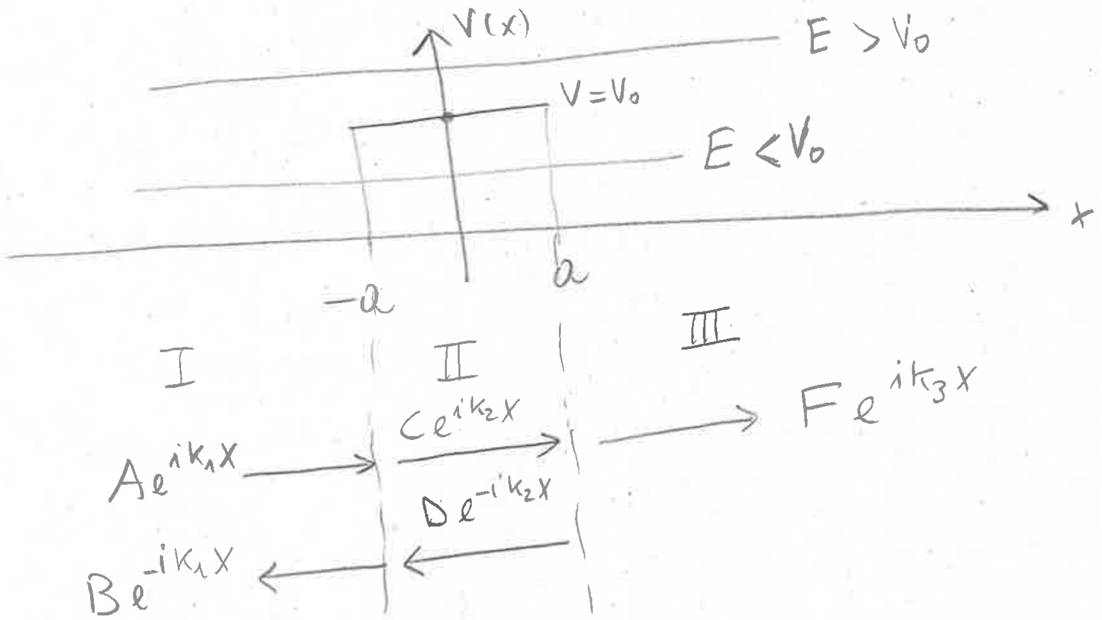
Exercises 08.06.2017

– Problem 1 –

Solve the rectangular barrier problem, with

$$V(x) = \begin{cases} 0, & x < -a \\ V_0 > 0, & -a \le x \le a \\ 0, & a < x \end{cases}$$



- Consider $E < V_0$ first.

As usual, the SE is:

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

We write

$$\psi(x,t) = \varphi(x)\exp\left(-\frac{iEt}{\hbar}\right)$$

Then

$$i\hbar \frac{\partial \psi}{\partial t} = i\hbar \varphi(x)\left(-\frac{iE}{\hbar}\right) e^{-iEt/\hbar}$$

$$= E\varphi(x) e^{-iEt/\hbar}$$

and the SE becomes

$$E\varphi(x)\cancel{e^{-iEt/\hbar}} = \left(-\frac{\hbar^2}{2m}\nabla^2\varphi + V\varphi\right)\cancel{e^{-iEt/\hbar}}$$

$$\Leftrightarrow \quad -\frac{2m}{\hbar^2}E\varphi(x) = \frac{d^2\varphi}{dx^2} - \frac{2mV}{\hbar^2}\varphi$$

$$\Leftrightarrow \quad \boxed{\frac{d^2\varphi}{dx^2} + \frac{2m}{\hbar^2}(E-V)\varphi = 0}$$

Since either $V=0$ or $V=V_0<E$, Then $E-V>0$

and I define:

region I: $\quad k_1^2 = \frac{2m}{\hbar^2}E$

region II: $\quad k_2^2 = \frac{2m}{\hbar^2}(E-V_0)$

region III: $\quad k_3^2 = k_1^2 = \frac{2m}{\hbar^2}E$

We know that the equation

$$\frac{d^2y}{dx^2} + K^2 y(x) = 0$$

has solution:

$$y(x) = \alpha e^{ikx} + \beta e^{-ikx}$$

Therefore in our case we have:

Region I: $\varphi_I(x) = A e^{ik_1x} + B e^{-ik_1x}$

Region II: $\varphi_{II}(x) = C e^{ik_2x} + D e^{-ik_2x}$

Region III: $\varphi_{III}(x) = F e^{ik_1X}$ (we <u>ASSUME</u> as initial condition that there are not waves impinging from right in region III)

The first derivatives are then:

$$\varphi_I'(x) = ik_1(A e^{ik_1x} - B e^{-ik_1x})$$

$$\varphi_{II}'(x) = ik_2(C e^{ik_2x} - D e^{-ik_2x})$$

$$\varphi_{III}'(x) = ik_1 F e^{ik_1x}$$

Now, as usual, we impose the continuity of the wave function and of its first derivative.

