Department of Applied Physics
Entrance Examination Booklet

Physics I

(Answer the 2 Problems in this Booklet)

August 26 (Tuesday) 9:30 – 11:30, 2014

REMARKS

1. Do not open this booklet before the start is announced.
2. Inform the staff when you find misprints in the booklet.
3. Answer the two problems in this booklet.
4. Use one answer sheet for each problem (two 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. You may use the blank sheet of this booklet to make notes, but you must not detach them.
7. Any answer sheet with marks or symbols irrelevant to your answers will be considered invalid.
8. Do not take this booklet and the answer sheets with you after the examination.

Examinee number	No.

Write down your examinee number above

Problem 1

As shown in Figure 1, a rotating rigid sphere with an angular velocity $\omega(>0)$ is vertically directed onto a flat horizontal floor and bounces, which results in a lateral velocity $v'(<0)$ and an angular velocity ω'. The rotation axis is parallel to the floor. The sphere has a mass m, a radius a, and is homogeneous in density. The positive directions of the x axis and of the rotation of the sphere are indicated by the arrows in Figure 1. For these conditions, answer the following questions.
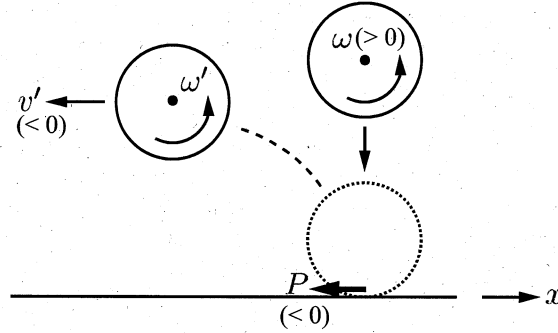

Figure 1

[1] Show that the moment of inertia I of this sphere about its central axis is given by $I = \frac{2}{5}ma^2$.

[2] Show the relation between v' and ω' under the condition that the sphere does not slip with respect to the floor on impact. This condition means that the lateral velocity of the sphere's contact point with the floor right after the impact is zero with respect to the floor.

[3] As shown in Figure 1, an impulse $P(< 0)$ acts laterally on the sphere at the impact due to friction. Write the relation between the momentum before and that after the impact using P. Write the relation for the angular momentum as well. Under the condition of [2], express the angular velocity ω' after the impact in terms of ω.

Next, consider that the same rigid sphere bounces repeatedly on the floor with friction as shown in Figure 2. The sphere has an initial lateral velocity v_0 (> 0) and angular velocity ω_0 (> 0). After the first impact on the floor, the lateral velocity and the angular velocity of the sphere become v_1 and ω_1, respectively, due to the impulse P_1 (< 0) acting laterally upon impact. Assume that the coefficient of restitution is less than unity. As time passes, the sphere ceases to bounce and rolls with a constant velocity v_f without slipping. The positive directions of the x axis and of the rotation of the sphere are indicated by the arrows in Figure 2. The axis of the rotation is parallel to the floor and perpendicular to the x direction.

[4] At the n-th bounce, the sphere impacts on the floor with the lateral velocity v_{n-1} and the angular velocity ω_{n-1}, resulting in the lateral velocity v_n and angular velocity ω_n due to the impulse P_n of friction. Write the relation between the momentum before and that after the impact using P_n. Write the relation for the angular momentum as well. Also show that the following quantity
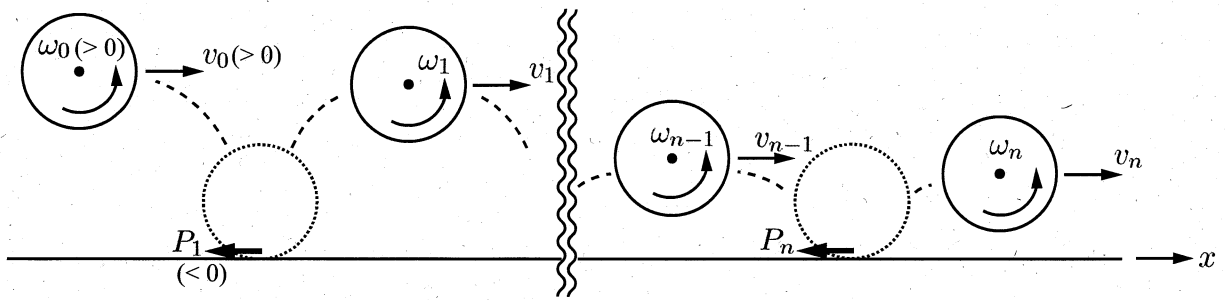
$$l = I\omega_n - amv_n$$

is constant, independent of n.

Figure 2

[5] Express the velocity v_{f} right after the bouncing ceases in terms of m, a, and l. Also write the relation between the velocity v_0 and angular velocity ω_0 for the case of $v_{\mathrm{f}} = 0$ without rolling when the bouncing ceases.

