Reflection operator

Is the operator that when it operates on such function it rotates around the origin

$\hat{R}\psi(x) = \psi(-x)$

Since $\psi(-x) = a\psi(x)$ as defined with parity relation

Then $\hat{R}\psi(x) = a\,\psi(x)$

And $\hat{R}\hat{R}\psi(x) = \hat{R}a\,\psi(x) = a^2\psi(x)$

$a^2 = 1 \quad and \quad a = \pm 1$

The eigenvalue of parity is ± 1

And the eigenfunction of the reflection operator will be

Even Function $\boldsymbol{f(-x) = f(x)}$

Examples: $f(x) = x^2$ then $f(-x) = (-x)^2 = x^2 = f(x)$

$y(x) = \cos x$

$y(-x) = \cos(-x)$

$y(-x) = \cos x = y(x)$

Odd Function $\boldsymbol{f(-x) = -f(x)}$

Examples: $f(x) = x^3$ then $f(-x) = (-x)^3 = -x^3 = -f(x)$

$y(x) = \sin x$

$y(-x) = \sin(-x)$

$y(-x) = -\sin x = -y(x)$

Exercise: If $\hat{H}(x) = \hat{H}(-x)$, Prove that the reflection operator commutes with the Hamiltonian operator, i.e. $[\hat{H}, \hat{R}] = 0$.

Solution: $\hat{R}\big(\hat{H}(x)\psi(x)\big) = \hat{H}(-x)\psi(-x) = \hat{H}(x)\psi(-x)$ because $\hat{H}(x) = \hat{H}(-x)$

Then $\hat{R}\big(\hat{H}(x)\psi(x)\big) = \hat{H}(x)\hat{R}\psi(x)$

And $\hat{R}\hat{H}\psi(x) - \hat{H}\hat{R}\psi(x) = 0$ or $(\hat{R}\hat{H} - \hat{H}\hat{R})\psi(x) = 0$

$\therefore\ [\hat{R}, \hat{H}] = [\hat{H}, \hat{R}] = 0$

Exercise: Prove that the Reflection operator $\hat{R}$ is Hermitian operator.

$\hat{R}$ to be a Hermitian operator it must satisfy the following relation,

$$\int \psi^*(\hat{R}\psi)\, dr = \int \psi(\hat{R}\psi)^* dr$$

By using x-direction then, the right-hand-side will be:

$$\int_{-\infty}^{\infty} \psi^*(x)\big(\hat{R}\psi(x)\big)\, dx = \int_{-\infty}^{\infty} \psi^*(x)(\psi(-x))\, dx$$

By changing the integration factor from x to $-x$ and $dx = -dx$

So, the integral will be,

$$\int_{-\infty}^{\infty} \psi^*(x)(\psi(-x))\, dx = -\int_{\infty}^{-\infty} \psi^*(-x)\big(\psi(x)\big)\, dx = -\int_{\infty}^{-\infty} \big(\psi(-x)\big)^* \psi(x) dx$$

$$= -\int_{\infty}^{-\infty} \big(\hat{R}\psi(x)\big)^* \psi(x) dx$$

Since $-\int_{\infty}^{-\infty} = \int_{-\infty}^{\infty}$

$$\int_{-\infty}^{\infty} \psi^*(x)\big(\hat{R}\psi(x)\big)\, dx = \int_{-\infty}^{\infty} \big(\hat{R}\psi(x)\big)^* \psi(x) dx$$

$\therefore$ $\hat{R}$ is Hermitian operator.

Exercise: Find the probability current density to the wave function $\psi(x,t) = 3k\, e^{ikx}$ where k is a constant.

probability current density is,

$$\boldsymbol{j}(\boldsymbol{r},t) = \frac{-i\hbar}{2m}(\Psi^*\boldsymbol{\nabla}\Psi - \Psi\boldsymbol{\nabla}\Psi^*)$$

$$\nabla\psi = \frac{d}{dx}\big(3k\, e^{ikx}\big) = 3ik^2 e^{ikx} \qquad \nabla\psi^* = \frac{d}{dx}\big(3k\, e^{-ikx}\big) = -3ik^2 e^{-ikx}$$

$$j = \frac{\hbar}{2mi}\Big(3k\, e^{-ikx}\big(3ik^2 e^{ikx}\big) - 3k\, e^{ikx}\big(-3ik^2 e^{-ikx}\big)\Big)$$

$$j = \frac{\hbar}{2mi}(9ik^3 + 9ik^3) = \frac{9\hbar k^3}{m}$$

Exercise: Show that, the linear momentum p_x of a free particle is a constant of motion.

