Physics 212: Lecture 14

Thursday, March 11, 1999
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1 Announcements

The two classes right after spring break (on Monday and Thursday, March 22 and 25) will be taught by Adam Wax, a 6th-year graduate student of the Physics Department. Besides filling in for me while I am out of town on the 22nd, this is a valuable opportunity for Adam to get some experience teaching an advanced undergraduate class (most graduate students miss having any teaching experience during their PhD training, a serious flaw). Please don't hesitate to ask him questions during and outside of class. He can also be reached via e-mail at awax@phy.duke.edu.

2 Reading

We will finish our discussion today of the single-particle three-dimensional Schrodinger equation with a spherically-symmetric potential. After spring break, we will start discussing the last important physical insight of this semester, that wave functions describing systems of identical particles must have special symmetries under permutation of the identical particles. This leads to the discovery of fermions, bosons, and the Pauli exclusion principle. The rest of the semester will then consist of applications of all that we have learned so far (e.g., to the electronic structure of periodic crystals, the shell theory of nuclei, neutron stars, etc.) plus a few lectures on some technical ways to solve the Schrodinger equation for these more complex problems (e.g., perturbation theory, the variational principle and Monte Carlo methods).

For the lectures starting after spring break, you should read:

1. Section 5.1 of Griffiths.
2. Sections 13.1-13-6 of French and Taylor

As usual, please read and think about this material *before* class so that you can participate in class discussions.

I would also encourage you to browse through some of the 212 course references in the reserved section of the Math-Physics library. You may find it interesting to see how Shankar or Landau/Lifshitz discuss this same material from a more advanced view point, both physically and mathematically. You should also dip into Feynman's Volume III of his lecture series, where Feynman works out his own unique way of explaining quantum mechanics in terms of amplitudes (he comes to the Schrodinger equation only at the end of his volume!).

3 Thought Questions

1. What is the physical meaning of the quantity $|Y_l^m(\theta, \phi)|^2$?
2. If $\psi(r, \theta, \phi) = R(r) Y_l^m(\theta, \phi)$ is a stationary wave function for a single particle in a spherically symmetric potential, what is the physical meaning of the quantity

$$\int_{r_1}^{r_2} |rR|^2 \, dr? \tag{1}$$

3. What is the degeneracy (number of linearly independent states of identical energy) for the $n = 5$ level of hydrogen?

4. The stationary hydrogen wave functions $\psi_{nlm} = R_{nl}(r)Y_l^m(\theta, \phi)$ have a complicated dependence on the coordinates r and θ. How can one test experimentally the details of this complicated dependence?

4 Concepts to Understand

1. Recall the following important point

$$0 = [H, L^2] = [H, L_z] = [L^2, L_z] = [H, S_z] = [L^2, S_z] = [L_z, S_z], \tag{2}$$

for an electron with Hamiltonian operator H, angular momentum squared operator L^2, z-orbital angular momentum component L_z, and z-spin angular momentum operator S_z. Since these four operators are all mutually commuting, one can find a complete set of eigenvectors that are simultaneously eigenvectors of all four operators. Further, experiment shows that there are no other operators that mutually commute with these four so that this gives a complete quantum description. (This set of operators is called "complete" which is quite a different meaning than saying that the eigenvectors of a given observable form a complete set.) Thus we can label the stationary states of the electron by four quantum numbers:

$$|n, l, m, s_z\rangle, \tag{3}$$

where n determines an energy level, l the magnitude-squared of the angular momentum, m the z-component of the angular momentum, and s_z the z-component of the spin angular momentum. Thus:

$$H|n, l, m, s_z\rangle = E_n \, |n, l, m, s_z\rangle, \tag{4}$$
$$L^2|n, l, m, s_z\rangle = l(l+1)\hbar^2 \, |n, l, m, s_z\rangle, \tag{5}$$
$$L_z|n, l, m, s_z\rangle = m\hbar \, |n, l, m, s_z\rangle, \tag{6}$$
$$S_z|n, l, m, s_z\rangle = s_z\hbar \, |n, l, m, s_z\rangle. \tag{7}$$

