PHYS 304 Review Notes

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General Forms for Solving Schrodinger Equations in Bound States

For a Schrodinger equation of the form:

$$-\frac{\hbar}{2m}\frac{\partial^2\psi}{\partial x^2} + V(x)\psi = i\hbar\frac{\partial\psi}{\partial t},$$

we can define a general solution for bound states to be of the following form:

$$\Psi(x,t) = \sum_{n=0}^{\infty} c_n\psi_n(x)\cdot\varphi_n(t),$$

where $\psi_n(x)$ is a stationery state for the given potential $V(x)$, and $\varphi_n(t)$ is the time-dependance of the solution, given by:

$$\varphi_n(t) = e^{-iE_nt/\hbar},$$

where E_n is the energy corresponding to the state. In addition, the bound state coefficients can be found according to:

$$c_n = \int_{-\infty}^{\infty}\psi_n(x)\Psi(x,0)dx.$$

These c_n values can be interpreted as the probabilities of each energy state:

$$P(E_n) = |c_n|^2$$

and as a consequence:

$$\sum_{n=1}^{\infty}|c_n|^2 = 1 \qquad \text{and} \qquad \langle H\rangle = \sum_{n=1}^{\infty}|c_n|^2E_n.$$

For the potentials that have been covered thus far in the course, there are two different stationery states corresponding to each potential. We can also define their energies:

Infinite Square Well

$$\psi_n = \sqrt{\frac{2}{a}}\sin\left(\frac{n\pi}{a}x\right)$$

$$E_n = \frac{\hbar^2k_n^2}{2m} = \frac{n^2\pi^2\hbar^2}{2ma^2}$$

where $k_n = \frac{n\pi}{a}$

Harmonic Oscillator

$$\psi_n = \left(\frac{m\omega}{\pi\hbar}\right)^{\frac{1}{4}}\frac{1}{\sqrt{2^nn!}}H_n(\xi)e^{-\xi^2/2}$$

$$E_n = \left(n+\frac{1}{2}\right)\hbar\omega$$

where $\xi = \sqrt{\frac{m\omega}{\hbar}}x$

The Hermite Polynomials are also important to note:

$$H_n(\xi) = \begin{cases} H_0(\xi) = 1 \\ H_1(\xi) = 2\xi \\ H_2(\xi) = 4\xi^2 - 2 \\ H_3(\xi) = 8\xi^3 - 12\xi \\ \dots \end{cases}$$

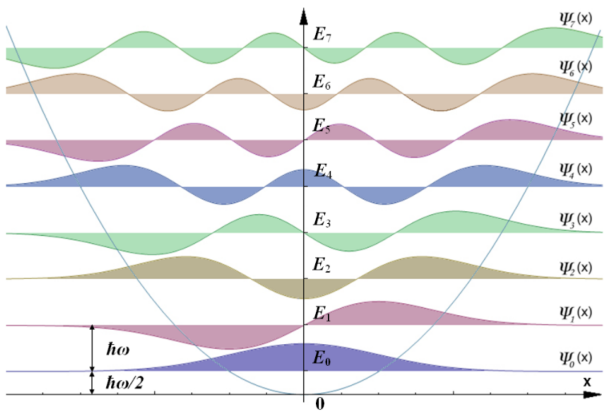
Stationery States: Stationery states are states in which:

1. All expectation values are independent of time.
2. Total energy is definite.
3. The general solution is a linear combination of stationery states.

Key features of the stationery states of the infinite square well:

- They are alternating even and odd.
- Each successive energy state gains an additional zero crossing (node)
- They are mutually orthogonal, which implies that $\int \psi_m^*(x)\psi_n(x) = 0, m \neq n$.

It is also useful to know what the bound states look like for the harmonic oscillator.



General Forms for Solving Free Particle Problems

For many potentials, particles appear in scattered states, instead of bound states. In these cases, energies are not quantized and general forms are computed over integrals, not sums.

For the case of the free particle, where the potential is zero everywhere, one can find the solution using the following procedure.

1. Identify $\phi(k)$, which is the distribution of states over the variable k, using a Fourier transform:

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

2. Transform the function out of the frequency domain using another Fourier transform:

$$\Psi(x,t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \psi(k)e^{i\left(kx - \frac{\hbar k^2}{2m}t\right)}dk.$$

The distribution of states $\phi(k)$ in the general solution is known as the wavepacket. There are two velocities that are important in this case.

- Phase Velocity: $v_{\text{phase}} = \frac{\omega}{k} = \frac{\hbar k}{2m} = \sqrt{\frac{E}{2m}}$
- Group Velocity: $v_{\text{group}} = 2v_{\text{phase}} = \frac{d\omega}{dk}$

In all of these forms, k is k_0, which is the fundamental frequency of the group.

