



The Schrödinger Cook Book



Plan

1. Learn to cook – the Schrödinger way!
2. Taste it (Understand Solution!)
3. Free Particle
4. Particle-in-Box



The Schrödinger Recipe

Question: I know the state of the system at time $t = 0$ is $\psi^0(x)$. What is the expectation value of A as a function of time? The Recipe:

1. Put down the Hamiltonian operator H
2. Find energy eigenstates, solve $H\psi = E\psi$; gives $\{\psi_n, E_n\}$
3. Expand ψ^0 in the basis given by $\{\psi_n\}$; get $\psi^0(x) = \sum_n a_n \psi_n(x)$
4. The state at time t : $\Psi(x, t) = \sum_n a_n \psi_n(x) e^{-\frac{iE_n t}{\hbar}}$
5. Expectation value $\langle A \rangle(t) = \int \Psi^*(x, t) A \Psi(x, t) dx$



Free Particle

Particle in a large box ($L \rightarrow \infty$)

1. Write down Hamiltonian Operator $H = \frac{P^2}{2m} = -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2}$

2. Solve $-\frac{\hbar^2}{2m} \frac{\partial^2 \psi}{\partial x^2} = E\psi$

(a) What are possible values of E ? ($E \geq 0$)

(b) Two possible eigenstates $\frac{1}{\sqrt{2\pi}}e^{ikx}$ and $\frac{1}{\sqrt{2\pi}}e^{-ikx}$

with $k = \frac{\sqrt{2mE}}{\hbar}$, $E(k) = \frac{\hbar^2 k^2}{2m}$

(c) Energy levels are degenerate! They are also continuous!



Free Particle

4. **Write** $\psi^0(x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \phi(k) e^{ikx} dk;$

$$\phi(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} e^{-ikx} \psi^0(x) dx$$

5. $\Psi(x, t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \phi(k) e^{ikx} e^{-\frac{iE(k)t}{\hbar}} dk$



Free Particle...the physics

- Suppose $\psi^0(x)$ is one of the eigenstates of H say k_0
- Then (in a box of length $2L$) $\Psi(x, t) = \frac{1}{\sqrt{2L}} e^{ik_0 x} e^{-i \frac{\hbar k_0^2}{2m} t}$
- What are $\langle H \rangle(t)$ and $\langle P \rangle(t)$?
- You see $\langle H \rangle(t) = \frac{\hbar^2 k_0^2}{2m}$ and $\langle P \rangle(t) = \hbar k_0$
- Interestingly $\langle P \rangle$ is independent of time! Momentum is conserved (just like in classical mechanics)!!
- When is a physical observable conserved? Answer: If an operator A commutes with the Hamiltonian, it will correspond to a conserved quantity



Particle-in-Box

Well, can we solve without “solving” ?

1. Write down Hamiltonian Operator

$$H = \frac{P^2}{2m} = -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + V(x)$$

● $V(x) = \infty$ if $x \leq 0, x \geq \ell$

● $V(x) = 0$ if $0 < x < \ell$

● Can consider only $0 < x < \ell$ with $\psi(0) = \psi(\ell) = 0$

2. Solve $-\frac{\hbar^2}{2m} \frac{\partial^2 \psi}{\partial x^2} = E\psi$ with $\psi(0) = \psi(\ell) = 0$ (Ah, same as the veena string!)

3. We see $E_n = n^2 E_0$, $n = 1, 2, 3\dots$ with $E_0 = \frac{\pi^2 \hbar^2}{2m\ell^2}$

4. The energy eigenstates are $\psi_n(x) = \sqrt{\frac{2}{\ell}} \sin\left(\frac{n\pi x}{\ell}\right)$

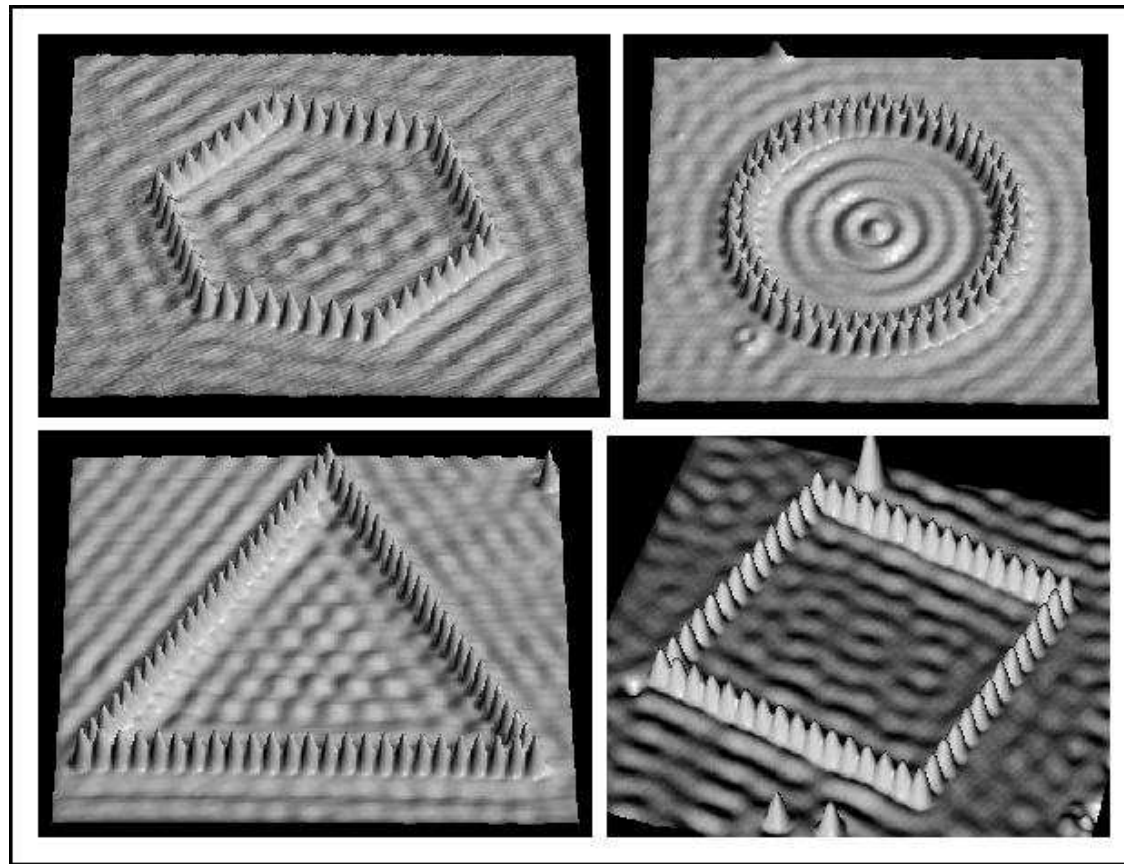


Tasting Particle-in-Box

- Examples : “Spectrum” of Butadiene molecule(??)
- What if ψ^0 is an eigenstate of H ?
- Suppose that we know the initial state $\psi^0(x) = \sum_n \alpha_n \psi_n(x)$, what is the meaning of α_n ?
- Understand this with two states ($|\alpha_n|^2$ is the probability that the measured energy will be E_n)
- Understand time evolution of the two-state superposition
- And, light? How? And, are there “boxes” around?

Boxes, really?

- Metals...lots of electron in a box!
- And real boxes with electrons..corrals (2D)



(IBM)



Summary

1. The Schrödinger recipe
2. Energy eigenstates...stationary states
3. Meaning of coefficients in an expansion of states
4. When is something conserved?
5. Next player...Paul Adrian Maurice Dirac