NATIONAL EXAMS
May 2015

Phys-A6: Solid State Physics

3 hours duration

NOTES:

1. If doubt exits as to the interpretation of any question, the candidate must submit with the answer paper, a clear statement of any assumption made.
2. Candidates may use one of two calculators, the Casio or Sharp approved models.
3. This is a CLOSED BOOK EXAM.
   Useful constants and equations have been annexed to the exam paper.
4. **Any FIVE (5) of the SEVEN (7)** questions constitute a complete exam paper.
   The first five questions as they appear in the answer book will be marked.
5. When answering questions, candidates must clearly indicate units for all parameters used or computed.

MARKING SCHEME

Questions	*Marks*				
1	(a) 2	(b) 5	(c) 5	(d) 5	(e) 3
2	(a) 3	(b) 3	(c) 8	(d) 6	
3	(a) 10	(b) 10			
4	(a) 4	(b) 6	(c) 4	(d) 6	
5	(a) 4	(b) 4	(c) 6	(d) 6	
6	(a) 6	(b) 2	(c) 3	(d) 9	
7	(a) 6	(b) 6	(c) 8		

1. Answer the following questions on crystal structures.

2 pts (a) How many three-dimensional *Bravais* lattices exist?

5 pts (b) What is the *packing fraction* of the body-centered-cubic lattice shown in Figure P1? [Note that the volume of a sphere or radius r is V = (4πr3)/3]

5 pts (c) Find the *primitive translation vectors* $\mathbf{a}_1$, $\mathbf{a}_2$ and $\mathbf{a}_3$ for the lattice of Figure P1 in terms of the cube edge a and Cartesian unit vectors **x**, **y**, and **z**.

5 pts (d) Calculate the volume of the *primitive cell* of the lattice shown in Figure P1?

3 pts (e) What are the Miller indices of the crystal plane containing the top eight atoms shown in Figure P1?

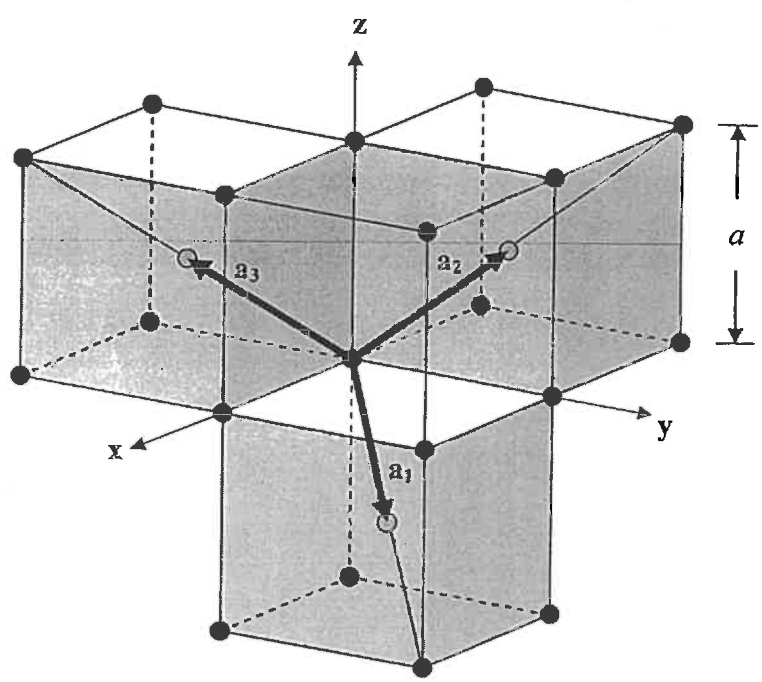


Figure P1

2. The solid curve in Figure P2a represents the total energy per molecule $U(R)$ as a function of ionic separation R for a typical ionic crystal such as KCl, NaCl, or ZnS. In these crystals, this energy is basically the sum of a repulsion contribution and a Coulomb contribution. Typical variations of these two components as a function of ionic separation R are shown in Figure P2a.

3 pts (a) Briefly explain the origin and impact of the repulsive energy contribution.

3 pts (b) Briefly explain the origin and impact of the Coulomb energy contribution.

8 pts (c) Determine the value for the equilibrium ionic separation R_o shown on the graph of Figure P2a.

