

PHY388 "Advanced Computational Physics"
Part II "Comparison of classical and quantum physics"
October 14 – December 9, 2011

<u>Goal</u>	The goal of part II of PHY388 is to strengthen the intuition for quantum mechanical and statistical concepts such as probability distributions and expectation values. We will compare the time evolution of the quantum mechanical wave function to the dynamics of classical ensembles.	
<u>Numerics</u>	Monte Carlo simulations of non-interacting classical ensembles, non-uniformly distributed random numbers, Box-Muller algorithm, rejection method, Fast Fourier transformation, split-operator techniques, Kaleidagraph graphics.	
<u>Class time</u>	MWF 2:00 – 2:50 Moulton 307B	
<u>Instructor</u>	Dr. R. Wagner, Moulton Hall 301B Phone: 438–2026	
<u>Office hours</u>	Officially MWF 10–11, but feel free to come by anytime	
<u>Textbooks</u>	None. Lecture notes will be provided instead.	
<u>References</u>	A recommended references includes: Paul L. DeVries, "A First Course in Computational Physics," John Wiley & Sons, Inc.	
<u>Homework</u>	A total of three homework assignments, each worth 50 points, will be distributed. The homework assignments will consist of some theoretical problems and some computer-based problems. The computer-based problems will generally require that you write computer programs in order to solve the problems. Though we will give examples in class using the Fortran programming language, you are welcome to work the problems in C++. Please consult one of your instructors to discuss the use of compilers for other languages. Homework assignments will have specific due dates. If the home work is turned in 1 msec after the due date, 50% of the total points will be subtracted. Homework turned in one week after the due date will not be accepted.	
<u>Exam</u>	There will be one exam during the final exam period for this course. Exact day/time will be announced when available. A make-up exam will not be given unless you can present a legitimate excuse.	
<u>Grades</u>	3 homework assignments (50 points each)	150 points
	Exam	183 points
		<u>TOTAL 333 points for PART I</u>

Your final letter grade for the entire course is based on the number of points you have gathered in both parts and it will be determined as follows:

A	90 – 100 %
B	80 – 89 %
C	70 – 79 %
D	60 – 69 %
F	59 % and below

We reserve the right to modify these boundaries downward if appropriate.

Tentative Table of Contents:

I Classical ensemble dynamics

- 1.1 Motivation: Classical versus quantum mechanics
- 1.2 Classical distribution function of particles in phase space
- 1.3 Average values, higher moments
- 1.4 The Liouville equation
 - 1.4.1 Multi-particle simulations
 - 1.4.2 Transformation of random variables
 - 1.4.3 Rejection method
 - 1.4.4 Box-Muller algorithm
 - 1.4.5 Analytical solution to the Liouville equation
 - 1.4.6 Example: Free-fall of Gaussian distribution
- 1.6 Time evolution of average values

II Quantum mechanical description

- 2.1 The Schrödinger equation
- 2.2 Exploiting linearity, decomposition into advantageous states
- 2.3 Free-time evolution using FFT
- 2.4 Example: Free-fall of a Gaussian wave packet
- 2.5 Iteration as a solution technique
 - 2.5.1 Second order split-operator scheme
 - 2.5.2 Third order split-operator scheme
 - 2.5.3 Error estimate of these schemes
- 2.6 Time evolution of expectation values
- 2.7 The Wigner quasi-probability function
 - 2.7.1 Microcanonical ensemble for the harmonic oscillator
 - 2.7.2 Wigner function for the harmonic oscillator
- 2.8 Quantum quasiperiod behavior

2.9 Temporally resolved scattering off a potential well

III Time-dependent methods to calculate spectra

3.1 Autocorrelation function

3.2 Lineshape fitting techniques

3.3 Integration in imaginary time