

Department of Applied Physics

Entrance Examination Booklet

Specialized Subjects

(Choose 3 Problems among the 4 Problems in this Booklet)

August 31 (Tuesday) 13:00 – 16:00, 2010

REMARKS

1. Do not open this booklet before the start is announced.
2. Inform the staff when you find misprints in the booklet.
3. Choose three problems among the four problems in this booklet, and answer the three problems.
4. Use one answer sheet for each problem (three answer sheets are given). You may use the back side of each answer sheet if necessary.
5. Write down the number of the problem which you answer in the given space at the top of the corresponding answer sheet.
6. Do not take this booklet and the answer sheets with you after the end of the examination.

Applicant Number	No.
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write down your applicant number above

Problem 1

Consider the ground state of an electron with a negative charge $-e$ bound to a positive point charge $+e$ fixed at the origin of the two- or three-dimensional space. The Hamiltonian is given by

$$H = -\frac{\hbar^2}{2m}\nabla^2 - \frac{e^2}{4\pi\epsilon_0 r},$$

where r is the distance between the electron and the point charge, \hbar is Planck's constant divided by 2π , m is the mass of the electron, and ϵ_0 is the vacuum permittivity. Using the variational method with a trial wave function $\psi(r) = N \exp(-\alpha r)$ for the ground state, answer the following problems. Here, α is the variational parameter and N is the normalization constant.

- [1] Obtain the optimal variational wave function and the energy expectation value in three-dimensional space. Note that the action of ∇^2 on $f(r)$ in three-dimensional space is as follows:

$$\nabla^2 f(r) = \frac{d^2}{dr^2} f(r) + \frac{2}{r} \frac{d}{dr} f(r)$$

- [2] Obtain the optimal variational wave function and the energy expectation value in two-dimensional space. Note that the action of ∇^2 on $f(r)$ in two-dimensional space is as follows:

$$\nabla^2 f(r) = \frac{d^2}{dr^2} f(r) + \frac{1}{r} \frac{d}{dr} f(r)$$

- [3] Based on the results of [1] and [2], discuss the physical meaning of the differences in spreads of the electron wave functions and in the energy expectation values.

Problem 2

Consider fermions with spin 1/2 in a cubic box with side length L and periodic boundary conditions to all three-side directions in contact with a heat reservoir and a particle source. The one-particle wave function obeys the Schrödinger equation,

$$\left[-\frac{\hbar^2}{2m} \frac{\partial^2}{\partial r^2} - \mu \right] \phi = E\phi, \quad (1)$$

irrespective of the spin state of the particle, where μ , \hbar , m and $\mathbf{r} = (x, y, z)$ denote the chemical potential, the Planck constant divided by 2π , the mass of each fermion, and the spatial coordinates whose axes are taken along the sides of the cubic box, respectively.

A one-particle eigenfunction of this system is $\phi = \exp[i(k_x x + k_y y + k_z z)]/\sqrt{L^3}$ and its energy eigenvalue is

$$E(\mathbf{k}) = \varepsilon(\mathbf{k}) - \mu, \quad \varepsilon(\mathbf{k}) = \frac{\hbar^2(k_x^2 + k_y^2 + k_z^2)}{2m} \quad (2)$$

where the components of the wave-number vector $\mathbf{k} = (k_x, k_y, k_z)$ take discrete values of $k_x = 2\pi\ell_x/L$, $k_y = 2\pi\ell_y/L$ and $k_z = 2\pi\ell_z/L$ with any integers ℓ_x , ℓ_y and ℓ_z .

Now we consider that a large number of ideal fermions, that is, non-interacting fermions, in this box are in thermal equilibrium at a temperature T . The chemical potential is μ . The grand-canonical (macro-canonical) partition function Ξ is expressed as a function of the set of $\Xi_1(\ell_x, \ell_y, \ell_z)$, where $\Xi_1(\ell_x, \ell_y, \ell_z)$ represents the contributions from each state, (ℓ_x, ℓ_y, ℓ_z) . The Boltzmann constant is k_B . Solve the following problems.

