

EXAM IN COURSE TFY4220 Solid State Physics

Monday 30. May 2011

Time: 9.00 – 13.00

DRAFT OF SOLUTION

Problem 1 (20%) Introductory Questions

a)

(1) Primitive unit cell: The minimum volume cell which will fill all space (without holes or overlap) when translated with all lattice vectors $\mathbf{R}$. Contains one lattice point.

(2) Crystal system: Bravais lattice point groups. We make a unit cell with three edges a, b, c and three angles α, β, γ , which will make up different crystal systems dependent on the restrictions on lengths a, b, c and angles α, β, γ . Examples of crystal systems are triclinic, monoclinic, orthorhombic...)

(3) Bravais lattice: A distinct lattice type /special lattice type. A special pattern of points which looks identical from each point.

There are 7 crystal systems and 14 Bravais lattices in 3 dimensions.

b) Phonon: quantum of energy of a lattice vibration; a collective excitation in a periodic, elastic arrangement of atoms in condensed matter.

Optical phonon: masses oscillate with opposite phase; opposite directions.

Acoustic phonon: masses oscillate with same phase; same directions.

See figure 10, page 98 in Kittel.

In total, with s atoms in basis, there are $3s$ modes, 3 acoustical and $3(s-1)$ optical modes.

c) The free electron model can describe heat capacity, thermal conductivity, electrical conductivity/ resistivity and electrodynamics of metals. And the Hall effect (but not the signs in the Hall constant!).

d) Metal: Fermi level lies in a partial filled energy band.

Insulator: An energy gap occurs (at $T=0$) between a filled lower band (valence band) and an empty higher band (conduction band), there is a gap >3 eV at the Fermi level.

Semiconductor: An insulator with a small band gap (<3 eV). Thermal excitations across gap are possible.

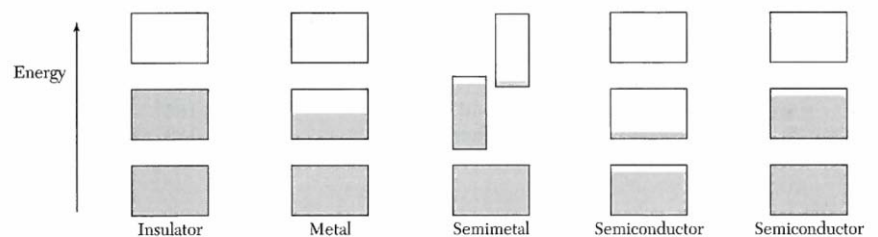


Figure 1 Schematic electron occupancy of allowed energy bands for an insulator, metal, semimetal, and semiconductor. The vertical extent of the boxes indicates the allowed energy regions; the shaded areas indicate the regions filled with electrons. In a **semimetal** (such as bismuth) one band is almost filled and another band is nearly empty at absolute zero, but a pure **semiconductor** (such as silicon) becomes an insulator at absolute zero. The left of the two semiconductors shown is at a finite temperature, with carriers excited thermally. The other semiconductor is electron-deficient because of impurities.

Electric conductivity of semiconductor and metal:

Semiconductor: A few mobile charge carriers available at room temperature= low conductivity. At higher T will there be more mobile electrons/holes and conductivity increases.

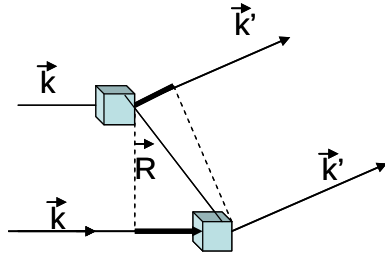
Metal: Many mobile electrons available. What limits the conductivity is impurities and phonons. Density of phonons increases with T , more phonon-electron collisions and less conductivity. This also happens for semiconductors, but here the effect of more charge carriers will be more important than the increase phonon-electron scattering.

Problem 2 (25%) Structure and Diffraction

a) Reciprocal lattice vector: $\vec{G}_{hkl} = h\vec{a}^* + k\vec{b}^* + l\vec{c}^*$ is a vector between lattice points in the reciprocal lattice, given by the sum of integers (h, k, l) of primitive vectors in the reciprocal lattice vectors ($\vec{a}^*, \vec{b}^*, \vec{c}^*$). The vector is normal to the lattice plane (hkl).

