Physics 327: Quantum Mechanics II

Course Overview, Schrödinger Equation in 3D

January 3, 2022

Prof. Russell Neilson

Syllabus

Prof. Russell Neilson
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Time:	Mon/Wed 12:00-1:50pm
In person location:	Curtis Hall 258
Remote synchronous link:	

https://drexel.zoom.us/meeting/register/tZYucO2upzkpGNcG3_ap3HDwfrAKFj4KIoSL

Required Text:	*Introduction to Quantum Mechanics*, 3rd Edition, by David J. Griffiths and Darrell F. Schroeter (2018).
In person help session:	TBD
Zoom help session:	By appointment using the same zoom session as class. Please email.

Course Description: Covers the three-dimensional Schrodinger equation, angular momentum, matrix mechanics, the hydrogen atom, and perturbation theory.

Course purpose within a program of study: This course will partially fulfill the requirement for core courses in the plan of study for a B.S. in Physics.

Prerequisites: PHYS 326.

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Statement of expected learning: This course will address the Drexel Learning Priorities, including Communication, Information Literacy, and Technology Use. By the end of this course, students will be able to do the following:

- Solve for the eigenstates and energies of a single particle in three dimensions for the case of central potential.
- Understand the detailed structure of the wave function for Hydrogen and hydrogen-like atoms.
- Compute properties of systems including orbital angular momentum and spin, including magnetic moments.
- Solve for the eigenstates and energies of multiple particle systems such as occur in simple atoms and solids.
- Find most probable configurations and energies of many-particle, many-level systems using quantum statistical mechanics.
- Use knowledge of the eigenstates and energies of simple systems and approximation methods to solve for energies of perturbed systems.

Grading matrix: Grades will be based on:

Homework: 35%
Midterm: 25%
Final: 40%

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Homework problems will be collected and graded most weeks. Homework may be submitted in class, or electronically on Learn. If submitting electronically, please submit a PDF file. Students are encouraged to work together on homework in the form of study groups and discussions, but copying is not acceptable. Exams will be open book and open notes, but sharing among students and use of additional online materials is strictly forbidden. Students in violation of these policies will receive no credit for the assignment.

Grade scale:
A 90-100, **B** 80-89, **C** 70-79, **D** 60-69, **F** 0-59

Late Homework policy: It is expected that homework will be submitted on time. Unexcused late homework will be subject to a 25% penalty. If you require an extension, please request by email before the due date.

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Course calendar: Students are expected to complete assigned readings before scheduled classes. Homework assignments will be posted on Learn and are due by the end of the day on Thursdays. Below is a rough guide of anticipated course content and due dates. Note, this is likely to vary.

Week	Textbook sections	Homework/Midterm
1/3-1/7*	4.1	
1/10-1/14*	4.2	HW #1 due
1/18-1/21	MLK, 4.3	HW #2 due
1/24-1/38	4.4	HW #3 due
1/31-2/4	Review, Midterm	Midterm 2/2
2/7-2/11	5.1	HW #4 due
2/14-2/18	5.2	HW #5 due
2/21-2/25	5.3	HW #6 due
2/28-3/4	7.1	HW #7 due
3/7-3/11	Review	HW #8 due

*Remote synchronous classes, following Drexel University COVID-19 policy.

Course policies: The instructor reserves the right to change the course as described in this syllabus at any time. Students will be notified of changes by email and class announcement

Schrödinger equation in 3D

To tackle most “real” problems, we need to work in three dimensions.

Fortunately, generalizing the Schrödinger equation to 3D is not too difficult. Solving it on the other hand will add some few complications…

Recall from QM-I (1D)

Time-dependent Schrödinger equation:

$$i\hbar\frac{\partial\Psi}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2\Psi}{\partial x^2} + V\Psi$$

or

$$i\hbar\frac{\partial\Psi}{\partial t} = \hat{H}\Psi$$

Where $H = \frac{1}{2}mv^2 + V = \frac{p^2}{2m} + V$ and we replace $p \rightarrow -i\hbar\frac{\partial}{\partial x}$

We found stationary states by solving the time-independent Schrödinger equation

$$\hat{H}\psi(\mathrm{x}) = \mathrm{E}\psi(x)$$

and tacked on a time-dependent phase factor (wiggle factor)

$$\Psi_n(x,t) = \psi_n(x)e^{-iE_n t/\hbar}$$

Generalizing to 3D

In 3D

$$H = \frac{1}{2}mv^2 + V = \frac{p^2}{2m} + V = \frac{1}{2m}\left(p_x^2 + p_y^2 + p_z^2\right) + V$$