At $x=-a$ we require:

$$\varphi_I(-a) = \varphi_{II}(-a) \qquad \Longleftrightarrow$$
$$\varphi'_I(-a) = \varphi'_{II}(-a)$$

$$\Longleftrightarrow \begin{cases} A e^{-ik_1 a} + B e^{ik_1 a} = C e^{-ik_2 a} + D e^{ik_2 a} \\ \cancel{i} k_1 \left(A e^{-ik_1 a} - B e^{+ik_1 a} \right) = \cancel{i} k_2 \left(C e^{-ik_2 a} - D e^{ik_2 a} \right) \end{cases}$$

At $x=a$ we instead obtain:

$$\begin{cases} C e^{ik_2 a} + D e^{-ik_2 a} = F e^{ik_1 a} \\ \cancel{i} k_2 \left(C e^{ik_2 a} - D e^{-ik_2 a} \right) = \cancel{i} k_1 F e^{ik_1 a} \end{cases}$$

If we divide both sides of these equations by A, we have four unknows $\frac{B}{A}, \frac{C}{A}, \frac{D}{A}, \frac{F}{A}$ to be determined.

The "mechanical" way to solve this problem is to put it in the matrix form (with $k_1 a \equiv \alpha$ and $k_2 a \equiv \beta$)

$$\begin{bmatrix} e^{i\alpha} & -e^{-i\beta} & -e^{i\beta} & 0 \\ -\alpha e^{i\alpha} & -\beta e^{-i\beta} & \beta e^{i\beta} & 0 \\ 0 & e^{i\beta} & e^{-i\beta} & -e^{i\alpha} \\ 0 & \beta e^{i\beta} & -\beta e^{-i\beta} & -\alpha e^{i\alpha} \end{bmatrix} \begin{bmatrix} B/A \\ C/A \\ D/A \\ F/A \end{bmatrix} = \begin{bmatrix} -e^{-i\alpha} \\ -\alpha e^{-i\alpha} \\ 0 \\ 0 \end{bmatrix} \Longleftrightarrow M\underline{u} = \underline{v} \Rightarrow$$
$$\Rightarrow \underline{u} = M^{-1}\underline{v}$$

The solutions are:

$$\frac{B}{A} = \frac{2i\sin(2k_2 a)(k_1^2 - k_2^2)}{\underbrace{e^{4ik_2 a}(k_1-k_2)^2 + (k_1+k_2)^2}_{\equiv d}}$$

$$\frac{C}{A} = -\frac{2e^{-i(k_1-k_2)a} k_1(k_1+k_2)}{d}$$

$$\frac{D}{A} = \frac{2e^{i(k_1-k_2)a} k_1(k_1-k_2)e^{-2ik_2 a}}{d}$$

$$\frac{F}{A} = -\frac{4e^{-2ia(k_1-k_2)} k_1 k_2}{d}$$

The transmission and reflection coefficient T and R are defined as:

$$T = \left|\frac{F}{A}\right|^2 ; \quad R = \left|\frac{B}{A}\right|^2$$

With $T+R=1$. Let us prove it:

Note that $d = 2ie^{i2ak_2}\left[(k_1^2+k_2^2)\sin(2ak_2) + 2i\cos(2ak_2)k_1k_2\right]$

Therefore $|d|^2 = 4\left[(k_1^2+k_2^2)^2\sin^2(2ak_2) + 4\cos^2(2ak_2)k_1^2k_2^2\right]$

and $T+R = \dfrac{|B|^2+|F|^2}{|A|^2}$

$$= \frac{4\sin^2(2k_2a)(k_1^2-k_2^2)^2 + 16k_1^2k_2^2}{|d|^2}$$

but $\frac{|d|^2}{4} = (k_1^2+k_2^2)^2\sin^2(2ak_2) + 4[1-\sin^2(2ak_2)]k_1^2k_2^2$

$$= \sin^2(2ak_2)(k_1^4+k_2^4+2k_1^2k_2^2-4k_1^2k_2^2) + 4k_1^2k_2^2$$

$$= (k_1^2-k_2^2)^2\sin^2(2ak_2) + 4k_1^2k_2^2 \Rightarrow$$

$$\Rightarrow T+R=1 \quad \text{and} \quad \frac{1}{T} = \left|\frac{A}{F}\right|^2 = 1 + \left(\frac{k_1^2-k_2^2}{2k_1k_2}\right)^2 \sin^2(2k_2a)$$