6 pts (d) Determine the Madelung constant α for the line of ions equally spaced shown in Figure P2b.

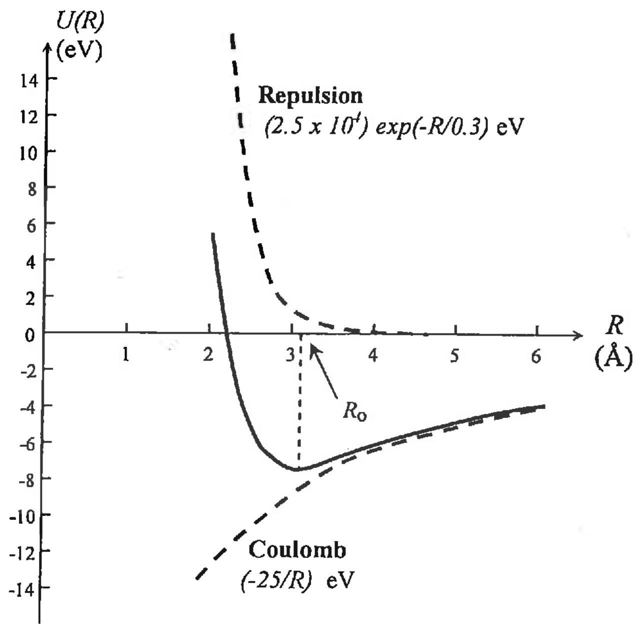


Figure P2a

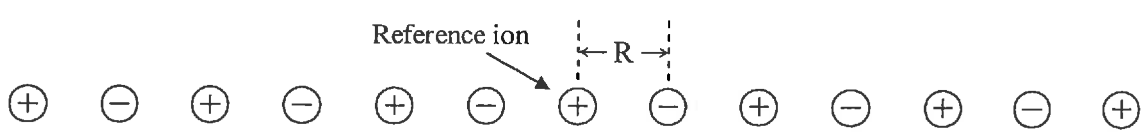


Figure P2b

3. Consider vibrations in a crystal with a monatomic basis where each atom has a mass M and a force constant C between nearest-neighbour lattice planes. Figure P3 shows the displacements of planes of atoms (grey circles) from their equilibrium positions (dashed lines) when vibrations are present. The normal spacing between planes at rest, a, depends on the direction of the wave vector **K**.

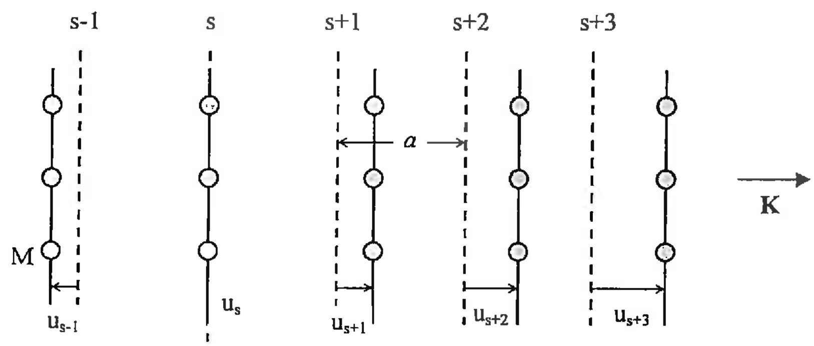


Figure P3

Assuming displacements of the form $u_s = u\ exp(isKa)$, all having the time dependence $exp(-i\omega t)$ and considering only nearest planes, the equation of motion of this system leads to the following formula:

$$M\omega^2 = -C[e^{iKa} + e^{-iKa} - 2]$$

10 pts (a) Show that the dispersion relation $\omega(K)$ is given by $\omega = \sqrt{\left(\frac{4C}{M}\right)}\left|\sin(\frac{Ka}{2})\right|$

and plot the dispersion relation for the *first Brillouin zone* defined by $-\pi/a \leq K \leq +\pi/a$.

10 pts (b) The transmission velocity of a wave packet (energy propagation) in this crystal is given by the *group velocity*

$$v_g = \frac{d\omega}{dK}$$

Find expressions for v_g at the edge of the Brillouin zone (where $K = \pm\pi/a$) and for long wavelengths (where $Ka << 1$).

Briefly discuss what each of the two results means.

