



MASSACHUSETTS INSTITUTE OF TECHNOLOGY  
DEPARTMENT OF CHEMISTRY  
CAMBRIDGE, MASSACHUSETTS 02139 USA

**5.73 Quantum Mechanics I**

Fall, 2003

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*Recommended Text:* Quantum Mechanics, Vols. I and II  
Cohen-Tannoudji, Diu, Laloë

*Library Reserve Text:* Quantum Mechanics, *Merzbacher*  
Group Theory and Quantum Mechanics, *Tinkham*  
Applied Wave Mechanics, *Golding*  
The Theory of Atomic Spectra, *Condon and Shortley*  
Atoms and Molecules, *Karplus and Porter*

*Lectures:* MWF, 10:00AM, Room 4-153

*“Recitation”:* Room 2-151, Wednesdays, 5:00PM (to be verified)

*Grading:*

Homework (weekly)	35%	(~ten problem sets)
Mid-Term Exam	20%	(open-book, take home)
Final Exam	30%	(open-book, take home)
In-Class Quizzes	15%	(approximately 30)

Tentative mid-term exam hand-in date: October 24, 2003

Tentative final exam hand-in date: December 10, 2003.

This is a course for users rather than admirers of Quantum Mechanics. It will wind its way, with a minimum of elegance and philosophical correctness, through a progression of increasingly complex (mostly) time-independent problems. We will begin with one-dimensional problems, treated in the Schrödinger  $\Psi(x)$  wavefunction picture. Then Dirac's bra-ket notation will be introduced and we will switch permanently to Heisenberg's matrix mechanics picture. In matrix mechanics all information resides in a collection of numbers called "matrix elements" and all sorts of trickery will be developed to find ways of deriving the values of all matrix elements without ever actually evaluating any integrals! One can never underestimate the importance of Perturbation Theory. Armed with matrices, we will turn to 3-D central force (spherical symmetry) problems, and discover that for all spherical systems (atoms), the angular factors of all matrix elements are trivially evaluable without approximation. Key topics are commutation rule definitions of scalar, vector, and spherical tensor operators, the Wigner-Eckart theorem, and 3-j (Clebsch-Gordan) coefficients. Finally, we deal with many-body systems, exemplified by many-electron atoms ("electronic structure"), anharmonically coupled harmonic oscillators ("Intramolecular Vibrational Redistribution: IVR"), and periodic solids.

The text is Quantum Mechanics, Volumes 1 and 2, by C. Cohen-Tannoudji, B. Diu, and F. Lalöe (CTDL). The point of view of the text is quite different from the lectures (the text is more elegant, analytical, and logical). Reading assignments are intended to *complement* the lectures. Most homework, but few exam problems, will be based on the CTDL text. Additional reading material will be handed out in class, much of which is notes prepared almost 50 years ago by Professor Dudley Herschbach of Harvard University (while he was an Assistant Professor at Berkeley).

There will be approximately ten weekly problem sets, ~30 in-class 5-minute quizzes, and two take-home, open-book exams. A key difference between problems and the exams is that out-of-class discussion of the problems, **but not of the exams**, is *expected*. Problem sets should be handed in at the start of class on the specified due date and will be graded (graders listed at top of syllabus). Course grades will be determined by the average of the ten problem set grades (35%), the exams (50%) and approximately 30 in-class quizzes (15%). The quizzes are intended to exercise important concepts or techniques immediately after they are introduced.

TENTATIVE LECTURE SCHEDULE AND TOPICS

<u>No. of Lectures</u>	<u>Topic</u>		
9	I.	(9/3 - 9/22)	<b>One Dimensional Problems (R. Field)</b>
	1.	9/3	Course Outline. Free Particle. Motion?
	2.	9/5	Infinite Box, $\delta(x)$ Well, $\delta(x)$ Barrier.
	3.	9/8	$ \Psi(x,t) ^2$ : Motion, Position, Spreading, Gaussian Wavepacket.
	4.	9/10	Information Encoded in $\Psi(x,t)$ . Stationary Phase.
	5.	9/12	Continuum Normalization.
	6.	9/15	Linear $V(x)$ . JWKB Approximation and Quantization.
	7.	9/17	JWKB Quantization Condition.
	8.	9/19	Rydberg-Klein-Rees: $V(x)$ from $E_{vJ}$ .
	9.	9/24	Numerov-Cooley Method.
11	II.	(9/24 - 10/20)	<b>Matrix Mechanics (R. Field)</b>
	10	9/26	Matrix Mechanics.
	11.	9/29	Matrix Solution of Harmonic Oscillator.
	12.	10/1	Eigenvalues and Eigenvectors. DVR Method.
	13.	10/3*	Creation ( $\mathbf{a}^\dagger$ ) and Annihilation ( $\mathbf{a}$ ) Operators.
	14.	10/6	Perturbation Theory I. Begin Cubic Anharmonic Perturbation.
	15.	10/8	Perturbation Theory II. Cubic and Morse Oscillators.
	16.	10/10	Perturbation Theory III. Transition Probability. Wavepacket. Degeneracy.
	17.	10/15	Perturbation Theory IV. Recurrences. Dephasing. Quasi-Degeneracy. Polyads.
	18.	10/17	Variational Method.
	19.	10/20	Density Matrices. Initial Non-Eigenstate Preparation, Evolution, Detection. Quantum Beats.

9	III.	(10/22 - 11/12)	<b>Central Forces and Angular Momentum (T. Van Voorhis)</b>
20.		10/20	Angular Momentum I: Commutation Relations
21.		10/22	Angular Momentum II: Matrix Representations
22.		10/24	Angular Momentum III: Tensors and the Wigner Eckart Theorem
23.		10/27	The Hydrogen Atom
24.		10/29	Perturbations I: The Spin-Orbit Effect
25.		10/31	Perturbations II: The Zeeman Effect
26.		11/3	Scattering From a Central Potential: The Scattering Wavefunction
27.		11/5	Differential Cross Sections and the Born Approximation
28.		11/7	The Partial Wave Expansion
29.		11/12	Lifetimes and Widths
10	IV.	(11/14 - 12/10)	<b>Many Particle Systems: Atoms, Coupled Oscillators, Periodic Lattice (T. Van Voorhis)</b>
30.		11/14	Product Bases and Identical Particles
31.		11/17	The Helium Atom: Singlets, Triplets and interactions
32.		11/19**	The Lithium Atom: Shielding and the aufbau principle
33.		11/21	The Born-Oppenheimer (or Adiabatic) Approximation
34.		11/24	The Sudden (or Diabatic) Approximation
35.		11/26	Non-Born-Oppenheimer effects
36.		12/1	Electronic Structure I: The Valence Bond Picture
37.		12/3	Electronic Structure II: The Molecular Orbital Picture
38.		12/5	Infinite Systems I: Band Structure
39.		12/8	Infinite Systems II: Conductors, Insulators and Excitons
40.		12/10†	Wrap-Up/Catch-Up

\* Add date

\*\* Drop date

† Exam Hand-In date.