Probabilities and Expectation Values

Heisenberg Uncertainty Principle:

$$\sigma_x \sigma_p \geq \frac{\hbar}{2}$$

Orthogonality

- The stationery states in the infinite square well are orthogonal.
- $\int_0^L \sin\left(\frac{n\pi x}{L}\right) \sin\left(\frac{m\pi x}{L}\right) dx = 0$
- $\int_0^L \cos\left(\frac{n\pi x}{L}\right) \cos\left(\frac{m\pi x}{L}\right) dx = 0$
- $\int_0^L \sin\left(\frac{n\pi x}{L}\right) \cos\left(\frac{m\pi x}{L}\right) dx = 0$
- $\int f_{\text{even}}(x) f_{\text{odd}}(x) dx = 0$
- $\int_0^L \sin\left(\frac{n\pi x}{L}\right) \sin\left(\frac{n\pi x}{L}\right) dx = \frac{L}{2}$
- $\int_0^L \cos\left(\frac{n\pi x}{L}\right) \cos\left(\frac{n\pi x}{L}\right) dx = \frac{L}{2}$

Probabilites and Such

We can define the probability of an event j given the total number of events N and the total number of times it occurs $N(j)$:

$$P(j) = \frac{N(j)}{N}.$$

In discrete variables, if we seek to find the average event j, denoted by $\langle j \rangle$, we can find it with:

$$\langle j \rangle = \frac{\sum j N(j)}{N} = \sum_{j=0}^{\infty} j P(j).$$

The standard deviation of an event is important to define:

$$\sigma = \sqrt{\langle j^2 \rangle - \langle j \rangle^2}$$

Similar formulae can also be applied to continuous variables. First, we define the probability density of some quantity as $\rho(x)dx$, that is $\rho(x)dx$ is the probability that an individual (chosen at random) lies between x and $(x + dx)$. Hence, it follows that:

$$P_{ab} = \int_a^b \rho(x) dx.$$

Expected Values

As alluded to prior, we can have certain expected values for quantities, that is, the average value for that quantity over all time. In general, for some quantity Q, this is given by:

$$\langle Q(x,p)\rangle = \int_{-\infty}^{\infty} \Psi^* \left[Q\left(x, -i\hbar\frac{\partial}{\partial x}\right)\right] \Psi dx$$

Where $Q(x,p)$ is some operator that can be described as a function of x and p.

Hence, we can define some common operators:

- Position Operator, x: x.
- Momentum Operator, $\hat{p}$: $\hat{p} = -i\hbar\frac{\partial}{\partial x}$.

Energy is another expected value, but obtaining it in bound states is a bit difficult. It can be obtained as follows:

$$\langle E\rangle = \sum_{n=1}^{\infty} |c_n|^2 E_n.$$

Important Integrals

There are some important integrals that often come up:

$$\int_{-\infty}^{\infty} e^{-\frac{x^2}{a^2}} dx = \sqrt{\pi}a \qquad \int_{-\infty}^{\infty} x^2 e^{-\frac{x^2}{a^2}} dx = \frac{\sqrt{\pi}a^3}{2}$$

Dirac Notation

Definitions:

- A ket, denoted as $|B\rangle$ defines notation for a vector. Hence, it can be interpreted that:

$$|B\rangle = \begin{bmatrix} b_1 \\ b_2 \\ \vdots \\ b_n \end{bmatrix}$$

- A bra, denoted as $\langle A|$ defines notation for the complex conjugate of a vector. Hence, it can be interpreted that:

$$\langle A| = \begin{bmatrix} a_1 \\ a_2 \\ \vdots \\ a_n \end{bmatrix}^\dagger = \begin{bmatrix} a_1^* & a_2^* & \cdots & a_n^* \end{bmatrix}$$

Mathematical Implications:

- Thus, it follows that the combination of a bra and ket in order yields the inner product of two vectors:

$$\langle A|B\rangle = \begin{bmatrix} a_1^* & a_2^* & \cdots & a_n^* \end{bmatrix} \begin{bmatrix} b_1 \\ b_2 \\ \vdots \\ b_n \end{bmatrix} = a_1^* b_1 + a_2^* b_2 + \cdots + a_n^* b_n$$

- We can also define the "ketbra" operation, which is the reverse order of the braket, and is also the outer product. This is especially useful in the case of finding the identity matrix for a system:

$$\sum_i = |e_i\rangle\langle e_i| = I$$

  Where e_i denote all of the possible basis vectors for a system.