We will show that $\vec{k} - \vec{k}' = \vec{G}_{hkl}$ has to be valid for constructive interference.

$\vec{k}$ and $\vec{k}'$ are the incoming and the scattered k-vector, respectively, for the X-ray scattering. $|\vec{k}| = |\vec{k}'| = k = \frac{2\pi}{\lambda}$. We look at scattering from two lattice points with a distance $\vec{R}$ and look at the path difference:



Difference in path (from figure):

$$\vec{R} \cdot \frac{\vec{k}'}{k} - \vec{R} \cdot \frac{\vec{k}}{k} = \vec{R}(\vec{k}' - \vec{k}) \cdot \frac{1}{k} = \vec{R}(\vec{k}' - \vec{k}) \cdot \frac{\lambda}{2\pi}$$

This has to be an integer number of λ if constructive interference. The equation over is valid for all $\vec{R}$.

$$\vec{R}(\vec{k}' - \vec{k}) \cdot \frac{\lambda}{2\pi} = n\lambda, \quad \vec{R}(\vec{k}' - \vec{k}) = 2\pi n \quad \text{this gives that } e^{i\vec{R}(\vec{k}' - \vec{k})} = 1. \quad \text{For this to be valid,}$$

$(\vec{k}' - \vec{k}) = \vec{G}_{hkl}$ has to be valid for all $\vec{R}$. This was what should be shown. QED.

b) The angle between $\vec{k}$ and $\vec{k}'$ is 2θ . For a cubic crystal we have

$$|\vec{a}^*| = |\vec{b}^*| = |\vec{c}^*| = \frac{2\pi}{a} \quad \text{which gives} \quad (\vec{k}' - \vec{k}) = \vec{G}_{hkl} = \frac{2\pi}{a}h + \frac{2\pi}{a}k + \frac{2\pi}{a}l$$

$$\text{Square both sides give: } (\vec{k})^2 - 2|\vec{k}||\vec{k}'|\cos(2\theta) + (\vec{k}')^2 = \left(\frac{2\pi}{a}\right)^2 (h^2 + k^2 + l^2)$$

$$2k^2[1 - \cos(2\theta)] = \left(\frac{2\pi}{a}\right)^2 (h^2 + k^2 + l^2)$$

$$2\left(\frac{2\pi}{\lambda}\right)^2 [1 - 1 + 2\sin^2 \theta] = \left(\frac{2\pi}{a}\right)^2 (h^2 + k^2 + l^2)$$

$$\frac{4}{\lambda^2} \cdot \sin^2 \theta = \frac{h^2 + k^2 + l^2}{a^2}$$

$$\frac{4a^2}{\lambda^2} \cdot \sin^2 \theta = h^2 + k^2 + l^2$$

$$\text{or } \sin^2 \theta = \left(\frac{\lambda}{2a}\right)^2 (h^2 + k^2 + l^2)$$

You will get full pot if you derive $\sin^2 \theta$ from Braggs law, starting from $2d \sin \theta = n\lambda$, introducing expression for d , and square this (and obtain the same result!).

c) This is what we did in the X-ray lab. We have to find the (hkl) values corresponding to the 5 lines. This can be solved in two ways:

1) Look at the lowest difference in $\sin^2 \theta$ from above and from this find the $h^2 + k^2 + l^2$ (N_i) in the equation above.

$$\sin^2 \theta = \left(\frac{\lambda}{2a} \right)^2 (h^2 + k^2 + l^2) = \left[\left(\frac{\lambda}{2a} \right)^2 N_i \right]$$

line	$\sin^2 \theta$	$\sin^2 \theta_{i-1} - \sin^2 \theta_i$	N_i	N	hkl
1	0.0433	0.0147	2.99	3	111
2	0.0580	0.0593	4	4	200
3	0.1173	0.0438	8.09	8	220
4	0.1611	0.0145	11.11	11	311
5	0.1756		12.11	12	222

