Comparisons of Development:
Quantum Theory for the Computer Age
versus
Standard Quantum Mechanics Texts

The text *Quantum Theory for the Computer Age (QTCA)* is a new and developing text with brand new material that is generally quite different from what is found elsewhere. The next few pages contain several listings and comparisons of the features and logical development of *QTCA* along with those of more conventional expositions.

This will also help to connect what is (or is not) available in *QTCA* with what is (or is not) available in conventional texts. One direct comparison is made between *Quantum Mechanics* by Merzbacher and *QTCA*.

One thing *not* mentioned here is the extensive (and growing) computer graphics simulation and animation library that comes with *QTCA*. These programs stimulated many of the new theoretical and conceptual developments found in *QTCA*. We are confident that this set of applications is currently quite unique in the world.

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Contents

- List of topics for a rigorous two-semester modern graduate quantum course for students of atomic, molecular, and optical physics (AMOP), nano-science, and classical and quantum computational theory.
  (Based on Text: *Quantum Theory for the Computer Age* by Harter (U of A 2001)
  UA Courses QM I 5413 and QMII 5423.

- Comparing Logical development and Approach of Standard Quantum Texts vs. *QTCA*

- Direct Comparison of *Quantum Mechanics* by Merzbacher and *QTCA*.

List of topics for a rigorous modern graduate quantum course for serious students of optics, nano-science, and classical and quantum computational theory. Heisenberg-Dirac-Feynman approach.
Based on Text: *Quantum Theory for the Computer Age* by Harter (U of A 2001)
Optional Topics (leading to the "wild-blue-yonder") are shaded

Quantum I

1. Quantum analyzers, their states, and quantum axioms (Uses optical or spin-1/2 polarization experiments and simulations)
    - Dirac notation and operator matrix representations
    - Transformation and transfer matrices

Matrix operator eigensolutions: Their algebra and geometry
- Spectral decomposition of commuting observables
    - Relation to Lagrange interpolation
- Unitary symmetry and group axioms. (With reasons why they work)
- Perturbation and variational techniques (Optional if done later)
    - Relation to permutation classes and Lagrange multipliers

2.Quantum wavefunctions and dynamics (Starts using 1D laser optics and derives matter waves and basic relativistic quantum theory. Uses wave simulations.)
- Waves described by space and time
    - Group and phase velocity
- Waves described by wavevector and frequency
    - Matter waves and relativistic dispersion. Classical connections
- Confined waves, wavepackets, and pulse trains
    - Bohr-ring waves. Heisenberg uncertainty
- Accelerated waves and gravity. (Optional)
    - Recoil effects. Pound-Rebka experiment

3. Quantum Fourier analysis and symmetry (Starts using plane waves, Bohr-waves, and develops discrete waves on quantum wells and nano-structures. Uses band simulations.)
- Fourier transform and transformation matrices. (Discrete versus continuous)
- Fourier symmetry analysis
- Time evolution operators, matrices, and Hamiltonian generators
    - Schrodinger time equation
    - Hamiltonian eigensolutions. Cyclic symmetry analysis.
- 2-State evolution and analogs. U(2) symmetry analysis. (Optional if done later.)
    - Euler angles and gauge. Operator angles. Relation to Hamilton quaternions

4. Quantum wave equations (Starts with free optical and matter waves and develops quantum bound and scattering resonant states. Uses wave simulations.)
- Difference and differential equations
    - Schrodinger in x-basis and Schrodinger in k-basis.
- Infinite well and Bohr-ring embedding
    - Quantum beats. (Optional) Revivals
- Finite wells and barriers
    - Transmission and admittance functions
    - C-matrices and S-matrix eigenchannels (optional if done in QM II)
- Introduction to harmonic oscillator (optional if done in QM II)
    - Coherent wavepackets and classical correspondence

Quantum II

1. Periodic potentials and symmetry (Optional if done in SS Phys)
    - Multiple barriers and S-matrix theory
        - Resonant and non-resonant eigenchannels
    - Non-Abelian symmetry analysis of periodic structure and states (Optional if in MMII)
        - Modern point group projection algebra
    - Fourier analysis of periodic structures and states (Optional)
        - Space group analysis (optional)