Problem 2

Consider the electrostatic potential due to infinitely long line charges with uniform charge densities placed in vacuum of permittivity ε_0.

[1] Calculate the electric field strength $E(r)$ at a point $(x, y) = (r \cos \theta, r \sin \theta)$ when a line charge with a linear charge density λ is placed on the z axis, as shown in Figure 1, and verify that the electrostatic potential $\phi(r, \theta)$ of this line charge is given by

$$\phi(r) = -\frac{\lambda}{2\pi\varepsilon_0} \ln \frac{r}{r_0}, \tag{1}$$

where the electrostatic potential is set to be zero at $r = r_0$.

[2] Calculate the electrostatic potential $\phi(r, \theta)$ at a point $(x, y) = (r \cos \theta, r \sin \theta)$ when a line charge with a linear charge density λ is placed at $(x, y) = (a, 0)$ and another line charge with a linear charge density $-\lambda$ is placed at $(b, 0)$ with $0 < a < b$ as shown in Figure 2. The line charges are parallel to the z axis.
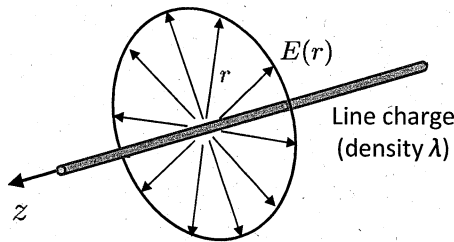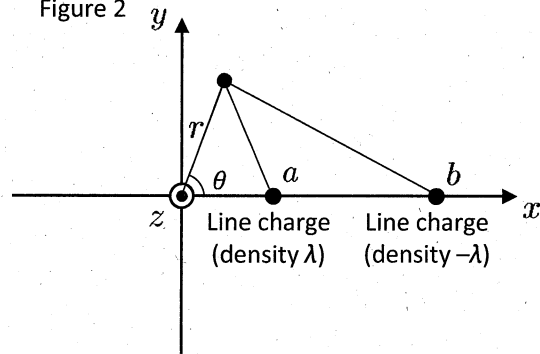
Figure 1

$E(r)$

r

Line charge (density λ)

z

Figure 2

y

r

θ a b

z Line charge (density λ) Line charge (density $-\lambda$)

x

Consider a conductor with an infinitely long cylindrical hollow of radius R centered on the z axis and an infinitely long line charge with a linear charge density λ placed parallel to the z axis within the hollow as shown in Figure 3. The conductor is connected to earth ground and is infinitely large. The line charge induces opposite charges on the inner surface of the conductor due to the electric field of the line charge. Consider the method of mirror images to calculate the distribution of the induced surface charges. Since the electrostatic potential is constant (independent of position) in the conductor, the image charge is placed such that the total electrostatic potential due to the line charge and the image charge becomes constant at the inner surface of the conductor. Consider a system of two line charges shown in Figure 4, where a line charge with a linear charge density λ is placed at $(x, y) = (d, 0)$ and an image line charge with a linear charge density $-\lambda$ is placed at $(x, y) = (D, 0)$ with $0 < d < R < D$.

[3] Calculate the electrostatic potential at a point $(x, y) = (r \cos \theta, r \sin \theta)$ assuming first that no conductor is present and verify that the condition for the electrostatic potential being constant at $r = R$ is given by $D = R^2/d$. By using this condition, express the electrostatic potential $\phi(r, \theta)$ within the cylindrical hollow $(r < R)$ without using D.

[4] The induced surface charge density σ on the inner surface of the conductor can be calculated by

$$\sigma = -\varepsilon_0 \frac{\partial \phi}{\partial n} = \varepsilon_0 \left(\frac{\partial \phi}{\partial r} \right)_{r=R}, \tag{2}$$

where $\partial\phi/\partial n$ is the partial derivative of the electrostatic potential with respect to the normal direction to the inner surface of the conductor. Calculate the induced surface charge density $\sigma(\theta)$ at a point $(x, y) = (R\cos\theta, R\sin\theta)$.
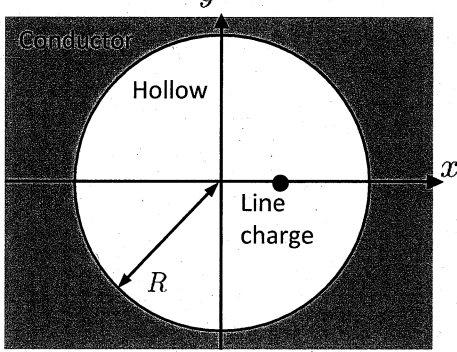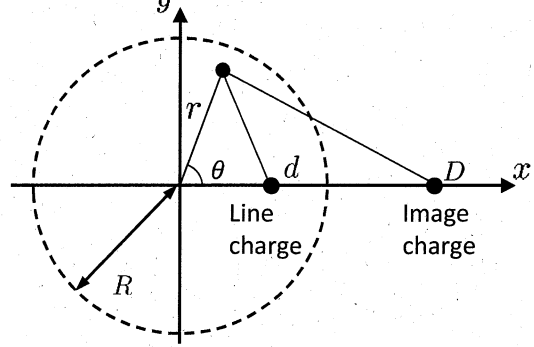
Figure 3

