$\boxed{\frac{\mathrm{d}}{\mathrm{d}t} < p_x >= -\left\langle \frac{\partial V(\vec{r},t)}{\partial x} \right\rangle}$$

Consider first the expression:

$$\frac{\mathrm{d}}{\mathrm{d}t} < p_x >= \frac{\mathrm{d}}{\mathrm{d}\,t}\int_V \Psi^*(\vec{r},t)\left(-\imath\hbar\frac{\partial}{\partial x}\right)\Psi(\vec{r},t)\mathrm{d}\vec{r}$$

$$\frac{\mathrm{d}}{\mathrm{d}t} < p_x >= -\imath\hbar\frac{\mathrm{d}}{\mathrm{d}\,t}\int_V \Psi^*(\vec{r},t)\frac{\partial}{\partial x}\Psi(\vec{r},t)\mathrm{d}\vec{r}$$

Using the the Liebnitz Integral Rule, and the chain integration rule, we can write:

$$\frac{\mathrm{d}}{\mathrm{d}t} < p_x >= -\imath\hbar\left[\int_V \frac{\partial}{\partial\,t}\Psi^*(\vec{r},t)\frac{\partial}{\partial x}\Psi(\vec{r},t)\mathrm{d}\vec{r} + \int_V \Psi^*(\vec{r},t)\frac{\partial}{\partial\,t}\frac{\partial}{\partial x}\Psi(\vec{r},t)\mathrm{d}\vec{r}\right]$$

exchanging the derivatives in the second integral on the RHS:

$$\frac{\mathrm{d}}{\mathrm{d}t} < p_x >= -\imath\hbar\left[\int_V \Psi^*(\vec{r},t)\frac{\partial}{\partial\,x}\frac{\partial}{\partial\,t}\Psi(\vec{r},t)\mathrm{d}\vec{r} + \int_V \frac{\partial}{\partial\,t}\Psi^*(\vec{r},t)\frac{\partial}{\partial\,x}\Psi(\vec{r},t)\mathrm{d}\vec{r}\right]$$

Using Eq. 3 and Eq. 4 and expanding the Hamiltonian operator we have:

$$\frac{\mathrm{d}}{\mathrm{d}t} < p_x >= \left[\int_V -\Psi^*(\vec{r},t)\frac{\partial}{\partial\,x}\left(-\frac{\hbar^2}{2\,m}\nabla^2\Psi(\vec{r},t) + V(\vec{r},t)\Psi(\vec{r},t)\right)\mathrm{d}\vec{r} + \int_V\left(-\frac{\hbar^2}{2\,m}\nabla^2\Psi^*(\vec{r},t) + V(\vec{r},t)\Psi^*(\vec{r},t)\right)\frac{\partial}{\partial\,x}\Psi(\vec{r},t)\mathrm{d}\vec{r}\right]$$

rearranging the terms associated to the potential $V(\vec{r},t)$, we have:

$$\frac{\mathrm{d}}{\mathrm{d}t} < p_x >= \frac{\hbar^2}{2\,m}\int_V\left[\Psi^*(\vec{r},t)\frac{\partial}{\partial\,x}\left(\nabla^2\Psi(\vec{r},t)\right) - \nabla^2\Psi^*(\vec{r},t)\frac{\partial}{\partial\,x}\Psi(\vec{r},t)\right]\mathrm{d}\vec{r} + \int_V\left[V(\vec{r},t)\Psi^*(\vec{r},t)\frac{\partial}{\partial\,x}\Psi(\vec{r},t) - \Psi^*(\vec{r},t)\frac{\partial}{\partial\,x}\left(V(\vec{r},t)\Psi(\vec{r},t)\right)\right]\mathrm{d}\vec{r}$$