Now we replace each component of p by its operator:

$$p_x \to -i\hbar\frac{\partial}{\partial x}, \qquad p_y \to -i\hbar\frac{\partial}{\partial y}, \qquad p_z \to -i\hbar\frac{\partial}{\partial z}$$

Which we can write in terms of the gradient operator (‘grad’, ’del’, ‘nabla’) $\nabla = \left(\frac{\partial}{\partial x}, \frac{\partial}{\partial y}, \frac{\partial}{\partial z}\right)$

$$\mathbf{p} \to -i\hbar\nabla$$

Then we get

$$H = -\frac{\hbar^2}{2m}\nabla^2 + V$$

Where we have the Laplacian

$$\nabla^2 \equiv \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}$$

Generalizing to 3D

So the Schrödinger equation is

$$i\hbar\frac{\partial\Psi}{\partial t} = -\frac{\hbar^2}{2m}\nabla^2\Psi + V\Psi$$

Ψ and V are now functions of $\boldsymbol{r} = (x, y, z)$ and t.

As in 1D, we can use separation of variables to find the time-*independent* Schrödinger equation:

$$-\frac{\hbar^2}{2m}\nabla^2\psi + V\psi = E\psi$$

with stationary state solutions. The general solution to the time-*dependent* equation is then:

$$\Psi(\mathbf{r}, t) = \sum_{n=1}^{\infty} c_n\psi_n(\mathbf{r})e^{-iE_n t/\hbar}$$

The normalization condition is now a 3D integral over all space

$$\int |\Psi|^2 d^3\mathbf{r} = 1$$

Spherical coordinates

It’s very common to have a spherical potential $V = V(r)$, where it is natural to work in spherical coordinates (r, θ, ϕ).

We can look up the Laplacian in spherical coordinates

$$\nabla^2 = \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right) + \frac{1}{r^2 \sin\theta}\frac{\partial}{\partial \theta}\left(\sin\theta\frac{\partial}{\partial \theta}\right) + \frac{1}{r^2 \sin^2\theta}\left(\frac{\partial^2}{\partial \phi^2}\right)$$

So, the time-independent Schrödinger equation becomes

$$-\frac{\hbar^2}{2m}\left[\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right) + \frac{1}{r^2 \sin\theta}\frac{\partial}{\partial \theta}\left(\sin\theta\frac{\partial}{\partial \theta}\right) + \frac{1}{r^2 \sin^2\theta}\left(\frac{\partial^2}{\partial \phi^2}\right)\right]\psi + V\psi = E\psi$$

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We'll define $k^2 = \frac{2m}{\hbar^2}(E - V)$ to get

$$\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2 \frac{\partial \psi}{\partial r}\right) + \frac{1}{r^2 \sin\theta}\frac{\partial}{\partial \theta}\left(\sin\theta \frac{\partial \psi}{\partial \theta}\right) + \frac{1}{r^2 \sin^2\theta}\left(\frac{\partial^2 \psi}{\partial \phi^2}\right) = -k^2\psi$$

Separation of variables

We'll look for a separable solution

$$\psi(r,\theta,\phi) = R(r)\Theta(\theta)\Phi(\phi)$$

Plug in to Schrödinger equation and divide by $R\Theta\Phi$

$$\frac{1}{Rr^2}\frac{d}{dr}\left(r^2\frac{dR}{dr}\right) + \frac{1}{\Theta r^2 \sin\theta}\frac{d}{d\theta}\left(\sin\theta\frac{d\Theta}{d\theta}\right) + \frac{1}{\Phi r^2 \sin^2\theta}\left(\frac{d^2\Phi}{d\phi^2}\right) = -k^2$$

Multiply by $r^2 \sin^2\theta$ and rearrange

$$\frac{1}{\Phi}\left(\frac{d^2\Phi}{d\phi^2}\right) = r^2\sin^2\theta\left[-k^2 - \frac{1}{Rr^2}\frac{d}{dr}\left(r^2\frac{dR}{dr}\right) - \frac{1}{\Theta r^2 \sin\theta}\frac{d}{d\theta}\left(\sin\theta\frac{d\Theta}{d\theta}\right)\right]$$

Since LHS is a function of ϕ only, and RHS is not a function of ϕ, both sides must be a constant, we'll call it $-m^2$

Φ equation

$$\frac{1}{\Phi}\left(\frac{d^2\Phi}{d\phi^2}\right) = -m^2$$

$$\left(\frac{d^2\Phi}{d\phi^2}\right) = -m^2\Phi$$

Solution:

$$\Phi = e^{im\phi}$$

(don’t worry about normalization for now)

Periodicity $\Phi(\phi + 2\pi) = \Phi(\phi)$ requires $m = 0, \pm 1, \pm 2, \ldots$