Solution: To be a constant of motion, it must satisfy the relation, $\frac{d}{dt}\langle p_x \rangle = 0$

$$\frac{d}{dt}\langle p_x \rangle = -i\hbar \frac{d}{dt}\int \psi^* \frac{\partial \psi}{\partial x}\, dr = -\, i\hbar \left[\int \psi^* \frac{\partial}{\partial x}\frac{\partial \psi}{\partial t}\, dr + \int \frac{\partial \psi^*}{\partial t}\frac{\partial \psi}{\partial x}\, dr\right]$$

By using the Schrödinger equation and its complex conjugate, where $V(x) = 0$ for a free particle,

$$i\hbar \frac{\partial \psi}{\partial t} = H\psi \Rightarrow \quad \frac{\partial \psi}{\partial t} = \frac{1}{i\hbar} H\psi \qquad\qquad -i\hbar \frac{\partial \psi^*}{\partial t} = (H\psi)^* \Rightarrow \quad \frac{\partial \psi^*}{\partial t} = \frac{-1}{i\hbar} H\psi^*$$

To replace $\frac{\partial \Psi}{\partial t}$ and $\frac{\partial \Psi^*}{\partial t}$, respectively, we get,

$$\frac{d}{dt}\langle p_x \rangle = -\left[\int \psi^* \frac{\partial}{\partial x}(H\psi)dx - \int (H\psi)^* \frac{\partial \psi}{\partial x}\, dx\right] = -\int \psi^* \frac{\partial}{\partial x}(E\psi)dx + \int (E\psi)^* \frac{\partial \psi}{\partial x}\, dx$$

$$\frac{d}{dt}\langle p_x \rangle = -E\left[\int \psi^* \frac{\partial \psi}{\partial x} dx - \int \psi^* \frac{\partial \psi}{\partial x}\, dx\right] = 0$$

Then $\langle p_x \rangle = constant\ of\ motion$

Exercise: Determine whether any of the following functions are physically acceptable in quantum mechanics.

1) e^{-x} in the interval $[0, \infty]$ *physically acceptable*

Because: Single Valued, Continuous, Finite,

2) e^{-x} in the interval $[-\infty, \infty]$ *not acceptable*

Because: It can't be normalized in the interval $[-\infty, \infty]$

3) $sin^{-1}(x)$ in the interval $[-1,1]$ *not acceptable*

Because: It is a multi-values function in this interval $\left(sin^{-1}(1) = \frac{\pi}{2}, \frac{\pi}{2} + 2\pi, \ldots\right)$

4) $\frac{\sin(x)}{x}$ in the interval $[0, \infty]$ *acceptable*

Because: $\lim_{x\to 0} \frac{\sin(x)}{x} = 1$,finite.

5) $e^{-|x|}$ in the interval $[-\infty, \infty]$ *not acceptable*

Because: The first derivative is not continuous.

Exercise: The wave function of particle rotates in a circular path is given by, $\psi_n(x) = \sqrt{\frac{1}{2\pi}} e^{in\theta}$ where $n = 0, \pm1, \pm2, \ldots$ and $0 \le \theta \le 2\pi$. Prove that, these functions are an orthonormal group.

Solution: The orthonormal condition is, $\int_0^{2\pi} \psi_m^* (\theta)\psi_n(\theta)d\theta = \delta_{mn}$

$\delta_{mn} = 0$ for $m \neq n$, $\delta_{mn} = 1$ for $m = n$

$$\int_0^{2\pi} \psi_m^* (\theta)\psi_n(\theta)d\theta = \int_0^{2\pi} \sqrt{\frac{1}{2\pi}} e^{-im\theta} \sqrt{\frac{1}{2\pi}} e^{in\theta}\, d\theta = \frac{1}{2\pi}\int_0^{2\pi} e^{-im\theta}\, e^{in\theta}\, d\theta$$

$$= \frac{1}{2\pi}\int_0^{2\pi} e^{-i(m-n)\theta}\, d\theta = \frac{1}{2\pi}\int_0^{2\pi} \cos(m-n)\,\theta\, d\theta + \frac{i}{2\pi}\int_0^{2\pi} \sin(m-n)\,\theta\, d\theta$$

For $m \neq n$ then

$$\delta_{mn} = \frac{1}{2\pi}\Big(\sin(m-n)\,\theta]_0^{2\pi} - \frac{i}{2\pi}(-\cos(m-n)\,\theta]_0^{2\pi} = 0$$ **Orthogonal condition**

For $m = n$ then

$$\frac{i}{2\pi}\int_0^{2\pi} \sin(0)\,\theta\, d\theta = 0$$

$$\delta_{mn} = \frac{1}{2\pi}\int_0^{2\pi} \cos(0)\,\theta\, d\theta = \frac{1}{2\pi}\int_0^{2\pi} d\theta = \frac{2\pi}{2\pi} = 1$$ **Normalization condition**

Home Works:

1- If the functions ψ_1 and ψ_2 are solutions of the Schrödinger equation for a particle, then show that $a_1\psi_1 + a_2\psi_2$, where a_1 and a_2 are arbitrary constants, is also a solution of the same equation.

2- Show that the expectation value of a physical quantity can be real only if the corresponding operator is Hermitian.

3- Show that the normalization integral is independent of time.