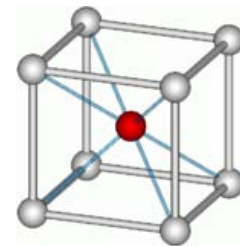
2) We can assume bcc or fcc and do a test and trial:

bcc				fcc			
hkl	$h^2+k^2+l^2$	a^2	a	hkl	$h^2+k^2+l^2$	a^2	a
110	2	27,4568591	5,239929	111	3	41,18529	6,417577
200	4	40,995931	6,402806	200	4	40,99593	6,402806
211	6	30,4061893	5,514181	220	8	40,54159	6,367227
220	8	29,5191061	5,433149	311	11	40,58877	6,370932
310	10	33,8519932	5,818247	222	12	40,62239	6,37357

In both cases we find that the reflections (with intensities) are 111, 200, 220, 311 and 222, corresponding to none reflections (extinctions) with mixed indices, and therefore a fcc structure, and that the lattice parameter is 6.37 Å.

d) This is a cubic primitive (P) cell with a basis of A in (000) and B in $(\frac{1}{2} \frac{1}{2} \frac{1}{2})$; corresponds to the CsCl structure (grey is A and red is B).

One AB molecule per Bravais lattice point.



This structure (P) will not give any extinctions:

$$\text{We have } S_G = F_{hkl} = \sum_j f_j e^{-i\vec{G}_{hkl} \cdot \vec{r}_j} = \sum_j f_j \cdot e^{-i2\pi(hx_j + ky_j + lz_j)} = f_A + f_B \cdot e^{-i2\pi(\frac{h}{2} + \frac{k}{2} + \frac{l}{2})}$$

Above T_c (statistically disorder on the atom positions) each lattice point will statistically have $\frac{1}{2}$ A and $\frac{1}{2}$ B and the two 'atoms' in the basis will be identical. We will have a base centred cubic (bcc) structure and observe extinctions as for the bcc:

$$F(hkl) = \sum_j f_j e^{-i\vec{G}_{hkl} \cdot \vec{r}_j} = \left(\frac{1}{2} f_A + \frac{1}{2} f_B \right) \left[1 + e^{-i2\pi(\frac{h}{2} + \frac{k}{2} + \frac{l}{2})} \right] = \begin{cases} \left(\frac{1}{2} f_A + \frac{1}{2} f_B \right) & \text{for } h+k+l=\text{even} \\ 0 & \text{for } h+k+l=\text{odd} \end{cases}$$

That means; extinctions if sum of hkl is an even integer.

Problem 3 (25%) Phonons

a) This derivation is done in Kittel pages 97-99 and also in the lecture. I therefore show it very brief here.

We put up the force on the atom, assuming only nearest neighbour interaction, and then Newton's second law for each of the two masses in the basis.

$F_m = K(v_{n-1} - u_n) + K(v_n - u_n)$ and $F_M = K(u_n - v_n) + K(u_{n+1} - v_n)$. With Newtons 2. law, we get the two coupled differential equations

$$m \frac{\partial^2 v_n}{\partial t^2} = K(u_{n+1} + u_n - 2v_n) \text{ and } M \frac{\partial^2 u_n}{\partial t^2} = K(v_n + v_{n-1} - 2u_n)$$

Then we use the solutions $u_n = u \cdot e^{i(nka - \omega t)}$ og $v_n = v \cdot e^{i(nka - \omega t)}$ and get

$$\begin{bmatrix} 2K - m\omega^2 & -K(1 + e^{-ika}) \\ -K(1 + e^{ika}) & 2K - M\omega^2 \end{bmatrix} \cdot \begin{pmatrix} u \\ v \end{pmatrix} = 0$$

The determinant has to be zero, which gives the equation

$$(2K - m\omega^2)(2K - M\omega^2) - K^2(1 + e^{ika})(1 + e^{-ika}) = 0$$

$$4K^2 - 2Km\omega^2 - 2KM\omega^2 + mM\omega^4 - K^2(1 + e^{ika})(1 + e^{-ika}) = 0$$

This is a second order equation in ω^2 ,

$$x = \frac{-b \pm \sqrt{b^2 - 4ac}}{2a}, \quad \begin{aligned} a &= mM \\ b &= -2K(m + M) \\ c &= 2K^2(1 + \cos ka) \end{aligned}$$

$$\omega^2 = \frac{2K(m + M) \pm \sqrt{4K^2(m + M)^2 - 4mM 2K^2(1 + \cos ka)}}{2mM}$$

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and gives the dispersion relationship

$$\omega^2 = \frac{K(m + M)}{mM} \left[1 \pm \sqrt{1 - \frac{4mM}{(m + M)^2} \cdot \sin^2 \frac{ka}{2}} \right] \quad (*)$$

as we were supposed to show.