2. Time-variable perturbations and transitions
    - Classical electromagnetic perturbations
        - A•p versus E•r
        - Problems with ignoring relativity
    - Transitions due to oscillatory perturbations
        - Fermi Golden rule
    - Two state resonant transitions
        - Fermi Golden rule broken

3. Quantum harmonic oscillators and multi-exciton states
    - 1D states and dynamics
        - Coherent and squeezed states
        - Classical correspondence (and lack thereof)
    - 2D – ND states and dynamics
        - Schwinger-Glauber analysis (optional)
    - Bose versus Fermi-Dirac permutational symmetry
        - Brown-Twiss and related experiments
    - Non-relativistic quantum field (optional if done in Laser Physics or QE)
        - Fock N-photon states versus coherent states (optional)
        - Jaynes-Cumming's model (optional)

4. Quantum rotation and angular momentum
    - Relations between rotation and 2D vibration. Wigner D-function analysis
        - Atomic and molecular beam polarization
    - Quantum rotor D-wavefunctions and special cases
        - Legendre P and associated Y-harmonics
        - Symmetric and asymmetric rotor states and dynamics (Optional if in AMP)
    - Coupled rotation and spin
        - Hyperfine (21 cm example) and spin-orbit states
        - Coupled rotors and centrifugal effects (optional if in AMP or QMIII)

5. Quantum orbitals and central force dynamics
    - Hydrogen-like electronic structure
        - O(4) analysis (optional)
        - Spectrum generating algebra (optional)
        - Rydberg states and MCQDT (optional)
    - Helium-like electronic structure
        - Herrick-Kellman-Berry analysis (optional)

Comparing Logic and Approach of Standard to Newer Quantum Texts

Standard "Wavefunction"QM Texts		**Newer "Matrix" QM Texts** (with QTCA Chapters)
Schiff, Merzbacher, .., extended by Sakauri		*Dirac, Feynman,..., extended by Harter*
Born-Fermi-Oppenheimer development		Heisenberg-Dirac-Feynman development
Differential equations first	Ch.1	Matrix equations first
Matrices an afterthought	Ch.11	Diff. eq's limiting case of matrix-eq's
Numerical analysis not discussed		Powerful numerical analysis exposed
Nano-structures not invented yet	Ch.8-14	Nano- and-micro structure models used
Modern molecular QM impractical	Ch.15,24	Powerful molecular theory developed
Foggy logic		Solid logic for both physics and mathematics
Little or no statement of axioms	Ch.2	Physics axioms 0-4 for $\langle x'\|x\rangle$ amplitudes
Wavefunctions and operators vague	Ch.1	Beam analyzer **T**-op gives $\langle x\|\Psi\rangle=\langle x\|T\|y\rangle$
Unitarity not explained well		Math. symmetry principles give $U^\dagger U=1$
Unitarity not applied well	Ch.1-3	Relates easily to physics axioms
Little motivation for Dirac notation		Compelling motivation for Dirac notation
Appears mysterious	Ch.1	Based on optics $\langle x'\|x\rangle=\cos\theta$, etc.
Mostly unmotivated		Based on geometry and linear algebra
Mostly real analysis at first		Complex analysis from the get-go
Little phase or phasor analysis	Ch.4	Powerful phasor visualization from start
No spectral decomposition algebra		Best-ever treatment of spectral decomposition
Orth-norm &completeness mysterious	Ch.3	Tied into axioms 0-4
Weak relations		Related to Lagrange interpolation
		Related to Lagrange multipliers
Poor motivation for eigensolutions		Beam analyzers make eigensolutions obvious
(Hard to do, with Diff'Equ!)	Ch.3	Analyzers have "own-vectors"
Weak examples		Clear beam polarization examples
Poor analysis of eigenvectors		Powerful spectral decomposition analysis
Laborious GrmSht. degeneracy treatment	Ch.3	Easy commuting-observable algebra
Weak development of symmetry	Ch.8,15	Compelling intro. to symmetry analysis
Voodoo-like "measurement theory"		Clear explanation using phase randomization
Poor intro to density ops	Ch.1,10	Motivated devel. of density matrices
Primitive treatment of wave dynamics		Elegant graphical wave analysis and visualization
Poor definition of V_{group} and V_{phase}	Ch.4	Precise definition of V_{group} and V_{phase}
No relation to special relativity	Ch.5	World's first wave derivation of SR
Silly (or no) deriv. of Schrodinger wave eq.		Lucid relativistic wave analysis using symmetry
DeBroglie relation is *axiom*	Ch.5	DeBroglie relation is *theorem*
Wave dispersion clumsy afterthought		Powerful relativistic dispersion theory
Convoluted classical connections		Concise and elegant classical connections
Schrodinger limitations unclear		Schrodinger limitations quite clear
Analogies are few and weak	Ch.11	Strong and revealing classical analogs

