Boltzmann equation in 2D SSL with cross magnetic and electric fields

Rev. 1

We start from following Boltzmann equation

$$\frac{\partial f}{\partial t} + \frac{e}{\hbar}\left(\mathbf{E} + \mathbf{v}\times\mathbf{B}\right)\frac{\partial f}{\partial \mathbf{k}} + \mathbf{v}(\mathbf{k})\frac{\partial f}{\partial r} = \left(\frac{\partial f}{\partial t}\right)_{st} \tag{1}$$

We consider case when $f(...)$ is spatially homogeneous, i.e. it depends only on $\mathbf{k}$, then

$$\frac{\partial f}{\partial t} + \frac{e}{\hbar}\left(\mathbf{E} + \mathbf{v}\times\mathbf{B}\right)\frac{\partial f}{\partial \mathbf{k}} = \frac{f_0 - f}{\tau} \tag{2}$$

Electric field is along x-axis and magnetic field is along z-axis.

$$\mathbf{E} = (E, 0, 0) \tag{3}$$
$$\mathbf{B} = (0, 0, B) \tag{4}$$
$$\mathbf{v}\times\mathbf{B} = (v_y B, -v_x B, 0)) \tag{5}$$

And will make following substitution

$$t \to \tau t \tag{6}$$

which gives following form to the Boltzmann equation

$$\frac{\partial f}{\partial t} - \frac{ed\tau}{\hbar}(E + v_y B)\frac{\partial f}{\partial (k_x d)} + \frac{ed\tau}{\hbar} v_x B \frac{\partial f}{\partial (k_y d)} = f_0 - f \tag{7}$$

where

$$\mathbf{v} = \frac{1}{\hbar}\frac{\partial \varepsilon}{\partial \mathbf{k}} \tag{8}$$

and ε is an energy of an electron in the zone, which in tight-binding apporiximation takes form in the first zone

$$\varepsilon = \frac{\hbar^2 k_y^2}{2m} - \frac{\Delta_1}{2}\cos(k_x d) \tag{9}$$

therefore

$$v_x = \frac{\Delta_1 d}{2\hbar}\sin(dp_x/h) \tag{10}$$
$$v_y = \frac{\hbar}{md}\phi_y \tag{11}$$

And Boltzmann equations now takes following form

$$\frac{\partial f}{\partial t} - \left(\frac{ed\tau}{\hbar}E + \frac{ed\tau}{m}k_y B\right)\frac{\partial f}{\partial (k_x d)} + \frac{\Delta_1 e d^2 \tau}{2\hbar^2} B \sin(k_x d)\frac{\partial f}{\partial (k_y d)} = f_0 - f \tag{12}$$

Now we can define

$$E_* = \frac{\hbar}{ed\tau} \tag{13}$$
$$m_x = \frac{2\hbar^2}{\Delta_1 d^2} \tag{14}$$
$$\tag{15}$$
$$\boxed{\alpha = m/m_x} \tag{16}$$

Then, with cyclotron frequency defined as

$$\omega_c = \frac{eB}{\sqrt{mm_x}} \tag{17}$$

we get following

$$\frac{\partial f}{\partial t} - \left(\frac{E}{E_*} + \frac{\omega_c \tau}{\sqrt{\alpha}} k_y d\right) \frac{\partial f}{\partial (k_x d)} + \sqrt{\alpha}\omega_c \tau \sin(k_x d) \frac{\partial f}{\partial (k_y d)} = f_0 - f \tag{18}$$

And if we know define

$$\phi_x = k_x d \tag{19}$$

$$\phi_y = \frac{k_y d}{\sqrt{\alpha}} \tag{20}$$

$$\tilde{E} = E/E_* \tag{21}$$

$$\tilde{B} = \omega_c \tau \tag{22}$$

Boltzmann equations takes form

$$\boxed{\frac{\partial f}{\partial t} - \left(\tilde{E} + \tilde{B}\phi_y\right) \frac{\partial f}{\partial \phi_x} + \tilde{B} \sin(\phi_x) \frac{\partial f}{\partial \phi_y} = f_0 - f} \tag{23}$$

Alternatively, if we define Bloch frequency as

$$\omega_B = \frac{edE}{\hbar} \tag{24}$$

it can be written as

$$\frac{\partial f}{\partial t} - (\omega_B \tau + \omega_c \tau \phi_y) \frac{\partial f}{\partial \phi_x} + \omega_c \tau \sin(\phi_x) \frac{\partial f}{\partial \phi_y} = f_0 - f \tag{25}$$

