FUNDAMENTAL PRINCIPLES OF QUANTUM MECHANICS
A NUMERICAL DEMONSTRATION

MAX PLANCK INSTITUTE FOR SOLID STATE RESEARCH
MPI-FKF OPEN DAY

*E*lectronic Structure Theory Department

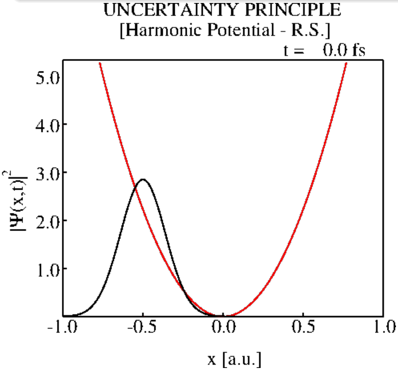
Prof. Alavi

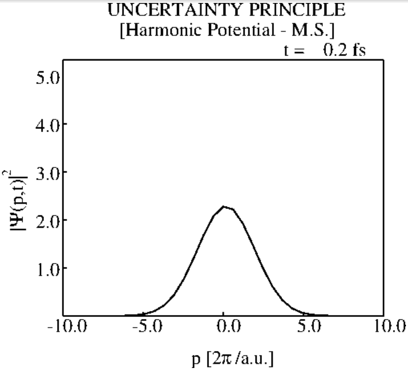
20 April 2024

Heisenberg's Uncertainty Principle

The laws of **Quantum Mechanics** do not follow our intuition!

We cannot measure the position (x) and the momentum (p) of a quantum particle at the same time with arbitrary precision.





J. J. Tanner, J. Chem. Education 67, 917 (1990)

Our Working Equation

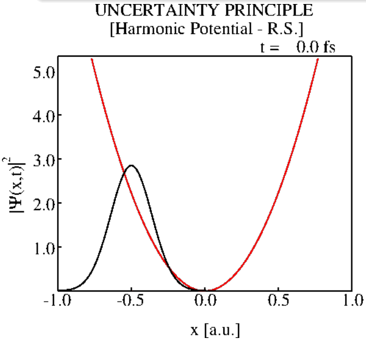
The **Schrödinger Equation**:

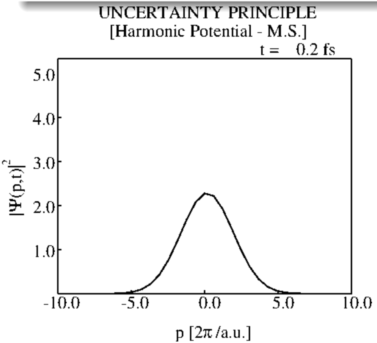
$$
\begin{aligned}
\mathrm{i}\frac{\partial \Psi(x,t)}{\partial t} &= \hat{H}(x,p)\Psi(x,t) \\
&= \left[\hat{T}(p) + \hat{V}(x)\right]\Psi(x,t)
\end{aligned}
$$

Heisenberg's Principle

$$\Delta x \Delta p \geq \frac{\hbar}{2}$$

$$V(x) = \frac{1}{2} m\omega^2 x^2$$





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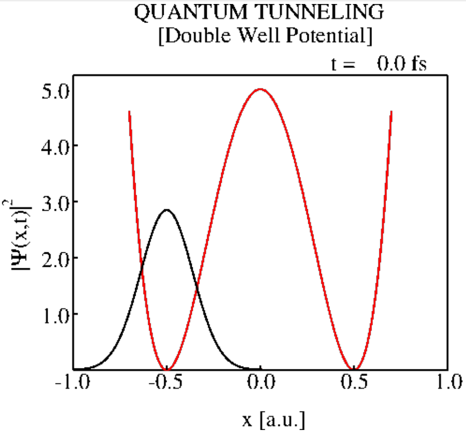
A Strange Phenomenon

There is a probability to find the particle on the other side of the barrier.

Quantum particles can pass through walls!



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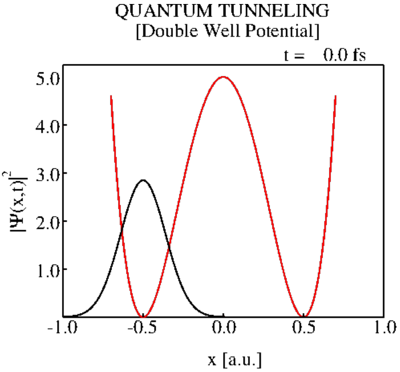
$$V(x) = V_o\,[16x^4 - 8x^2 + 1]$$

$$E_o < V_o$$



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