**PHY 741 Quantum Mechanics**
**12-12:50 PM MWF Olin 103**

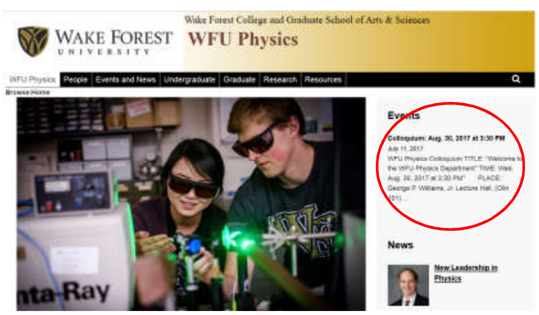
**Plan for Lecture 1:**

1. **Welcome & overview**
2. **Class structure & announcements**
3. **Overview of Mathematical Tools (Chapter 1 of our textbook)**
   a. **Notation**
   b. **Vector spaces**



Comment about Physics Colloquia

http://www.physics.wfu.edu






WFU Physics Colloquium

**TITLE:** "Welcome to the WFU Physics Department"
**TIME:** Wed. Aug. 30, 2017 at 3:30 PM*
**PLACE:** George P. Williams, Jr. Lecture Hall, (Olin 101)
* Note: early starting time.

Refreshments will be served at 3:00 PM in the lounge. All interested persons are cordially invited to attend.

PROGRAM

The purpose of this first seminar is to help new, returning, and prospective students (including both undergraduate and graduate students), faculty, and staff to become acquainted with each other and with the Physics Department. After refreshments in the lounge in the lobby of Olin Physical Laboratory (starting at 3:00), we will meet in the George P. Williams, Jr. Lecture Hall (Olin 101) at 3:30 PM for some announcements followed by presentations by some undergraduate students, highlighting their summer research experiences.

**Fall 2017 Schedule**
**for N. A. W. Holzwarth**

| | Monday | Tuesday | Wednesday | Thursday | Friday |
|---|---|---|---|---|---|
| 9:00-10:00 | Classical Mechanics PHY711 | | Classical Mechanics PHY711 | | Classical Mechanics PHY711 |
| 10:00-12:00 | Lecture Preparation/ Office Hours | | Lecture Preparation/ Office Hours | | Lecture Preparation/ Office Hours |
| 12:00-1:00 | Quantum Mechanics PHY741 | Physics Research | Quantum Mechanics PHY741 | Physics Research | Quantum Mechanics PHY741 |
| 1:00-2:15 | Condensed Matter Theory Journal Club | | Physics Research | | |
| 2:15-3:30 | | | | | Physics Research |
| 3:30-5:00 | Physics Research | | Physics Colloquium | | |

email: natalie@wfu.edu office: Olin 300

8/28/2017 PHY 741 Fall 2017 -- Lecture 1 4

Course webpage: http://www.wfu.edu/~natalie/f17phy741

## PHY 741 Quantum Mechanics

| | | |
|---|---|---|
| MWF 12 PM - 12:50 PM | OPL 103 | http://www.wfu.edu/~natalie/f17phy741/ |

| | | | |
|---|---|---|---|
| **Instructor:** Natalie Holzwarth | **Phone:**758-5510 | **Office:**300 OPL | **e-mail:**natalie@wfu.edu |

- General information
- Syllabus and homework assignments
- Lecture Notes

Last modified: Saturday, 26-Aug-2017 01:02:32 EDT

8/28/2017 PHY 741 Fall 2017 -- Lecture 1 5

Course webpage:
http://www.wfu.edu/~natalie/f17phy741/info

## PHY 741 Quantum Mechanics

| | | |
|---|---|---|
| MWF 12 PM - 12:50 PM | OPL 103 | http://www.wfu.edu/~natalie/f17phy741/ |

| | | | |
|---|---|---|---|
| **Instructor:** Natalie Holzwarth | **Phone:**758-5510 | **Office:**300 OPL | **e-mail:**natalie@wfu.edu |

### General Information

This course is the first semester of a two semester survey of Quantum Mechanics at the graduate level, using the textbook: **Principles of Quantum Mechanics (Second Edition)** by R. Shankar (Springer, 1994).

It is likely that your grade for the course will depend upon the following factors:

| | |
|---|---|
| Problem sets* | 40% |
| Computational project | 20% |
| Exams | 40% |

*In general, there will a new assignment after each lecture, so that for optimal learning, it would be best to complete each assignment before the the next scheduled lecture. According to the honor system, all work submitted for grading purposes should represent the student's own best efforts.