Figure 4

[5] Using the result of [4], verify that the amount of induced charges on the inner surface of the conductor per unit length along the z axis coincides with $-\lambda$ by integrating $\sigma(\theta)$ around a circle on the inner surface of the conductor. If necessary you may use the following formula:

$$\frac{1 - a^2}{1 - 2a\cos x + a^2} = 1 + 2\sum_{n=1}^{\infty} a^n \cos nx, \quad \text{when } |a| < 1. \tag{3}$$

The position of the line charge can be estimated by measuring the inner surface charge density. Consider a system of a line charge at $(x_0, y_0) = (d\cos\psi, d\sin\psi)$ with $d < R$ and four detectors to measure the inner surface charge density at $\theta = 0$, $\pi/2$, π, and $3\pi/2$ on the conductor, as shown in Figure 5. The size of the detector can be ignored and the detectors will not influence the electrostatic potential.

[6] Express the position of the line charge (x_0, y_0) using R and the inner surface charge density σ_1, σ_2, σ_3, and σ_4 measured at $\theta = 0$, $\pi/2$, π, and $3\pi/2$, respectively. The distance between the line charge and the z axis is small enough to neglect any higher order terms than d/R when you use equation (3).

Figure 5
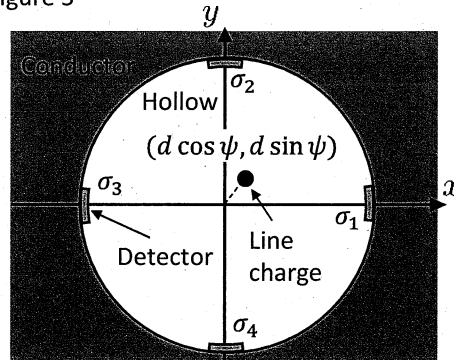
Department of Applied Physics

Entrance Examination Booklet

Physics II

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

August 26 (Tuesday) 13:00 – 16:00, 2014

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.
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Problem 1

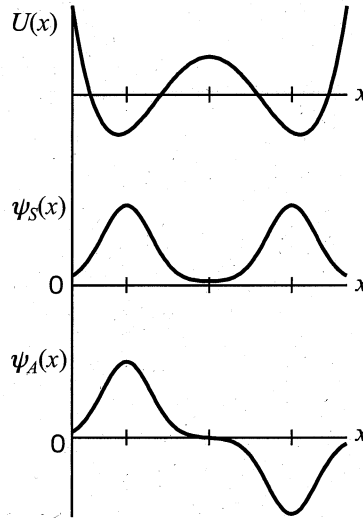Consider the one-dimensional potential $U(x)$ with two mimima shown in Figure 1.

Figure 1: The potential $U(x)$ and its eigenstates $\psi_S(x)$ and $\psi_A(x)$.

Consider a system where one particle is confined in the potential $U(x)$. Normalized eigenstates of $\psi_S(x)$ and $\psi_A(x)$ are obtained as the two lowest energy solutions of the Schrödinger equation. The energies of these two eigenstates are $\pm J$ ($J > 0$). Assume that the transition of the particle to states other than $\psi_S(x)$ and $\psi_A(x)$ is negligible and that dissipation can be neglected. The Planck constant divided by 2π is denoted by $\hbar$. Answer the following questions.

[1] Which of the two eigenstates ($\psi_S(x)$ or $\psi_A(x)$) corresponds to lower energy ($= -J$)? Explain the reason.

Next, $\psi_L(x)$ and $\psi_R(x)$ are defined as follows: $\psi_L(x) = \frac{1}{\sqrt{2}}(\psi_S(x) + \psi_A(x))$, $\psi_R(x) = \frac{1}{\sqrt{2}}(\psi_S(x) - \psi_A(x))$.

[2] Show that $\psi_L(x)$ and $\psi_R(x)$ are mutually orthogonal. Write down the Hamiltonian of the system as a 2×2 matrix using $\psi_L(x)$ and $\psi_R(x)$ as the basis.

From here, we express $\psi_L(x)$ as "the state where the particle exists in the left well", and $\psi_R(x)$ as "the state where the particle exists in the right well."

[3] At the time $t = 0$, the particle exists in the left well. Find the time-dependent probability that the particle exists in the right well.

