

Intermediate Quantum Mechanics

Lecture 12 Notes (3/2/15)

Simple Harmonic Oscillator I

The Simple Harmonic Oscillator Potential

- We want to solve for a particle in a simple harmonic oscillator potential:

$$V(x) = \frac{1}{2} m\omega^2 x^2$$

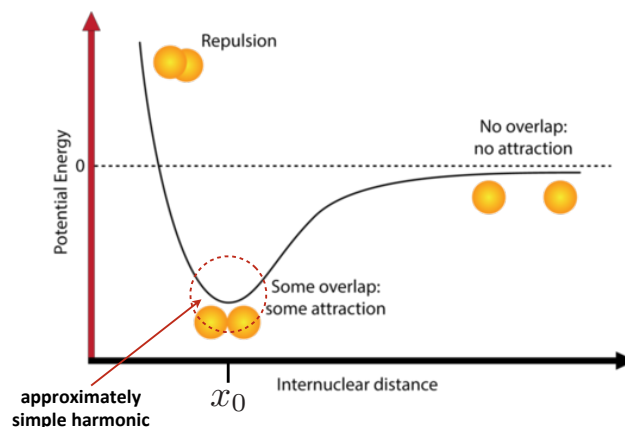
- Classically, this describes a mass, m , on the end of spring with spring constant, $k = m\omega^2$. The equation of motion is:

$$m\ddot{x} = -kx \qquad \ddot{x} = -\frac{k}{m}x = -\omega^2 x$$

and has the solution: $x = A \cos(\omega t + \phi)$ where A and ϕ are just constants of integration that depend on the initial conditions. The mass oscillates with angular frequency ω .

Importance of the Simple Harmonic Oscillator potential

- There are two reasons why the simple harmonic oscillator potential is uniquely important. It gives a very good approximation to a system that is close to equilibrium and, more importantly, it is the basis of quantum field theory, the full theory of relativistic quantum mechanics.
- No matter how complicated the potential energy of a system, when the system is near equilibrium the potential energy can be approximated as a simple harmonic oscillator potential. The figure below shows the example of the molecular binding potential of two hydrogen atoms.



- If $V(x)$ is analytic, it can be expanded as a power series about the equilibrium point.

$$V(x) = a_0 + a_1(x - x_0) + a_2(x - x_0)^2 + \dots$$

A constant term in the energy can always be ignored so the a_0 term can be dropped. Since at equilibrium the force is zero:

$$F(x_0) = -\frac{d}{dx}V(x_0) = 0 \quad \Rightarrow \quad a_1 = 0$$

The lowest order term is then $V(x_0) \approx a_2(x-x_0)^2$. For separation distances not far from the equilibrium separation x_0 , the potential energy can be approximated as a quadratic (simple harmonic oscillator) potential.

- In the hydrogen molecule, as long as it is not perturbed too much from its equilibrium separation, we can treat the two hydrogen atoms as if they were bound together by a spring. The same is true of the vibrational modes of all diatomic molecules. It's also true of polyatomic molecules and for solids.
- The simple harmonic oscillator potential is an essential part of quantum field theory. In order to formulate the combination of quantum mechanics with the special theory of relativity, x must be demoted from being an operator to being just a parameter like time. Then, the quantities that are wave functions in non-relativistic quantum mechanics become the operators, $\hat{\psi}(x, t)$. They are field operators, they depend on x and t .
- Consider a standing wave on a string fixed at both ends. For a given normal mode (harmonic), each point on the string oscillates up and down all with the frequency of the given harmonic. Each point on the string acts like a simple harmonic oscillator.
- Electromagnetic waves are analogous to waves on a string. [A difference is that it is a wave in three dimensions and it is a vector wave (the electric field is an arrow) rather than a scalar wave like the wave on a string.] Just as for a wave on a string, the normal modes of an electromagnetic field inside a cavity, consist of a set of simple harmonic oscillators one for each point in space. Each point in space acts like a simple harmonic oscillator. The quantum field operators contain creation and annihilation operators that create and annihilate photons, the quanta of these simple harmonic oscillators.
- We will here solve just a single quantum harmonic oscillator. In quantum field theory, space consists of a large or infinite number of quantum simple harmonic oscillators.