- [1] Derive $\Xi_1(\ell_x, \ell_y, \ell_z)$ and explain the relation between its form and Fermi-Dirac statistics. Beware of the spin degree of freedom of the fermion. Furthermore, write an expression of Ξ with $\Xi_1(\ell_x, \ell_y, \ell_z)$.
- [2] Consider the averaged number of particles $\langle n_{\mathbf{k}} \rangle$ with the wave-number vector \mathbf{k} . How is $\langle n_{\mathbf{k}} \rangle$ related to Ξ_1 ? Express $\langle n_{\mathbf{k}} \rangle$ in terms of μ , \hbar , m , \mathbf{k} , T , and k_B . Draw a graph of $\langle n_{\mathbf{k}} \rangle$ versus $|\mathbf{k}|$, and describe a characteristic feature of its temperature dependence.

In the thermodynamic limit ($L \rightarrow \infty$), the sum over integers (ℓ_x, ℓ_y, ℓ_z) becomes an integration as

$$\sum_{\ell_x, \ell_y, \ell_z} \rightarrow \frac{L^3}{(2\pi)^3} \int dk 4\pi k^2 = L^3 \int d\varepsilon D(\varepsilon) \quad (3)$$

where $D(\varepsilon)$ denotes the density of states per volume. Treat this thermodynamic limit in the following. You may use eq.(3) if necessary.

- [3] By using $D(\varepsilon)$, give an expression for a thermodynamic function, $J = -k_B T \ln \Xi$, derived from the grand-canonical partition function. Hereafter, do not forget the contribution from the two degrees of freedom of the spin.
- [4] By using β defined as $\beta = 1/(k_B T)$, derive the average energy per volume, $\langle E \rangle$ at T from Ξ . From this expression, derive the expression for $\langle E \rangle$ in terms of β and $D(\varepsilon)$.
- [5] Derive the explicit form of the density of states per volume, $D(\varepsilon)$, as a function of ε .

- [6] By using the results of problems [4] and [5], derive E_g , the energy per volume at the absolute zero temperature, as a function of the chemical potential μ .
- [7] With the expectation value of the number density $\langle \rho \rangle = \langle N \rangle / L^3$, the density susceptibility κ is defined by $\kappa = d\langle \rho \rangle / d\mu$, where N denotes the number of particles in the system. Give the expression to derive $\langle \rho \rangle$ from $D(\varepsilon)$ at arbitrary temperature. Further, when the chemical potential μ is changed at absolute zero temperature, derive $\langle \rho \rangle$ and κ as functions of μ . Give the expressions for $\mu > 0$ and for $\mu < 0$ separately. In addition, describe the relationship between κ and the density of states when $\varepsilon = \mu$, $D(\mu)$. Explain why this relation holds.
- [8] Derive an expression for the particle-number fluctuation $\langle \rho^2 \rangle - \langle \rho \rangle^2$ by using Ξ or J , and discuss how it is related to the density susceptibility κ .

Problem 3

Consider the motion of a particle with mass m and positive charge q in three-dimensional space with a static and uniform magnetic field of magnetic flux density B in the positive z direction. The time-dependent position of the particle is given by $\mathbf{r} = (x(t), y(t), z(t))$. The particle is subject to a centripetal force towards the origin $\mathbf{F} = -kr$. Provided that the velocity of the particle is slow compared to the speed of light, answer the following problems.

- [1] Write down the equations of motion for the particle and derive the angular frequency ω_0 of the harmonic oscillation along the z axis.
- [2] Consider the motion of the particle projected to the xy plane. The motion is a superposition of two harmonic oscillations. By assuming $x(t) = a \cos \Omega t$ and $y(t) = b \sin \Omega t$, obtain the angular frequencies Ω s for the two harmonic oscillations.
- [3] Provided that the angular frequency ω_0 obtained under [1] satisfies the inequality relation $\omega_0 \gg qB/m$, schematically illustrate the B -dependence of Ω .
- [4] Explain the physical reason for the occurrence of the two different angular frequencies obtained under [3].

In addition to the above conditions, the particle is subject to a damping force $\mathbf{f} = -m\gamma d\mathbf{r}/dt$ (γ is a positive constant and $\gamma \ll \omega_0$). Answer the following questions.