In the following, consider the system where two indistinguishable particles are confined in the potential $U(x)$. Assume that the particles obey Bose statistics and have no internal degrees of freedom. Consider the following states labeled as $|0\rangle$, $|1\rangle$, and $|2\rangle$:

- The state in which both particles exist in the left well is denoted as $|0\rangle$.

- The state in which one particle exists in the left well and the other one in the right well is denoted as $|1\rangle$.

- The state in which both particles exist in the right well is denoted as $|2\rangle$.

The wave function of the system can be expressed as $|\Psi(t)\rangle = c_0(t)|0\rangle + c_1(t)|1\rangle + c_2(t)|2\rangle$. Answer the following questions.

[4] Assume that there are no interactions between the particles.

[4.1] Show that the Hamiltonian $\mathcal{H}$ of this system can be expressed as follows:

$$\mathcal{H} = \begin{pmatrix} 0 & -\sqrt{2}J & 0 \\ -\sqrt{2}J & 0 & -\sqrt{2}J \\ 0 & -\sqrt{2}J & 0 \end{pmatrix}. \tag{1}$$

[4.2] Find all eigen energies of this system.

[4.3] At the time $t = 0$, both particles exist in the left well. Find the probability $P_n(t)$ ($n = 0, 1, 2$) as a function of t and J that n particles exist in the right well. Show $P_n(t)$ ($n = 0, 1, 2$) on a graph.

[5] Assume that there is strong attractive interaction between the particles so that the energy of the system decreases by A ($A \gg J > 0$) when both particles exist in the same well.

[5.1] Find the Hamiltonian of this system by modifying the diagonal elements of $\mathcal{H}$ in equation (1).

[5.2] Find all eigen energies of this system. Expand them to the order of J^2/A, using $A \gg J$.

[5.3] At the time $t = 0$, both particles exist in the left well. From Figures 2(a)-(e), choose the graph that shows the probability $P_n(t)$ ($n = 0, 1, 2$) that n particles exist in the right well at a time t. Indicate which of the lines (solid, dotted, or dashed-dotted) corresponds to $n = 0$, 1, and 2 in the figure you have chosen. For this chosen figure, derive an expression for the period T.

[6] Assume that there is strong repulsive interaction between the particles so that the energy of the system increases by B ($B \gg J > 0$) when both particles exist in the same well. From Figures 2(a)-(e), choose the graph that shows the probability $P_n(t)$ ($n = 0, 1, 2$) that n particles exist in the right well at a time t. Indicate which of the lines (solid, dotted, or dashed-dotted) corresponds to $n = 0$, 1, and 2 in the figure you have chosen. For this chosen figure, derive an expression for the period T.

[7] Explain whether there is an overall difference in the time dependences of the probabilities $P_n(t)$ ($n = 0, 1, 2$) between the cases of attractive ([5.3]) and repulsive ([6]) interactions.
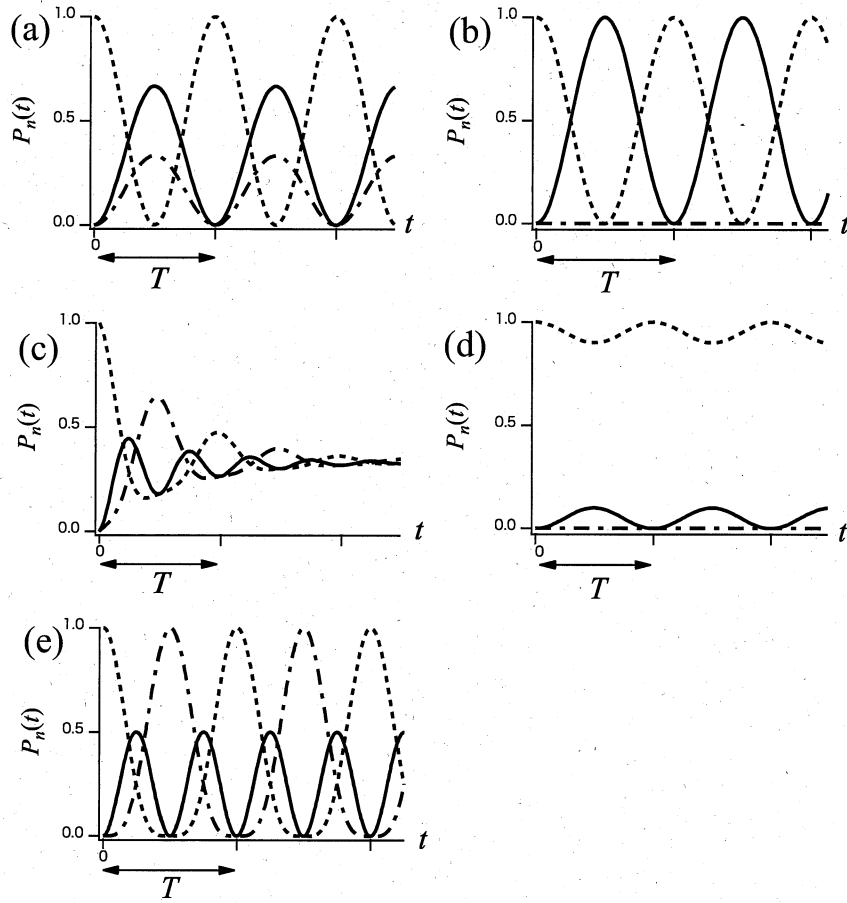
Figure 2: Time dependence of $P_n(t)$. In each Figure (a)-(e), the solid, dotted, and dashed-dotted lines correspond to either $n = 0$, 1, or 2.

