CS 294-2 tions. Fall 2004 Hamiltonians, Schrodinger's Equation, Uncertainty Rela-10/26/04 Lecture 15

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1 1-D Random Walk

1.1 Classical

Each time step, go one step in a random direction.

If you call the distance travelled in time step i by x_i , then

$$x_i = \begin{cases} +1 & w.p. \ 1/2 \\ -1 & w.p. \ 1/2 \end{cases}$$

and the total distance travelled in *n* steps is $X = x_1 + ... + x_n$. Now, $E(X) = nE(x_i) = 0$ so it is expected that you end up where you started from. However, $var(X) = n(var(x_i)) = nE[(x_i - E(x_i))^2] = nE(x_i^2) = n$, and so in *n* time steps you have covered a distance of $O(\sqrt{n})$. Alternately, it takes $O(k^2)$ time to go a distance *k*.

1.2 Probabilistic

We have $X \in \mathbb{Z}$ representing the total distance travelled, and a coin $b \in \{0,1\}$. Every step of the walk we update our position depending on the coin, then flip the coin in preparation for the next step. That is, WALK : $X \leftarrow X + (-1)^b$; pick new *b* randomly; repeat.

The (binomial) probability distribution for X is maximum at X = 0 and trails off farther away.

1.3 Quantum

Similar to the probabilistic random walk, we have $X \in \mathbb{Z}$ representing the total distance travelled, but now our coin $|b\rangle \in \mathbb{C}^2$ is a quantum bit. The coin flip is implemented as some unitary operator U (e.g. the Hadamard transform H). That is,

 $\mathsf{WALK}: \left| X, b \right\rangle \leftarrow \left| X + (-1)^b, b \right\rangle; \left| b \right\rangle \leftarrow U \left| b \right\rangle; \mathsf{repeat.}$

The quantum walk takes O(k) time to go a distance k. There are naturally many different ways to reach 0 after k time steps, but each of those ways is likely to carry a different phase, so they interfere destructively. Correspondingly, there are fewer ways to get outside some distance away from the start, so there is more constructive interference. The probability distribution for X after k time steps is small at X = 0 with two peaks centered at $\pm ck$ for some constant c.

2 Schrodinger's Equation

This equation gives how a quantum state $|\psi\rangle$ evolves over time. In natural units where $\hbar = c = 1$, Schrödinger's equation is

$$i\frac{d\left|\psi\right\rangle}{dt}=H\left|\psi\right\rangle$$

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where H is the Hamiltonian operator. The Hamiltonian is a hermitian operator, and so corresponds to an observable, namely energy.

Because the Hamiltonian is hermitian, it has an orthonormal set of eigenstates $|v_i\rangle$ with eigenvalues (energies) λ_i . A state in one of these eigenstates evolves as follows:

$$|\psi(t=0)\rangle = |v_i\rangle \implies |\psi(t)\rangle = e^{-i\lambda_i t}|v_i\rangle.$$

Thus in the energy eigenstate basis, the unitary time evolution operator U(t): $|\psi(t)\rangle = U(t)|\psi(0)\rangle$ is given by

$$U(t) = e^{-iHt} = \begin{bmatrix} e^{-i\lambda_1 t} & 0 \\ & \ddots & \\ 0 & e^{-i\lambda_n t} \end{bmatrix}$$

3 1-D particle

In the case of a 1-D particle, the state $|\psi\rangle = \psi(x,t)$ is the amplitude of the particle at position x at time t. In this case, the Hamiltonian operator $H = \frac{\partial^2}{\partial x^2}$, so Schrödinger's equation reads

$$i\frac{\partial\psi}{\partial t} = \frac{\partial^2\psi}{\partial x^2}.$$

A state with velocity $\sim k$ is given by $\psi(x) = e^{ikx}$, so the amplitude with which an arbitrary state ϕ has velosity k is given by

$$\left\langle \psi \right| \phi \right\rangle = \left\langle e^{ikx} \right| \phi \right\rangle = \int_{-\infty}^{\infty} e^{ikx} \phi(x,t) dx$$

This is similar to the Fourier transform of the wavefunction, that is, we can describe another wavefunction in velocity space as the F.T. of the position wave function:

$$\hat{\phi}(k,t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} e^{ikx} \phi(x,t) dx.$$

4 Uncertainty Relations

As we saw, the position and velocity of a 1-D particle are Fourier transforms of one another. Thus, localizing one comes at the expense of a wider spread in the other. The minimum standard deviation spread comes when both are of Gaussian form, then $\Delta x \Delta v = \Omega(1)$.

Similarly, consider a finite abelian group G. Starting with a distribution $D = \sum_{g} \alpha_{g} |g\rangle$, it's Fourier transform becomes a distribution $\hat{D} = \sum_{g} \hat{\alpha}_{g} |g\rangle$. We have the following uncertainty relations about these distributions:

$$\sum_{g} |lpha_{g}| + \sum_{g} |\hat{lpha}_{g}| \ge \sqrt{|G|}$$
 $S(D) + S(\hat{D}) \ge \log |G|$

where S(D) is the entropy of the distribution D.

5 Dirac Equation

Classically, the energy *E* of a 1-D particle is given by $E = p^2/2m$, where *p* is its momentum and *m* is its mass. The quantum analog of this relationship can be obtained by the translating the observables *E* and *p* into their respective operators (again in natural units) $E \rightarrow \hat{H} = i\partial/\partial t$ and $p \rightarrow \hat{p} = -i\partial/\partial x$, yielding Schrodinger's equation

$$i\frac{\partial\psi}{\partial t} = \frac{1}{2m}\frac{\partial^2\psi}{\partial x^2}.$$

Relativistically, the energy of a particle is given by $E^2 = p^2 + m^2$, so the quantum analog should satisfy $\hat{H}^2 = \hat{p}^2 + m^2 \hat{I}$. Consider instead a tensor product of the particle state with an additional qubit state. Then, in matrix form we could have

$$\hat{H} = \begin{bmatrix} \hat{p} & m\hat{l} \\ \hline m\hat{l} & -\hat{p} \end{bmatrix} = \begin{bmatrix} \hat{p} & 0 \\ \hline 0 & -\hat{p} \end{bmatrix} + m\begin{bmatrix} \hat{0} & \hat{l} \\ \hline \hat{l} & \hat{0} \end{bmatrix}$$

such that

$$\hat{H}^{2} = \begin{bmatrix} \frac{\hat{p}^{2} + m^{2}\hat{l} & 0}{0 & \hat{p}^{2} + m^{2}\hat{l}} \end{bmatrix}.$$