NB! In the exercise the root stopped before the sin... I hope all got the message about this correction!

b) When $k \rightarrow 0$ we get

$$\omega^2 = \begin{cases} 2K\left(\frac{1}{m} + \frac{1}{M}\right) & \text{optical branch} \\ \frac{1}{2}(ka)^2 K \frac{1}{M + m} & \text{acoustical branch} \end{cases}$$

On the BZ we have $k = \frac{\pi}{a}$ and this gives, when inserted into (*);

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$$\omega^2 = \begin{cases} \frac{2K}{m} \\ \frac{2K}{M} \end{cases} \quad \text{Which is corresponding to acoustical and optical depends on which mass is heaviest.}$$

Group velocity for long wavelengths:

$$v_g = \frac{\delta\omega}{\delta k} = 0 \quad \text{for optical branch}$$

$$v_g = \frac{\delta\omega}{\delta k} = a \sqrt{\frac{K}{2(m+M)}} \quad \text{for } k \rightarrow 0 \text{ acoustic branch..}$$

If the material is exposed to waves with ω_i , the wave will be damped very quickly; no propagation.

c) When $M = m$ the forbidden gap disappears. We are back to the result for the monoatomic lattice; the two branches will be one folded into the 1 Brilluin zone (1BZ). The acoustic

velocity is $\frac{a}{2} \sqrt{\frac{K}{m}}$, the same as for the monoatomic lattice with lattice constant $a/2$, as expected. The dispersion relation becomes as for the monoatomic chain:

$$\omega^2 = \frac{4K}{m} \sin^2 \frac{ka}{4} \quad \text{figure!}$$

d) We can measure the sound velocity in ionic materials by sending in IR light and look at the resonance curve. We did in the lattice vibration lab for SiC.

figure!

Problem 4 (30%) Free-electron model, energy bands and semiconductors

a) Free electron model: Assume conduction electrons are a free electron gas. No interaction with ions or lattice, or interaction between conduction electrons. Charged particles; follow the

Pauli principle. $E(k) = \frac{\hbar^2}{2m} k^2$. The Fermi energy is the highest occupied energy,

corresponding to the Fermi energy wave vector k_F , corresponding to a sphere in 3D. The number of states inside the sphere with radius k_F is N. The volume in k-space which is occupied by one state is given so that the size of the material is $L \cdot L \cdot L = L^3 = V$ in real space;

which is $\left(\frac{2\pi}{L^3}\right)$. There is one allowed wave vector for each $\left(\frac{2\pi}{L^3}\right)$ this will then give:

$$N = 2 \frac{\frac{4}{3} \pi k_F^3}{\left(\frac{2\pi}{L}\right)^3} = \frac{k_F^3 V}{3\pi^2} \text{ which gives } k_F = \left(\frac{N 3\pi^2}{V}\right)^{1/3}.$$

This gives the Fermi energy $E_F = \frac{\hbar^2}{2m} \left(\frac{3N\pi^2}{V}\right)^{2/3}.$

From this expression we can now find the number of states less than E , given by $N(E)$:

$$E_F = \frac{\hbar^2}{2m} \left(\frac{3N(E)\pi^2}{V}\right)^{2/3} \text{ gives } N(E) = \frac{V}{3\pi^2} \left(\frac{E 2m}{\hbar^2}\right)^{3/2}$$

Then we can find $D(E) = \frac{dN}{dE} = \frac{V}{3\pi^2} \left(\frac{2m}{\hbar^2}\right)^{3/2} \cdot \frac{3}{2} E^{1/2} = \frac{V}{2\pi^2} \left(\frac{2m}{\hbar^2}\right)^{3/2} E^{1/2}$

