PHY356: Quantum Mechanics

Jonah Chen

Fall 2022

1 Introduction

Schrodinger's Equation:

$$i\hbar\frac{\partial}{\partial t}\psi(x,t) = \left(\frac{p^2}{2m} + V(x,t)\right)\psi(x,t) \tag{1}$$

Conservation of Probability:

$$\frac{\partial(\psi^*\psi)}{\partial t} = \frac{\partial\psi^*}{\partial t}\psi + \psi^*\frac{\partial\psi}{\partial t} = -\mathrm{div}J \tag{2}$$

We can use the Schrodinger's equation and its complex conjugate to get the following:

$$\frac{\partial\psi^*}{\partial t}\psi = \tag{3}$$

$$\psi^*\frac{\partial\psi}{\partial t} = \tag{4}$$

Probability Current is then

$$J = -\frac{i\hbar}{2m}\left(\psi^*\nabla\psi - \psi\nabla\psi^*\right) \tag{5}$$

This requires the wave function ψ to be continuously differentiable (for non-singular potentials), unlike the electric field which can be discontinuous on surfaces.

Question: How does the wave mechanics recapture the notion of a classical particle?

Superposition Principle: If ψ_1 and ψ_2 are two solutions to the Schrodinger equation, then $\alpha\psi_1 + \beta\psi_2$ is also a solution for $\alpha, \beta \in \mathbb{C}$.

Simple Example:

$$\cos k_1 x + \cos k_2 x = 2\cos\left(\frac{k_1+k_2}{2}x\right)\cos\left(\frac{k_1-k_2}{2}x\right) \tag{6}$$

Let $k_1 = k_0 + \Delta k$ and $k_2 = k_0 - \Delta k$, assume $\Delta k \ll k_0$.

Fourier Decomposition: General solution of the free-particle schrodinger equation

$$\psi(\mathbf{r}, t) = (2\pi)^{-3/2} \int \mathrm{d}^3\mathbf{k}\, g(\mathbf{k}) \exp\left(i(\mathbf{k}\cdot\mathbf{r} - \omega t)\right) \psi_k \tag{7}$$

For simplicity, we will use $t = 0$ and 1 dimension, with a normal distribution of frequencies $g(k) = \exp\left\{-\frac{(k-k_0)^2}{2(\Delta k)^2}\right\}$. We can perform the fourier transform to get $\psi(x) = \exp\{i\Delta k^2 x^2\}$

Stationary States: These are eigenvectors of the hamiltonian, $H = -\frac{\hbar^2}{2m}\nabla^2 + V(x)$.

We will analyze the finite square well

$$V(x) = \begin{cases} -V_0 & \text{if } |x| < a/2 \\ 0 & \text{otherwise} \end{cases} \tag{8}$$

For bound states, plane waves will solve the schrodinger equation within the well $\phi_k(x) = A_1 e^{ikx} + A_2 e^{-ikx}$. Outside the well, exponentials will solve the schrodinger equation $\phi_k(x) = B_1 e^{qx} + B_2 e^{-qx}$.

Note how there is a nonzero probability to find the particle outside the well, which is classically disallowed. This is one case of tunneling.

Also note the symmetry of the potential, then the bound states must be either odd or even. Then, we only need to solve for one side of the well. We will focus on the even states first.

For even states, $\psi'(0) = 0$ so $ikA_1 - ikA_2 = 0 \implies A_1 = A_2 \equiv A$. Also note the boundary condition $\psi(a/2), \psi'(a/2)$ must be continuous.

$$A \cos\frac{ka}{2} = Be^{-qa/2} \tag{9}$$

$$Ak \sin\frac{ka}{2} = Bqe^{-qa/2} \tag{10}$$

We can divide the equations by each other and obtain

$$\cot\frac{ka}{2} = \frac{k}{q} \tag{11}$$

We know $k = \sqrt{2m(E + V_0)}/\hbar > 0$ and $q = \sqrt{-2mE}/\hbar > 0$. We define $k^2 + q^2 = 2mV_0/\hbar^2 \equiv k_0^2$. Then, $k/k_0 = |cos(ka/2)$.

We can non dimensionalize the equation by letting $x = ay$. Then, $a = \sqrt{2mV_0/\hbar^2}$. We can then solve for y:

$$\left(\frac{-\hbar^2}{2ma^2}\frac{d^2}{dy^2} - V_0\right)\psi = E\psi \tag{12}$$

Recapture the classical limit for step, smooth out the potential step.

