INFINITE SQUARE WELL - AVERAGE ENERGY

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Reference: Griffiths, David J. (2005), Introduction to Quantum Mechanics, 2nd Edition; Pearson Education - Problem 2.9.

The average or expectation value of the energy of a particle in an infinite square well can be worked out either by using the series solution in the form

$$\langle H\rangle=\sum_{n}|c_{n}|^{2}E_{n} \tag{1}$$

or directly using an integral, using $H=p^{2}/2m$ and $p=(\hbar/i)(d/dx)$:

$$\langle H\rangle=-\frac{\hbar^{2}}{2m}\int_{0}^{a}\Psi^{*}(x,t)\frac{d^{2}}{dx^{2}}\Psi(x,t)dx \tag{2}$$

Since $\Psi(x,t)$ in the general case is a sum over stationary states, as in

$$\Psi(x,t)=\sum_{n}c_{n}\psi_{n}(x)e^{-iE_{n}t/\hbar} \tag{3}$$

and the $\psi_{n}(x)$ functions are orthogonal, all the terms of the form

$$-\frac{\hbar^{2}}{2m}\int_{0}^{a}c_{n}^{*}\psi_{n}^{*}(x)e^{iE_{n}t/\hbar}c_{m}\psi_{m}(x)e^{-iE_{m}t/\hbar}dx \tag{4}$$

where $m\neq n$ in the integral evaluate to zero, and the remaining terms where $n=m$ are all independent of time since the complex exponentials cancel out, so $\langle H\rangle$ is independent of time. Thus if we know the wave function at any given time, we can use it to work out $\langle H\rangle$ at all times.

For example, if we have a parabolic wave function at $t=0$

$$\Psi(x,0)=Ax(a-x) \tag{5}$$

for $0\leq x\leq a$, we can work out $\langle H\rangle$ directly from it. Applying the normalization condition we can find A.

$$|A|^2 \int_0^a x^2(a-x)^2 dx = 1 \tag{6}$$

$$A = \sqrt{\frac{30}{a^5}} \tag{7}$$

We get for $\langle H \rangle$:

$$\langle H \rangle = \frac{30}{a^5} \int_0^a x(a-x) \left(-\frac{\hbar^2}{2m} \frac{d^2}{dx^2} x(a-x) \right) dx \tag{8}$$

Working out the second derivative and then the integral (use Maple or do by hand) we get $\langle H \rangle = 5\hbar^2 / ma^2$.