FYS.425 EXAM-PROBLEMS

0. Introduction and orientation

Explain briefly

three historical experimental observations, whose interpretation called for quantum theory.

duality of matter

1. Foundations of quantum mechanics

Explain briefly

observables in classical mechanics and quantum mechanics

nature and relevance of hermitian operators

interpretation of the wavefunction

the uncertainty principle

stationary quantum state and time dependent part of its wavefunction

time dependent and time independent Schrödinger equation

Ehrenfest's theorem

Consider

Explain quantum mechanical description of the outcome of a single experimental measurement and measurement of the value of an observable

From the general Schrödinger equation derive the differential equations for stationary state and time evolution. What are the conditions of separability.

Time evolution of expectation values and conservation laws in quantum mechanics: Constants of motion and Ehrenfest's theorem.

2. Linear motion and harmonic oscillator

Explain briefly

free particle dynamics in quantum mechanics

linear momentum and wave length

traveling and standing waves

Consider

Particle-in-a-box as a quantum dot model

Zero-point energy of harmonic oscillator

Virial theorem

3. Rotational motion and hydrogen atom

Explain briefly

hamiltonian of particle-on-a-ring

hamiltonian of particle-in-a-circle

hamiltonian of particle-on-a-sphere
atomic units
s, p, d, ... orbitals of hydrogen atom

Consider

Angular momentum in a plane and space

Angular momentum and spherical harmonics

Energy quantization of a particle in a sphere

Separation of simple rigid rotor hamiltonian

Rotationally symmetric quantum dot models: list three, but elaborate one

Schrödinger equation of hydrogenic atoms and the nodal structure of solutions

4. Angular momentum

Explain briefly

angular momentum
commutation relations of angular momenta (around perpendicular axes)
shift or ladder operators
spin
orbital angular momentum
Clebsh–Gordan coefficients

Consider

Coupling of angular momenta, case: two spins in coupled and uncoupled states

Coupling of angular momenta, case: orbital angular momentum and spin

a) Define the angular momentum in classical mechanics and in quantum mechanics.
b) Prove, that $\mathbf{j}_1 + \mathbf{j}_2$ is an angular momentum, but $\mathbf{j}_1 - \mathbf{j}_2$ is not, if $\mathbf{j}_1$ and $\mathbf{j}_2$ both are quantum mechanical angular momenta

5. Group theory

Explain briefly

symmetry operations and symmetry elements
point groups and space groups
the five point group operators
matrix representation of point group symmetry operators
reducible and irreducible representations
character of representation
irreducible representations of the point group C_{3v}

irreducible representations of the point group C_{4v}

symmetry and degeneracy

Consider

Characters and classes of point groups. Define the concepts and make analyses with two examples, C_{2v} and C_{3v}

6. Perturbation theory

Explain briefly

reference system and perturbation in perturbation theory

Hellman–Feynman theorem

Rabi oscillations

Fermi's golden rule

selection rules of quantum transitions

Einstein transition probabilities

lifetime and spectral line width

Consider

Time-independent two-level perturbation theory

First order correction to the ground state energy

Variation theorem

Rayleigh–Ritz variational method

Hellmann–Feynman theorem

Rabi oscillations of two-level system

Derive Planck distribution from Einstein transition probabilities and Boltzmann distribution

7. Atomic spectra and atomic structure

Explain briefly

selection rule of the electric dipole transition

spin–orbit coupling

closed shells and coupling of holes

Pauli principle

term symbol

central-field and orbital approximations

Slater determinant

Hund's rules

Zeeman effect

Stark effect

Consider

Consequences of indistinguishability of identical electrons

b) What are the LS-coupled states in case of two electrons of an atom in the same p-orbital or different p-orbitals.
c) Consequently, what are the states of four electrons of an atom in the same p-orbital?

Self-consistency and SCF calculations of electronic structure

Essentials of
a) Hartree–Fock (HF) approach,
b) restricted and unrestricted HF approach, and
c) self-consistent field (SCF) method.

Explain Stark effect

8. Molecular structure

Explain briefly

BornOppenheimer approximation

bonding, non-bonding and antibonding orbital

semiempirical and *ab initio* (or *first-principles*) electronic structure approaches

conjugated molecules

π-bonding

free electron model

Consider

Molecular orbital method and valence bond method.

Molecular orbitals of diatomic homonuclear molecules.

9. First-principles methods

Explain briefly

primitive GTO functions

basis set superposition error

electronic correlation
Hartree–Fock limit
Kohn–Sham equations

Consider

Slater type (STO) and gaussian type (GTO) basis sets in electronic structure calculations.

One-electron picture and its break-down: what is it and why it breaks down?

Hartree–Fock limit, Configuration interaction (CI) and full CI.

Examine **A- or B-case, only**, and use He atom and/or H_2 molecule as examples, where relevant.
A) Origin, nature and appearance of exchange and correlation phenomena of electrons.
B) Describe how the exchange and correlation energies of electrons can be evaluated. Use some usual approach as an example.

Electronic correlation: Choose one of the conventional approaches and explain the main points.

Density Functional Theory (DFT) and Local-Density Approximation (LDA).

Description of many-body effects or correlation interaction in
a) Hartree–Fock or wave function methods, (3p)
b) Density Functional Theory (DFT) and (3p)
c) Quantum Monte Carlo (QMC) methods. (3p)

QD. Quantum dots extra

Explain briefly

LS-coupling and jj-coupling

Consider

Particle-in-a-box as a quantum dot model

Particle-on-a-sphere as a quantum dot model

the state of an electron in spherical quantum dot with confinement $V(r) = \frac{1}{2}r^2$

Quantum states of electrons
a) in a finite quantum well and
b) in sc. superlattice

a) Define typical nanostructure models, *i.e.,* potentials confining the electrons, and
b) choose one of those, and then, describe properties of the electronic quantum states (orbitals) and properties of the nanostructure.

List a few quantum dot structures for confinement of electrons (and holes, if relevant)
Then, choose your favourite quantum dot and consider
b) its one-electron states and
c) other relevant properties, manufacture or applications

Special features of the electronic structure in low-dimensional (< 3) nanostructures:
a) Compare the densities-of-states.
b) Compare the quantum dots in cases of "weak confinement" and "strong confinement"