Standard QM Texts (contd)		**Newer QM Texts (contd)**
Clumsy treatment of Fourier theory	Ch.7-9	Powerful and elegant treatment of Fourier theory
Continuum related poorly to discrete	Ch.7,11,16	Mechanical analogies clarify *Cn-C*∞ relation
Poor topological discussions	Ch.11	Bounded (Bnd) vs. Unbounded (Unb) combined with Discrete (Dis) vs. Continuous (Con) give four topologies
(Serious		(1) (Unb)-(Con)-x with (Unb)-(Con)-k *(Banach* $\langle x\|k\rangle$*)*
missed		(2) (Unb)-(Dis)-x with (Bnd)-(Con)-k *(Bohr* $\langle x\| k_m\rangle$ *)*
distinctions		(3) (Bnd)-(Con)-x with (Unb)-(Dis)-k *(Bloch* $\langle x_p\|k\rangle$*)*
here.)		(4) (Bnd)-(Dis)-x with (Bnd)-(Dis)-k *(Hilbert* $\langle x_p\|k_m\rangle$*)*
Old and inapplicable examples	Ch.7-9	Cn-symm-analysis of Q-dots and photon band-gap
Practically no quantum dynamics	Ch.9,12	New wave revival and quantum beat theory
Difficult treatment of time evol**U**tion op.		Time evolution **U** just another “analyzer” operator
Limited examples of Hamiltonian **H**-ops		Unlimited and interesting nano-structure examples
H-op e-analysis difficult		Symmetry makes e-analysis/calc. simple & powerful
Possible **H**-structure unclear	Ch.9	Complete classification of all possible **H**-operators
Possible solutions unclear		Complete classification of all possible **H**-solutions
Obscure development of 2-state systems		Precise clear analogy with 2D-oscillator & opt. polariz’n
2D oscillator not exploited fully	Ch.10	Classical 2D oscillator *ABCD* theory developed
Schwinger U(2) algebra not used	Ch.21-24	Quantum 2D *ABCD*-oscillator U(2) theory used
No derivation of Pauli spinor ops. σ_μ		How Hamilton developed σ_μ more completely in 1843
Clumsy application of 2-state Hamiltonian		Cool classification scheme by “*ABCD*” mnemonics
Mysterious Pauli-*X*,*Y*,*Z* ops.	Ch.10	*AD* Type-Hamiltonians *(Asymmetric-Diagonal)*
		B-Type Hamiltonians *(Bilateral-Balanced)*
		C-Type Hamiltonians *(Circular-Chiral-Coriolis)*
Unclear & incomplete spin state analysis		Lucid analysis of **H** operator and state dynamics
Few visualization aids	Ch.10	U(2) hardware & software analogs
Spin angles unrelated to geometry		Euler angle state coordinates
Operator labeling incomplete		Axis angle operator coordinates
Unclear how to control spin/phase		Complete and clear spin/phase control
Weak Schrodinger wave analysis		Powerful U(2) **C**-matrix vs. **S**-matrix scattering theory
Poor for modern nano-structures		Designed for modern superlattice and Q-dots
Even square wells made difficult	Ch.12	Simple and extensible theory for square PE’s
Failures of SW not noticed		Effects of “infinite force” PE’s clarified
Over-emphasis of bound states	Ch.12-14	Development based to resonances
Little on scattering channels	Ch.14	New channel-eigenchannel transformation theory
Poor Schrodinger numerical analysis		Powerful numerics and analysis based on simple analogs
Tunneling is mysterious	Ch.11	Tunneling clarified by “curtain-resonance” analog
Little about wave dynamics	Ch.4,9	Designed to analyze pulses, packets, and revivals
Clumsy development of periodic PE		Powerful symmetry-based analysis
Bloch waves mysterious	Ch.9-16	Bloch waves clearly analyzed (and animated)
Clumsy angular momentum development	Ch.23-24	Best QTAM treatment available

