PHY 742 Quantum Mechanics II
1-1:50 AM MWF Olin 103

Plan for Lecture 1

1. **Structure of the course**
2. **Review of main concepts from Quantum Mechanics I**
3. **Preview of topics for Quantum Mechanics II**
4. **Quantum particle interacting with classical electromagnetic fields**
   Reading: Chapter 9 in Carlson's textbook

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PHY 742 Quantum Mechanics II>

MWF 1-1:50 PM	**OPL 103**	**http://www.wfu.edu/~natalie/s20phy742/**

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- General information
- Syllabus and homework assignments
- Lecture notes

Last modfied: Saturday, 04-Jan-2020 01:14:28 EST

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General Information

This course is a continuation of Quantum Mechanics II, using the textbook written by Professor Eric Carlson Quantum Mechanics. Note that by request of Professor Carlson, the textbook is available to all WFU students and staff through his password controlled link. WFU students and staff are welcome to download the full pdf file of the textbook, but are requested to not distribute it outside of WFU. The course material for PHY 742 will start approximately with Chapter 9 of the textbook. Students may also wish to consult the following additional texts:

- L. D. Landau and E. M. Lifshitz, **Quantum Mechanics (Non-relativistic theory)**
- Eugen Merzbacher, **Quantum Mechanics**
- Leonard I. Schiff, **Quantum Mechanics**
- Claude Cohen-Tannoudji, Bernard Diu, and Franck Laloë, **Quantum Mechanics, Vol. one, Vol. two**
- J. J. Sakurai, **Modern Quantum Mechanics**
- J. J. Sakurai, **Advanced Quantum Mechanics**

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

Problem sets*	45%
Presentation	10%
Exams	45%

*The schedule notes the "due" date for each assignment. Homeworks may be turned in 1 lecture past their due date without grade penalty. After that, the homework grade will be reduced by 10% for each succeeding late date. According to the honor system, all work submitted for grading purposes should represent the student's own best efforts. This means that students who work together on homework assignments should all contribute roughly equally and independently verify all derivations and results.

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Course schedule for Spring 2020

(Preliminary schedule -- subject to frequent adjustment.)

	Lecture date	Reading	Topic	HW	Due date
1	Mon: 01/13/2020	Chap. 9	Quantum mechanics of electromagnetic forces	#1	01/22/2020
2	Wed: 01/15/2020	Chap. 9			
3	Fri: 01/17/2020	Chap. 9			
	Mon: 01/20/2020	No class	Martin Luther King Holiday		
4	Wed: 01/22/2020				
5	Fri: 01/24/2020				
6	Mon: 01/27/2020				
7	Wed: 01/29/2020				
8	Fri: 01/31/2020				
9	Mon: 02/03/2020				
10	Wed: 02/05/2020				

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Discussion points on course structure –

1. **Where/how to keep supplemental texts?**
2. **Take home exams**
   a. **Mid-term during the week of Mar. 2-6**
   b. **Final during the week of May 1-8**
3. **Presentations?**
   How to interface with PHY 712 presentations?

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Summary of topics covered in Quantum Mechanics I

Topic	Chapters in EC Text
Fundamentals and formalism of QM	1,3,4,11
Solution of S. E. for simple 1-dim potentials	2
Quantum mechanics of harmonic oscillator	5
Angular momentum	7
Addition and rotation of angular momentum including spin	8
Hydrogen atom	7
Time-independent perturbation theory methods	12

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Topics for Quantum Mechanics II

Single particle analysis

- Single particle interacting with electromagnetic fields – EC Chap. 9
- Scattering of a particle from a spherical potential – EC Chap. 14
- More time independent perturbation methods – EC Chap. 12, 13
- Single electron states of a multi-well potential ➔ molecules and solids – EC Chap. 2,6
- Time dependent perturbation methods – EC Chap. 15
- Relativistic effects and the Dirac Equation – EC Chap. 16

Multiple particle analysis

- Quantization of the electromagnetic fields – EC Chap. 17
- Photons and atoms – EC Chap. 18
- Multi particle systems; Bose and Fermi particles – EC Chap. 10
- Multi electron atoms and materials
  - Hartree-Fock approximation
  - Density functional approximation

Interaction of a particle with an electromagnetic field
Ref: Chapter 9 of Professor Carlson's text
Additional references: L&L #22, XVI