RHS of the equation

$$r^2 \sin^2\theta \left[-k^2 - \frac{1}{Rr^2}\frac{d}{dr}\left(r^2\frac{dR}{dr}\right) - \frac{1}{\Theta r^2 \sin\theta}\frac{d}{d\theta}\left(\sin\theta\frac{d\Theta}{d\theta}\right)\right] = -m^2$$

Divide by $\sin^2\theta$ and rearrange:

$$\frac{1}{R}\frac{d}{dr}\left(r^2\frac{dR}{dr}\right) + r^2k^2 = -\frac{1}{\Theta\sin\theta}\frac{d}{d\theta}\left(\sin\theta\frac{d\Theta}{d\theta}\right) + \frac{m^2}{\sin^2\theta}$$

Now LHS depends only on r and RHS depends only on θ, so both must be constant (remember k depends on $V(r)$). We'll call that constant $l(l+1)$.

Θ equation

$$-\frac{1}{\Theta \sin\theta}\frac{d}{d\theta}\left(\sin\theta \frac{d\Theta}{d\theta}\right) + \frac{m^2}{\sin^2\theta} = l(l+1)$$

$$\frac{1}{\sin\theta}\frac{d}{d\theta}\left(\sin\theta \frac{d\Theta}{d\theta}\right) - \frac{m^2}{\sin^2\theta}\Theta + l(l+1)\Theta = 0$$

Solutions for this are the **associated Legendre functions**

$$\Theta(\theta) = AP_l^m(\cos\theta)$$

which are related to the **Legendre polynomials** $P_l(x)$:

$$P_l^m(x) = (-1)^m(1-x^2)^{m/2}\left(\frac{d}{dx}\right)^m P_l(x) \qquad (m \geq 0).$$

$$P_l^{-m}(x) = (-1)^m\frac{(l-m)!}{(l+m)!}P_l^m(x)$$

Legendre Polynomials

The Legendre polynomials themselves can be found by the Rodrigues formula:

$$P_l(x) = \frac{1}{2^l l!}\left(\frac{d}{dx}\right)^l (x^2 - 1)^l$$

Examples:

$$P_0 = 1$$

$$P_1 = \frac{1}{2}\frac{d}{dx}(x^2 - 1) = x$$

etc

Legendre Polynomials

$$P_0 = 1$$

$$P_1 = x$$

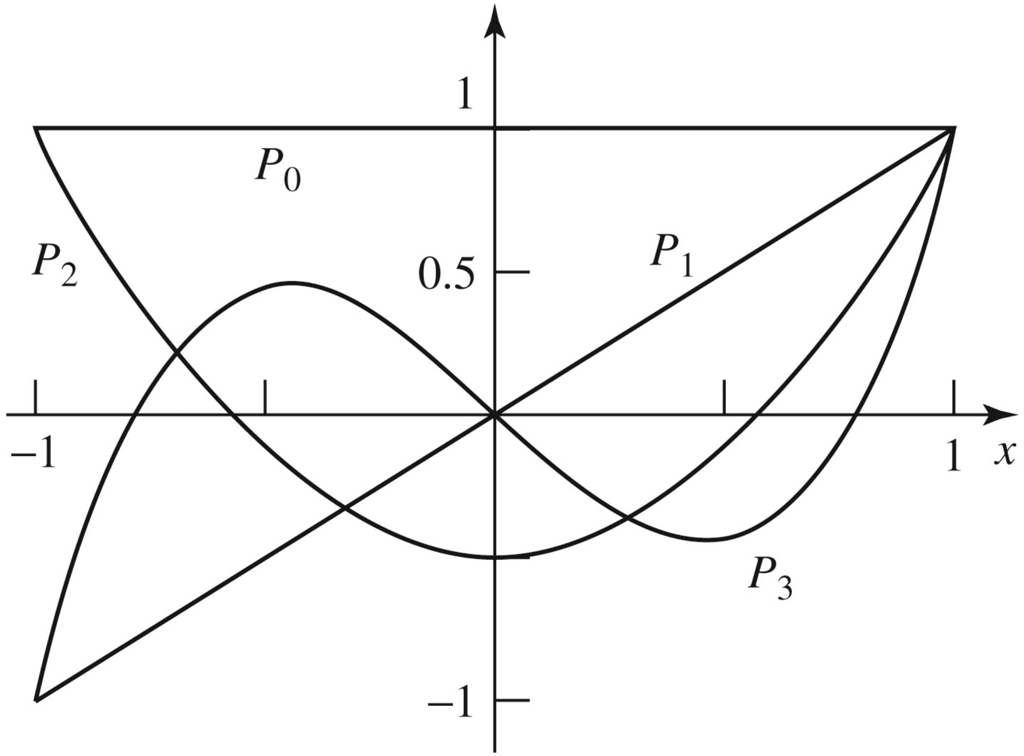
$$P_2 = \frac{1}{2}(3x^2 - 1)$$

$$P_3 = \frac{1}{2}(5x^3 - 3x)$$

$$P_4 = \frac{1}{8}(35x^4 - 30x^2 + 3)$$

$$P_5 = \frac{1}{8}(63x^5 - 70x^3 + 15x)$$

(a)



(b)

$P_l(x)$ is a polynomial of degree l, and alternates even and odd. l must be a non-negative integer.