Time independent Schrodinger Equation

- The time dependent Shrodinger Equation is: $i\hbar \frac{d}{dt} |\psi(t)\rangle = \hat{H} |\psi(t)\rangle$.

In the x -representation this becomes:

$$i\hbar \frac{d}{dt} \langle x | \psi(t) \rangle = \langle x | \hat{H} | \psi(t) \rangle$$

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

- The energy eigenstates are given by:

$$\langle x | E \rangle = \psi_E(x, t) = e^{-iEt/\hbar} u(x)$$

Plugging this into the time dependent Schrodinger Equation, we get the time independent Schrodinger equation.

$$E u(x) = \left(-\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + V(x) \right) u(x)$$

For a given $V(x)$, the solution of this differential equation gives the spatial dependence of the energy eigenstates, while imposing boundary conditions on $u(x)$, determines the allowed energy eigenvalues.

- Typically, a course in quantum mechanics first solves for an infinite potential well, a potential energy that is zero inside some region and is infinite outside of that region and then next solves for the finite potential well, a potential energy that is zero inside some region and is constant but finite outside of that region. These are interesting problems that illustrate the idea of quantized energy levels, but we are going to jump right to the simple harmonic oscillator potential that, as discussed above, is by far the most important.
- For the simple harmonic oscillator potential, the time independent Schrodinger Equation is:

$$E u(x) = \left(-\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + \frac{1}{2} m\omega^2 x^2 \right) u(x)$$

We could solve this differential equation. Instead we will solve for the energy eigenvalues and energy eigenstates using just operator algebra.

- For those interested, here are the steps in solving the differential equation.
 - 1) Assume a solution of the form of a power series times a Gaussian:

$$u(x) = \sum_i a_i (x')^i e^{-x'^2/2}$$

- 2) Substitute this into the differential equation and determine a recursion relation for the coefficients of the power series.

$$\frac{a_{i+2}}{a_i} = f(i)$$

- 3) Find that the recursion relation for the power series must terminate for some term n in order that $u(x)$ satisfy the condition of a physical state:

$$u(x) \rightarrow 0 \quad \text{as} \quad x \rightarrow \pm \infty$$

- 4) This gives solutions for $u(x)$ that are finite polynomials times a Gaussian and that have discrete (quantized) eigenvalues.

Operator Solution

- In operator form, the Hamiltonian is:

$$\hat{H} = \frac{\hat{p}^2}{2m} + \frac{1}{2} m\omega^2 \hat{x}^2$$

- When solving this equation, the physical constants: \hbar , m , ω are a nuisance. We can get rid of them by writing the Hamiltonian in a unit less form.

$$\frac{\hat{H}}{\hbar\omega} = \frac{1}{2m\hbar\omega} \hat{p}^2 + \frac{m\omega}{2\hbar} \hat{x}^2$$

- Now define: $\hat{p}' \equiv \frac{1}{\sqrt{m\hbar\omega}} \hat{p}$ and $\hat{x}' \equiv \sqrt{\frac{m\omega}{\hbar}} \hat{x}$

The Hamiltonian is then:
$$\hat{H} = \frac{\hbar\omega}{2} (\hat{p}'^2 + \hat{x}'^2)$$

- The commutator of \hat{x}' with \hat{p}' is: $[\hat{x}', \hat{p}'] = \frac{[\hat{x}, \hat{p}]}{\hbar} = i$

- Define two new operators:

$$\hat{a} \equiv \frac{1}{\sqrt{2}} (\hat{x}' + i\hat{p}') \quad \text{and} \quad \hat{a}^\dagger \equiv \frac{1}{\sqrt{2}} (\hat{x}' - i\hat{p}')$$