This gives

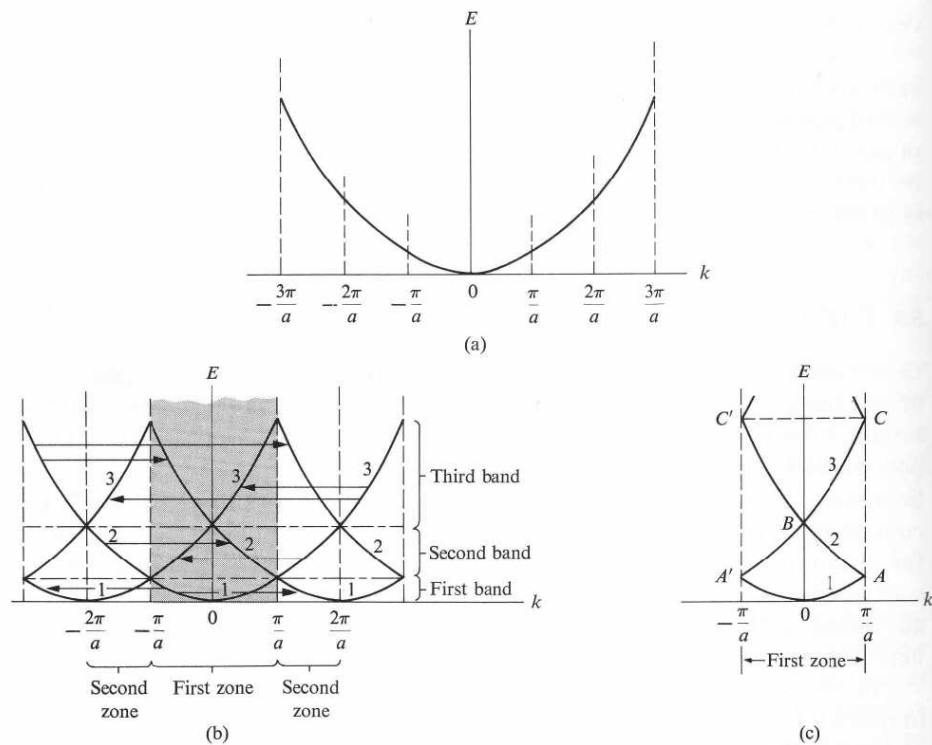
$$C = \frac{V}{2\pi^2} \left(\frac{2m}{\hbar^2}\right)^{3/2}$$

b) Empty lattice approximation; the parabola for free electrons are made above each reciprocal lattice point, as shown in figure (b) under, the 'bands' can be numbered from where they cross the BZ boundaries.

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The figure shows the three different schemes used:

- (a) extended zone scheme
- (b) periodical zone scheme
- (c) reduced zone scheme



All three descriptions are fully equivalent.

c) In words: We start with the Schrödinger equation; use a potential in this which is periodic with the lattice and also a sum of Bloch functions as the wave function. Bloch functions are plane waves multiplied with a function with period as the lattice. When the periodic potential and the Bloch functions are put into the S-equation, (both as Fourier sums) we get the Central equation -coupled set of equations. Everything happens in the 1BZ, energy band, $2N$ states in each band, we get an electronic band structure; forbidden energies, Bragg scattering is the

reason Standing waves on BZ boarder; the same k gives different energies. The energy gap is proportional to the first Fourier component of the potential.

Mathematically (from lectures) (I don't expect all this!!!)

(1)

ELECTRONS IN PERIODIC
~ POTENTIAL ~

Periodic potential: $U(\vec{r}+\vec{T})=U(\vec{r})$

Schrodinger equation:

⊗ $H\psi(\vec{r}) = \left[-\frac{\hbar^2}{2m} \nabla^2 + U(\vec{r}) \right] \psi(\vec{r}) = E\psi(\vec{r})$

(1) $\psi(\vec{r}) = \sum_{\vec{k}} C_{\vec{k}} e^{i\vec{k}\cdot\vec{r}}$ plane waves, F-series
Summed over $\vec{k}$ given
from periodic boundary
conditions. Quasi-continuous.