Problem 2

Consider the canonical distribution of N identical particles with mass m in a cubic box of side length L. The reduced Planck constant $\hbar$ is equal to the Planck constant h divided by 2π. The Boltzmann constant is k_{B}. The temperature and the volume of the system are T and $V = L^3$, respectively. The system obeys the Boltzmann statistics, in which the probability of a particle to have an energy E is proportional to $\exp(-\frac{E}{k_{\mathrm{B}}T})$. Ignore any internal degrees of freedom of the particles and any relativistic effects. Solve the following problems and show how you derive your answers.

Consider an ideal gas, where the interaction between the particles can be ignored.

[1] Calculate the partition function Z of this system. If necessary, you may use the following formula:

$$\int_{-\infty}^{\infty} \exp(-x^2)dx = \sqrt{\pi}. \tag{1}$$

[2] Calculate the internal energy U and the specific heat C of this system.

[3] Derive the equation of state by calculating the pressure P using the following equation:

$$P = -\frac{\partial F}{\partial V}, \tag{2}$$

where F is the Helmholtz free energy.

Now consider that interactions between the particles take place, which include a long-range attractive part and a short-range repulsive part. The attractive interaction can be taken into account by assuming a uniform attractive potential, that is, the energy of one particle can be replaced by $E = \frac{p^2}{2m} - \alpha\frac{N}{V}$, where α is a positive constant and p is the momentum of the particle. Because of short-range repulsive interaction, each particle prohibits other particles from entering into a volume b centered around it. This exclusion effect can be taken into account by replacing V with $V - Nb$.

[4] Calculate the partition function Z of this system. Calculate the pressure P and derive the equation of state.

Next consider $A(V) = F(T, N, V) + PV$, a function of V, at a given temperature T and pressure P. At the volume V that gives local extrema of $A(V)$, the equation of state is satisfied as provided by equation (2). Now we define the Gibbs free energy $G(T, N, P)$ at a given temperature and pressure as the minimum of $F(T, N, V) + PV$, which is also a function of V:

$$G(T, N, P) = \min_V[F(T, N, V) + PV]. \tag{3}$$

At a particular temperature T and pressure P, the function $F(T, N, V) + PV$ has two equal minima as shown in the following figure.
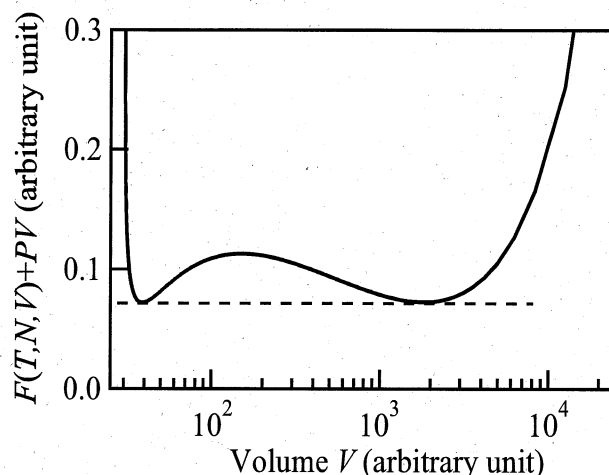

Figure 1: $F(T, N, V) + PV$ as a function of V (solid curve). The dashed line is a guide to the eye.

[5] Which point(s) in Figure 1 at which the equation of state is satisfied is (are) stable in thermal equilibrium? Which is (are) unstable? Describe the reason by considering the sign of $\dfrac{\partial P}{\partial V}$.

[6] Draw $F(T, N, V) + PV$ as a function of V when the pressure P either increases or decreases from Figure 1 at a constant temperature T. For both cases explain the physical reason for the changes by pressure P.

[7] Draw the isothermal curve derived from the equation of state on the P-V plane at this temperature by considering the behavior of the function $F(T, N, V) + PV$ discussed above. Draw the isothermal curve of the equilibrium state on the P-V plane, based on the definition of the Gibbs free energy in equation (3).