- Case #2: $E < V$

Everything is as before, with the modification

$$ik_2 \to k \quad \text{where} \quad k^2 = \frac{2m}{\hbar^2}(V_0 - E) > 0$$

Remembering that

$$\sin(iz) = i\sinh z$$

and noticing that <u>all</u> the previous algebra does not change, we find:

$$\frac{1}{T} = 1 + \left(\frac{k_1^2+k^2}{2k_1k}\right)^2 \sinh^2(2ka)$$: $T \neq 0$ TUNNELLING!

The quantum particle can cross the barrier!

In the case $E > V$, notice that

$$\frac{1}{T} = 1 \quad \text{when} \quad \sin(2K_2 a) = 0$$

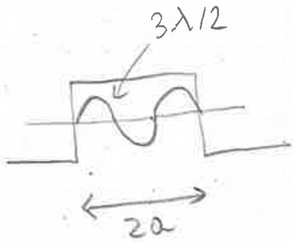
That is: $$2aK_2 = n\pi \qquad (n = 1, 2, \ldots)$$

with $$K_2 = \frac{\sqrt{2m(E-V_0)}}{\hbar}$$

If we introduce the new parameter λ defined as:

$$K_2 = \frac{2\pi}{\lambda} \qquad (\lambda = \text{wavelength})$$

then we have $$2a = n\left(\frac{\lambda}{2}\right)$$



This means that the resonant transmission is achieved when $2a$ is an integral number of half-wavelengths.

From $2aK_2 = n\pi$ and $K_2^2 = \frac{2m(E-V_0)}{\hbar^2}$ we find that at resonance:

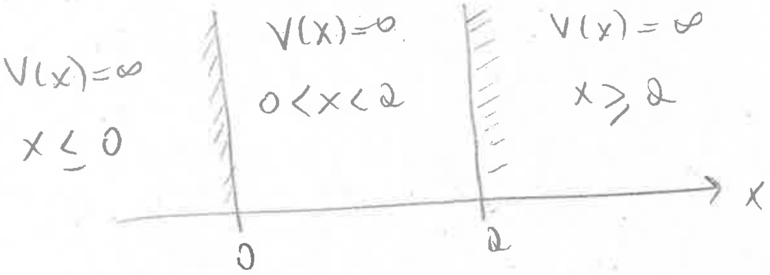
$$E - V_0 = n^2\left(\frac{\pi^2\hbar^2}{8a^2 m}\right) = n^2 E_1$$

E_1 = ground-state energy of a 1-D box of width $2a$.

- Problem 2 -

E8)

For the particle in a box:



we have find:

$$\hat{H} = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2}$$

$$\hat{H} u_n = E_n u_n \qquad \begin{cases} E_n = n^2 \dfrac{\hbar^2 \pi^2}{2ma^2} \\ u_n(x) = \sqrt{\dfrac{2}{a}} \sin\left(\dfrac{n\pi x}{a}\right) \end{cases}$$

let $\psi(x) = Ax(a-x)$. with $A>0$.

$$\|\psi(x)\|^2 = A^2 \int_0^a x^2(a-x)^2 dx = \frac{a^5}{30} A^2$$

Impose $\|\psi(x)\|^2 = 1 \Rightarrow \frac{a^5}{30} A^2 = 1 \Leftrightarrow A^2 = \frac{30}{a^5} = \frac{30\,a}{a^6} \Rightarrow$

$$\Rightarrow A = \sqrt{30}\,\frac{a^{1/2}}{a^3} = \frac{\sqrt{30}}{a^{5/2}}$$

So $\boxed{\psi(x) = \frac{\sqrt{30}}{a^{5/2}} x(a-x)}$

Write $\psi(x) = \sum_{n=1}^{\infty} b_n u_n(x)$

where $b_n = \int_0^a u_n^*(x)\psi(x) = \sqrt{\frac{2}{a}}\frac{\sqrt{30}}{a^{5/2}} \int_0^a x(a-x)\sin\left(\frac{n\pi x}{a}\right)dx$

$$= \frac{4\sqrt{15}}{\pi^3 n^3}(1-\cos(n\pi)) = \frac{4\sqrt{15}}{\pi^3 n^3}\underbrace{(1-(-1)^n)}_{=\begin{cases}0, & n \text{ even} \\ 2, & n \text{ odd}\end{cases}}$$