Ratio of Bloch and cyclotron oscillation frequencies will be important to us down the road. For f_0 we use Boltzmann distribution

$$f_0 \propto e^{-\dfrac{\varepsilon}{k_b T}} \tag{26}$$

which in our variables ϕ_x and ϕ_y takes form

$$f_0 = C \exp\left\{\mu \cos(\phi_x) - \frac{\mu}{2}\phi_y^2\right\} \tag{27}$$

$$\boxed{\mu = \frac{\Delta_1}{2k_b T}} \tag{28}$$

Now, constant C must be such that dimensionless norm of f_0 is 1. Therefore

$$\frac{1}{C} = \frac{d^2}{\hbar^2} \int_{-\infty}^{+\infty} \mathrm{d}p_y \int_{p_x \in \mathrm{BZ}} \mathrm{d}p_x \exp\left\{\mu \cos(\phi_x) - \frac{\mu}{2}\phi_y^2\right\} \tag{29}$$

$$= \sqrt{\alpha} \int_{-\infty}^{+\infty} e^{-\mu \phi_y^2/2} \mathrm{d}\phi_y \int_{-\pi}^{\pi} e^{\mu \cos(\phi_x)} \mathrm{d}\phi_x \tag{30}$$

$$= 2\pi I_0(\mu) \sqrt{\frac{2\pi\alpha}{\mu}} \tag{31}$$

Thus full form of equilibrium distribution is

$$\boxed{f_0 = \frac{1}{2\pi I_0(\mu)} \sqrt{\frac{\mu}{2\pi\alpha}} \exp\left\{\mu \cos(\phi_x) - \frac{\mu}{2}\phi_y^2\right\}} \tag{32}$$

This way, in total, we have four free parameters defining our system, μ and α that characterize lattice parameters such as lattice period and band width and temperature, and $\tilde{E}$, $\tilde{B}$ that specify external fields. One of the parameters that we will be calculating is drift velocity v_{dr}, which we will define like this

$$v_{dr} =\frac{2d}{\Delta_1 \hbar}\int\int \frac{\partial \varepsilon}{\partial p_x} f(p_x,p_y)\mathrm{d}p_x\mathrm{d}p_y \tag{33}$$

$$=\sqrt{\alpha}\int_{-\pi}^{\pi}\mathrm{d}\phi_x\int_{-\infty}^{+\infty}\mathrm{d}\phi_y \sin(\phi_x)f(\phi_x,\phi_y) \tag{34}$$

When magentic field is 0 and E is constant, i.e. E_{dc}, analytic solution Boltzmann equation is well known and as well as expression for drift velocity

$$v_{dr} = \left\{\sqrt{\alpha}\int_{-\pi}^{\pi}\mathrm{d}\phi_x\int_{-\infty}^{+\infty}\mathrm{d}\phi_y \sin(\phi_x)f_0(\phi_x,\phi_y)\right\}\frac{E_{dc}/E_*}{1+(E_{dc}/E_*)^2} \tag{35}$$

$$=\frac{I_1(\mu)}{I_0(\mu)}\frac{E_{dc}/E_*}{1+(E_{dc}/E_*)^2} \tag{36}$$

From which follows that peak value of v_{dr} is at $E_{dc}/E_* = 1$ and is

$$v_p = \frac{I_1(\mu)}{2I_0(\mu)} \tag{37}$$

Later, down the road, we will be plotting not v_{dr}, but v_{dr}/v_p, which for dc electric field only take very simple form

$$\frac{v_{dr}}{v_p} = 2\frac{E_{dc}/E_*}{1+(E_{dc}/E_*)^2} \tag{38}$$

Now dew to periodicty of $f(\phi_x,\phi_y)$ along ϕ_x with period 2π and additionally $f_0(-\phi_x,\phi_y) = f_0(\phi_x,\phi_y)$, it makes sense for us to expand f and f_0 into Fourier series.

$$f_0 =a_0^{(0)} + \sum_{n=1}^{\infty} a_n^{(0)}\cos(n\phi_x) \tag{39}$$

$$f =a_0 + \sum_{n=1}^{\infty} a_n\cos(n\phi_x) + b_n\sin(n\phi_x) \tag{40}$$

where coeffients $a_n^{(0)}$, a_n and b_n in general will depend on ϕ_y and last two also on t. And with the from of f_0 as selected above $a_n^{(0)}$ becomes

$$a_n^{(0)} =\frac{1}{\pi}\int_{-\pi}^{\pi} f_0(\phi_x,\phi_y)\cos(n\phi_x)\mathrm{d}\phi_x \tag{41}$$

$$=\frac{\sigma(n)I_n(\mu)}{\pi I_0(\mu)}\sqrt{\frac{\mu}{2\pi\alpha}}\exp\left\{-\frac{\mu}{2}\phi_y^2\right\} \tag{42}$$

where

$$\sigma(n) = \begin{cases} 1/2 & : n = 0 \\ 1 & : n \neq 1 \end{cases} \tag{43}$$

Norm of $f(\phi_x,\phi_y)$ must always be one, i.e.

$$\sqrt{\alpha}\int_{-\pi}^{\pi}\mathrm{d}\phi_x\int_{-\infty}^{+\infty}\mathrm{d}\phi_y f(\phi_x,\phi_y) = 1 \tag{44}$$

which in fourier representation takes form

$$2\pi\sqrt{\alpha}\int_{-\infty}^{+\infty} a_0(\phi_y)\mathrm{d}\phi_y = 1 \tag{45}$$

Once we move on to the numerical calculations this equation can be used to check correctness. And calculation of v_{dr} is done through following equation

$$v_{dr} = \pi\sqrt{\alpha}\int_{\pi}^{\pi} b_1(\phi_y)\mathrm{d}\phi_y \tag{46}$$

and

$$\frac{v_{dr}}{v_p} = \frac{2I_0(\mu)\pi\sqrt{\alpha}}{I_1(\mu)}\int_{\pi}^{\pi} b_1(\phi_y)\mathrm{d}\phi_y \tag{47}$$