Results from Classical Mechanics: (cgs Gaussian units)

General treatment of particle of mass m and charge q moving in 3 dimensions in a potential $V(\mathbf{r})$ as well as electromagnetic scalar and vector potentials $U(\mathbf{r},t)$ and $\mathbf{A}(\mathbf{r},t)$:

Lagrangian: $$L(\mathbf{r},\dot{\mathbf{r}},t)=\frac{1}{2}m\dot{\mathbf{r}}^2-V(\mathbf{r})-qU(\mathbf{r},t)+\frac{q}{c}\dot{\mathbf{r}}\cdot\mathbf{A}(\mathbf{r},t)$$

Hamiltonian: $$\mathbf{p}=\frac{\partial L}{\partial\dot{\mathbf{r}}}=m\dot{\mathbf{r}}+\frac{q}{c}\mathbf{A}(\mathbf{r},t)$$

$$H(\mathbf{r},\mathbf{p},t)=\mathbf{p}\cdot\dot{\mathbf{r}}-L(\mathbf{r},\dot{\mathbf{r}},t)$$

$$=\frac{1}{2m}\left(\mathbf{p}-\frac{q}{c}\mathbf{A}(\mathbf{r},t)\right)^2+V(\mathbf{r})+qU(\mathbf{r},t)$$

Results from Classical Mechanics, (cgs Gaussian units) continued

Some details: $L(\mathbf{r},\dot{\mathbf{r}},t)=\frac{1}{2}m\dot{\mathbf{r}}^2-V(\mathbf{r})-qU(\mathbf{r},t)+\frac{q}{c}\dot{\mathbf{r}}\cdot\mathbf{A}(\mathbf{r},t)$

Hamiltonian: $\mathbf{p}=\frac{\partial L}{\partial\dot{\mathbf{r}}}=m\dot{\mathbf{r}}+\frac{q}{c}\mathbf{A}(\mathbf{r},t)$

$$H(\mathbf{r},\mathbf{p},t)=\mathbf{p}\cdot\dot{\mathbf{r}}-L(\mathbf{r},\dot{\mathbf{r}},t)$$

$$=\left(m\dot{\mathbf{r}}+\frac{q}{c}\mathbf{A}(\mathbf{r},t)\right)\cdot\dot{\mathbf{r}}-\left(\frac{1}{2}m\dot{\mathbf{r}}^2-V(\mathbf{r})-qU(\mathbf{r},t)+\frac{q}{c}\dot{\mathbf{r}}\cdot\mathbf{A}(\mathbf{r},t)\right)$$

$$=\frac{1}{2}m\dot{\mathbf{r}}^2+V(\mathbf{r})+qU(\mathbf{r},t)$$

$$H(\mathbf{r},\mathbf{p},t)=\frac{1}{2m}\left(\mathbf{p}-\frac{q}{c}\mathbf{A}(\mathbf{r},t)\right)^2+V(\mathbf{r})+qU(\mathbf{r},t)$$

Canonical form

Interaction of a particle of mass *m* and charge *q* with an electromagnetic field:

Classical Hamiltonian in SI units:

$$H(\mathbf{r},\mathbf{p},t)=\frac{1}{2m}(\mathbf{p}-q\mathbf{A}(\mathbf{r},t))^2+V(\mathbf{r})+qU(\mathbf{r},t)$$

Quantum Hamiltonian in SI units and in coordinate representation:

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

$$H(\mathbf{r},t)=\frac{1}{2m}(-i\hbar\nabla-q\mathbf{A}(\mathbf{r},t))^2+V(\mathbf{r})+qU(\mathbf{r},t)$$

Note: In EC's text, $q\leftrightarrow -e$

Relationship of scalar and vector potentials to electric and magnetic fields:

Electric field: $\mathbf{E}(\mathbf{r},t)=-\frac{\partial\mathbf{A}(\mathbf{r},t)}{\partial t}-\nabla U(\mathbf{r},t)$

Magnetic field: $\mathbf{B}(\mathbf{r},t)=\nabla\times\mathbf{A}(\mathbf{r},t)$

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Quantum mechanical treatment of interaction of particle of mass m and charge q with classical electromagnetic fields in terms of scalar and vector potentials *U*(r,*t*) and A(r,*t*)