E9)

Calculate $\langle \hat{H} \rangle$ in two ways

1) $\langle \hat{H} \rangle = \sum_{n=1}^{\infty} |b_n|^2 E_n$

$$= \frac{16 \cdot 15}{\pi^{\cancel{6}4}} \frac{\hbar^2 \cancel{\pi^2}}{2ma^2} \sum_{n=1}^{\infty} \frac{[1-(-1)^n]^2}{n^{\cancel{6}4}} \cancel{n^2} = \frac{5\hbar^2}{ma^2}$$

$$(1-\cos(n\pi))^2 = 1 + \cos^2(n\pi) - 2\cos n\pi$$
$$= 2(1-\cos n\pi)$$

$$1-(-1)^n = \begin{cases} 0, & n \text{ even} \\ 2, & n \text{ odd} \end{cases} \Rightarrow$$

$$\Rightarrow \sum_{n=1}^{\infty} \frac{[1-(-1)^n]^2}{n^4} = 4 \underbrace{\sum_{n=1}^{\infty} \frac{1}{(2n-1)^4}}_{= \frac{\pi^4}{96}}$$

Gradshteyn and Ryzhik 0.234-5 p8

$$\frac{16 \cdot 15 \cdot 4}{96} = 10$$

2) $\langle \hat{H} \rangle = \int_0^a \psi^*(x) (\hat{H}\psi)(x)\, dx$

$$\frac{d^2}{dx^2}[x(a-x)] = -2$$

$$= \frac{30}{a^5} \int_0^a x(a-x) \left[\left(-\frac{\hbar^2}{2m} \frac{d^2}{dx^2} \right) x(a-x) \right] dx$$

$$= \frac{30}{a^5} \frac{\hbar^2}{\cancel{2}m} \cancel{2} \underbrace{\int_0^a x(a-x)\, dx}_{= \frac{a^3}{6}} = \frac{\cancel{6} \cdot 5}{a^{\cancel{5}2}} \frac{\hbar^2}{m} \frac{\cancel{a^3}}{\cancel{6}} = \frac{5\hbar^2}{ma^2}$$

✓

Now, calculate $\langle \hat{H}^2 \rangle$ in the two manners.

1) $\langle \hat{H}^2 \rangle = \sum_{n=1}^{\infty} |b_n|^2 E_n^2$

$$= \sum_{n=1}^{\infty} \left\{ \frac{\cancel{240}\,60}{\pi^{\cancel{6}}{}_2 n^{\cancel{6}}{}_2} [1-(-1)^n]^2 \frac{\cancel{n^4}\hbar^4 \cancel{\pi^4}}{\cancel{4} m^2 a^4} \right\}$$

$$= \frac{60\hbar^4}{\pi^2 m^2 a^4} \underbrace{\sum_{n=1}^{\infty} \frac{[1-(-1)^n]^2}{n^2}}_{= 4 \underbrace{\sum_{n=1}^{\infty} \frac{1}{(2n-1)^2}}_{= \frac{\pi^2}{8}} = \frac{\pi^2}{2}}$$

$$= \frac{30\hbar^4}{m^2 a^4}$$

2) $$\langle \hat{H}^2 \rangle = \int_0^a \psi^*(x) \underbrace{(\hat{H}^2 \psi)(x)}_{=0} dx = 0!$$

Note that $\hat{H}\psi = \frac{\sqrt{30}\,\hbar^2}{a^{5/2} m} \Rightarrow \|\hat{H}\psi\|^2 = \frac{30\hbar^4}{a^5 m^2} \int_0^a dx$

$$= \frac{30\hbar^2}{m^2 a^4}$$

What is the origin of this problem?

$$b_n = \langle u_n | \psi \rangle$$

$$\langle \hat{H}^2 \rangle = \sum_{n=1}^{\infty} |b_n|^2 E_n^2$$

$$= \sum_n \langle \psi | u_n \rangle \langle u_n | \psi \rangle E_n^2$$

$$= \sum_n \langle \psi | \underbrace{\hat{H} | u_n \rangle}_{= E_n | u_n \rangle} \overbrace{\langle u_n | \hat{H}}^{= E_n | u_n \rangle} | \psi \rangle$$

$$= \langle \psi | \hat{H} \underbrace{\left(\sum_n | u_n \rangle \langle u_n | \right)}_{= \hat{I}} \hat{H} | \psi \rangle$$

$$= \begin{cases} \| \hat{H} | \psi \rangle \|^2 = \dfrac{30 \hbar^2}{m^2 a^4} \\ \\ \langle \psi | \hat{H}^2 | \psi \rangle = 0 \end{cases} \quad !$$

