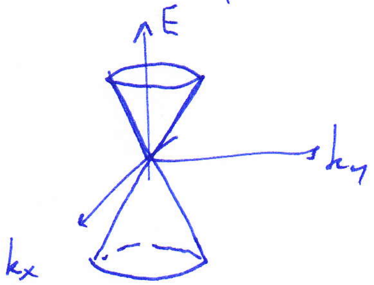
séries 8 - 2011

Probleme 30.

a) Graphene has a dispersion relation like:

$$E = \hbar v_F |\vec{k}|.$$

in the space $(E, \vec{k_x}, \vec{k_y})$ we can draw



0.25 pts

b) Let's calculate the density of state $\rho_{2D}(E)$.

Graphene is 4-fold degenerate : spin + orbital.

$$\rho_{2D}(E) \times L^2 dE = 4 \times g(k) d^2k \text{ in 2D}$$

↳ density of states in k-space.

$$g(k) = \left(\frac{L}{2\pi}\right)^2 \quad \& \quad d^2k = 2\pi k\, dk.$$

using the dispersion relation we get $k = \frac{E}{\hbar v_F}$ and $dk = \frac{dE}{\hbar v_F}$

then $\rho_{2D}(E)\, dE = \frac{4}{L^2} \times \left(\frac{L}{2\pi}\right)^2 2\pi \frac{E}{\hbar v_F} \frac{dE}{\hbar v_F}.$ 1 pts

$$\rho_{2D}(E) = \frac{\cancel{4}}{\cancel{4}\pi^{\cancel{2}}} \times \frac{2\pi E}{(\hbar v_F)^2} = \frac{2E}{\pi(\hbar v_F)^2}$$

Graphene density of states is linearly proportional to energy.

For parabolic dispersion $E = \frac{\hbar^2 k^2}{2m}$ we get $k = \left(\frac{2mE}{\hbar^2}\right)^{1/2}$ and $dk = \frac{1}{2}\sqrt{\frac{2m}{\hbar^2}}\, E^{-1/2} dE$

and finally $\rho_{2D}^{para}(E) = g \cdot \frac{m}{2\pi\hbar^2}$ which is energy independent.

degeneracy

0,25 pt

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Problème 31.

a) we want to calculate the fermi energy.

By definition $E_F = \dfrac{\hbar^2 k_F^2}{2m_e}$

Now we have to determine k_F depending on the electrons density n.

What I know is that N (total number of électrons) is ~~equal~~ within my Fermi sphere of radius k_F. Then I can write

$$N = \underset{\text{spin}}{2} \int_{k=0}^{k=k_F} \rho_k \, d^3k = 2\int_0^{k_F} \frac{V}{(2\pi)^3} 4\pi k^2 dk = \frac{V}{3\pi^2} k_F^3$$

finally $k_F = (3n\pi^2)^{1/3}$ which leads to $\boxed{E_F = \dfrac{\hbar^2}{2m_e}(3\pi^2 n)^{2/3}}$ 0.5 pt

b). we want to calculate the total energy.

the energy of one electron is given as $E = \dfrac{\hbar^2 k}{2m_e}$

we can write $E_{tot} = 2\int_0^{k_F}$ density of state (k space) × energy × d^3k.

$$E_{tot} = 2\int_{k=0}^{k=k_F} \rho_k \times E(k) \times 4\pi k^2 dk = 2\int_0^{k_F} \frac{V}{(2\pi)^3} \frac{\hbar^2 k^4}{2m} 4\pi \, dk$$

$$= \frac{V\hbar^2 k_F^5}{10\pi^2 m_e}$$

BUT $N = \dfrac{4/3\pi k_F^3}{\frac{(2\pi)^3}{V}} = \dfrac{V}{3\pi^2} k_F^3$

Finally we get $E_{tot} = \dfrac{3N\hbar^2 k_F^2}{10 m_e}$

$= \dfrac{3}{5} N E_F$ with $E_F = \dfrac{\hbar^2 k^2}{2m_e}$. 0,5 pts

c) Al has a density of $2.70 \times 10^3 kg/m^3$ and a molar mass of $26,98 g/mol$

$$\frac{\text{atom}}{nm^3} = \frac{\text{density}}{\text{molar mass}} \times N_A \times \underset{(nm)^3}{(10^{-9})^3} = \frac{2,7 \cdot 10^6}{26,98} \times 6,02 \times 10^{23} \times (10^{-9})^3$$

$= 60,24$ atoms/nm^3 0,25 pts

d) from a) $E_F = \dfrac{\hbar^2}{2m_e}(3\pi^2 n)^{2/3} \Rightarrow (n 3\pi^2)^{2/3} = \dfrac{2m_e E_F}{\hbar^2} \Rightarrow n = \left(\dfrac{2m_e E_F}{\hbar^2}\right)^{3/2} \times \dfrac{1}{3\pi^2}$

0,25 pt

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Probleme 31. Suite.

e) if we combine c) and d) we get

$$\frac{\text{electron}}{\text{atom}} = \left(\frac{\text{atom}/nm^3}{\text{electron}/nm^3}\right)^{-1} = \frac{180.1}{60.24} = \underbrace{2.99}_{\simeq 3} \text{ electrons/atom}.$$