Schrödinger equation:

$$i\hbar\frac{\partial\Psi(\mathbf{r},t)}{\partial t}=H(\mathbf{r},t)\Psi(\mathbf{r},t)$$

$$H(\mathbf{r},t)=\frac{1}{2m}(-i\hbar\nabla-q\mathbf{A}(\mathbf{r},t))^2+V(\mathbf{r})+qU(\mathbf{r},t)$$

Note that, as shown in EC's text and as we will also see in classical electrodynamics, the scalar and vector coordinates are ambiguous wrt a "gauge" transformation

$$\mathbf{A}'(\mathbf{r},t)=\mathbf{A}(\mathbf{r},t)+\nabla\chi(\mathbf{r},t)\qquad U'(\mathbf{r},t)=U(\mathbf{r},t)-\frac{\partial\chi(\mathbf{r},t)}{\partial t}\qquad \text{where } \nabla^2\chi(\mathbf{r},t)-\frac{1}{c^2}\frac{\partial^2\chi(\mathbf{r},t)}{\partial t^2}=0$$

Schrödinger equation for gauge transformed Hamiltonian: $i\hbar\frac{\partial\Psi'(\mathbf{r},t)}{\partial t}=H'(\mathbf{r},t)\Psi'(\mathbf{r},t)$

It can be shown that: $\Psi'(\mathbf{r},t)=\Psi(\mathbf{r},t)e^{iq\chi(\mathbf{r},t)/\hbar}$

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Recap: $i\hbar\frac{\partial\Psi(\mathbf{r},t)}{\partial t}=H(\mathbf{r},t)\Psi(\mathbf{r},t)$ and $i\hbar\frac{\partial\Psi'(\mathbf{r},t)}{\partial t}=H'(\mathbf{r},t)\Psi'(\mathbf{r},t)$

where $H(\mathbf{r},t)=\frac{1}{2m}(-i\hbar\nabla-q\mathbf{A}(\mathbf{r},t))^2+V(\mathbf{r})+qU(\mathbf{r},t)$

and $H'(\mathbf{r},t)=\frac{1}{2m}(-i\hbar\nabla-q\mathbf{A}'(\mathbf{r},t))^2+V(\mathbf{r})+qU'(\mathbf{r},t)$

$$\mathbf{A}'(\mathbf{r},t)=\mathbf{A}(\mathbf{r},t)+\nabla\chi(\mathbf{r},t)\qquad U'(\mathbf{r},t)=U(\mathbf{r},t)-\frac{\partial\chi(\mathbf{r},t)}{\partial t}$$

$\Rightarrow \Psi'(\mathbf{r},t)=e^{iq\chi(\mathbf{r},t)/\hbar}\Psi(\mathbf{r},t)$ ←**differs only by phase factor**

PHY 742 -- Assignment #1

January 13, 2020

Read Chapter 9 in **Professor Carlson's QM textbook**..

1. Verify the gauge transformation for the particle wavefunction shown in slide 11 of Lecture 1. Note that some useful steps for this verification are given on page 146 of the text.

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Properties of the "kinetic momentum operator" $\boldsymbol{\pi} \equiv -i\hbar\nabla - q\mathbf{A}(\mathbf{r},t)$

Note that not all of the components of the kinetic momentum operator commute.
In terms of the magnetic field $\mathbf{B} = \nabla\times\mathbf{A}$, the non-trivial commutation relationships are:

$$[\pi_x,\pi_y] \equiv iq\hbar B_z$$
$$[\pi_y,\pi_z] \equiv iq\hbar B_x$$
$$[\pi_z,\pi_x] \equiv iq\hbar B_y$$

This means that for a charged particle moving in a magnetic field, the there is uncertainty in the simultaneous measurement of the three components of the kinetic momentum.

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Effects of the electromagnetic field on the particle current operator.

