Physics 143a – Workshop 6

Solving Time-Independent Schrödinger Equation in One-Dimension

Week Summary

- **Particle in an infinite potential well:** For a particle in an infinite potential well, the potential energy is

$$V(x) = \begin{cases} 0 & \text{for } 0 < x < L \\ \infty & \text{otherwise} \end{cases}. \tag{1}$$

The energy eigenstates (in position space) and eigenvalues are, respectively,

$$\psi_n(x) \equiv \langle x|E_n\rangle = \sqrt{\frac{2}{L}} \sin\frac{n\pi}{L}x, \qquad E_n = \frac{\hbar^2\pi^2}{2mL^2}n^2, \tag{2}$$

where $n = 0, 1, 2, \ldots$.

- **Algorithm for Solving Schrödinger Equation (in 1d):** When we claim to have "solved" the Schrödinger equation for a system, we mean that we have computed the energy eigenstates (in position space) and energy eigenvalues for that system. The general procedure for solving the Schrödinger equation is as follows:

1. Write down the (possibly piecewise) potential $V(x)$ for the entire domain of x.
2. Divide your piecewise potential into distinct regions each defined by a non-piecewise function.
3. Determine the boundary conditions connecting the wavefunctions adjoining each potential region, and the asymptotic conditions ensuring finiteness at long distances.
   (a) For finite potentials, we require the wavefunction and its derivative to be continuous at the boundary.
4. For finite potential wells choose whether your particle energy E is greater than or less than V_{max}.
5. Find the general solution to the Schrödinger equation

$$\left(\frac{d^2}{dx^2} + \frac{2m}{\hbar^2}(E - V(x))\right)\varphi(x) = 0, \tag{3}$$

   in each region identified in step $\#2$ given the energy condition of step $\#4$.
6. Impose the boundary conditions of step $\#3$ to obtain a system of equations in the coefficients of the general solution.
7. Solve the system of equations to find $\varphi(x)$ in each region, and, for bound state problems, the allowed values of the energies as functions of system parameters. **Bound state** problems are those where $|\varphi(x)|^2 \to 0$ as $x \pm \infty$; Otherwise the problem is considered a **scattering** problem.

1 Problems

1. **Transition Amplitudes**
   Billy asks his fellow students Susan and Sally a question about probabilities: If a system defined by Hamiltonian $\hat{H}$ is initially in the state $|\phi\rangle$, what is the probability that the system transitions to the state $|\alpha\rangle$ in a time t?

   Susan answers:

   > The probability that $|\phi\rangle$ transitions to $|\alpha\rangle$ in a time t is $|\langle\alpha|\phi\rangle|^2$.

   Sally answers:

   > The probability that $|\phi\rangle$ transitions to $|\alpha\rangle$ in a time t is $|\langle\alpha|e^{-i\hat{H}t/\hbar}|\phi\rangle|^2$.

   Who is correct and why? What does the other answer represent? What if $|\alpha\rangle = |E_n\rangle$ (i.e., $|\alpha\rangle$ is an energy eigenstate with energy eiegnvalue E_n.)?

2. **The Postulates of Quantum Mechanics (or close to them)**
   Jamie wrote down the following postulates of quantum mechanics, but they're not quite right:

   (i) The state of any quantum system is represented by a wave function $\Psi(x,t)$.

   (ii) Physical observables are mathematically represented by unitary operators with the property $\hat{A}^\dagger = \hat{A}^{-1}$

   (iii) When we perform a measurement on a quantum system, the state of the system is multiplied by a phase $e^{-i\hat{H}t/\hbar}$ corresponding to the state's energy

   (iv) If we measure the observable Φ in a system defined by the state $|\psi\rangle$, the possible values we can obtain are $\langle\phi_j|\psi\rangle$ with probability $\langle\phi_j|\psi\rangle^2$ where $|\phi_j\rangle$ are the eigenkets of the operator corresponding to Φ

   (v) The time evolution of a system is given by the equation

   $$\hbar\frac{d}{dt}|\psi\rangle = -\hat{H}|\psi\rangle,$$

   where $\hat{H}$ is the unitary operator for energy.

   For each postulate

   (a) Consider and/or calculate some of its implications.

   (b) State the correct version.

3. **Infinite Square Well Potential**
   A particle of mass m is confined to a one-dimensional region $0 \le x \le a$. At $t = 0$, its normalized wave function is

   $$\psi(x, t=0) = \sqrt{\frac{8}{5a}}\left[1 + \cos\left(\frac{\pi x}{a}\right)\right]\sin\left(\frac{\pi x}{a}\right). \tag{4}$$

   (a) What is the wave function at a later time $t = t_0$?

   (b) If you measure the energy of this particle, what values might you get, and what is the probability of getting each of them?

   (c) What is the average energy of the system at $t = 0$ and again at $t = t_0$? How does it compare to the possible energy measurement values above?

2 Solutions

1. Sally is right. If we begin in a state $|\phi\rangle$, then the probability to be in a state $|\alpha\rangle$ after a time t is $|\langle\alpha|e^{-i\hat{H}t/\hbar}|\phi\rangle|^2$. The quantity $\langle\alpha|\phi\rangle$, on the other hand, represents the overlap between the $|\phi\rangle$ and $|\alpha\rangle$ state. The quantity $|\langle\alpha|\phi\rangle|^2$ does not have a clear physical meaning unless either $|\alpha\rangle$ or $|\phi\rangle$ are energy eigenstates.