- [5] A spatially uniform alternating electric field $\mathbf{E} = (E_0 \cos \omega t, 0, 0)$ is additionally applied. After the forced oscillation reaches its steady state, estimate $\overline{x(t)^2 + y(t)^2}$, the average of $x(t)^2 + y(t)^2$ over one cycle $2\pi/\omega$.
- [6] Schematically illustrate the ω -dependence of $\overline{x(t)^2 + y(t)^2}$ obtained under [5] for the following two cases, $\gamma \ll qB/m \ll \omega_0$ and $qB/m \ll \gamma \ll \omega_0$.

Problem 4

In crystals of transition-metal compounds, a 3d transition-metal cation feels an electric field from surrounding anions. This electric field is called crystal electric field. Under influence of this field, 3d electron orbitals (principal quantum number $n = 3$, angular momentum quantum number $l = 2$, and magnetic quantum number $m = -2, \dots, 2$), which are five-fold degenerated in a spherical potential, will split into several energy levels. This splitting is called crystal-electric-field splitting. A 3d transition-metal cation with one electron in the 3d orbitals ($3d^1$) is surrounded by the anions as shown in Fig. 1. Answer the following questions on the crystal-electric-field splitting of the 3d orbitals of this transition-metal cation. It is sufficient to take account of the nearest-neighbor anions shown in Fig. 1 as the origin of the crystal electric field. Ignore the spin splitting and spin-orbit coupling, and assume that hybridization with other orbitals than the 3d orbitals can be neglected because of the small crystal-electric-field splitting.

To answer the questions, use the fact that the directional part of the 3d one-electron wave-function in the spherical potential is given by the spherical harmonics $Y_{2m}(\theta, \phi) = \Theta_{2m}(\theta)\Phi_m(\phi)$, where θ and ϕ are the spherical coordinate variables defined in Fig. 1, $\Phi_m(\phi) = \frac{1}{\sqrt{2\pi}}e^{im\phi}$, and $\Theta_{2m}(\theta)$ is given as follows (double sign in same order):

$$\begin{aligned}\Theta_{20} &= \frac{\sqrt{5}}{2\sqrt{2}}(3\cos^2\theta - 1), \\ \Theta_{2\pm 1} &= \mp \frac{\sqrt{15}}{2}\sin\theta\cos\theta, \\ \Theta_{2\pm 2} &= \frac{\sqrt{15}}{4}\sin^2\theta.\end{aligned}$$

- [1] When $a = c$ in Fig. 1, the arrangement of anions becomes a regular octahedron, and the symmetry around the 3d transition-metal cation is cubic. In the cubic symmetry, it is known that the 3d electron orbitals will energy-split into two-fold-degenerated $d\gamma$ and three-fold-degenerated $d\epsilon$ orbitals, and their directional dependence is given as follows:

$$\begin{array}{c} \underbrace{\hspace{10em}}_{d\gamma} \qquad \underbrace{\hspace{10em}}_{d\epsilon} \\ \text{(a)}Y_{20} \quad \text{(b)}Y_{22} + Y_{2-2} \quad \text{(c)}Y_{21} + Y_{2-1} \quad \text{(d)}Y_{21} - Y_{2-1} \quad \text{(e)}Y_{22} - Y_{2-2} \end{array}$$

Assign the above (a-e) wave functions to the isosurfaces shown in Fig. 2(i-v). In addition, determine the energetic order of the $d\gamma$ and $d\epsilon$ orbitals.

- [2] Next, let us consider the energy splitting of the 3d orbitals in the anion octahedron that is slightly distorted along the z axis ($0 < 1 - \frac{c}{a} \ll 1$). Because of this slight distortion, the symmetry lowers to tetragonal, and the two-fold and three-fold degeneracies of the $d\gamma$ and the $d\epsilon$ orbitals will be further removed. Nevertheless, you may assume that the forms of the wave functions remain unchanged. From the directional dependence of the wave functions, qualitatively consider the energy splitting of the orbitals in this tetragonal environment, and put in order the (a-e) orbital energy levels. (Explicitly specify any remaining degeneracy.)