4. Using classical theory, the interpretation of the properties of metals in terms of the motion of free electrons had notable successes. However, it failed to explain the heat capacity and the magnetic susceptibility of electrons, and their remarkable long mean free path. It took quantum mechanics and the Fermi-Dirac distribution to better understand the properties of metals.

4 pts (a) Give the two main reasons why metals are so transparent to free electrons.

6 pts (b) Figure P4 shows the first three energy levels and associated wave functions for a free electron of mass m confined to a line of length L inside infinite barriers. For each energy level n, the wave function must be of the form $\psi_n = A \sin\left(\frac{2\pi}{\lambda_n}x\right)$ and meet the boundary conditions that $\psi_n(0) = \psi_n(L) = 0$ at the barriers.

Given that each wave function is a solution to Schrödinger equation

$$-\frac{\hbar^2}{2m}\frac{d^2\psi_n}{dx^2} = \epsilon_n \psi_n$$

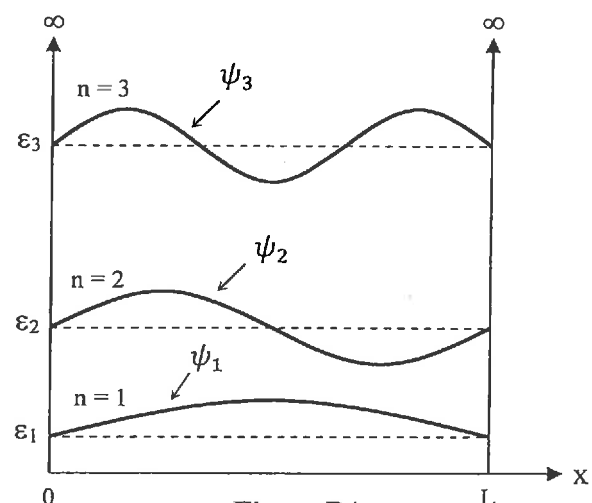
show that for each level n the energy is given by:

$$\epsilon_n = \frac{\hbar^2}{2m}\left(\frac{n\pi}{L}\right)^2$$

4 pts (c) Briefly describe what the term ***Fermi energy*** means for a system of N electrons such as the one shown in Figure P4.

6 pts (d) If an even number N of electrons must be accommodated on the line of Figure P4, show that the value of the Fermi energy is given by:

$$\epsilon_F = \frac{\hbar^2}{2m}\left(\frac{N\pi}{2L}\right)^2$$



<u>**Figure P4**</u>

5. Figure P5 shows the energy band and Fermi-Dirac distribution for an *extrinsic* semiconductor. Measurements on *intrinsic* samples of this semiconductor lead to an *effective mass* of 1.2*m* for electrons and 0.6*m* for holes.

4 pts (a) For the *intrinsic* semiconductor at T = 300 °K, calculate how far above the top of the valence band E_v the Fermi level is situated.

4 pts (b) State if the *extrinsic* semiconductor is of type N or type P, and briefly explain your answer.

6 pts (c) If, at T = 300 °K, the hole concentration in the *extrinsic* semiconductor is 2.25×10^3 /cm^3, what is the electron concentration?

6 pts (d) If, at T = 300 °K, the Fermi level in Figure P5 is situated 0.15 eV below the bottom of the conduction band E_c, calculate the probability for an electron to occupy an energy level situated 0.1 eV above E_c.

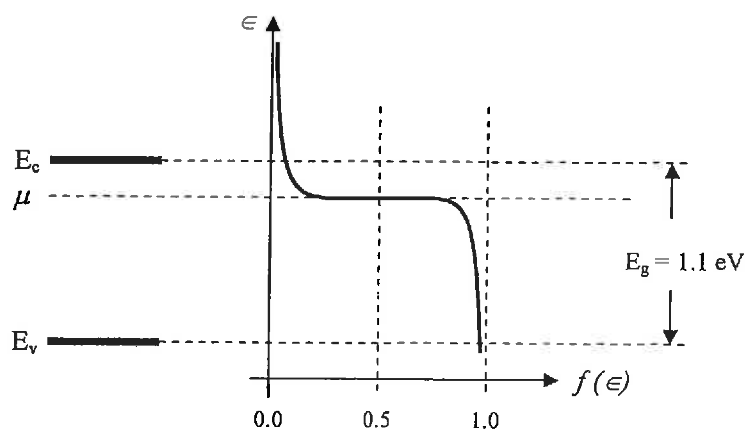


Figure P5

6. The following questions refer to magnetism present or induced in crystal lattices. Note that Figure P6 shows experimental data on the variation of the inverse of the magnetic susceptibility with temperature for a complex crystal involving a rare earth element.

