PHYS 304 Review Notes

Reese Critchlow

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 <u>stationery state</u> for the given potential V(x), and $\varphi_n(t)$ is the time-dependence of the solution, given by:

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

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:

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

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

Harmonic Oscillator

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

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

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

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

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

The Hermite Polynomials are also important to note:

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

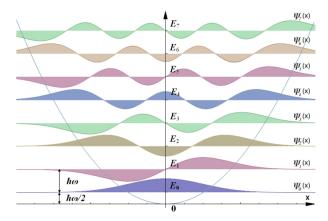
Stationery States: Stationery states are states in which:

- 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 <u>scattered states</u>, 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 <u>free particle</u>, 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 <u>wavepacket</u>. There are two velocities that are important in this case.

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• 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:

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

Orthogonality

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

Probabilities 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 <u>probability density</u> 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:

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