Lecture 6: Physics 212

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H. S. Greenside

1 Reading

1. French and Taylor: Sections 5-1 through 5-4, Chapter 10, Sections 11-1, 11-2, 11-4, and the Appendix on pages 506-509.
2. Griffiths: Sections 4.1, 4.3, and 4.4.

2 Questions

1. Why is it important to know whether a potential $V(x, y, z)$ is only a function of radius $r = \sqrt{x^2 + y^2 + z^2}$ so that V and be written as $V(r)$?
2. Can one measure experimentally the azimuthal coordinate ϕ of a quantum mechanical particle and simultaneously its x-component of angular momentum?

3 Concepts to Understand

1. To generalize the Schrodinger equation to three space dimensions of a single particle of mass m, one has to determine the operator corresponding to the Hamiltonian (total energy as a function of momentum and position):

$$H = \frac{\mathbf{P}^2}{2m} + V(x, y, z) \tag{1}$$

$$= \frac{1}{2m}\left(p_x^2 + p_y^2 + p_z^2\right) + V(x, y, z). \tag{2}$$

The intuitive guess that one simply replaces p_y and p_z by the generalization of what we have already discussed for $p_x = (\hbar/i)\partial_x$ turns out to be correct so that the three-dimensional single-particle time-dependent Schrodinger equation is then:

$$i\hbar\,\partial_t \Psi(t, x, y, z) = \left(\frac{-\hbar^2}{2m}\left(\partial_x^2 + \partial_y^2 + \partial_z^2\right) + V(x, y, z)\right)\Psi. \tag{3}$$

$$= \left(\frac{-\hbar^2}{2m}\nabla^2 + V\right)\Psi, \tag{4}$$

where we have used the usual abbreviation for the Laplacian operator $\nabla^2 = \triangle = \partial_x^2 + \partial_y^2 + \partial_z^2$. Just as was the case for the one-dimensional Schrodinger equation, we can solve Eq. (3) by separation of variables $\Psi(t, x, y, z) = f(t)\psi(x, y, z)$ in which case we find that a solution can be written in the form

$$\Psi(t, x, y, z) = e^{-iEt/\hbar}\psi(x, y, z), \tag{5}$$

where the stationary wave function ψ satisfies the time-independent Schrodinger equation:

$$\left(\frac{-\hbar^2}{2m}\nabla^2 + V(x, y, z)\right)\Psi = E\Psi. \tag{6}$$

The general solution to the single-particle three-dimensional time-dependent Schrodinger equation is then a superposition over all energy states:

$$\Psi(t,x,y,z) = \sum_n c_n e^{-iE_n t/\hbar} \psi_n(x,y,z), \tag{7}$$

where the amplitudes $c_n = \langle \psi_n | \Psi \rangle$ (generally complex-valued!) are determined by the initial state $\Psi(0,x,y,z)$:

$$c_n = \int_{-\infty}^{\infty} dx \int_{-\infty}^{\infty} dy \int_{-\infty}^{\infty} dz \, \psi_n(x,y,z) \Psi(0,x,y,z). \tag{8}$$

This integral can also be written in spherical coordinates as:

$$c_n = \int_0^{\infty} \int_0^{\pi} \int_0^{2\pi} \psi_n(r,\theta,\phi) \Psi(0,r,\theta,\phi) \, r^2 \sin(\theta) \, dr \, d\theta \, d\phi, \tag{9}$$

since I hope that you remember and know that an infinitesimal volume dV in spherical coordinates is given by $dV = r^2 \sin(\theta) dr \, d\theta \, d\phi$.

2. Know how to derive and use various commutation relations involving the operator vector angular momentum $\mathbf{L}$:

$$\mathbf{L} \times \mathbf{L} = i\hbar \mathbf{L}, \qquad [L^2, \mathbf{L}] = 0, , \qquad [L^2, f(r)] = 0. \tag{10}$$

3. Review your chain rule so that you understand why the z-component of the angular momentum operator

$$L_z = x p_y - y p_z, \tag{11}$$

turns into

$$L_z = \frac{\hbar}{i} \frac{\partial}{\partial \phi}, \tag{12}$$

when one changes coordinates from Cartesian to cylindrical, $(x,y,z) \to (r,\phi,z)$, or from Cartesian to spherical, $(x,y,z) \to (r,\theta,\phi)$.