- The product of \hat{a}^\dagger and \hat{a} is:

$$\begin{aligned} \hat{a}^\dagger \hat{a} &= \frac{1}{2} (\hat{x}' - i\hat{p}') (\hat{x}' + i\hat{p}') = \frac{1}{2} (\hat{x}'^2 + \hat{p}'^2) + \frac{i}{2} [\hat{x}', \hat{p}'] \\ &= \frac{1}{2} (\hat{x}'^2 + \hat{p}'^2) - \frac{1}{2} = \frac{\hat{H}}{\hbar\omega} - \frac{1}{2} \end{aligned}$$

- The Hamiltonian is then:
$$\hat{H} = \hbar\omega \left(\hat{a}^\dagger \hat{a} + \frac{1}{2} \right)$$

- If $|E_n\rangle$ is an eigenstate of \hat{H} with eigenvalue E_n then, from the above equation, it is also a eigenstate of $\hat{a}^\dagger \hat{a}$:

$$\hat{H} |E_n\rangle = E_n |E_n\rangle \quad \hat{a}^\dagger \hat{a} |E_n\rangle = n |E_n\rangle \quad \text{with} \quad E_n = n\hbar\omega + \frac{\hbar\omega}{2}$$

n will turn out to be an integer but we haven't shown that yet.

Raising and Lowering Operators

- The commutation of \hat{a} and \hat{a}^\dagger is:

$$[\hat{a}, \hat{a}^\dagger] = \frac{1}{2} [(\hat{x}' + i\hat{p}'), (\hat{x}' - i\hat{p}')] = i$$

$$= -\frac{i}{2}[\hat{x}', \hat{p}'] + \frac{i}{2}[\hat{p}', \hat{x}'] = -i[\hat{x}', \hat{p}'] = 1$$

- We now use this commutator to find $\hat{a}^\dagger |E_n\rangle$:

$$\hat{a}^\dagger |E_n\rangle = \hat{a}^\dagger[\hat{a}, \hat{a}^\dagger] |E_n\rangle = \hat{a}^\dagger(\hat{a}\hat{a}^\dagger - \hat{a}^\dagger\hat{a}) |E_n\rangle = \hat{a}^\dagger\hat{a}\hat{a}^\dagger |E_n\rangle - n\hat{a}^\dagger |E_n\rangle$$

$$\Rightarrow \hat{a}^\dagger\hat{a}(\hat{a}^\dagger |E_n\rangle) = (n+1)\hat{a}^\dagger |E_n\rangle$$

$$\Rightarrow \hat{a}^\dagger |E_n\rangle \text{ is an eigenstate of } \hat{a}^\dagger\hat{a} \text{ with eigenvalue } n+1.$$

$$\Rightarrow \hat{a}^\dagger |E_n\rangle \text{ is an eigenstate of } \hat{H} \text{ with eigenvalue: } (n+1)\hbar\omega + \frac{\hbar\omega}{2} = E_n + \hbar\omega$$

$$\Rightarrow \hat{a}^\dagger |E_n\rangle = \alpha |E_{n+1}\rangle \quad \text{with} \quad \hat{H} |E_{n+1}\rangle = E_{n+1} |E_{n+1}\rangle$$

- In a similar manner, we find:

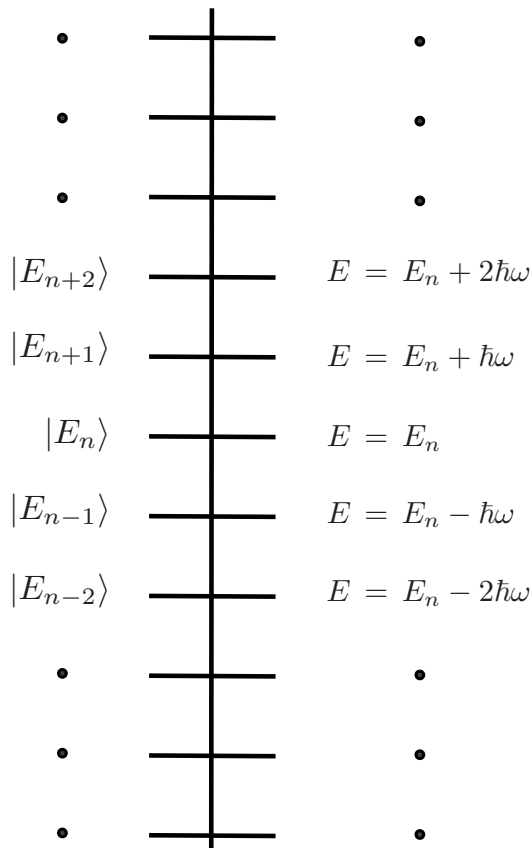
$$\hat{a} |E_n\rangle \text{ is an eigenstate of } \hat{a}^\dagger\hat{a} \text{ with eigenvalue } n-1.$$

$$\Rightarrow \hat{a} |E_n\rangle \text{ is an eigenstate of } \hat{H} \text{ with eigenvalue: } (n-1)\hbar\omega + \frac{\hbar\omega}{2} = E_n - \hbar\omega$$

$$\Rightarrow \hat{a} |E_n\rangle = \beta |E_{n-1}\rangle \quad \text{with} \quad \hat{H} |E_{n-1}\rangle = E_{n-1} |E_{n-1}\rangle$$

Energy eigenstates

- Starting with an energy eigenstate $|E_n\rangle$ with energy eigenvalue E_n and operating successively with \hat{a}^\dagger , creates other eigenstates each with an energy eigenvalue of one additional unit of $\hbar\omega$. Similarly, starting with an energy eigenstate $|E_n\rangle$ with energy eigenvalue E_n and operating successively with \hat{a} , creates other eigenstates each with an energy eigenvalue of one less unit of $\hbar\omega$. We then have a ladder of energy eigenvalues separated from each other by an integral number units of $\hbar\omega$ of energy.



- In the direction of increasing energy this raising can continue to infinity. In the direction of decreasing energy the lowering must terminate at a lowest energy state since the energy eigenvalues of the harmonic oscillator potential must be positive definite.

The ground state

- It is easy to show that the eigenvalues of the harmonic oscillator Hamiltonian must be greater than or equal to zero.

$$\hat{H} = \frac{\hbar\omega}{2} (\hat{p}'^2 + \hat{x}'^2)$$

Let $|E\rangle$ be an eigenstate of \hat{H} and define $|A\rangle \equiv \hat{p}'|E\rangle$ and $|B\rangle \equiv \hat{x}'|E\rangle$

$$E = \langle E|\hat{H}|E\rangle = \frac{\hbar\omega}{2} (\langle E|\hat{p}'\hat{p}'|E\rangle + \langle E|\hat{x}'\hat{x}'|E\rangle) = \frac{\hbar\omega}{2} (\langle A|A\rangle + \langle B|B\rangle)$$

Since the inner product of a vector with itself is positive definite, we have:

$$\langle A|A\rangle \geq 0 \quad \text{and} \quad \langle B|B\rangle \geq 0 \quad \Rightarrow \quad E \geq 0$$

- This means that we can't just keep lowering. There must be a lowest energy state with positive definite energy. This is the ground state $|E_0\rangle$. The lowering operator \hat{a} acting on this state gives the null vector: $\hat{a}|E_0\rangle = |\emptyset\rangle$.

- The ground state $|E_0\rangle$ has energy $E = \hbar\omega/2$. The other eigenstates $|E_n\rangle$ then have energies:

$$E_n = n\hbar\omega + \frac{\hbar\omega}{2}$$

where we now have that n is a positive integer or zero: $n = 0, 1, 2, \dots$