We note that:

$$\frac{\partial}{\partial x}\nabla^2\Psi \;=\; \frac{\partial}{\partial x}\left[\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}+\frac{\partial^2}{\partial z^2}\right]\Psi \;=\; \left[\frac{\partial^3}{\partial x^3}+\frac{\partial}{\partial x}\frac{\partial^2}{\partial y^2}+\frac{\partial}{\partial x}\frac{\partial^2}{\partial z^2}\right]\Psi$$

$$\frac{\partial}{\partial x}\nabla^2\Psi \;=\; \left[\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}+\frac{\partial^2}{\partial z^2}\right]\frac{\partial}{\partial x}\Psi \;=\; \nabla^2\left[\frac{\partial}{\partial x}\Psi\right]$$

consequently

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}t} < p_x > = \frac{\hbar^2}{2\,m}\int_V \left[\Psi^*(\vec{r},t)\nabla^2\left(\frac{\partial}{\partial x}\Psi(\vec{r},t)\right) \;-\; \nabla^2\Psi^*(\vec{r},t)\frac{\partial}{\partial x}\Psi(\vec{r},t)\right]\mathrm{d}\vec{r}\,+ \\ \int_V \left[V(\vec{r},t)\Psi^*(\vec{r},t)\frac{\partial}{\partial x}\Psi(\vec{r},t) \;-\; \Psi^*(\vec{r},t)\frac{\partial}{\partial x}\left(V(\vec{r},t)\Psi(\vec{r},t)\right)\right]\mathrm{d}\vec{r}\end{aligned} \tag{18}$$

using Eq. 7 with $u = \Psi^*$ and $v = \frac{\partial}{\partial x}\Psi$, we have modify the first integral on the RHS of the equation above:

$$\begin{aligned}&\int_V \left[\Psi^*(\vec{r},t)\nabla^2\left(\frac{\partial}{\partial x}\Psi(\vec{r},t)\right) \;-\; \nabla^2\Psi^*(\vec{r},t)\frac{\partial}{\partial x}\Psi(\vec{r},t)\right]\mathrm{d}\vec{r} \\ &= \\ &\int_S \left[\Psi^*(\vec{r},t)\overrightarrow{\nabla\left(\frac{\partial}{\partial x}\Psi(\vec{r},t)\right)} \;-\; \frac{\partial}{\partial x}\Psi(\vec{r},t)\overrightarrow{\nabla\Psi^*(\vec{r},t)}\right]\mathrm{d}\vec{r} \\ &= 0\end{aligned}$$

Since we know that $\lim_{|\vec{r}|\to\infty}\Psi(\vec{r},t) = 0$ and $\lim_{|\vec{r}|\to\infty}\frac{\partial}{\partial x}\Psi(\vec{r},t) = 0$, then the surface integral is zero. Consequently Eq. 18 becomes:

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}t} < p_x > &= \int_V \left[V(\vec{r},t)\Psi^*(\vec{r},t)\frac{\partial}{\partial x}\Psi(\vec{r},t) \;-\; \Psi^*(\vec{r},t)\frac{\partial}{\partial x}\left(V(\vec{r},t)\Psi(\vec{r},t)\right)\right]\mathrm{d}\vec{r} \\ &= -\int_V \Psi^*(\vec{r},t)\left[\frac{\partial}{\partial x}\left(V(\vec{r},t)\Psi(\vec{r},t)\right) \;-\; V(\vec{r},t)\frac{\partial}{\partial x}\Psi(\vec{r},t)\right]\mathrm{d}\vec{r}\end{aligned} \tag{19}$$

Since

$$\frac{\partial}{\partial x}\left(V(\vec{r},t)\Psi(\vec{r},t)\right) \;=\; V(\vec{r},t)\frac{\partial}{\partial x}\Psi(\vec{r},t) \;+\; \Psi(\vec{r},t)\frac{\partial}{\partial x}V(\vec{r},t)$$

then

$$\frac{\mathrm{d}}{\mathrm{d}t} < p_x > = -\int_V \Psi^*(\vec{r},t)\frac{\partial}{\partial x}V(\vec{r},t)\Psi(\vec{r},t)\mathrm{d}\vec{r} \tag{20}$$

that is the final result:

$$\frac{\mathrm{d}}{\mathrm{d}t} < p_x > = -\left\langle \frac{\partial V(\vec{r},t)}{\partial x} \right\rangle \tag{21}$$