Problem 3

Suppose a monochromatic, x-polarized, plane electromagnetic wave with an angular frequency ω, travelling in the $+z$ direction, is incident onto the interface ($z = 0$) between the vacuum and a medium with electric conductivity that follows Ohm's law, as shown in Figure 1. This gives rise to a reflected wave and a transmitted wave, of which the latter travels further in the $+z$ direction. In the following, we consider the propagation of this transmitted electromagnetic wave inside the medium. Suppose that the electric field $\boldsymbol{E}(\boldsymbol{r}, t)$ and the magnetic flux density $\boldsymbol{B}(\boldsymbol{r}, t)$ at position $\boldsymbol{r}$ and time t inside the medium are governed by the following equations:

$$\nabla \times \boldsymbol{E} = -\frac{\partial \boldsymbol{B}}{\partial t}, \qquad \nabla \cdot \boldsymbol{E} = 0, \qquad \nabla \times \boldsymbol{B} = \varepsilon\mu\frac{\partial \boldsymbol{E}}{\partial t} + \mu\sigma\boldsymbol{E}, \qquad \nabla \cdot \boldsymbol{B} = 0.$$

Here ε, μ, and σ, denoting the electric permittivity, magnetic permeability, and electric conductivity of the medium, respectively, are all positive and real-valued constants. Then, the wave equations for the electromagnetic wave propagating in the $+z$ direction inside the medium read as follows:

$$\frac{\partial^2 \boldsymbol{E}}{\partial z^2} - \varepsilon\mu\frac{\partial^2 \boldsymbol{E}}{\partial t^2} - \mu\sigma\frac{\partial \boldsymbol{E}}{\partial t} = 0, \qquad (1) \qquad\qquad \frac{\partial^2 \boldsymbol{B}}{\partial z^2} - \varepsilon\mu\frac{\partial^2 \boldsymbol{B}}{\partial t^2} - \mu\sigma\frac{\partial \boldsymbol{B}}{\partial t} = 0. \qquad (2)$$

Assuming that the electric field of the electromagnetic wave oscillates in the x-direction in the medium as well, answer the following questions.
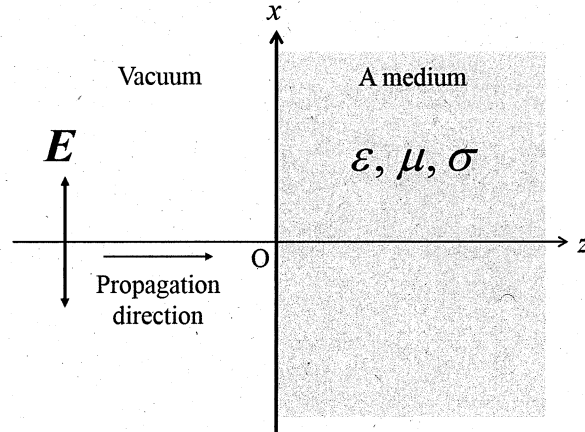

Figure 1

[1] The plane-wave solution of equation (1) is given in the complex form:

$$\boldsymbol{E}(z, t) = \mathrm{Re}\left[\tilde{\boldsymbol{E}}_0 \exp\left\{i\left(\tilde{k}z - \omega t\right)\right\}\right], \qquad (3)$$

where $\tilde{\boldsymbol{E}}_0$ is a complex vector and $\tilde{k} = k_1 + ik_2$ is a complex number (k_1 and k_2 are both real). Express the phase velocity (the velocity of the wave front) v of the plane wave in equation (3), using any necessary quantities among k_1, k_2, and ω.

[2] At a certain travelling distance d from the interface ($z = 0$), the amplitude of the electric field has become attenuated to $1/e$ of its value at the interface (e is the base of the natural logarithm). Express this characteristic distance d, using any necessary quantities among k_1, k_2, and ω.

[3] Express k_1 and k_2 using the quantities ε, μ, σ, and ω.

[4] Show how the distance d, defined in [2], depends on the conductivity σ, for the two extreme cases of large conductivity ($\sigma \gg \varepsilon\omega$) and small conductivity ($\sigma \ll \varepsilon\omega$).

[5] The oscillation of the magnetic flux density is delayed with respect to that of the electric field by the phase delay ϕ ($0 \le \phi < 2\pi$). Express ϕ using any necessary quantities among k_1, k_2, and ω. Also, calculate the value of ϕ in the limit of large conductivity $\left(\dfrac{\sigma}{\varepsilon\omega} \to \infty\right)$ as well as in the limit of small conductivity $\left(\dfrac{\sigma}{\varepsilon\omega} \to 0\right)$.

[6] Express the magnitude $|\langle \boldsymbol{S} \rangle|$ of the time-average $\langle \boldsymbol{S} \rangle$ of the Poynting vector $\boldsymbol{S} = (1/\mu)\, \boldsymbol{E} \times \boldsymbol{B}$ of the electromagnetic wave just after penetration ($z = 0$), using any necessary quantities among ε, μ, σ, ω, ϕ, and $|\tilde{\boldsymbol{E}}_0|$.