(The above list contains only a fraction of the new features in QTCA.)

NA=Not Available in QTfCAr

Merzbacher *Quantum Mechanics*

Merzbacher		QTfCA
Chapter 1 Intro	QTfCA	1
Wavefunction... meaning		1
Chapter 2 Wave packets..Wave Equation		4,11
Princ of Superposition , Uncertainty ,		1,12
Wave Equation for Free Particle		4,9,11
Chapter 3 Schrodinger Equation..Operator Algebra		2,5,11
Wave Equation		11
Momentum Space		7,8
Expectation values		11,12
Stationary states		1,9,10
Virial Th		18,20
Chapter 4 Principles of Wave Mechanics	QTfCA	1-13
Hermitian operators		2,3
Completeness of eigenstates		3
Continuous spectrum		4,7
Unitary operators		1-3
Charged particle in B-field		10
Galilean transformation		4,17
Chapter 5 Linear Harmonic Oscillator	QTfCA	20-21
Eigenvalues and eigenfunctons		3,20
Motion of wavepackets		9,20
Chapter 6 Piecewise Constant Potentials	QTfCA	12-16
Step, Barrier, Square Well		13
Chapter 7 The WKB Approximation		NA
Bound states		12-13
Barrier transmission		12-16
Exponential decay		14
Chapter 8 Variational Methods and Perturbation		3
Calculus of Variations		3,5
Rayleigh Ritz		3,18
Double oscillator	NA	14
Molecular states		24,35
Periodic potential		14-16
Chapter 9 Vector Spaces in Quantum Mechanics		1-3
(Intro to Dirac notation and operators)		1-3
Chapter 10 Eigenvalues and Eigenvectors		3
(Intro to eigensolutions of normal operators)		3
Commuting observables		3
Harmonic oscillator... and coherent states		20
Chapter 11 Angular Momentum in QM		23-25
Orbital Ang. Mom.		24
Spherical Harmonics		24
Chapter 12 Spherical Potentials		24.26
Square well		NA
Radial equation		24,26
Coulomb Potential and bound eigenfunctions		26
Chapter 13 Scattering	NA	
Green's functions		11
Born approx		18
Coulomb scattering		NA
Chapter 14-15 Quantum Dynamics		9-12
Quantization		5
Forced oscillator		17-18
Density operator		1,10
Chapter 16 Spin		10,24
Spin polarization		1,10,19
Rotations, Spin operators		1,10,19
Spin dynamics		1,10,19
Chapter 17 Rotations and Symmetry Ops		10,24
Group representations		8-10,15
(Clebsch Gordan ology)		24
Chapter 18-19 Bound & Time Dep Perturbation		17-19
Fermi Golden rule		18
Chapter 120 Formal Theory of Scattering		NA
Chapter 121-22 Identical Particle, n-BodySys.		27-31
Chapter 123 Photons and em Fields		22
Chapter 24.Relativistic Electron THeory		NA...yet!