As shown in Chapter 2, we still expect that the particle charge density ρ and current density $\mathbf{j}$, satisfy the continuity equation: $\frac{\partial\rho}{\partial t} + \nabla\cdot\mathbf{j} = 0$

Particle charge density: $\rho(\mathbf{r},t) = q\left|\Psi(\mathbf{r},t)\right|^2$

Particle current density $\mathbf{j}$:

$$\mathbf{j}(\mathbf{r},t) = \frac{qi\hbar}{2m}\left(\Psi(\mathbf{r},t)\nabla\Psi^*(\mathbf{r},t) - \Psi^*(\mathbf{r},t)\nabla\Psi(\mathbf{r},t)\right) - \frac{q^2}{m}\mathbf{A}(\mathbf{r},t)\left|\Psi(\mathbf{r},t)\right|^2$$

Note that with this form of the current density, the continuity equation is consistent with the Schrödinger Eq: $i\hbar\frac{\partial\Psi(\mathbf{r},t)}{\partial t} = H(\mathbf{r},t)\Psi(\mathbf{r},t)$

where $H(\mathbf{r},t) = \frac{1}{2m}\left(-i\hbar\nabla - q\mathbf{A}(\mathbf{r},t)\right)^2 + V(\mathbf{r}) + qU(\mathbf{r},t)$

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Effects of the electromagnetic field on the particle current operator -- continued

$$i\hbar\frac{\partial\Psi(\mathbf{r},t)}{\partial t} = \left[\frac{1}{2m}\left(-i\hbar\nabla - q\mathbf{A}(\mathbf{r},t)\right)^2 + V(\mathbf{r}) + qU(\mathbf{r},t)\right]\Psi(\mathbf{r},t)$$

$$\frac{\partial\rho(\mathbf{r},t)}{\partial t} = q\left(\Psi^*(\mathbf{r},t)\frac{\partial\Psi(\mathbf{r},t)}{\partial t} + \Psi(\mathbf{r},t)\frac{\partial\Psi^*(\mathbf{r},t)}{\partial t}\right)$$

$$= \frac{q}{2mi\hbar}\left(\Psi^*(\mathbf{r},t)\left(-i\hbar\nabla - q\mathbf{A}(\mathbf{r},t)\right)^2\Psi(\mathbf{r},t) - \Psi(\mathbf{r},t)\left(i\hbar\nabla - q\mathbf{A}(\mathbf{r},t)\right)^2\Psi^*(\mathbf{r},t)\right)$$

$$= \frac{q}{2mi\hbar}\left(-\hbar^2\left(\Psi^*(\mathbf{r},t)\nabla^2\Psi(\mathbf{r},t) - \Psi(\mathbf{r},t)\nabla^2\Psi^*(\mathbf{r},t)\right)\right)$$
$$+ \frac{2i\hbar q^2}{2mi\hbar}\left(\nabla\cdot\mathbf{A}(\mathbf{r},t)\left|\Psi(\mathbf{r},t)\right|^2 + \mathbf{A}(\mathbf{r},t)\cdot\left(\Psi^*(\mathbf{r},t)\nabla\Psi(\mathbf{r},t) + \Psi(\mathbf{r},t)\nabla\Psi^*(\mathbf{r},t)\right)\right)$$

$$= \frac{qi\hbar}{2m}\left(\nabla\cdot\left(\Psi^*(\mathbf{r},t)\nabla\Psi(\mathbf{r},t) - \Psi(\mathbf{r},t)\nabla\Psi^*(\mathbf{r},t)\right)\right) + \frac{q^2}{m}\left(\nabla\cdot\left(\mathbf{A}(\mathbf{r},t)\left|\Psi(\mathbf{r},t)\right|^2\right)\right)$$

$$= -\nabla\cdot\mathbf{j}(\mathbf{r},t)$$

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Summary of results --

Schrödinger equation:

$$i\hbar\frac{\partial\Psi(\mathbf{r},t)}{\partial t}=H(\mathbf{r},t)\Psi(\mathbf{r},t)$$

$$H(\mathbf{r},t)=\frac{1}{2m}\left(-i\hbar\nabla-q\mathbf{A}(\mathbf{r},t)\right)^2+V(\mathbf{r})+qU(\mathbf{r},t)$$

Particle charge density: $\rho(\mathbf{r},t)=q\left|\Psi(\mathbf{r},t)\right|^2$

Particle current density $\mathbf{j}$:

$$\mathbf{j}(\mathbf{r},t)=\frac{qi\hbar}{2m}\left(\Psi(\mathbf{r},t)\nabla\Psi^*(\mathbf{r},t)-\Psi^*(\mathbf{r},t)\nabla\Psi(\mathbf{r},t)\right)-\frac{q^2}{m}\mathbf{A}(\mathbf{r},t)\left|\Psi(\mathbf{r},t)\right|^2$$

Continuity equation: $\frac{\partial\rho}{\partial t}+\nabla\cdot\mathbf{j}=0$

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