Study Guide for chapter 11

1. Blackbody radiation.
    a. What is blackbody radiation? What quantity does the total energy or energy density of the radiation depend on? Do they dependent on the type of objects?

    b. We discussed several theories: Stefan-Boltzmann law, Wien equation, Planck equation, and Rayleigh-Jeans equation. Which ones give the exact description of the energy of blackbody radiation? You need to know the approximate form of the relationships. Draw the curves of radiation energy density vs. wavelength or frequency over temperature at different temperatures using Planck's equation. How does it change if Wien equation or Rayleigh-Jeans equation is used? What is ultra- violet catastrophe? How do you convert wavelength to frequency?

    c. Origin of Planck's equation. What are the two theoretical considerations for deriving the Planck equation? Under what assumptions does Planck's equation reduce to Rayleigh-Jeans equation?

2. Photoelectric effect. What are the observations? How does the theory developed by Einstein explain them?

3. The particle nature of light can be explained using the concept of a photon. Remember the relationship between wavelength (wave property) and linear momentum (particle property).

4. Electron diffraction. What is the de Broglie wavelength of particles? Which particle is more wave-like, a) electron; b) neutron; or c) atom?

5. Wave-particle duality. What is the relationship that reconciles the wave and particle nature of matter?

6. Heisenberg's uncertainty principle. In the electron diffraction experiment, narrowing the slit results in an increased accuracy in our knowledge of the position of electrons, but a decreased accuracy in the knowledge of the momentum in the same direction.

7. **Time-dependent Schrödinger equation**. Write down the equation in the general form (in three dimensions) and the equation for a free electron. What is the variable? What are the operators? What is the unknown? What information does the solution offer?

8. **Time-independent Schrödinger equation**.

    a. Derive the time-independent Schrödinger equation from the time-dependent form   assuming that the external field (or potential) is time invariant. Hint: express the time- dependent wave function as a product of the time-independent wave function and an exponential function (Eq. 11.83).

    b. Write down the equation in three dimension and point out the variable, operator. What are the unknowns?

    c. Write down the probability density and the probability of finding a particle in a space element dxdydz and in the entire space. What is $|f|^2$ for a real function f and a complex function $f=af_1+ibf_2$?

9. **Eigenvalue equation**. Given an example of eigenvalue equation and point out the operator, eigenfunction and

eigenvalue.

10. **Postulates III**. Quantum mechanical operators perform two types of operations. What are they? Remember: position operator, linear momentum operator, kinetic energy operator and potential energy operator.

11. **General understanding of "particle in a one-dimensional box"**. Write down the two Schrödinger equations for describing the particle in a one-dimensional box (for both inside and outside of the box)? What is the total energy and wavefunction obtained from solving these two equations?

12. More on "particle in a one-dimensional box".

a. Write down the probability density of finding the particle inside the box.

b. Draw a plot showing the wavefunction and probability density for the state n=2?

c. What is the total energy of the particle in state n=4? On how many positions can the particle vanish inside the box in this state?

d. Is the energy gap between two adjacent energy levels, n and n+1 the same? Give the expression for this energy gap.

e. What is probability of finding the particle between position x and x+dx?

f. What is the total probability of finding the particle in the box?

13. **Contrast "particle in a one-dimensional box" with "tennis ball in a one-dimensional box"**. Suppose we give the tennis ball an initial velocity in the x direction. No friction or other forces are present. Point out two major differences. Hint: energy levels and probability of finding the particle or ball.

14. **Particle in a box** – three dimensional form.

    a. Write down the wave function and energy of the particle. There is one quantum number for each dimension.

    b. What is the degree of degeneracy for the energy level $E_{2,3,4}$? What is the number of wave functions for this energy level?