5 Generalization of the Ehrenferst Theorems

Consider an observable $\mathcal{A}$ represented by an operator A, we can evaluated in Dirac's notation as:

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}t}\langle \mathrm{A}\rangle &= \frac{\mathrm{d}}{\mathrm{d}t}\langle \Psi|\mathrm{A}|\Psi\rangle \\ &= \left\langle \frac{\mathrm{d}}{\mathrm{d}t}\Psi \middle| \mathrm{A} \middle| \Psi \right\rangle + \left\langle \Psi \middle| \frac{\mathrm{d}}{\mathrm{d}t}\mathrm{A} \middle| \Psi \right\rangle + \left\langle \Psi \middle| \mathrm{A} \middle| \frac{\mathrm{d}}{\mathrm{d}t}\Psi \right\rangle \\ &= \int_V \frac{\mathrm{d}}{\mathrm{d}t}\Psi^*\mathrm{A}\Psi\mathrm{d}\vec{r} + \int_V \Psi^*\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{A}\Psi\mathrm{d}\vec{r} + \int_V \Psi^*\mathrm{A}\frac{\mathrm{d}}{\mathrm{d}t}\Psi\mathrm{d}\vec{r}\end{aligned} \tag{22}$$

The expression above cointains the time derivative of the operator A. The value of this derivative depends on the *representation* used.

• – **Schrödinger Representation** In the Schrödinger Representation the time dependence of the system is embeddedin the wavefunctions $\Psi(\vec{r},t)$ and the operators A are time-independent.

• – **Heisemberg Representation** In the Heisemberg Representation the time dependence of the system is embedded in the operators $\mathrm{A}(t)$ and wavefunctions $\Psi(\vec{r})$ are time-independent.

• – **Interaction Representation** In the Interaction Representation the time dependence of the system is embedded both in the operators $\mathrm{A}(t)$ and the wavefunctions $\Psi(\vec{r},t)$.

Using Eq. 3 and Eq. 4 we can write Eq.25 as:

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}t}\langle \mathrm{A}\rangle &= -\frac{1}{\imath\hbar}\langle \mathrm{H}\Psi|\mathrm{A}|\Psi\rangle + \left\langle \Psi \middle| \frac{\mathrm{d}}{\mathrm{d}t}\mathrm{A} \middle| \Psi \right\rangle + \frac{1}{\imath\hbar}\langle \Psi|\mathrm{A}|\mathrm{H}\Psi\rangle \\ &= \left\langle \Psi \middle| \frac{\mathrm{d}}{\mathrm{d}t}\mathrm{A} \middle| \Psi \right\rangle + \frac{1}{\imath\hbar}\left[\langle \Psi|\mathrm{A}|\mathrm{H}\Psi\rangle - \langle \mathrm{H}\Psi|\mathrm{A}|\Psi\rangle\right]\end{aligned} \tag{23}$$

since the Hamiltonia operator H is hermitian:

$$\langle \mathrm{H}\Psi|\mathrm{A}|\Psi\rangle = \langle \Psi|\mathrm{H}\mathrm{A}\Psi\rangle \tag{24}$$

we can write:

$$\frac{\mathrm{d}}{\mathrm{d}t}\left\langle \mathrm{A}\right\rangle \,=\, \left\langle \Psi \middle| \frac{\mathrm{d}}{\mathrm{d}t}\mathrm{A} \middle| \Psi \right\rangle \,+\, \frac{1}{\imath\hbar}\left[\langle\Psi|\mathrm{AH}|\Psi\rangle - \langle\Psi|\mathrm{HA}|\Psi\rangle\right] \tag{25}$$

or:

$$\frac{\mathrm{d}}{\mathrm{d}t}\left\langle \mathrm{A}\right\rangle \,=\, \left\langle \frac{\mathrm{d}}{\mathrm{d}t}\mathrm{A} \right\rangle \,+\, \frac{1}{\imath\hbar}\left\langle[\mathrm{A},\mathrm{H}]\right\rangle \tag{26}$$