Next, let us think how to experimentally determine the energy levels of the 3d electron orbitals in the tetragonal symmetry obtained in [2] by measuring light absorption spectra. Since the wavelength of the light is sufficiently longer than the dispersions of the 3d orbital wave functions, the interaction Hamiltonian between the light and the 3d electron can be assumed as follows:

$$\mathcal{H}' = -\mathbf{P} \cdot \mathbf{E} - \mathbf{M} \cdot \mathbf{H}, \quad (1)$$

where $P = -er$ and $M \simeq -\mu_B l$. Here, e , r and l are the elementary charge, the position and angular-momentum operators of the 3d electron, respectively, and μ_B stands for the Bohr magneton. E and H represent the electric and magnetic field vectors, respectively. In \mathcal{H}' , the first term stands for the electric dipole transition, the second one for the magnetic dipole transition.

- [3] Discuss the possibility of electric dipole transitions between the energy levels obtained in [2].
- [4] From here, consider only the magnetic dipole transition. Imagine that the two light absorption spectra in Figs. 3(A) and (B) were obtained at zero temperature. In this experiment, linearly polarized light proceeding in the x direction is incident on the system, where the electric field vector is parallel to the y axis, or to the z axis. Which polarization condition is used when Fig. 3(A) or 3(B) is obtained? Explain why you think so. Here, you may use angular momentum raising and lowering operators $l_{\pm} = l_x \pm il_y$.

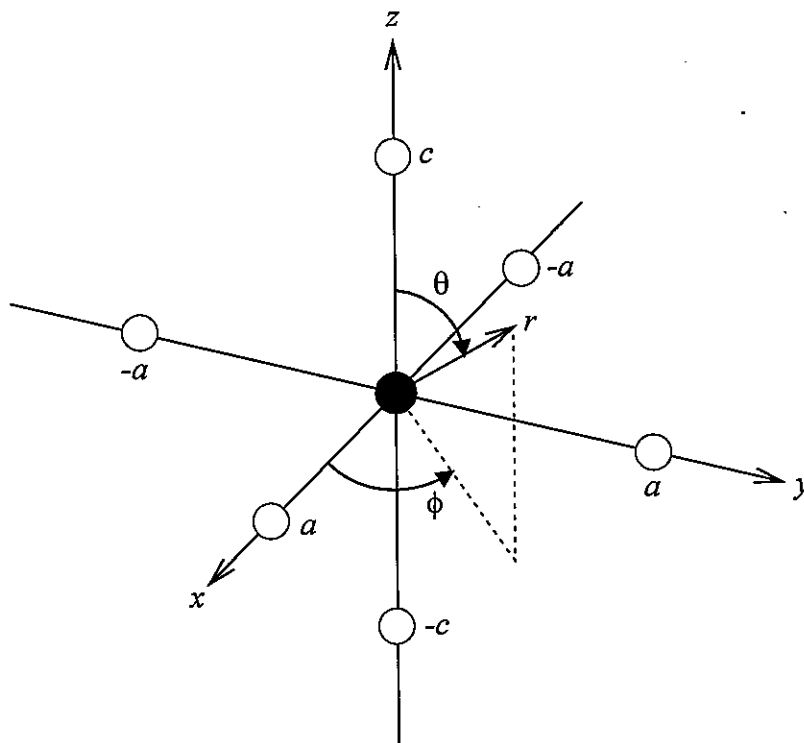


Figure 1: A 3d transition metal cation in the anion octahedron. The cation (filled circle) is located at the origin, whereas the anions (open circles) are on the x , y , and z axes. The distances between the cation and anions are a for the x and y directions, and c for the z direction.