15. **Harmonic Oscillator** – classical energy and quantum description.

    a. Write down the classical expression for the total energy of a system consisting of two balls connected by a massless spring. Point out the kinetic energy and potential energy.

    b. What is the corresponding Hamiltonian?

    c. What is the Schrodinger equation that describes the system?

    d. What is the quantum mechanical energy of a harmonic oscillator? Explain all terms. What is the lowest energy? Are the energy levels degenerate?

    e. Point out two differences between the classical and quantum description of harmonic oscillator. Hint: energy and probability density.

16. **Vibrational spectroscopy**.

a. Which energy level is most populated at room temperature? What is the most probable transition between vibrational energy levels? Write down the transition energy and explain all terms. What is the frequency of emitted or absorbed light?

b. Name one useful quantity one can obtain from measuring the vibrational spectrum of a molecule.

c. In which wavelength region can a vibrational transition be observed? a) Infrared; b) Ultra-violet; c) X-ray; or d) visible?

17. **Commutator**.

a. Use the commutation relation (commutator) between the two operators z and p_z to prove that z and p_z cannot be simultaneously determined, e.g., $\Delta z \Delta p_z \neq 0$.

b. Use the commutation relation to prove that energy and time cannot be simultaneously determined, e.g., $\Delta t \Delta E \neq 0$.

c. Can we simultaneously determine z and p_z of two particles?

d. Bonus. Can x and kinetic energy be simultaneously determined?

18. **Requirements for an acceptable wave function**.

a. Give the definition for wave function.

b. Name three requirements for an acceptable wave function.

c. Which of the following functions cannot be a wave function? a) kx; b) sin(ax); c) e^{ax}; d) $\sin^2(ax)$

19. **Quantum description of hydrogen-like atoms**

a. Write down the Hamiltonian for a system consisting of one electron and one nucleus. Point out the kinetic energy operator and potential energy operator.

b. What is the electronic energy of H atom? Which quantum number does it depend on? What the degree of degeneracy?

c. What is the spacing between two adjacent levels? Does the spacing increase, decrease or remain the same with the quantum number?

20. **Orbitals**

a. The electronic wave function is also known as orbital. An orbital is specified by what quantum numbers?

b. Write down the quantum numbers for the following orbitals: 3s, $4p_y$, $4d_{x2-y2}$, $5d_{z2}$.

c. How many nodes do the above orbitals have?

d. Draw these orbitals in Cartesian coordinate.

21. **Radial function**.

a. What is a radial function? What is a radial distribution function?

b. For the orbital $5d_{z2}$, write down the expression for the radial distribution function.

22. **Angular momentum** – classical form and quantum mechanical operator.

a. Write down the classical equation for the angular momentum (L_z) of a mass rotating about z axis. Explain the terms.

b. What is the corresponding quantum mechanical operator?

23. **Rigid rotor** – classical energy and quantum description.

a. Write down the classical expression for the kinetic energy of a rigid rotor.

b. What is the corresponding Hamiltonian?

c. What is the Schrodinger equation that describes a rigid rotor? What are the quantum numbers?

d. Write down the quantum mechanical energy of a rigid rotor. Are the energy levels degenerate? If yes, what is the degree of degeneracy?

24. **Rotational spectroscopy**.

a. What are the allowed transitions between rotational energy levels? Write down the transition energy and explain all terms. What is the frequency of emitted or absorbed light?

b. Name one useful quantity one can obtain from measuring the rotational spectrum of a molecule.

c. What is the wavelength range of rotational spectra?

25. **Orbital angular momentum operators**

a. Write down the classical form and quantum mechanical operator of angular momentum in Cartesian coordinate.

b. What is the advantage of transforming to a spherical coordinate?

c. What are the eigenvalues and eigenfunctions of L_z and L^2 operators? Point out the quantum numbers and the values they can take on.

d. What values can L have?

26. **Spin angular momentum operators**

a. No classical counterpart.

b. What are the eigenvalues and eigenfunctions for of S_z and S^2 operators?

c. What is the spin for photons, neutrons and electrons?