0,25 pt

f). with b) we find

$$E_{tot} = \frac{3}{5} N E_F \quad \text{and with a) we get} \quad E_F = \frac{\hbar^2}{2m_e}(3\pi^2 n)^{2/3}$$

finally $E = \frac{3}{5} N \frac{\hbar^2}{2m_e}\left(3\pi^2 \frac{N}{V}\right)^{2/3}$

at $T=0$ $\quad p = -\frac{\partial E}{\partial V}\Big)_N = \frac{2}{3} \times \frac{(3\pi^2)^{2/3}\hbar^2}{5 \times 2m_e}\left(\frac{N}{V}\right)^{5/3}$

$$= \frac{(3\pi^2)^{2/3}}{5}\frac{\hbar^2}{m_e}\left(\frac{N}{V}\right)^{5/3}$$

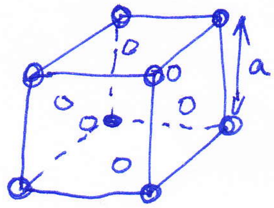
The bulk modulus is defined as $B = -V\frac{\partial P}{\partial V}\Big)_N$

$$B = +\frac{5}{3}\frac{(3\pi^2)^{2/3}}{5}\frac{\hbar^2}{m_e}\left(\frac{N}{V}\right)^{5/3}$$

$$= \boxed{\frac{(3\pi^2)^{2/3}}{3}\frac{\hbar^2}{m_e} n^{5/3}}$$

0,5 pt

Aluminum is a cristal with fcc structure



there are 8 atoms • that share 8 unit cell each. ⇒ 1 atom.

there are 6 atoms o that share 2 unit cell each ⇒ 3 atom

Finally Al had 4 atoms per unit cell.

e) gives us: $3e^-$ per atom ⇒ $12e^-$ per unit cell.

we can get now the density $n = \frac{N}{V} = \frac{12}{a^3}$

$$B = \frac{(3\pi^2)^{2/3}}{3} 12^{5/3} \frac{\hbar^2}{m_e a^5} \sim 2{,}25 \times 10^{11}\ N.m^{-2}.$$

0,25 pt

$$\boxed{\text{Compressibility} = \frac{1}{B} = \frac{1}{2{,}25} \times 10^{-11}\ \frac{m^2}{N}}$$

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Probleme 32.

We know $\mu = \int g(\varepsilon) f(\varepsilon)\varepsilon\, d\varepsilon$ & $n = \int g(\varepsilon) f(\varepsilon) d\varepsilon$.

with $f(\varepsilon) = \dfrac{1}{1 + e^{(\varepsilon - \mu)/k_B T}}$

we remark the following $g(\varepsilon) = \begin{cases} \varepsilon > 0 = \dfrac{m}{\hbar^2 \pi^2}\sqrt{\dfrac{2mE}{\hbar^2}} \\ \varepsilon < 0 \quad = 0 \end{cases}$

$$n = \int_{-\infty}^{\mu} g(\varepsilon) dE + \frac{\pi^2}{6}(k_B T)^2 \left.\frac{dg(E)}{dE}\right|_{E=\mu} + O\left(\frac{k_B T}{\mu}\right)^4$$

$$n \simeq \int_0^{E_F} g(\varepsilon)\, d\varepsilon + \underbrace{\int_{E_F}^{\mu} g(\varepsilon) d\varepsilon}_{(\mu - E_F) g(\varepsilon)} + \frac{\pi^2}{6}(k_B T)^2 g(\varepsilon_F)'$$

↳ constant around E_F.

since n = Constant with T

we can write $\mu = \varepsilon_F - \dfrac{\pi^2}{6}(k_B T)^2 \dfrac{g(\varepsilon_F)'}{g(\varepsilon_F)}$

*Problem 33

The current from the left to the right contact with the respective electro-chemical potentials μ_L, R reads:

$$I_{L\to R} = \int_{-\infty}^{\infty} T(E) f(E-\mu_L) \cdot [1 - f(E-\mu_R)]\, dE,$$

where $T(E)$ is the energy-dependent tunneling probability and f is the Fermi distribution. $T(E)$ also contains the density of states in both contacts, $T(E) = D_L(E) D_R(E) t(E)$ with $t(E)$ the tunnel matrix element. The formula simply means that the electrons have to tunnel from a filled state (there should be an electron that can tunnel!) into an empty state (the Pauli principle suppresses tunneling into a filled state). Similarly, one obtains for the electrons tunneling back from the right to the left contact

$$I_{R\to L} = \int_{-\infty}^{\infty} T(E) f(E-\mu_R) \cdot [1 - f(E-\mu_L)]\, dE.$$

The total current is the sum of the two contribution:

$$\begin{aligned} I_{\text{tot}} &= I_{L\to R} - I_{R\to L} \\ &= \int_{-\infty}^{\infty} T(E) \left[f(E-\mu_L) - \cancel{f(E-\mu_L) f(E-\mu_R)} - f(E-\mu_R) + \cancel{f(E-\mu_L) f(E-\mu_R)} \right]. \end{aligned}$$

The required result follows if we assume an energy-independent tunneling matrix element and energy independent densities of states.