Associated Legendre functions

For $l = 0$: $P_0 = 1, P_0^0 = 1$, and can't have $m \neq 0$ because $\frac{d}{dx} P_0 = 0$.

For $l = 1$: $P_1 = x, P_1^0 = x, P_1^1 = -\sqrt{1 - x^2}$

For $l = 2$

$$P_2^0 = \frac{1}{2}(3x^2 - 1)$$

$$P_2^1 = -\sqrt{1 - x^2}\frac{d}{dx}\left[\frac{1}{2}(3x^2 - 1)\right] = -3x\sqrt{1 - x^2}$$

$$P_2^2 = (1 - x^2)\left(\frac{d}{dx}\right)^2\left[\frac{1}{2}(3x^2 - 1)\right] = 3(1 - x^2)$$

Note, if $m > l$ then $P_l^m = 0$.

So, we have $l = 0,1,2, \ldots$ and $m = -l\,, -l + 1\,, \ldots 0\,, \ldots\; l - 1\,, l$

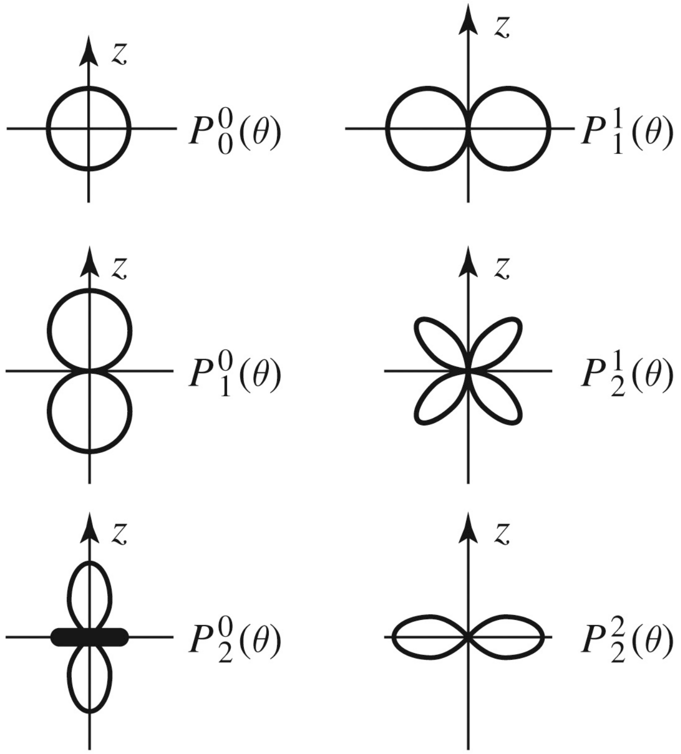
Associated Legendre functions

Note, we want $P_l^m(\cos\theta)$ instead of $P_l^m(x)$.

Conveniently, the $\sqrt{1-x^2}$ terms that appear become $\sqrt{1-\cos^2\theta} = \sin\theta$

$P_0^0 = 1$	$P_2^0 = \frac{1}{2}(3\cos^2\theta - 1)$
$P_1^1 = -\sin\theta$	$P_3^3 = -15\sin\theta(1-\cos^2\theta)$
$P_1^0 = \cos\theta$	$P_3^2 = 15\sin^2\theta\cos\theta$
$P_2^2 = 3\sin^2\theta$	$P_3^1 = -\frac{3}{2}\sin\theta(5\cos^2\theta - 1)$
$P_2^1 = -3\sin\theta\cos\theta$	$P_3^0 = \frac{1}{2}(5\cos^3\theta - 3\cos\theta)$

(a)



(b)

Plots of $r = |P_l^m(\cos\theta)|$. Each figure should be rotated about the z-axis

Spherical harmonics

We can combine the angular parts of $\Psi = R\Theta\Phi$ into one function

$$Y(\theta, \phi) = \Theta(\theta)\Phi(\phi).$$

These are called spherical harmonics.

$$Y_l^m(\theta, \phi) = A_l^m P_l^m(\cos\theta)e^{im\phi}$$

Where A_l^m is some normalization constant.