2. The angular dependence of the three-dimensional Laplacian in spherical coordinates is exactly the angular momentum operator squared:

$$\nabla^2 = \partial_x^2 + \partial_y^2 + \partial_z^2 \tag{8}$$
$$= \frac{1}{r^2}\partial_r\left(r^2\partial_r\cdot\right) + \frac{1}{r^2\sin(\theta)}\partial_\theta\left(\sin(\theta)\partial_\theta\cdot\right) + \frac{1}{r^2\sin^2(\theta)}\partial_\phi^2$$
$$= \frac{1}{r^2}\partial_r\left(r^2\partial_r\cdot\right) - \frac{1}{\hbar^2 r^2}L^2$$
$$= \frac{1}{r}\partial_r^2(r\cdot) - \frac{1}{\hbar^2 r^2}L^2. \tag{9}$$

This allows one to reduce the single-particle Schrodinger equation for a spherically symmetric potential $V = V(r)$ to a single-particle one-dimensional Schrodinger equation for the radial part of the wave function. If we use separation of variables for a stationary state:

$$\psi(r, \theta, \phi) = R(r)\, Y_l^m(\theta, \phi), \tag{10}$$

and use the fact that:

$$L^2 Y_l^m = l(l+1)\hbar^2 \, Y_l^m, \tag{11}$$

and if we denote $rR(r)$ by the function $u(r)$, then we can show that u satisfies the following single-particle one-dimensional Schrodinger equation for $r \geq 0$:

$$\frac{-\hbar^2}{2m}\frac{d^2u}{dr^2} + \left[\frac{\hbar^2}{2m}\frac{l(l+1)}{r^2} + V(r)\right] u = Eu. \tag{12}$$

This is known as the *radial equation*. It corresponds to a particle of mass m moving in an effective one-dimensional potential:

$$V_{1d}(r) = V(r) + \frac{\hbar^2}{2m}\frac{l(l+1)}{r^2}. \tag{13}$$

The solution $u(r)$ to the radial equation satisfies the condition:

$$u(0) = 0. \tag{14}$$

This follows from $u = rR$ and the fact that R is continuous and finite everywhere since the wavefunction $\psi = RY_l^m$ is. Since the spherical harmonics are already normalized over the surface of the unit sphere, you should be able to see easily that the condition for the radial function $u = rR$ to be normalized is:

$$\int_0^\infty |u|^2\, dr = 1. \tag{15}$$

3. A simple application of the radial equation is for the infinite spherical well, which has a potential V that is zero out to radius r_0 and infinite beyond:

$$V(r) = \begin{cases} 0, & \text{for } r \le r_0, \\ \infty, & \text{for } r > r_0. \end{cases} \tag{16}$$

For $l = 0$, the radial equation reduces to the single-particle one-dimensional Schrodinger equation for an infinite well of width $L = r_0$ and we can write down immediately the infinitely many energy states:

$$E_{n,l=0} = \frac{n^2\pi^2\hbar^2}{2mr_0^2}. \tag{17}$$

The corresponding wave functions are:

$$\psi_{n,l=0,m=0} = \frac{1}{\sqrt{2\pi r_0}}\frac{\sin(n\pi r/a)}{r}. \tag{18}$$

Griffiths discusses the solutions for the more general case with $l > 0$. One gets radial functions that are expressed in terms of the spherical Bessel functions of order l, $j_l(x)$ plus the positions of their roots.