More generally, you should make sure you understand the important skill of representing operators in different coordinate systems, e.g., how to derive expressions for ∇f, $\nabla \cdot \mathbf{v}$, $\nabla \times \mathbf{v}$, $\nabla^2 f$ in cylindrical and spherical geometries.

Challenge: Given a stationary state $\psi(x,y,z) = \psi(r,\theta,\phi)$, write down an expression for the probability of finding an electron a distance r from the origin where $r_1 \le r \le r_2$.

Challenge: Give a stationary state $\psi(x,y,z)$, deduce and write down a criterion for this wavefunction to be normalizable, in terms of its asymptotic (far-from-the-origin) behavior.

Considering various operators in cylindrical or spherical coordinate systems is natural since angular momentum classically corresponds to rotation of some object around an axis and one is then motivated to see how various equations appear when the coordinate system is based on this rotation axis.

4. From the generalized uncertainty principle that we discussed last semester (see Section 3.4 of Griffiths):

$$\sigma_A^2 \sigma_B^2 \ge \left(\frac{1}{2i} [A,B] \right)^2, \tag{13}$$

we see from Eq. (12) that one can not know the angular position ϕ of a quantum particle simultaneously with its z-component of angular momentum since:

$$[\phi, L_z] \neq 0. \tag{14}$$

This has some interesting implications, e.g., it implies in principle that one can not balance a pencil on its point since one would then have zero uncertainty in its angular position (it is exactly vertical) and zero uncertainty in its angular momentum around the pencil point. I'll let you figure out how to estimate how long a pencil can stay balanced if you take into account quantum mechanics.

5. By solving an operator-eigenvalue problem $L_z f = \lambda f$ and by assuming that the amplitude (not the probability) is single-valued everywhere in space, you should understand how to show that the z-component of the angular momentum is discretized and takes on the values $k\hbar$ for $k = 0, \pm 1, \pm 2, \cdots$. The integer denoting the multiple of $\hbar$ is traditionally denoted "m" and is called the "magnetic quantum number" An eigenstate of the z-component of angular momentum can then be written $|m\rangle$ which means that $L_z|m\rangle = m|m\rangle$.

6. In Section 4.3.1 of Griffiths, understand how one can use the raising/lowering operators $L_\pm = L_x \pm i L_y$ to deduce the eigenvalues
$$l(l+1)\hbar^2, \qquad l = 0, 1/2, 1, 3/2, \cdots. \tag{15}$$
of L^2, the magnitude-squared angular momentum operator. The number l is called the "orbital" or "azimuthal" quantum number.

   Since $[L^2, L_z] = 0$, one can find a set of kets that are simultaneously eigenvectors of both L^2 and L_z. These can be labeled as $|l, m\rangle$ where l is the orbital quantum number and m is the *magnetic quantum number* and, for given l, takes on the $2l + 1$ values
$$m = -l, -(l-1), -(l-2), \cdots, -1, 0, 1, \cdots, l-1, l. \tag{16}$$

   If one sees M beams coming out of a Stern-Gerlach device, we would have $2l + 1 = M$ and so the azimuthal quantum number would be $l = (M-1)/2$. If this value is half-integer (e.g., $M = 2$), then we conclude that the particles coming out of the Stern-Gerlach device must have part of their angular momentum coming from an intrinsic spin since orbital angular momenta can only lead to integer values of l.

   If you remember our theorem from Physics 211, that eigenvectors corresponding to different eigenvalues are orthogonal (I sure hope you remember this and also remember how to prove it with a few lines of algebra), then you can see immediately that:
$$\langle l, m | l', m' \rangle = \delta_{l,l'} \delta_{m,m'}, \tag{17}$$
i.e., kets having different orbital and magnetic quantum numbers are orthogonal. The Stern-Gerlach device shows this directly: if you take an output beam in a particular state $|l, m\rangle$ and send it into an identical Stern-Gerlach device, the same beam emerges with full intensity, i.e., a pure beam has no projection onto any other beam with differing m values.

7. We will discuss and derive the fact that the eigenvectors $f_{m,n}(\theta, \phi) = \langle \theta, \phi | m, n \rangle$ of the operator L^2 are the spherical harmonic functions $Y_l^m(\theta, \phi)$, which are extremely important in many areas of physics and applied mathematics. The geometric shape of the spherical harmonics for different values of quantum numbers m and n will turn out to be the key for understanding the shapes of various orbitals of atoms (but not molecules which generally lack a spherical symmetry and so have a potential that can not be written as $V = V(r)$ for some radial coordinate r).