8/28/2017 PHY 741 Fall 2017 -- Lecture 1 6

Course webpage:
http://www.wfu.edu/~natalie/f17phy741/info

## PHY 741 Quantum Mechanics

| MWF 12 PM - 12:50 PM | OPL 103 | http://www.wfu.edu/~natalie/f17phy741/ |
|---|---|---|

| Instructor: Natalie Holzwarth | Phone:758-5510 | Office:300 OPL | e-mail:natalie@wfu.edu |
|---|---|---|---|

### Computational Project

The purpose of this assignment is to provide an opportunity for you to study a topic of your choice in greater depth. The general guideline for your choice of project is that it should have something to do with quantum mechanics, and there should be some degree of computation associated with the project. The completed project will include a short write-up and a ~20min presentation to the class. You may design your own project or use one of the following list (which will be updated throughout the term).

- Consider a scattering experiment in which you specify the spherically symetric interaction potential V(r). Write a computer program (using your favorite language) to evaluate the scattering phase shifts and cross section for your system. Or you can use the Born approximation to estimate the scattering cross section.
- Use the variation method to find the lowest eigenstate of a Schödinger equation of your choice.
- Using degenerate perturbation theory, analyze the spin splitting of your favorite open shell atom in the presence of a magnetic field B, showing both the Zeeman and Paschen-Back limits.



Course webpage: http://www.wfu.edu/~natalie/f17phy741/homework

## PHY 741 Quantum Mechanics

| MWF 12 PM - 12:50 PM | OPL 103 | http://www.wfu.edu/~natalie/f17phy741/ |
|---|---|---|

| Instructor: Natalie Holzwarth | Phone:758-5510 | Office:300 OPL | e-mail:natalie@wfu.edu |
|---|---|---|---|

### Course schedule

(Preliminary schedule -- subject to frequent adjustment.)

| | Date | F&W Reading | Topic | Assignment | Due |
|---|---|---|---|---|---|
| 1 | Mon, 8/28/2017 | Chap. 1 | Review of basic principles | #1 | 9/6/2017 |
| 2 | Wed, 8/30/2017 | | | | |
| 3 | Fri, 9/01/2017 | | | | |
| 4 | Mon, 9/04/2017 | | | | |
| 5 | Wed, 9/06/2017 | | | | |
| 6 | Fri, 9/08/2017 | | | | |
| 7 | Mon, 9/11/2017 | | | | |
| 8 | Wed, 9/13/2017 | | | | |
| 9 | Fri, 9/15/2017 | | | | |
| 10 | Mon, 9/18/2017 | | | | |



## PHY 741 – Assignment #1

08/28/2017

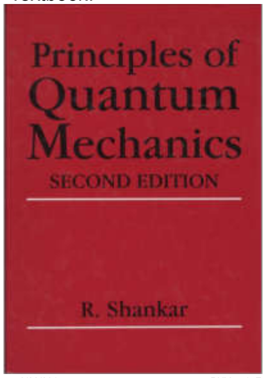
Read Chapter 1 of **Shankar**.

1. Consider a 3-dimensional vector space with three non-orthogonal vectors $|v_1\rangle$, $|v_2\rangle$, and $|v_3\rangle$, where

$$|v_1\rangle = \hat{\mathbf{x}} + \hat{\mathbf{y}} + \hat{\mathbf{z}}$$
$$|v_2\rangle = \hat{\mathbf{x}} + \hat{\mathbf{y}} - \hat{\mathbf{z}}$$
$$|v_3\rangle = \hat{\mathbf{x}} - \hat{\mathbf{y}} + \hat{\mathbf{z}}.$$

Use the Gram-Schmidt procedure to form 3 orthonormal vectors $|w_1\rangle$, $|w_2\rangle$, and $|w_3\rangle$. Determine expressions for $|w_1\rangle$, $|w_2\rangle$, and $|w_3\rangle$ in terms of $\hat{\mathbf{x}}$, $\hat{\mathbf{y}}$, and $\hat{\mathbf{z}}$.

Textbook:

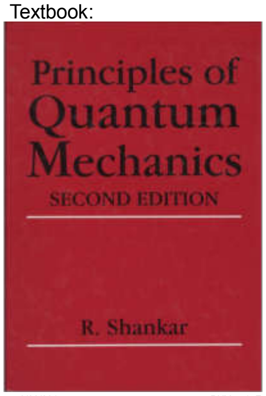



Topics

- Mathematical introduction
- Review of classical mechanics and emergence of quantum effects
- Simple one-dimensional systems in the quantum and classical treatments
- The harmonic oscillator
- Feynman's path integrals
- Multi-dimensional systems
- Angular momentum
- The hydrogen atom
- Spin
- Approximation methods
- Time-dependence



Textbook:




Topics -- continued

- Time-dependent perturbation theory
- Scattering theory
- The Dirac equation
- More about path integrals