2 Postulates of QM

- Take for example, a 3-dimensional vector $\mathbf{v} = (v_1, v_2, v_3)$. The components v_1, v_2, v_3 is dependent on your basis. Somebody else can represent the same vector with different v_1, v_2, v_3. In quantum mechanics, the wavefunction $\psi(x) : \mathbb{R} \to \mathbb{C}$ is just a representation of the more abstract state-vector $|\psi\rangle$ in the position basis.
- We will eventually show that the stationary states forms an orthonormal basis for this abstract vector space.
- Project operator $|\phi\rangle\langle\phi|$ is related to the act of observation.

2.1 Mathematical Tools

- We will declare that these state vectors belong to L^2 hilbert space, and inherit its inner product.
$$\langle\phi|\psi\rangle = \int \phi^* \psi \mathrm{d}\mu \tag{13}$$
and its norm
$$|\psi| = \sqrt{\langle\psi|\psi\rangle} \tag{14}$$
- Note that these state vectors are now independent of the choice of basis.
- Consider the momentum eigenstates $\frac{1}{\sqrt{2\pi}}e^{ikx}$, then a wave function $\psi(x)$ can be written as a linear combination of these states.
$$\psi(x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \mathrm{d}k\, g(k) e^{ikx} \tag{15}$$
By the fourier transform, we can find $g(k)$ by taking the inverse transform
$$g(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \mathrm{d}x\, \psi(x) e^{-ikx} \tag{16}$$
- The completeness relation states that given any function $f(x)$, it can be written as a superposition of the given basis. They can be written as
  - Discrete case:
$$\sum_{n=1}^{N} |\phi_n\rangle\langle\phi_n| = \mathbf{1} \tag{17}$$
  - Continuous case:
$$\int \mathrm{d}\mu\, |\phi\rangle\langle\phi| = \mathbf{1} \tag{18}$$

  where $\mathbf{1}$ is the identity operator.

- The fourier transform generalizes to n dimensions with

$$\psi(\mathbf{r}) = \frac{1}{(2\pi)^{n/2}} \int \mathrm{d}^n k \, g(\mathbf{k}) e^{i\mathbf{k}\cdot\mathbf{r}} \tag{19}$$

$$g(\mathbf{k}) = \frac{1}{(2\pi)^{n/2}} \int \mathrm{d}^n x \, \psi(\mathbf{r}) e^{-i\mathbf{k}\cdot\mathbf{r}} \tag{20}$$

- We will show later that the eigenvectors to a hermitian operator forms an orthonormal basis of the state space.

2.2 Dirac Notation

- For any $\psi(x)$ wavefunction, we can write it as $\psi(x) = \sum_n c_n \phi_n(x)$ where $\phi_n(x)$ is a set of basis. We can convey the same information with just the set of coefficients. This is like the coordinate representation of a vector.
- In this light, the fourier transform is a unitary change of basis. We can show it's unitary by the fact it preserves norms.

$$|g|^2 = \int_{-\infty}^{\infty} \mathrm{d}k \, g^*(k) g(k) = \int_{-\infty}^{\infty} \mathrm{d}k \int_{-\infty}^{\infty} \mathrm{d}x \int_{-\infty}^{\infty} \mathrm{d}x' \, \psi^*(x') e^{-ikx'} \psi(x) e^{ikx} \tag{21}$$

$$= \int_{-\infty}^{\infty} \mathrm{d}x \int_{-\infty}^{\infty} \mathrm{d}x' \, \psi^*(x') \psi(x) \delta(x - x') \tag{22}$$

$$= \int_{-\infty}^{\infty} \mathrm{d}x \, \psi^*(x) \psi(x) = |\psi|^2 \tag{23}$$

- We will define the **dual space** in the linear algebra sense, which is denoted as **bra** vectors $\langle x|$. Then, the inner product of $|x\rangle$ and $|f\rangle$ can be written as $\langle x|f\rangle$, which is the wavefunction (as that's the representation of f in the position basis).

$$\langle x|f\rangle = \int_{-\infty}^{\infty} \mathrm{d}x' \, f(x') \langle x|x'\rangle \tag{24}$$

$$= \int_{-\infty}^{\infty} \mathrm{d}x' \, f(x') \delta(x - x') \tag{25}$$

$$= f(x) \tag{26}$$