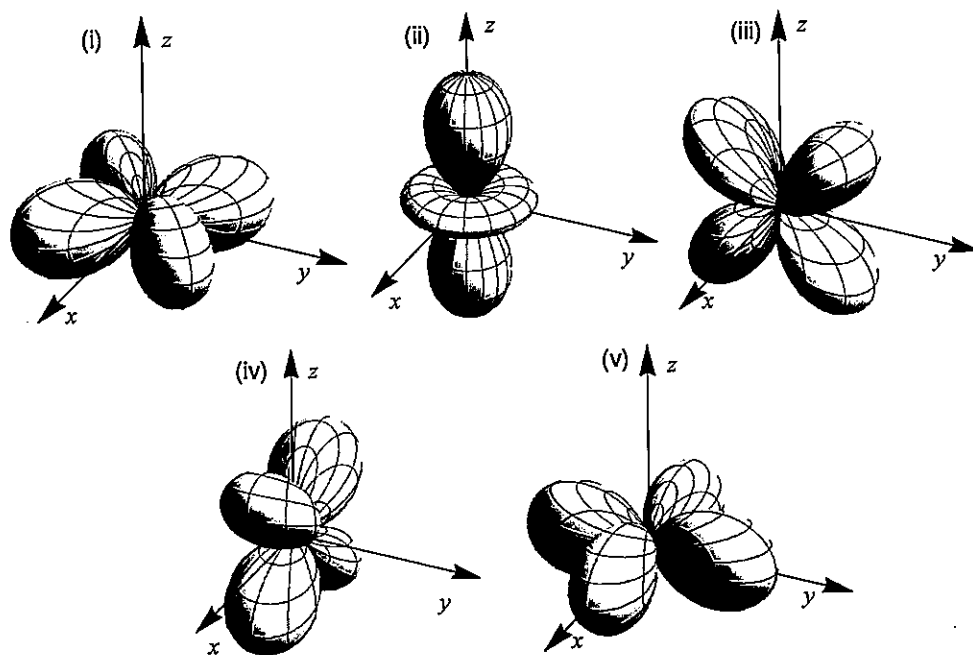


Figure 2: Schematic illustration of the spatial distribution of the directional part of the $d\epsilon$ and $d\gamma$ wave functions. The isosurfaces illustrate the amplitudes of the directional part of the wave functions as distances from the origin.

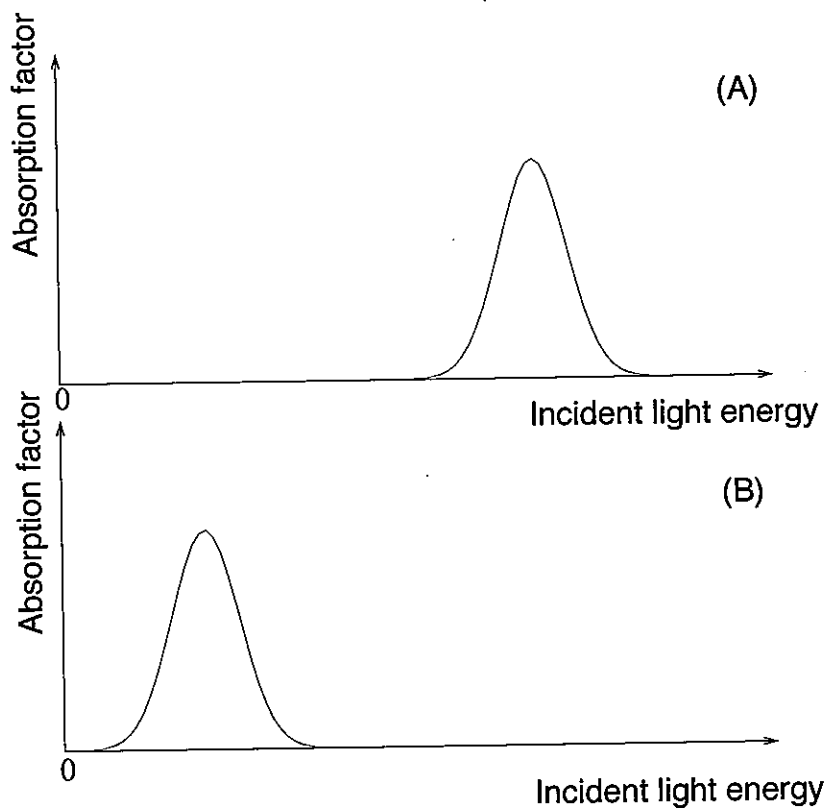


Figure 3: (A, B) Schematic light absorption spectra. The two measurements are performed in the same energy range, but the vertical scales are not identical.