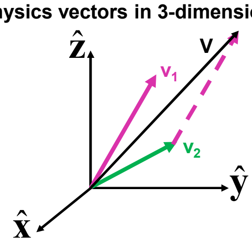


Read Chapter 1 -- (1.1-1.4)

Mathematical tools useful for studying quantum mechanics

Notion of generalized linear vector space

**Physics vectors in 3-dimensional space**




$$\mathbf{V} = \mathbf{v}_1 + \mathbf{v}_2$$

## Abstract linear vector space

*Definition 1. A linear vector space* $\mathbb{V}$ *is a collection of objects* $|1\rangle$, $|2\rangle, \ldots, |V\rangle, \ldots, |W\rangle, \ldots$, called vectors, for which there exists

1. A definite rule for forming the vector sum, denoted $|V\rangle + |W\rangle$
2. A definite rule for multiplication by scalars $a, b, \ldots$, denoted $a|V\rangle$ with the following features:

- The result of these operations is another element of the space, a feature called *closure*: $|V\rangle + |W\rangle \in \mathbb{V}$.
- Scalar multiplication is *distributive in the vectors*: $a(|V\rangle + |W\rangle) = a|V\rangle + a|W\rangle$.
- Scalar multiplication is *distributive in the scalars*: $(a+b)|V\rangle = a|V\rangle + b|V\rangle$.
- Scalar multiplication is *associative*: $a(b|V\rangle) = ab|V\rangle$.
- Addition is *commutative*: $|V\rangle + |W\rangle = |W\rangle + |V\rangle$.
- Addition is *associative*: $|V\rangle + (|W\rangle + |Z\rangle) = (|V\rangle + |W\rangle) + |Z\rangle$.
- There exist a *null vector* $|0\rangle$ obeying $|V\rangle + |0\rangle = |V\rangle$.
- For every vector $|V\rangle$ there exists an *inverse under addition*, $|-V\rangle$, such that $|V\rangle + |-V\rangle = |0\rangle$.



## Comment on bra and ket notation

For an $n$ dimensional vector space, $|V\rangle = \begin{pmatrix} v_1 \\ v_2 \\ v_3 \\ v_4 \\ \vdots \\ v_n \end{pmatrix}$

$$\langle W| = \begin{pmatrix} w_1^* & w_2^* & w_3^* & w_4^* & \cdots & w_n^* \end{pmatrix}$$

$$\langle W|V\rangle = w_1^* v_1 + w_2^* v_2 + \cdots w_n^* v_n$$



## Notion of linear independence

The next concept is that of *linear independence* of a set of vectors $|1\rangle, |2\rangle \ldots |n\rangle$. First consider a linear relation of the form

$$\sum_{i=1}^{n} a_i |i\rangle = |0\rangle \qquad (1.1.1)$$

We may assume without loss of generality that the left-hand side does not contain any multiple of $|0\rangle$, for if it did, it could be shifted to the right, and combined with the $|0\rangle$ there to give $|0\rangle$ once more. (We are using the fact that any multiple of $|0\rangle$ equals $|0\rangle$.)

*Definition 3.* The set of vectors is said to be *linearly independent* if the only such linear relation as Eq. (1.1.1) is the trivial one with all $a_i = 0$. If the set of vectors is not linearly independent, we say they are *linearly dependent*.

Note that linear independence does not necessarily imply that the vectors are orthogonal.

**Gram–Schmidt Theorem**

Let us now take up the Gram–Schmidt procedure for converting a linearly independent basis into an orthonormal one. The basic idea can be seen by a simple example. Imagine the two-dimensional space of arrows in a plane. Let us take two nonparallel vectors, which qualify as a basis. To get an orthonormal basis out of these, we do the following:

- Rescale the first by its own length, so it becomes a unit vector. This will be the first basis vector.
- Subtract from the second vector its projection along the first, leaving behind only the part perpendicular to the first. (Such a part will remain since by assumption the vectors are nonparallel.)
- Rescale the left over piece by its own length. We now have the second basis vector: it is orthogonal to the first and of unit length.