Applications in Quantum Physics:

In quantum mechanics, we introduce the concept of Hilbert Space, which under the viewpoint that a function can be described as an abstract vector, is defined as the vector space of all square-integrable functions on specified intervals:

$$\left\{ f(x) : \int_a^b |f(x)|^2 dx < \infty \right\}$$

Since most functions are map continuous functions to continuous functions in quantum physics, we can use braket notation and Hilbert Space to express the inner product for two functions:

$$\langle f(x)|g(x)\rangle = \int_a^b f(x)^* g(x) dx$$

where a and b denote endpoints of the $f(x)$ and $g(x)$ abstract vectors. Oftentimes, these bounds are infinite. A corollary of this is that if both f and g are square integrable functions, then the inner product between f and g $\langle f|g\rangle$ is guaranteed to exist.

There are some important implications that arise from these definitions:

- A function is said to be normalized when its inner product with itself evaluates to 1.
- Two functions are orthogonal to each other when their inner product is zero.
- Two functions are orthonormal if their inner product is zero and they are normalized.
- A set of functions is complete if **any** other function f in Hilbert Space can be expressed as a linear combination of the two:

$$f = \sum_{n=1}^{\infty} c_n f_n(x)$$

  where for an orthonormal set, $c_n = \langle f_n | f \rangle$.

  - Infinite Square Well states are complete on $(0, a)$.
  - Harmonic Oscillator states are complete on $(-\infty, \infty)$.

Observables: If we state that wavefunctions can be represented as abstract vectors, then we can state that observables correspond to linear transformations on wavefunctions. Hence, to compute an observable, we can imagine the process as:

1. Transform the original wavefunction Ψ using some linear transformation representing the observable: $Q \left|\Psi\right\rangle$
2. Project the original wavefunction onto the transformed space to obtain the magnitude of the observable: $\left\langle\Psi\right| Q \left|\Psi\right\rangle$

Hence, we can state that for some observable Q:

$$\langle Q \rangle = \langle \Psi | Q | \Psi \rangle = \int_{-\infty}^{\infty} \Psi^* \hat{Q} \Psi dx$$

It is important to note that since we require observables to be real quantities, that all operators for an observable must be hermetian, that is that $\hat{Q} = \hat{Q}^\dagger$, or for the purpose of proofs:

$$\left\langle f \middle| \hat{Q} f \right\rangle = \left\langle \hat{Q} f \middle| f \right\rangle$$

Determinate States and Eigenfunctions:

It is known that determinate states of Q are eigenfunctions of $\hat{Q}$, that is:

$$\hat{Q}\psi = q\psi$$

where $q = \langle Q \rangle$. From this, we obtain two important definitions:

- Spectrum: the collection of all of the eigenvalues for a given wavefunction.
- Degenerate Spectrums: spectrums where two or more linearly independent eigenfunctions share the same eigenvalue.

It is to be noted that there exists two types of spectra:

- Discrete Spectra: Eigenvalues are separated from each other
  - Eigenfunctions lie in Hilbert space (normalizable) and constitute physically realizable states.
  - Eigenvalues are real.
  - Eigenfunctions are orthonormal to each other.
- Continuous Spectra: Eigenfunctions are non-countable, continuous, and are not normalizable. As a result, they do not represent possible wavefunctions, however, a linear combination of them *might* be.
  - Eigenfunctions with real eigenvalues are said to be Dirac Normalizable (notes on this later) and complete.

Axiom ($\star$): The eigenfunctions of an observable operator are complete.

Generalized Statistical Interpretation

Core Concepts:

1. If you measure a measure an observable $Q(x, p)$ on a particle in the state $\Psi(x, t)$, you are certain to get one of the eigenvalues of the Hermetian operator $\hat{Q}$ $(\star\star)$.

   (a) If the spectrum is discrete, then the probability of getting the particular eigenvalue q_n associated with an orthonormal eigenfunction $f_n(x)$ is:

   $$|c_n|^2 \qquad \text{where} \qquad c_n = \langle f_n|\Psi\rangle\,, n \in \mathbb{N}$$

   (b) If the spectrum is continuous, with *real* eigenvalues $q(z)$ and associated [Dirac-Normalized] eigenfunctions $f_z(x)$, the probability of getting a result in the range dz is:

   $$|c(z)|^2 dz \qquad \text{where} \qquad c(z) = \langle f_z|\Psi\rangle\,, z \in \mathbb{R}$$

2. By means of $(\star)$ and $(\star\star)$, it is implied that Ψ is a linear combination of functions for some basis:

   $$\Psi = \sum_n c_n(t) f_n \qquad \text{or} \qquad \Psi = \int_{-\infty}^{\infty} c(z,t) f_z dz$$

   (a) Combined with the fact that $\sum_n |c_n|^2 = 1$, it is also implied that we can describe expectation values in terms of generalized probabilities:

   $$\langle Q\rangle = \sum_n q_n |c_n|^2$$

Given this, we can hypothesize what various different basis functions might look like for different observables. Some examples (in position space) include:

- Momentum-Space Eigenfunctions: $f_p(x) = \frac{1}{\sqrt{2\pi\hbar}} e^{\frac{ipx}{\hbar}}$
- Position-Space Eigenfunctions: $g_y(x) = \delta(x - y)$

The existence of a momentum-space eigenfunction in position space provides us with the ability to find the momentum space wavefunction. It is denoted as:

$$\Phi(p,t) = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} e^{\frac{-ipx}{\hbar}} \Psi(x,t) dx$$

Which, if we look closer at, is actually a bra-ket in disguise:

$$\Phi(p,t) = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} e^{\frac{-ipx}{\hbar}} \Psi(x,t) dx = \langle f_p(x)|\Psi(x,t)\rangle$$

This serves as a nice segue into the next concept, which are bases in Hilbert space.

Bases in Hilbert Space: Since the Hilbert space is a space of functions which can be expressed as abstract vectors, then there must be an arbitrary abstract vector in Hilbert space corresponding to every possible wavefunction. This is denoted by $|\mathcal{S}(t)\rangle$.

Before we move deeper, it is important to define some vectors that will be used frequently in the following text:

- $|x\rangle$: eigenfunction of $\hat{x}$ with arbitrary eigenvalue x...*
- $|p\rangle$: eigenfunction of $\hat{p}$ with arbitrary eigenvalue p...*
- $|n\rangle$: eigenfunction (E_n [constant]) of $\hat{H}$ with arbitrary eigenvalue E...*

*... I wrote ellipses in my notes and think I'm missing something here.

Which leads to the important property that the inner product/projection of one bases eigenfunctions with the arbitrary $\mathcal{S}(t)$ function yields the wavefunction in that respective basis:

- $\langle x|\mathcal{S}(t)\rangle = \Psi(x,t)$
- $\langle p|\mathcal{S}(t)\rangle = \Phi(p,t)$
- $\langle n|\mathcal{S}(t)\rangle = c_n(t)$

Hence, it is also to be noted that different operators "look different" in different bases:

$$\hat{x} \to \begin{cases} x & \text{in position space} \\ i\hbar\frac{\partial}{\partial p} & \text{in momentum space} \end{cases} \qquad \hat{p} \to \begin{cases} -i\hbar\frac{\partial}{\partial x} & \text{in position space} \\ p & \text{in momentum space} \end{cases}$$

Remark: We can determine the coefficients for a function in its basis by:

$$\langle f_n'|f_n\rangle$$

for some arbitrary eigenfunction f_n for some observable $\hat{Q}$.

Moving backwards, we can also find $|\mathcal{S}(t)\rangle$ for various bases:

- $\langle \Psi(p,t)^*|p\rangle = \int \Psi(p,t)\,|p\rangle\,dp$
- $\langle \Phi(x,t)^*|x\rangle = \int \Phi(x,t)\,|x\rangle\,dx$

However, since $\Phi(p,t) = \langle p|\mathcal{S}(t)\rangle$ and $\Psi(x,t) = \langle x|\mathcal{S}(t)\rangle$, we can generalize:

$$|\mathcal{S}(t)\rangle = \int_{-\infty}^{\infty} \langle O_z|\mathcal{S}(t)|O_z\rangle\,dz$$

for some arbitrary basis $\{|O_z\rangle\}$.

Change of Bases in Dirac Notation: Given everything that we know, it should make sense that we can measure observables in different bases. To generalize, we can write that:

$$\langle \text{basis}|\,\text{operator}\,|\text{state}\rangle$$

Examples:

- $\langle x|\,\hat{x}\,|\mathcal{S}(t)\rangle = x\Psi(x,t)$: application of position operator in x basis.
- $\langle p|\,\hat{x}\,|\mathcal{S}(t)\rangle = i\hbar\frac{\partial\Phi}{\partial p}$: application of position operator in p basis.

Notes on the concept of Dirac Orthonormality: In the case that eigenvalues are discrete, the condition holds that:

$$\langle f_n|f_m\rangle = \delta_{nm} = \begin{cases} 0 & \text{if } n \neq m \\ 1 & \text{if } n = m \end{cases}$$

However, since continuous states don't obey this kind of orthonormality with the Kronecker-Delta function, they still are able to find a sort of orthonormality with the Dirac-Delta function:

$$\left\langle f_q'\middle|f_q\right\rangle = \delta(q - q')$$

This makes sense, since the physical solution for systems with discrete eigenvalues is obtained under discrete summation, the Kronecker-Delta function fits the use case. Similarly, since the physical solution for systems with continuous eigenvalues is obtained by integration, the Dirac-Delta function fits the use case.