If with $\hat{D}$ we denote the differential operator

$$\hat{D} \equiv \frac{d}{dx}$$

Then $\hat{H} = -\dfrac{\hbar^2}{2m} \hat{D}^2$

and the <u>DOMAIN</u> of $\hat{H}$ is given by the functions that vanishes at $x=0$ and $x=a$:

$$\mathcal{D}(\hat{H}) = \{ \phi : \hat{H}\phi \in L^2(0,a) , \ \phi(0) = \phi(a) = 0 \}$$

In this domain $\hat{H}$ is self-adjoint

First, we recall that 2 operators $\hat{A}$ and $\hat{B}$ with domains $\mathcal{D}(\hat{A})$ and $\mathcal{D}(\hat{B})$, respectively, are equal if:

$$\hat{A}\varphi = \hat{B}\varphi \quad \text{for all } \varphi \in \mathcal{D}(\hat{A}) = \mathcal{D}(\hat{B})$$

In this case we write $\hat{A} = \hat{B}$. So, two operators are equal if both the operation:

$$\hat{A}\varphi = \psi \;;\; \hat{B}\varphi = \psi$$

and the domains: $\mathcal{D}(\hat{A}) = \mathcal{D}(\hat{B})$, are equal.

-Definition 1-

The operator $\hat{A}$ is HERMITIAN if

$$(\varphi, \hat{A}\psi) = (\hat{A}\varphi, \psi) \quad \text{for all } \varphi, \psi \in \mathcal{D}(\hat{A})$$

in our case $\hat{A} = \hat{H}$.

$$\Leftrightarrow \quad (\varphi, \hat{A}\psi) - (\hat{A}\varphi, \psi) = 0$$

$$\Leftrightarrow \quad \int_0^a \left[\underbrace{\varphi^*(x) \frac{d^2\psi}{dx^2}} - \left(\frac{d^2\varphi}{dx^2}\right)^* \psi(x) \right] dx$$

$$= \int_0^a \varphi^* d\left(\frac{d\psi}{dx}\right) = \varphi^*(x)\psi'(x)\Big|_0^a - \underbrace{\int_0^a \frac{d\psi}{dx}\frac{d\varphi^*}{dx}dx}$$

$$= \int_0^a \frac{d\varphi^*}{dx} d(\psi) = \varphi'^*(x)\psi(x)\Big|_0^a - \int_0^a \psi \frac{d^2\varphi^*}{dx^2} dx$$

Therefore:

$$(\varphi,\hat{H}\psi)-(\hat{H}\varphi,\psi)=\overset{=0}{\varphi^*(a)}\psi'(a)-\overset{=0}{\varphi^*(0)}\psi'(0)+$$

$$-\varphi'^*(a)\overset{=0}{\psi(a)}+\varphi'^*(0)\overset{=0}{\psi(0)}$$

$$\underbrace{+\int_0^a\psi(x)\frac{d^2\varphi^*}{dx^2}dx-\int_0^a\left(\frac{d^2\varphi}{dx^2}\right)^*\psi(x)dx}_{=0}$$

Therefore $\hat{H}$ is hermitian for all the functions φ,ψ that vanishes at end points.

— <u>Definition 2</u> —

Given the operator $\hat{A}$ defined on the domain $\mathcal{D}(\hat{A})$, the <u>ADJOINT</u> operator $\hat{A}^+$ is defined via the identity:

$$(\varphi,\hat{A}\psi)=(\hat{A}^+\varphi,\psi)\quad\text{for all }\psi\in\mathcal{D}(\hat{A})$$
$$\text{on }\varphi\in\mathcal{D}(\hat{A}^+)$$

The operator $\hat{A}$ is <u>SELF-ADJOINT</u> if it is Hermitian and $\mathcal{D}(\hat{A})=\mathcal{D}(\hat{A}^+)$.