Let $|I\rangle, |II\rangle, \ldots$ be a linearly independent basis. The first vector of the orthonormal basis will be

$$|1\rangle = \frac{|I\rangle}{|I|} \quad \text{where} \quad |I| = \sqrt{\langle I|I\rangle}$$

Clearly

$$\langle 1|1\rangle = \frac{\langle I|I\rangle}{|I|^2} = 1$$

As for the second vector in the basis, consider

$$|2'\rangle = |II\rangle - |1\rangle\langle 1|II\rangle$$

which is $|II\rangle$ minus the part pointing along the first unit vector. (Think of the arrow example as you read on.) Not surprisingly it is orthogonal to the latter:

$$\langle 1|2'\rangle = \langle 1|II\rangle - \langle 1|1\rangle\langle 1|II\rangle = 0$$

We now divide $|2'\rangle$ by its norm to get $|2\rangle$ which will be orthogonal to the first and normalized to unity



Summary of Gram-Schmidt procedure:

$$|1\rangle = \frac{|I\rangle}{\sqrt{\langle I|I\rangle}}$$

$$|2\rangle = \frac{|2'\rangle}{\sqrt{\langle 2'|2'\rangle}} \quad \text{where } |2'\rangle = |II\rangle - |1\rangle\langle 1|II\rangle$$

$$|3\rangle = \frac{|3'\rangle}{\sqrt{\langle 3'|3'\rangle}} \quad \text{where } |3'\rangle = |III\rangle - |1\rangle\langle 1|III\rangle - |2\rangle\langle 2|III\rangle$$

Note that, the orthonormal basis set is not unique

## Other methods of finding orthonormal basis from linearly independent vectors.

Suppose you have an n-dimensional set of non-orthogonal basis functions:

$$|V\rangle = \begin{pmatrix} v_1 \\ v_2 \\ v_3 \\ v_4 \\ \vdots \\ v_n \end{pmatrix}.$$

Form an $n \times n$ overlap matrix $O = \begin{pmatrix} \langle v_1|v_1\rangle & \langle v_1|v_2\rangle & \langle v_1|v_3\rangle & \langle v_1|v_4\rangle & \cdots & \langle v_1|v_n\rangle \\ \langle v_2|v_1\rangle & \langle v_2|v_2\rangle & \langle v_2|v_3\rangle & \langle v_2|v_4\rangle & \cdots & \langle v_2|v_n\rangle \\ \langle v_3|v_1\rangle & \langle v_3|v_2\rangle & \langle v_3|v_3\rangle & \langle v_3|v_4\rangle & \cdots & \langle v_3|v_n\rangle \\ \langle v_4|v_1\rangle & \langle v_4|v_2\rangle & \langle v_4|v_3\rangle & \langle v_3|v_4\rangle & \cdots & \langle v_4|v_n\rangle \\ \vdots & \vdots & \vdots & \vdots & \cdots & \vdots \\ \langle v_n|v_1\rangle & \langle v_n|v_2\rangle & \langle v_n|v_3\rangle & \langle v_n|v_4\rangle & \cdots & \langle v_n|v_n\rangle \end{pmatrix}$



## Other methods of finding orthonormal basis from linearly independent vectors -- continued

$$O = \begin{pmatrix} \langle v_1|v_1\rangle & \langle v_1|v_2\rangle & \langle v_1|v_3\rangle & \langle v_1|v_4\rangle & \cdots & \langle v_1|v_n\rangle \\ \langle v_2|v_1\rangle & \langle v_2|v_2\rangle & \langle v_2|v_3\rangle & \langle v_2|v_4\rangle & \cdots & \langle v_2|v_n\rangle \\ \langle v_3|v_1\rangle & \langle v_3|v_2\rangle & \langle v_3|v_3\rangle & \langle v_3|v_4\rangle & \cdots & \langle v_3|v_n\rangle \\ \langle v_4|v_1\rangle & \langle v_4|v_2\rangle & \langle v_4|v_3\rangle & \langle v_3|v_4\rangle & \cdots & \langle v_4|v_n\rangle \\ \vdots & \vdots & \vdots & \vdots & \cdots & \vdots \\ \langle v_n|v_1\rangle & \langle v_n|v_2\rangle & \langle v_n|v_3\rangle & \langle v_n|v_4\rangle & \cdots & \langle v_n|v_n\rangle \end{pmatrix}$$

It can be shown that:

- ***O*** is a Hermitian, positive definite matrix
- Its eigenvectors can be put into orthonormal form



## Other methods of finding orthonormal basis from linearly independent vectors -- continued

Suppose we find the eigenvalues and eigenvectors of $\mathbf{O}$:

$$\mathbf{O}|w_1\rangle = \lambda_1|w_1\rangle$$
$$\mathbf{O}|w_2\rangle = \lambda_2|w_2\rangle$$
$$\vdots$$
$$\mathbf{O}|w_n\rangle = \lambda_n|w_n\rangle$$

It follows that $\langle w_i|w_j\rangle = 0$ for $i \neq j$

If eigenfunctions are normalized in the usual way then,

$$\langle w_i|w_j\rangle = \delta_{ij}$$

$\Rightarrow \{|w_i\rangle\}$ can be used as orthonormal basis with the same span as $\{|v_i\rangle\}$.