(2) $U(\vec{r}) = \sum_{\vec{G}} U_{\vec{G}} e^{i\vec{G}\cdot\vec{r}}$ plane waves with periodicity
as the reciprocal lattice

(1) and (2) into ⊗:

$$\sum_{\vec{k}} \left[-\frac{\hbar^2}{2m} \nabla^2 - E + \sum_{\vec{G}} U_{\vec{G}} e^{i\vec{G}\cdot\vec{r}} \right] C_{\vec{k}} e^{i\vec{k}\cdot\vec{r}} = 0$$

$$\sum_{\vec{k}} \left(\frac{\hbar^2 k^2}{2m} - E \right) C_{\vec{k}} e^{i\vec{k}\cdot\vec{r}} + \sum_{\vec{k}} \sum_{\vec{G}} U_{\vec{G}} C_{\vec{k}} e^{i\vec{G}\cdot\vec{r} + i\vec{k}\cdot\vec{r}} = 0$$

(2)

last part: $\sum_{\vec{k}' \rightarrow \vec{k}} \sum_{\vec{G}} U_{\vec{G}} C_{\vec{k}} e^{i(\vec{G}+\vec{k})\cdot\vec{r}}$
new variable; $\vec{k} = \vec{k}' + \vec{G}$

$$= \sum_{\vec{G}} \sum_{\vec{k}-\vec{G}} U_{\vec{G}} C_{\vec{k}-\vec{G}} e^{i\vec{k}\cdot\vec{r}} = \sum_{\vec{G}} \sum_{\vec{k}} U_{\vec{G}} C_{\vec{k}} e^{i\vec{k}\cdot\vec{r}}$$

→ As long as the sum is infinite,
 $\sum_{\vec{k}-\vec{G}} = \sum_{\vec{k}}$!

to S-equation:

$$\sum_{\vec{k}} \left[\left(\frac{\hbar^2 k^2}{2m} - E \right) C_{\vec{k}} + \sum_{\vec{G}} U_{\vec{G}} C_{\vec{k}-\vec{G}} \right] e^{i\vec{k}\cdot\vec{r}} = 0$$

$$\left(\frac{\hbar^2 k^2}{2m} - E \right) C_{\vec{k}} + \sum_{\vec{G}} U_{\vec{G}} C_{\vec{k}-\vec{G}} = 0$$

to be valid at every point $\vec{r}$.

This set of algebraic equations ~~are~~ is a
reexpression of the wave equation for
a periodic lattice.

d)

Intrinsic: undoped, no states in band.

Extrinsic: doped, energy level of impurity states in band gap

p-doping: empty states near the top of the valence band

n-doping: filled electron states near the bottom of the conduction band

Explained in Kittel page 209-213.

Effective mass of electron or hole reflects that the properties of semiconductors also depend on band structure near the gap, not only on the gap. The electron in a periodic potential will be accelerated relative to the lattice as if it has another mass. It is inversely proportional to the curvature of the energy band. In general a tensor. Explained in lecture and Kittel page 200-201.

e)

Expression for the density of states $D(E)$ with the lowest energy conduction band equal to E_c :

$$D(E) = \frac{V}{2\pi^2} \left(\frac{2m}{\hbar^2} \right)^{3/2} (E - E_c)^{1/2} \quad (\text{this can be taken from problem 4 a}).$$

We can do this $f(E) = \frac{1}{e^{(E-\mu)/k_B T} + 1} \approx e^{-(E-\mu)/k_B T}$ because the band gap in semiconductors (~ 1 eV) is usually much larger than $k_B T$ and therefore $(E - \mu) \gg k_B T$.

Concentration n of electrons in the conduction band:

$$n = \frac{N}{V} \int_{E_C}^{\infty} f(E) \cdot D(E) dE = \frac{1}{V} \int_{E_C}^{\infty} e^{-(E-\mu)/k_B T} \cdot \frac{V}{2\pi^2} \left(\frac{2m}{\hbar^2} \right)^{3/2} (E - E_C)^{1/2} dE$$

$$n = \frac{1}{2\pi^2} \left(\frac{2m}{\hbar^2} \right)^{3/2} e^{\frac{\mu}{k_B T}} \int_{E_C}^{\infty} e^{-E/k_B T} \cdot (E - E_C)^{1/2} dE$$

This was done in the lectures and in Kittel on page 206.

We have to use the integral $\int_0^{\infty} u^{1/2} e^{-u} du = \sqrt{\frac{\pi}{2}}$ (This is the Gammafunction of 3/2)

(<http://no.wikipedia.org/wiki/Gammafunksjonen>) and can be found in Rottmann.

The answer becomes:

$$n = 2 \left(\frac{mk_B T}{2\pi\hbar^2} \right)^{3/2} e^{\frac{(\mu - E_C)}{k_B T}}$$