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:

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

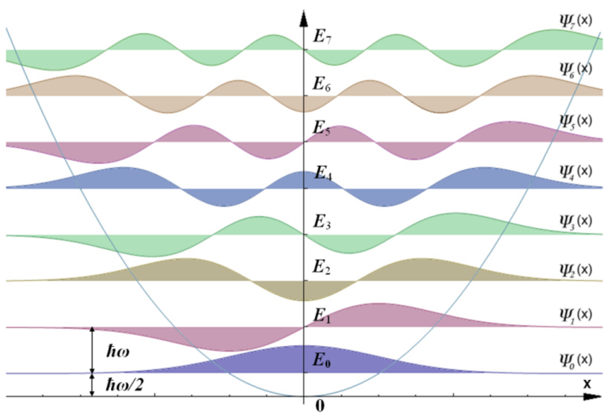
Stationery States: Stationery states are states in which:

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.
- $\displaystyle\int_0^L \sin\left(\frac{n\pi x}{L}\right) \sin\left(\frac{m\pi x}{L}\right) dx = 0$
- $\displaystyle\int_0^L \cos\left(\frac{n\pi x}{L}\right) \cos\left(\frac{m\pi x}{L}\right) dx = 0$
- $\displaystyle\int_0^L \sin\left(\frac{n\pi x}{L}\right) \cos\left(\frac{m\pi x}{L}\right) dx = 0$
- $\displaystyle\int f_{\text{even}}(x) f_{\text{odd}}(x) dx = 0$
- $\displaystyle\int_0^L \sin\left(\frac{n\pi x}{L}\right) \sin\left(\frac{n\pi x}{L}\right) dx = \frac{L}{2}$
- $\displaystyle\int_0^L \cos\left(\frac{n\pi x}{L}\right) \cos\left(\frac{n\pi x}{L}\right) dx = \frac{L}{2}$

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:

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

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:

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