CHEM 3420-pchem II, Quantum Mechanics
Review Sheet for Final

Time period designated for final: Tuesday, Dec. 8, 9 AM

Material covered: This study sheet is a guideline to help you sort through the numerous topics that we have covered. This review sheet is not all inclusive. You are also responsible for anything that we discussed in class; that is in the text and notes; and the material covered by our quizzes, in-class worksheets, and homework. A helpful hint when studying is to ask ourselves "Why is this? Where did it come from?", "What does this mean?", "How can I work a problem with this?", "What is the practical application of this?"

The make-up of the test: multi-match, short-answer, discussion, short and long problems

Information that you will have at your disposal:
-Periodic table, scratch paper, various integral solutions, spherical harmonic table, radial function table
-You may also bring each of your notecards from the tests.

From test #1

I. The history of Quantum Mechanics

A. The people of QM

You need to know who they were, what they did (in word and formulae), and how what they did contributed to QM.

Balmer
Bohr
Schrodinger
Einstein
Pauli
Heisenberg
Dulong
Petit
Dirac
Planck
Wien
deBroglie
Rydberg
Angstrom
Rayleigh

B. The events leading up to/phenomena involved in the discovery of QM

II. Math

A. Concepts that we have used

Be able to use these and manipulate them.

Complex numbers, complex conjugate
Rules of exponents
Eigenfunctions, eigenvalues
Operators
Derivatives
Integrals
Partial derivatives
Triple integrals
Coordinate systems

B. Specific things we need to know

How to take the derivative of any function
How to do simple integrals (e.g. $\int x dx$, $\int \sin(x)dx$, $\int e^x dx$), etc.
How to look up integrals in an integral table
Any math involved in any homework problem.

IV. QM concepts

These are general topics. Many of them include definitions, formulas, problems, etc. <u>We need to know it all!</u>

<u>Schrodinger's equation:</u>
1-D PIB: the Hamiltonian, the wavefunction, the energy
2-D PIB: the Hamiltonian, the wavefunction, the energy
3-D PIB: the Hamiltonian, the wavefunction, the energy
Be able to find the energy by operating on the wavefunction with the Hamiltonian given a wavefunction.
Heisenberg uncertainty principle
Normalization of a function
Expectation values
Orthogonalization of a function
Wave-particle duality
The postulates of QM
Orthonormal complete set
Requirements for a good wavefunction
Separation of variables

<u>From test #2</u>

I. Degeneracy = g, (9.2b and handouts from Noggles text)

Definition and physical interpretation as it applies to the 3D PIB
How to determine g for the 3D PIB
How to determine the E of a degenerate state in terms of the 3D PIB
Definition and physical interpretation as it applies to a real atom.

II. Harmonic oscillator (9.4 and 9.5 and various handouts)

The background/derivation of the HO: Classical Mechanics (CM) motion
- Hooke's law
  - Simple harmonic motion
  - Hooke's law
    - Be able to explain Hooke's law using a diagram.
    - Spring constant, restoring force, etc.
  - How does the F of hooke's law change with K and m?

Be familiar with the classical analogy of the spring related to a diatomic molecule's vibrations.
Know what a force constant is.
Know H, ψ, and E for the HO and how to use them and how to work problems with them.
Be able to find ψ_v when v is any reasonable number. (This means being able to use Hermite polynomials and the normalization expression.)
Know the relationship between frequency and angular frequency.
Know the relationship between angular frequency and the force constant.
What is a reduced mass and why is it used?
QM expressions for the Hamiltonian (both kinetic and potential)
Be familiar with and know how to explain all meanings of the HO energy diagram for both QM and CM and any differences therein (including the energy diagrams from Noggles' book that had a) wavefunctions and b) probability densities).

