Wavefunction Evolution

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August 2019

1 Wavefunction Evolution

For this project I wanted to create an animation that showed how the probablity density evolved as a function of time given some initial conditions and constraints.
The set up is a particle of mass m kg confined to flat 2D space. The potential in which it is situated is an infinite potential well, dimensionality of a square of length L.

2 Theory

In the case for which I have made my animation the parameters where:

Parameter	Value
L/m	10^{-9}
m/kg	10^{-27}

From these parameters we can construct our theory and make prediction on what we expect to happen.
For non relativistic quantum mechanics, the wavefunction obeys the Schrodinger equation, that is in Dirac notation:

$$\hat{\mathcal{H}}|\Psi\rangle = \hat{E}|\Psi\rangle$$

In co-ordinate representation:

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

The potential of our system is $V = \big(0 \in 0 < x, y < L,\, otherwise\, \infty\ \big)$. We can represent our state vector as a linear combination of energy eigenstates;
$|\Psi\rangle = \sum_{n=1}^{\infty} c_n|E_n\rangle$ where $|E_n\rangle$ denotes the nth energy eigenstate.

When acting on these energy eigenstates the Hamiltonian becomes

$$-\frac{\hbar^2}{2m}\nabla^2\psi_n = E_N\psi_n$$

Which has simple complex exponent solutions. Imposing the boundary conditions we obtain

$$\psi_{nm}(x, y) \propto \sin(n\pi x/L)\sin(m\pi y/L)$$

Now for modelling the time evolution of the probability density. The initial state will be a Gaussian surface positioned at the centre of the square and its amplitude decreases $\propto r^2$ until it reaches the edge of the square in which its amplitude drops to zero. Because of the $x-y$ symmetry of the setup and the separability of the coordinates the motion can be modelled by solving for one dimension, say x, and then multiplying by the y component, which will have the same solution.
Once we have the C_n coefficients we can derive the time dependence through:

$$\hat{\mathcal{H}}|\Psi\rangle = i\hbar\frac{\partial}{\partial t}|\Psi\rangle$$

$$\hat{\mathcal{H}}C_n|E_n\rangle = i\hbar\frac{\partial}{\partial t}C_n|E_n\rangle$$

$$C_nE_n|E_n\rangle = i\hbar\dot{C_n}|E_n\rangle$$

Integrating for each independent $|E_n\rangle$

$$C_n = C_{n0}e^{-iE_nt/\hbar}$$

Thus the overall wavefunction in one dimension is

$$|\Psi_x\rangle = C_{n0}e^{-iE_nt/\hbar}|E_n\rangle$$

So as the x and y components take the same form

$$|\Psi\rangle = |\Psi_x\rangle|\Psi_y\rangle = \sum_n C_{n0}e^{-iE_nt/\hbar}\sum_m C_{m0}e^{-iE_mt/\hbar}|E_{mn}\rangle$$

Solving the one dimensional case, the initial wavefunction will take the form

$$\phi_0 = \Lambda e^{-(x-L/2)^2/(2\sigma^2)}$$

Where Λ is the normalization constant that we will get python code to calculate and σ which describes the standard deviation or the spread of the initial wavefunction. To represent the initial statevector in terms of the energy eigenstates:

$$|\Psi_0\rangle = C_{n0}|E_n\rangle$$

$$\langle E_m|\Phi_0\rangle = \delta_{nm}C_{n0} = C_{m0}$$

$$C_{m0} = \int_{-\infty}^{\infty}\langle E_m|\mathbf{x}\rangle\langle\mathbf{x}|\Phi_0\rangle dx$$

$$C_{m0} = \int_{-\infty}^{\infty}\psi_m^*\phi_0 dx$$

Putting these results together will give us the probability density, $|\psi|^2$. Actually determining this will be done on python due to the very large amount of cross terms that arise from the calculation.
The overall probability density takes the form

$$|\psi|^2 = \sum_{mnop} C_{mnop0} e^{-iE_m t/\hbar} e^{-iE_n t/\hbar} e^{iE_o t/\hbar} e^{iE_p t/\hbar} \psi_{nm} \psi^*_{op}$$

The animation shows the behaviour of the probability density as a function of time.

The total energy of ψ_{mn} is given by the sum of the individual spatial function as if they were separate systems, $E_{nm} = (n^2 + m^2)\frac{\hbar^2\pi^2}{2mL^2}$. This means the higher energy oscillation frequencies are integer multiples of the ground state frequency, thus the periodic behaviour of the time varying probability density will be determined by the ground state frequency which due to symmetry is $|2, 2\rangle$ ie $\omega_{22} = E_{22}/\hbar = \frac{4\hbar\pi^2}{mL^2}$. Thus we should see a time period of oscillation of $1.5 \times 10^{-12} s$ which is what we see in the animation.