6 pts (a) The magnetic moment of a free atom arises due to three main factors:

① Spin of the electrons
② Orbital momentum of electrons
③ Change of the orbital angular momentum of electrons due to an externally applied magnetic field.

Briefly explain how these factors are involved in *diamagnetic* and/or *paramagnetic* materials.

2 pts (b) To a lesser extent, nuclear magnetic moments can also give rise to paramagnetism. Give the approximate ratio between the strength of nuclear paramagnetism and the strength of electronic paramagnetism.

3 pts (c) Briefly explain how the *magnetic susceptibility* χ is defined and what types of units are used.

9 pts (d) Based on the graph of Figure P6,

i. State if the crystal is *paramagnetic* or *diamagnetic* and briefly justify why.

ii. Briefly explain why the susceptibility decreases with temperature.

iii. Evaluate the *Currie constant* of the crystal.

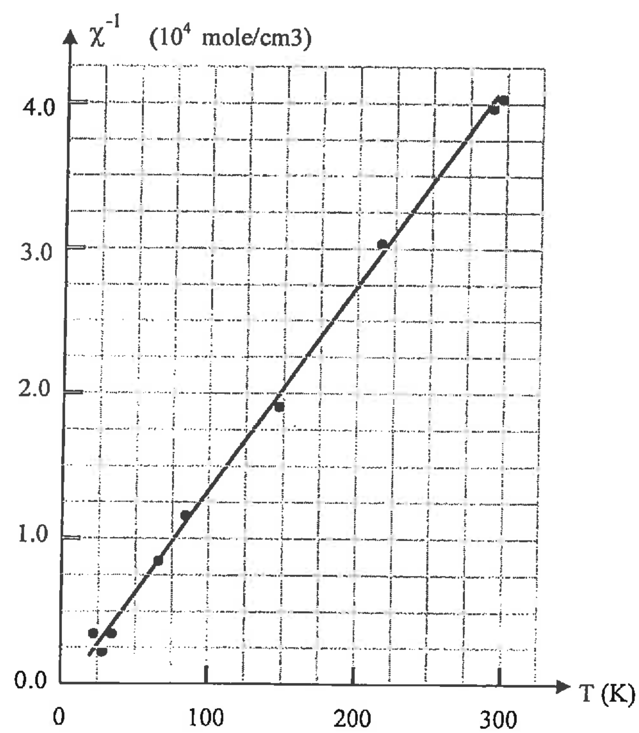


Figure P6

7. The following questions refer to the presence of defects and the diffusion of impurities in crystal lattices.

6 pts (a) Briefly explain what each of the following terms means:

i. Schottky defect

ii. Frenkel defect

iii. Color center

6 pts (b) If the energy to take an atom of sodium (Na) from its normal lattice site to a lattice site at the surface of the crystal is 1.0 eV, calculate the required temperature T (in °K) to obtain a bulk defect concentration of 1 vacancy per 100,000 atoms of Na.

8 pts (c) Figure P7 shows experimental results on the diffusion of zinc (Zn) atoms in a copper (Cu) host crystal. From the graph, determine values of the *diffusion constant* D_0 and *activation energy E* involved in the diffusion process.