   If $|\alpha\rangle = |E_n\rangle$, then Sally's and Susan's answers are the same and both represent the probability of getting the eigenvalue E_n upon measuring the energy of the system.

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2. (i) If the state of every quantum system were represented by a wave function $\Psi(x, t)$, then it would not be possible to describe systems which do not have a clear one-dimensional position space interpretation. For example, it would not be possible to describe spin systems or generally any system (like the NH_3 molecule) with a finite-number of energy levels and no sensible position basis representation.

   The correct postulate: *The state of every quantum system can be represented by a ket* $|\psi\rangle$*.*

   (ii) If physical observables were represented by unitary operators, then such operators would be dimensionless and they would only have eigenvalues of the form $e^{i\alpha}$ where α is a real quantity. Thus, we could not interpret the eigenvalues of such operators as connected to physical quantities because those eigenvalues would be both complex and without physical units.

   The correct postulate: *Physical observables are mathematically represented by Hermitian operators with the property* $\hat{A}^\dagger = \hat{A}$*.*

   (iii) A phase appended to a state ket does not change the physical properties of the state ket. Thus if measuring a state yielded a new state which was simply the former state multiplied by $e^{-i\hat{H}t/\hbar}$ with $\hat{H}$ corresponding to the system's energy, then measuring a state would yield the same state multiplied by a phase. We would also need to specify what t represents in this formula and replace $\hat{H}$ with $\langle E\rangle = \langle\psi|\hat{H}|\psi\rangle$ where $|\psi\rangle$ is the state of the system. In any case, such a phase multiplication would allow for the simultaneous measurement of physical observables defined by operators which do not commute.

   The correct postulate: *When we perform a measurement on a quantum system, the state of the system collapses to the eigenstate corresponding to the eigenvalue obtained from the measurement.*

   (iv) The quantity $\langle\phi_j|\psi\rangle$ does not have the correct dimensions to be associated with a measurement of the physical quantity Φ. Also, as an inner product, it can be complex and thus cannot correspond to a physical quantity. The stated probability $\langle\phi_j|\psi\rangle^2$ is also complex and cannot represent a real probability.

   The correct postulate: *If we measure the observable* Φ *in a system defined by the state* $|\psi\rangle$*, the possible values we can obtain are* ϕ_j *with probability* $|\langle\phi_j|\psi\rangle|^2$ *where* $|\phi_j\rangle$ *and* ϕ_j *are the eigenkets and eigenvalues, respectively, of the operator corresponding to the observable* Φ*.*

   (v) The given time-evolution equation would result in a quantum system which does not conserve probability. Also, defining the Hamiltonian as a unitary operator introduces all the previous problems (cited in (ii)) associated with have physical quantities defined by unitary operators.

The correct postulate: *The time evolution of a system is given by the equation*

$$i\hbar\frac{d}{dt}|\psi\rangle = \hat{H}|\psi\rangle,$$

where $\hat{H}$ is the Hermitian operator for energy.

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3. (a) To determine the time-dependence of the wave function, we first need to expand $\psi(x,0)$ in term of its energy eigenfunctions. Given Eq.(2), we find

$$\begin{aligned}\psi(x,t=0) &= \sqrt{\frac{8}{5a}}\left[1+\cos\left(\frac{\pi x}{a}\right)\right]\sin\left(\frac{\pi x}{a}\right)\\ &= \frac{2}{\sqrt{5}}\sqrt{\frac{2}{a}}\sin\left(\frac{\pi x}{a}\right) + \frac{1}{\sqrt{5}}\sqrt{\frac{2}{a}}\sin\left(\frac{2\pi x}{a}\right)\\ &= \frac{2}{\sqrt{5}}\psi_1(x) + \frac{1}{\sqrt{5}}\psi_2(x) \qquad (5)\end{aligned}$$

Thus the time-dependent wave function is

$$\begin{aligned}\psi(x,t_0) &= \frac{2}{\sqrt{5}}\psi_1(x)e^{-iE_1t_0/\hbar} + \frac{1}{\sqrt{5}}\psi_2(x)e^{-iE_2t_0/\hbar}\\ &= \sqrt{\frac{8}{5a}}\left[1+\cos\left(\frac{\pi x}{a}\right)e^{-i\hbar\pi^2t_0/ma^2}\right]\sin\left(\frac{\pi x}{a}\right)e^{-i\hbar\pi^2t_0/ma^2}, \qquad (6)\end{aligned}$$

where we used $E_n = \hbar^2\pi^2n^2/2ma^2$.

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(b) If you measure the energy of the particle you will get either E_1 and E_2 each with probability defined by the modulus squared of their corresponding state. Namely

$$\text{Prob}(E=E_1) = \frac{4}{5}, \qquad (7)$$

$$\text{Prob}(E=E_2) = \frac{1}{5}. \qquad (8)$$

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(c) The average of the energy is independent of time. Computing this average, we find

$$\langle E\rangle = \frac{4}{5}E_1 + \frac{1}{5}E_2 = \frac{4}{5}\cdot\frac{\hbar^2\pi^2}{2ma^2} + \frac{1}{5}\cdot\frac{2\hbar^2\pi^2}{ma^2} = \frac{4\hbar^2\pi^2}{5ma^2}. \qquad (9)$$

This average is between the two values we computed in (b).

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