III. Rigid Rotor (RR) and Angular Momentum (represented by L or J)

What does the rigid rotor represent?
Know H, ψ, and E for the 2D RR and how to use them and how to work problems with them.
Be able to find $\psi_{m\text{-}\ell}$ when m_ℓ is any reasonable number.
Know the difference between angular frequency and velocity and frequency
Moment of inertia
Reduced mass
angular momentum (J)

What types of motions have we studied as they relate to the motions of atoms and molecules? What are the models we have developed to study these motions? (So far, we've studied three types.) Which of these models have a zero-point energy and why?

What is the energy expression of the RR as pertains to the particle-in-a ring lab?
How would we calculate the energy of benzene or some other "ring" molecule using the particle-in-a-ring model?

What other questions could be asked?

<u>From test #3</u>

What scientists and their contributions have we studied in these sections?

Ch. 9, Sections 7&8
The 3-D Rigid Rotor

- Energy, Hamiltonian, wavefunction
  - Use the separation of variable technique when using the wavefunction.
  - r is constant.
  - Have ℓ and m_ℓ quantum numbers.
  - Magnitude of orbital angular momentum
  - z-component of orbital angular momentum
  - Be able to discuss meanings of Figures 9.37 and 9.40.
  - Stern Gerlach experiment

Spin

- Spin quantum number
  - Know difference between bosons and fermions and which apply to e-, p+, neutrons, mesons, photons.
  - Magnitude of spin angular momentum
  - z-component of spin angular momentum
  - Be able to discuss meanings of Figure 9.41.
  - Stern Gerlach experiment

Ch. 10

Hydrogenic atoms
- Hamiltonian, energy, wavefunction
  - Terms within and approximations to the Hamiltonian and why
  - Separation of variable technique for wavefunction
    - Radial component of wavefunction
    - Angular component of wavefunction
    - How to use both
    - Most probable radius
    - Average radius
    - Bohr radius
  - Quantum numbers involved with hydrogenic atoms
    - Shells and subshells
    - Principle quantum number
    - Physical representation of radial wavefunctions

Many-electron atoms
- All information for hydrogenic wavefunctions…and the differences between the two systems..
- Hamiltonian, energy, wavefunction
  - Terms within and approximations to the Hamiltonian and why
  - Separation of variable technique for wavefunction
    - Radial component of wavefunction
    - Angular component of wavefunction
    - How to use both
  - Quantum numbers involved with hydrogenic atoms
    - Shells and subshells
    - Principle quantum number
    - Physical representation of radial wavefunctions
- Pauli principle
- Hunds rule
- Aufbau principle
- Z-effective
- Shielding
- Electron configurations and orbital diagrams

Selction rules for hydrogenic and multi-electron atoms
- For ℓ and m-ℓ as well as L, S, and J.
- Grotrian diagrams

Singlet and Triplet states
- Physical interpretations
- Be able to compare and contrast: e- configurations, energies, spin and orbital angular momentum
- Grotrian diagrams

Spin-orbit Coupling and Term Symbols
- Physical interpretations
- Vector addition diagrams (be able to explain, e.g. Fig. 10.28)
- Fine structure
  - Energy calculations
  - Coupling constant and calculations
  - Be able to explain diagrams like Fig. 10.29 and 10.30
- L, S, and J and determining term symbols for them.

Ch. 11 Molecular Structure
The material from Ch. 11 covers pages 362 through 386. Please omit section "c The Variation Principle" and "d two simple cases" on pages 380 through 384.

- Please pay special attention to concepts and theory excluding wavefunctions. (Please be able to give a generic wavefunction such as Equation 11.1 and 11.2 and explain what it means.)
- Valence Bond Theory
  - What is the theory?
  - How and why is it used?
  - What are problems with it?
  - Hybridization
- Molecular Orbital Theory
  - What is the theory?
  - How and why is it used?
  - What are problems with it?
  - Bonding and antibonding orbitals
  - Molecular orbital energy diagrams: both homonuclear diatomics and heteronuclear diatomics
  - Covalent and polar covalent bonds
  - Electronegativity
- Please be able to understand and explain the following figures:
  - 1, 2, 23, 24, 31, 33, 36, 37

Suggested problems to work…
Chapter 11
Exercises: 1, 2, 3, 4, 5
Problems: none