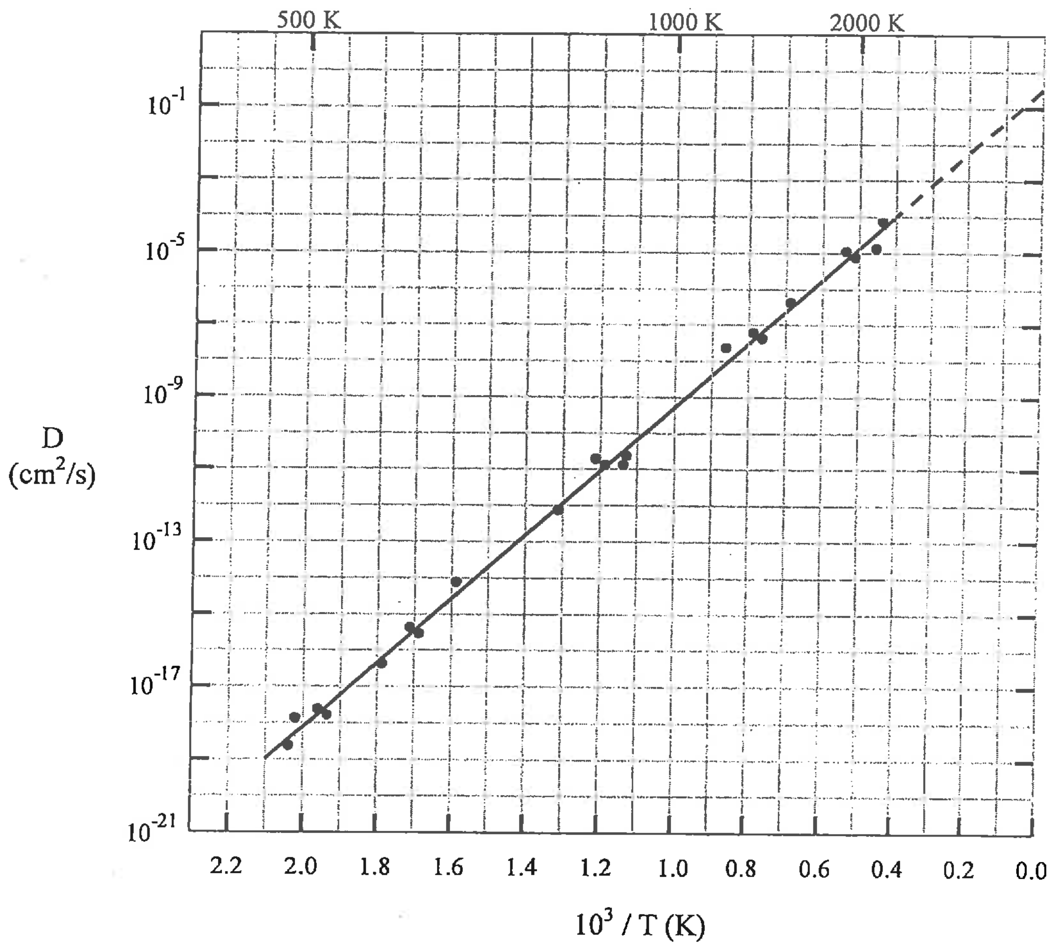


Figure P7

--- **END** ---

USEFUL EQUATIONS

---

(1) $sin^2\theta = \frac{1}{2}(1-\cos 2\theta)$

(2) $cos\theta = \frac{1}{2}[\exp(i\theta)+\exp(-i\theta)]$

(3) For $\theta << 1$: $\cos\theta \cong 1-\frac{1}{2}\theta^2$ and $\sin\theta \cong \theta$

(4) $\boldsymbol{T} = u_1\boldsymbol{a}_1 + u_2\boldsymbol{a}_2 + u_3\boldsymbol{a}_3$

(5) $\boldsymbol{G} = v_1\boldsymbol{b}_1 + v_2\boldsymbol{b}_2 + v_3\boldsymbol{b}_3$

(6) $\boldsymbol{p} = \boldsymbol{r}\times\boldsymbol{t} = \begin{pmatrix} p_1 \\ p_2 \\ p_3 \end{pmatrix}(\boldsymbol{x}\,\boldsymbol{y}\,\boldsymbol{z}) = \begin{pmatrix} r_2t_3 - r_3t_2 \\ r_3t_1 - r_1t_3 \\ r_1t_2 - r_2t_1 \end{pmatrix}(\boldsymbol{x}\,\boldsymbol{y}\,\boldsymbol{z})$ where $\boldsymbol{r} = r_1\boldsymbol{x} + r_2\boldsymbol{y} + r_3\boldsymbol{z}$, $\boldsymbol{t} = t_1\boldsymbol{x} + t_2\boldsymbol{y} + t_3\boldsymbol{z}$