Recalling that Ohm's law $\boldsymbol{J}(\boldsymbol{r}, t) = \sigma \boldsymbol{E}(\boldsymbol{r}, t)$, where $\boldsymbol{J}(\boldsymbol{r}, t)$ is the current density, holds in the medium, answer the following questions.

[7] Express the power $Q(\boldsymbol{r}, t)$ exerted on the medium per unit volume by the electromagnetic wave with an electric field $\boldsymbol{E}(\boldsymbol{r}, t)$ and a magnetic flux density $\boldsymbol{B}(\boldsymbol{r}, t)$, using any necessary quantities among $\boldsymbol{E}(\boldsymbol{r}, t)$, $\boldsymbol{B}(\boldsymbol{r}, t)$, and $\boldsymbol{J}(\boldsymbol{r}, t)$.

[8] Calculate $\displaystyle\int_0^{+\infty} \langle Q(z, t) \rangle dz$, where $\langle Q(z, t) \rangle$ denotes the time average of the power $Q(z, t)$ exerted on the medium per unit volume by the electromagnetic wave considered in [1]-[6], and show the relation between this result and $|\langle \boldsymbol{S} \rangle|$ calculated in [6]. Also, explain what this relation physically tells.

Problem 4

Consider the electronic state of a two-dimensional crystal with a unit cell length of a, as shown in Figure 1. The primitive unit vectors are $\boldsymbol{a}_1 = (\sqrt{3}a/2,\, a/2)$ and $\boldsymbol{a}_2 = (-\sqrt{3}a/2,\, a/2)$. Answer the following questions.

[1] Derive the primitive translation vectors $\boldsymbol{b}_1$ and $\boldsymbol{b}_2$ in the reciprocal space $(k_x,\, k_y)$, and sketch the first Brillouin zone with these vectors. In addition, find the coordinates of the points P and Q where the first Brillouin zone boundary crosses the axes of k_x (> 0) and k_y (> 0), respectively.

[2] Now consider that the electrons are free by ignoring the periodic potential. Derive the radius of the Fermi surface, k_F, in the case that there are two electrons per unit cell, considering the spin degrees of freedom.

[3] Sketch the schematic Fermi surface derived in [2] together with the first Brillouin zone arranged in an appropriate manner.

Next, consider the electronic states of the two-dimensional crystal shown in Figure 2, by taking a periodic potential into account. The two-dimensional crystal contains two atoms of different species, A and B, in the same unit cell shown in Figure 1. Each atom has three nearest neighbors at the same distance. The eigen wave function of the electrons, $\psi_{\boldsymbol{k}}(\boldsymbol{r})$, in the whole crystal satisfies the Schrödinger equation,

$$\mathcal{H}\psi_{\boldsymbol{k}}(\boldsymbol{r}) = E(\boldsymbol{k})\psi_{\boldsymbol{k}}(\boldsymbol{r}). \tag{1}$$

Here, $\mathcal{H}$ and $E(\boldsymbol{k})$ represent the Hamiltonian and the eigenvalue of the system, respectively. $\boldsymbol{k}$ is the quantum number specifying the eigen state. We shall assume that $\psi_{\boldsymbol{k}}(\boldsymbol{r})$ can be written as the sum of the functions contributed by the orbitals of the atoms A, $\psi_{\boldsymbol{k}}^A(\boldsymbol{r})$, and of the atoms B, $\psi_{\boldsymbol{k}}^B(\boldsymbol{r})$, with the coefficients, $\lambda_{\boldsymbol{k}}^A$ and $\lambda_{\boldsymbol{k}}^B$, as follows:

$$\psi_{\boldsymbol{k}}(\boldsymbol{r}) = \lambda_{\boldsymbol{k}}^A \psi_{\boldsymbol{k}}^A(\boldsymbol{r}) + \lambda_{\boldsymbol{k}}^B \psi_{\boldsymbol{k}}^B(\boldsymbol{r}). \tag{2}$$

$\psi_{\boldsymbol{k}}^A(\boldsymbol{r})$ and $\psi_{\boldsymbol{k}}^B(\boldsymbol{r})$ can be expressed by the outermost atomic orbitals of A and B, $\phi_A(\boldsymbol{r})$ and $\phi_B(\boldsymbol{r})$ (these are real functions), as follows:

$$\psi_{\boldsymbol{k}}^A(\boldsymbol{r}) = \sum_i \exp(i\boldsymbol{k}\cdot\boldsymbol{r}_i^A)\phi_A(\boldsymbol{r} - \boldsymbol{r}_i^A), \tag{3}$$

$$\psi_{\boldsymbol{k}}^B(\boldsymbol{r}) = \sum_j \exp(i\boldsymbol{k}\cdot\boldsymbol{r}_j^B)\phi_B(\boldsymbol{r} - \boldsymbol{r}_j^B). \tag{4}$$

Here, $\boldsymbol{r}_i^A$ and $\boldsymbol{r}_j^B$ represent the positions for i-th atom A and j-th atom B, respectively. In the following we neglect all atomic orbitals other than $\phi_A(\boldsymbol{r})$ and $\phi_B(\boldsymbol{r})$ and neglect interactions between the electrons as well.