So, for our function

$$\psi(x)=\frac{\sqrt{30}}{a^{5/2}}x(a-x)$$

we have

$$\tilde{\varphi}(x)\equiv\hat{H}\psi(x)=-\frac{\hbar^2}{2m}(\hat{D}^2\psi)(x)=\frac{\sqrt{30}\,\hbar^2}{a^{5/2}m}=\text{const.}$$

Therefore

$$\tilde{\varphi}(0) = \tilde{\varphi}(a) = \frac{\sqrt{30}\,\hbar^2}{a^{5/2} m} \neq 0$$

and $\tilde{\varphi}(x) \notin \mathcal{D}(\hat{H})$

This means that

$$(\hat{H}\psi, \hat{H}\psi) = (\hat{H}\psi, \tilde{\varphi}) \neq (\psi, \hat{H}\tilde{\varphi}) = (\psi, \hat{H}^2\psi)$$

because $\tilde{\varphi} \notin \mathcal{D}(\hat{H})$

But why

$$(\psi, \hat{H}^2\psi) = 0$$

is wrong? What about our rule for the average value of the generic observable f with associated operator $\hat{f}$:

$$\langle \hat{f} \rangle_\psi \equiv \int \psi^* (\hat{f}\psi)\, dq$$

Actually, this formula was given without derivation. If I prepare a system in a state represented by $\psi(q)$ and I measure an observable f such that:

$$\hat{f}|u_n\rangle = f_n|u_n\rangle$$

with $\langle u_n|u_m\rangle = \delta_{nm}$ and $\sum_n u_n(q) u_m^*(q') = \delta(q-q')$

Then the probability P_n to get the result $f = f_n$ is given by:

$$P_n = |\langle u_n|\psi\rangle|^2$$
$$= \left|\int u_n^*(q)\,\psi(q)\,dq\right|^2$$

Therefore, the expectation value of the "random variable" f is, according to probability theory,

$$\langle f\rangle = \sum_n f_n P_n$$

This is the correct definition of $\langle f\rangle$.

Now we are going to show that:

$$\langle f\rangle = \sum_n f_n P_n = \langle\hat{f}\rangle_\psi = \int \psi^*(\hat{f}\psi)\,dq$$

if and only if the operator $\hat{f}$ is self-adjoint.

So
$$\langle f\rangle = \sum_n f_n P_n$$
$$= \sum_n f_n |\langle u_n|\psi\rangle|^2$$
$$= \sum_n \big(f_n \langle\psi|u_n\rangle\big)\langle u_n|\psi\rangle$$
$$= \sum_n \langle\psi|u_n\rangle\big(f_n\langle u_n|\psi\rangle\big)$$

If $\hat{f}$ is self-adjoint and $\psi \in \mathcal{D}(\hat{f}) = \mathcal{D}(\hat{f}^\dagger)$, then

$f_n\langle\psi|u_n\rangle = (\psi, \hat{f}u_n)$ and $f_n\langle u_n|\psi\rangle = (\hat{f}u_n, \psi)$

This means that I can write either

$$\langle f \rangle = \sum_n f_n \langle \psi | u_n \rangle \langle u_n | \psi \rangle$$

$$= \sum_n \langle \psi | \hat{f} | u_n \rangle \langle u_n | \psi \rangle$$

$$= \sum_n \langle \psi | \hat{f} | \psi \rangle = \langle \hat{f} \rangle_\psi$$

or

$$\langle f \rangle = \sum_n \langle \psi | u_n \rangle \langle u_n | \hat{f} | \psi \rangle$$

$$= \sum_n \langle \psi | \hat{f} | \psi \rangle = \langle \hat{f} \rangle_\psi$$

– Another way to see how to calculate $\langle \hat{f} \rangle_\psi$ is to use the spectral decomposition of $\hat{f}$:

From $\hat{f}|u_n\rangle = f_n |u_n\rangle$ it follows that:

$$\hat{f} = \hat{I} \cdot \hat{f} \cdot \hat{I} = \left(\sum_n |u_n\rangle\langle u_n| \right) \hat{f} \left(\sum_m |u_m\rangle\langle u_m| \right)$$

$$= \sum_{n,m} |u_n\rangle\langle u_m| \underbrace{\langle u_n | \hat{f} | u_m \rangle}$$

$$= f_n \langle u_n | u_m \rangle = f_n \delta_{nm}$$

$$= \sum_n f_n |u_n\rangle\langle u_n|$$

Therefore:

$$\langle \hat{f} \rangle_\psi = \langle \psi | \hat{f} | \psi \rangle = \sum_n f_n |\langle u_n | \psi \rangle|^2$$ which gives the correct result.