Another example is the finite spherical well,

$$V(r) = \begin{cases} V_0 < 0, & \text{for } r \le r_0, \\ 0, & \text{for } r > r_0. \end{cases} \tag{19}$$

The radial equation now corresponds to *odd* parity solutions of a one-dimensional box of length $2r_0$ and, as we saw from the fall semester, such one-dimensional boxes don't have a stationary state unless the well is sufficiently deep (see Section 4-2 of French and Taylor). It turns out that the deuteron, the nuclear particle consisting of a bound proton and neutron, is known experimentally to have just a single bound state with binding energy $E = 2.2\,\text{MeV}$. Using the known size of the deuteron (about 10^{-13} cm and the fact that there is just one bound state of known value, and assuming the potential is a finite spherical well, one can deduce that the depth V_0 must be about 50 MeV. This is similar in magnitude to what one would get just by applying the uncertainty principle (if you can remember the homework problem you did from French and Taylor last semester: if $\triangle x \approx 10^{-13}$ cm and $\triangle x \triangle p \ge \hbar$ and $E \approx (\triangle p)^2/2m$.)

4. The hydrogen atom is a special case of a single electron in a spherical potential, namely the Coulomb inverse-r potential $V(r) = -e^2/r$ (CGS units). The general wave function can be written:

$$\psi(r,\theta,\phi) = R(r)Y_l^m(\theta,\phi), \tag{20}$$

where the radial part of the wave function $u = rR$ satisfies the one-dimensional single-particle Schrodinger equation

$$-\frac{\hbar^2}{2m}\frac{d^2u}{dr^2} + \left[\frac{\hbar^2}{2m}\frac{l(l+1)}{r^2} - \frac{e^2}{r}\right]u = Eu. \tag{21}$$

Before analyzing this equation further, it is helpful to set various coefficients to one by rescaling distance and energy (units of Bohr radius $r_0 = \hbar^2/(me^2)$ and ionization energy $E_0 = me^4/(2m\hbar^2)$. We then get:

$$\partial_r^2 u + \left(\frac{2}{r} - \frac{l(l+1)}{r^2}\right) u = \epsilon u, \tag{22}$$

where we have called $\epsilon = -E/E_0$ the rescaled energy.

We can then proceed analytically just as we did for the harmonic oscillator in Physics 211, by looking for a Taylor series expansion of the solution $u(r)$, after factoring out the asymptotic behaviors in the limit $r \to 0$ and $r \to \infty$. The details are given in Griffiths and in French/Taylor. One discovers that the radial function has the form:

$$u(r) = u_{nl}(r) = r^{l+1} e^{-r} p_{n,l}(r), \tag{23}$$

of a power of r times a decaying exponential times a polynomial of order $n-l-1$ for some integer $n \geq 1$ called *the principle quantum number*, which identifies the number of nodes in the radial wave function. This corresponds to an energy level:

$$E_n = -\frac{E_1}{n^2}. \tag{24}$$

One has the important inequality:

$$l \leq n - 1, \tag{25}$$

i.e., for a given energy level n of the hydrogen atom, the angular momentum number l (which determines the magnitude squared of $\mathbf{L}$) can not be larger than $n-1$. Thus the lowest energy state of the hydrogen atom has $n = 1$, $l = m = 0$.

5. The fact that the energy of the hydrogen atom does not depend on the orbital angular momentum number l is unique among spherically-symmetric potentials, it holds only for the Coulomb $1/r$ potentials. It is related to the fact that orbits of particles in such a potential are closed, which in turn is related to the conservation of a vector quantity called the Runge-Lenz vector, which classically is given by

$$\mathbf{n} = \frac{1}{m}\mathbf{p} \times \mathbf{l} - \frac{e^2}{r}\mathbf{r}, \tag{26}$$

or quantum mechanically by the operator

$$\mathbf{N} = \frac{1}{2m}[\mathbf{P} \times \mathbf{L} - \mathbf{L} \times \mathbf{P}] - \frac{e^2}{r}\mathbf{r}. \tag{27}$$

You can read more about the links between conservation, symmetry, and degeneracy in the more advanced text book "Principles of Quantum Mechanics, 2nd Edition" by R. Shankar.