(7) $V_{min} = |\boldsymbol{a}_1\cdot(\boldsymbol{a}_2\times\boldsymbol{a}_3)|$

(8) $\boldsymbol{b}_1 = 2\pi\frac{\boldsymbol{a}_2\times\boldsymbol{a}_3}{\boldsymbol{a}_1\cdot(\boldsymbol{a}_2\times\boldsymbol{a}_3)}$ $\quad \boldsymbol{b}_2 = 2\pi\frac{\boldsymbol{a}_3\times\boldsymbol{a}_1}{\boldsymbol{a}_1\cdot(\boldsymbol{a}_2\times\boldsymbol{a}_3)}$ $\quad \boldsymbol{b}_3 = 2\pi\frac{\boldsymbol{a}_1\times\boldsymbol{a}_2}{\boldsymbol{a}_1\cdot(\boldsymbol{a}_2\times\boldsymbol{a}_3)}$

(9) $2d\sin\theta = n\lambda$ $\quad \Delta\boldsymbol{k} = \boldsymbol{G}$ $\quad 2\boldsymbol{k}\cdot\boldsymbol{G} = \boldsymbol{G}^2$

(10) $U(R) = 4\epsilon\left[\left(\frac{\sigma}{R}\right)^{12} - \left(\frac{\sigma}{R}\right)^{6}\right]$ $\quad F(R) = -\,dU(R)/dR$

(11) $U_{tot} = -(2.15)(4N\varepsilon)$

(12) $U(R) = N\left[z\lambda e^{-R/\rho} - \frac{\alpha q^2}{R}\right]$ (CGS) [for SI, replace q^2 by $q^2/4\pi\varepsilon_o$]

(13) $\frac{\alpha}{R} = \sum_j \frac{(+/-)}{r_j}$

(14) $F_s = M\frac{d^2u_s}{dt^2} = C(u_{s+1}-u_s) - C(u_{s-1}-u_s)$

(15) $f(\epsilon) = \frac{1}{exp\left[\frac{\epsilon-\mu}{k_BT}\right]+1}$

(16) $k_F = \left(\frac{3\pi^2N}{V}\right)^{1/3}$

(17) $\epsilon_F = \frac{\hbar}{2m}\left(\frac{3\pi^2N}{V}\right)^{2/3}$

(18) $m^* = \hbar^2\Big/\left(\frac{d^2\epsilon}{dk^2}\right)$

(19) $np = 4\left(\frac{k_BT}{2\pi\hbar^2}\right)^3 (m_em_h)^{3/2}\exp\left(\frac{-E_g}{k_BT}\right)$

(20) $n_i = p_i = 2\left(\frac{k_B T}{2\pi\hbar^2}\right)^{3/2} (m_e m_h)^{3/4} \exp\left(\frac{-E_g}{2k_B T}\right)$

(21) $\mu = \frac{E_g}{2} + \frac{3}{4}\, k_B T\, \ln\,(m_h/m_e)$

(22) $\chi = -\frac{\mu_o N Z e^2}{6m}\langle r^2\rangle$

(23) $\chi = \frac{C}{T}$

(24) $\frac{n}{N-n} = exp\left(\frac{-E_V}{k_B T}\right)$

(25) $D = D_o exp\left(\frac{-E}{k_B T}\right)$

USEFUL PARAMETERS

Quantity	Symbol	Value	CGS	SI
Light velocity	c	2.998	10^{10} cm/s	10^{8} m/s
Proton's charge	e	1.602		10^{-19} C
Planck's constant	h	6.626	10^{-27} erg · s	10^{-34} J · s
	$\hbar = h/2\pi$	1.055	10^{-27} erg · s	10^{-34} J · s
Avogadro's number	N	6.022 x 10^{23} /mole		
Atomic mass unit	amu	1.66	10^{-24} g	10^{-27} kg
Electron's mass	m	9.11	10^{-28} g	10^{-31} kg
Proton's mass	M_p	1.67	10^{-24} g	10^{-27} kg
Bohr radius: $\hbar^2/me^2$	r_o	5.292	10^{-9} cm	10^{-11} m
Bohr magneton: $e\hbar/2mc$	μ_B	9.274	10^{-21} erg/G	10^{-24} J/T
Energy (electron volt)	eV	1.602	10^{-12} erg	10^{-19} J
Boltzmann's constant	k_B	1.38	10^{-16} erg/K	10^{-23} J/K
		0.862	10^{-4} eV/K	
	eV/k_B	1.16 x 10^{4} K		
Permittivity (free space)	ϵ_o		1	$10^7/4\pi c^2$ F/m
Permeability (free space)	μ_o		1	4π x 10^{-7} N/A^2