NAM=Not Available in Merzbacher NAAE=Not Avail. Anywhere Else

Harter *Quantum Theory for Computer Age*

Harter		Merzbacher
Unit 1 Introduction to Wave Amplitudes		
Chapter 1 Quantum Amplitudes and Analyzers		NAAE
Chapter 2 Transformation and Transfer Operators		NAM
Chapter 3 Operator Eigensolutions and Perturbations		9-10
Determinants, permanants, and permutation classes		NAM
Unit 2 Introduction to Wave Dynamics		
Chapter 4 Waves Viewed by Space and Time: Relativity		NAAE
Chapter 5 Waves Viewed by Wavevector and Frequency: Dispersion		NAAE
Chapter 6 Multidimensional Waves and Modes	Mostly	NAM
An "Old-Fashioned" classical approach to relativity		NAM
Unit 3 Introduction to Fourier Analysis and Symmetry		
Chapter 7 Fourier Transformation Matrices	Mostly	NAM
Chapter 8 Fourier Symmetry Analysis		NAAE
Chapter 9 Time Evolution and Fourier Dynamics	3,5 14-15	
Chapter 10 Two-State Evolution, Coupled Oscillation, and Spin		16
Optical ellipsometry and "Spin-control" using U(2) analysis		NAM
Unit 4 Introduction to Wave Equations		
Chapter 11 Difference Equations and Differential Operators	NAM and 3-4	
Chapter 12 Infinite-Well States and Dynamics	6 , NAAE and NAM	
Chapter 13 Step Potential Barriers and Wells		6
Scattering and "Quantum well control" using U(2) analysis		NAAE
Unit 5 Introduction to Periodic Potentials and Symmetry		
Chapter 14 Multiple Barriers, Eigenchannels, and Resonance Bands	8 and NAM	
Chapter 15 Non-Abelian Symmetry Analysis of Periodic Systems		NAAE
Chapter 16 Fourier Analysis of Periodic Potentials and States		NAM
Molecular symmetry control inside and out		NAAE
Unit 6 Introduction to Time-Variable Perturbations & Transitions		
Chapter 17 Classical Electromagnetic Perturbations		22,NAAE
Chapter 18 Transitions Due to Time-Variable Perturbation		18-19
Chapter 19 Two-State Resonant Transitions		16 NAM
The observer becomes the observed		NAM
Unit 7 Quantum Harmonic Oscillators		
Chapter 20 One-Dimensional Oscillator States and Dynamics		5, 10, 15
Chapter 21 Two-Dimensional Oscillator States and Dynamics		NAM
Chapter 22† Quantum Electromagnetic Field		22
Bose-Einsein and Fermi-Dirac symmetries		21
Unit 8 Quantum Rotation and Angular Momentum		
Chapter 23 Two-Dimensional Oscillator and Quantum Rotation		NAM
Chapter 24 Quantum Theory of Molecular and Nuclear Rotors		NAAE
Chapter 25 Quantum Theory of Coupled Spins and Rotors		17, NAM
The quantum frame inside and out: Mach's conundrum		NAAE
Unit 9 Quantum Orbitals and Central force dynamics		
Chapter 26 Hydrogen-like States and Dynamics		12
Chapter 27† Helium-like States and Dynamics		18, 22 NAM
Chapter 28† Rydberg States		NAM
Fano's multichannel quantum defect theory		NAM
Unit 10 Multiparticle States and Interactions		
Chapter 29† Unitary-Permutation Symmetry Projection		NAM
Chapter 30† U(m)xU(n) Analysis of Correlation (Entanglement)		NAM
Chapter 31† Atomic ℓn Configurations and Excitation		NAM
Xray photoelectron spectroscopy (XPS)		NAM
Unit 11 Polyatomic Molecules		
Chapter 32† Molecular Orbitals and Vibration		8, NAM
Chapter 33† Rovibrational Fine and Superfine Structure		NAAE
Chapter 34† Nuclear Hyperfine Structure		NAAE
Superhyperfine spectroscopy		NAAE

Notes

Many of Merzbacher's 145 sub-Chapter Headings are listed

Due to lack of space none of Harter's 136 sub-chapter headings or 400 sub-sub-chapter headings are listed here. See Tables of Contents at the beginning of each Chapter.

† Currently in *Princ. Symm. Spect. & Dyn*. Vol. I or Vol. II and being rewritten for QTfCA