[4] Derive the simultaneous equations with regard to $\lambda_{\boldsymbol{k}}^A$ and $\lambda_{\boldsymbol{k}}^B$, by calculating $\int \phi_A(\boldsymbol{r} - \boldsymbol{r}_i^A)\mathcal{H}\psi_{\boldsymbol{k}}(\boldsymbol{r})d\boldsymbol{r}$ and $\int \phi_B(\boldsymbol{r} - \boldsymbol{r}_j^B)\mathcal{H}\psi_{\boldsymbol{k}}(\boldsymbol{r})d\boldsymbol{r}$ and so on, and by considering the fact that $\psi_{\boldsymbol{k}}(\boldsymbol{r})$ satisfies equation (1). Note that we can neglect all overlap integrals between the atomic orbitals except those between identical atomic orbitals,

$$\int \phi_A(\boldsymbol{r} - \boldsymbol{r}_i^A)\phi_A(\boldsymbol{r} - \boldsymbol{r}_i^A)d\boldsymbol{r} = \int \phi_B(\boldsymbol{r} - \boldsymbol{r}_j^B)\phi_B(\boldsymbol{r} - \boldsymbol{r}_j^B)d\boldsymbol{r} = 1.$$

With regard to the matrix elements of the Hamiltonian $\mathcal{H}$, those between identical atomic orbitals can be written as

$$\int \phi_A(r - r_i^A)\mathcal{H}\phi_A(r - r_i^A)dr = \epsilon_A,$$

$$\int \phi_B(r - r_j^B)\mathcal{H}\phi_B(r - r_j^B)dr = \epsilon_B,$$

(here, we consider the case $\epsilon_A > \epsilon_B$), and those between atomic orbitals at different positions become a nonzero value as,

$$\int \phi_A(r - r_i^A)\mathcal{H}\phi_B(r - r_j^B)dr = \int \phi_B(r - r_j^B)\mathcal{H}\phi_A(r - r_i^A)dr = \tau,$$

only when a pair of the orbitals belongs to the nearest neighboring atoms of A and B ($|r_i^A - r_j^B| = a/\sqrt{3}$).

[5] Solve the simultaneous equations derived in [4], and find all energy eigen values $E(k)$ expressed as functions of k_x and k_y.

[6] The system has a finite energy gap, when a unit cell contains two outermost electrons on average. In this case, the wave vector of a highest-energy occupied state (E_1) and that of a lowest-energy unoccupied state (E_2) coincide at a point X on the axis k_y. Find the coordinates of the point X and calculate the energy gap, $E_g = E_2 - E_1$.

In the following, let the situation be limited to the case $k_x = 0$.

[7] Derive the k_y dependence of $E(k)$ near the point X. Assuming the relation $E_g \gg |\tau|$, calculate the effective mass along k_y.

[8] Provided that all B atoms are replaced by A atoms, derive the k_y dependence of $E(k)$ near the point X and calculate E_g.
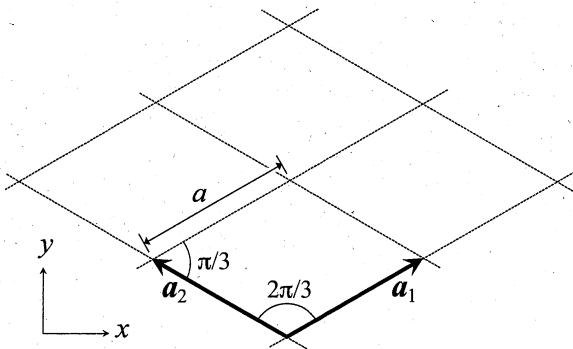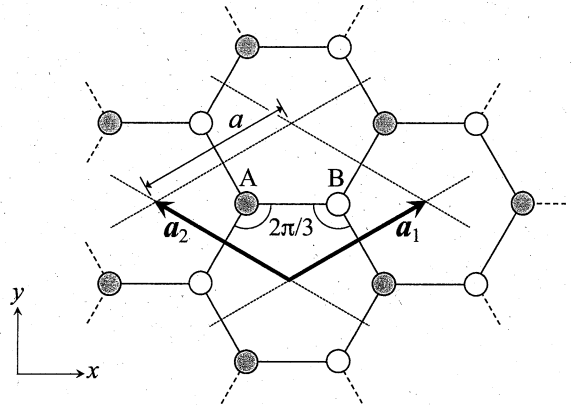

Figure 1: Two-dimensional lattice.

Figure 2: Two-dimensional crystal consisting of two kinds of atoms, A and B.