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

Rev. 4

1 Analytical treatment

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

$$\omega_c = \frac{eB}{\sqrt{m m_x}} \tag{17}$$

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

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

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

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

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

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

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

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

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, known as "Esaki-Tsu" equation

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

In general we will be applying a/c emf in the form

$$\tilde{E} = \tilde{E}_{dc} + \tilde{E}_{\omega} \cos(\omega t) \tag{39}$$

and in case when magnetic field is not applied we also have analitic expression for v_{dr}, which is known as "Tien-Gordon" equation. Analytic expression, "Taker formulae", is also known for absorption, which we will define like this

$$A = \left\langle \frac{v_{dr}}{v_p} \cos(\omega t) \right\rangle_t \tag{40}$$

In case when magnetic field is appied, however, analytic expression for absorption is not known. And that is the quantity we are most interested in.

Now due 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.

$$f_0 = \sum_{n=0}^{\infty} a_n^{(0)} \cos(n\phi_x) \tag{41}$$

$$f = \sum_{n=0}^{\infty} a_n \cos(n\phi_x) + b_n \sin(n\phi_x) \tag{42}$$

where coeffients $a_n^{(0)}$, a_n and b_n in general will depend on ϕ_y and last two also on time t. Note, that $a_{n<0} \equiv 0$ and $b_{n<1} \equiv 0$. And with the from of f_0, as selected above, $a_n^{(0)}$ becomes

$$a_n^{(0)} = \frac{\sigma(n)}{\pi} \int_{-\pi}^{\pi} f_0(\phi_x, \phi_y) \cos(n\phi_x) \mathrm{d}\phi_x \tag{43}$$

$$= \frac{\sigma(n) I_n(\mu)}{\pi I_0(\mu)} \sqrt{\frac{\mu}{2\pi\alpha}} \exp\left\{ -\frac{\mu}{2} \phi_y^2 \right\} \tag{44}$$

where

$$\sigma(n) = \begin{cases} 1/2 & : n = 0 \\ 1 & : n \neq 1 \end{cases} \tag{45}$$

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

$$\sqrt{\alpha} \int_{-\pi}^{\pi} \mathrm{d}\phi_x \int_{-\infty}^{+\infty} \mathrm{d}\phi_y f(\phi_x, \phi_y) = 1 \tag{46}$$

which in fourier representation takes form

$$\boxed{2\pi\sqrt{\alpha} \int_{-\infty}^{+\infty} a_0(\phi_y)\mathrm{d}\phi_y = 1} \tag{47}$$

Once we move on to the numerical calculations this equation can be used to check correctness. And from equation (34) it is clear that only b_1 will survice. And calculation of v_{dr} is done through following equation

$$v_{dr} = \sqrt{\alpha} \int_{-\infty}^{+\infty} \mathrm{d}\phi_y \int_{-\pi}^{+\pi} \mathrm{d}\phi_x \sin(\phi_x) b_1(\phi_y) \sin(\phi_y) \tag{48}$$

$$= \pi\sqrt{\alpha} \int_{-\infty}^{+\infty} b_1(\phi_y)\mathrm{d}\phi_y \tag{49}$$

and in view of definition of peak value of v_{dr} in eq. (37)

$$\boxed{\frac{v_{dr}}{v_p} = \frac{2I_0(\mu)\pi\sqrt{\alpha}}{I_1(\mu)} \int_{-\infty}^{+\infty} b_1(\phi_y)\mathrm{d}\phi_y} \tag{50}$$

In addition to drift velocity along x-axis we can look at drift velocity alogn y-axis, which we will define like this

$$v_y = \frac{2}{\Delta_1} \iint \frac{\partial \varepsilon}{\partial p_y} f(\phi_x, \phi_y)\mathrm{d}p_x\mathrm{d}p_y \tag{51}$$

$$= \int_{-\pi}^{\pi} \mathrm{d}\phi_x \int_{-\infty}^{+\infty} \phi_y f(\phi_x, \phi_y)\mathrm{d}\phi_y \tag{52}$$

$$= 2\pi \int_{-\infty}^{+\infty} a_0(\phi_y)\phi_y\mathrm{d}\phi_y \tag{53}$$

However just as with drift velocity along x-axis we will be working with ratio of v_y and peak velocity v_p.

$$\boxed{\frac{v_y}{v_p} = \frac{4\pi I_0(\mu)}{I_1(\mu)} \int_{-\infty}^{+\infty} a_0(\phi_y)\phi_y\mathrm{d}\phi_y} \tag{54}$$

This way we accounted for meaning of a_0 and b_1. Let us now take a look at a_1. Effective mass of an electron in the x direction is given by

$$m_{x,\mathbf{k}}^{-1} = \frac{1}{\hbar^2} \frac{\partial^2 \varepsilon}{\partial k_x^2} \tag{55}$$

We will be working however with ratio of electron mass to $m_{x,\mathbf{k}}$. And in our approximation of energy (9) that takes form

$$\frac{m}{m_{x,\mathbf{k}}} = \frac{\Delta_1 d^2 m}{2\hbar^2} \cos(k_x d) \tag{56}$$

$$= \alpha \cos(\phi_x) \tag{57}$$

To gather back this value from $f(\phi_x,\phi_y)$ we have to integrate over $\{p_x,p_y\}$ and to maintain dimensionlessness of ratio of these masses, this integration will take form

$$\frac{m}{m_{x,\mathbf{k}}} =\alpha^{3/2}\frac{d^2}{\hbar^2}\iint f(\phi_x,\phi_y)\cos(k_x d)\mathrm{d}p_x\mathrm{d}p_y \tag{58}$$

$$=\alpha^{3/2}\int_{-\pi}^{\pi}\mathrm{d}\phi_x\int_{-\infty}^{+\infty}\mathrm{d}\phi_y f(\phi_x,\phi_y)\cos(\phi_x) \tag{59}$$

$$=\alpha^{3/2}\int_{-\pi}^{\pi}\mathrm{d}\phi_x\int_{-\infty}^{+\infty}\mathrm{d}\phi_y a_1(\phi_y)\cos(\phi_x)\cos(\phi_x) \tag{60}$$

Finally giving us following

$$\boxed{\frac{m}{m_{x,\mathbf{k}}} = \pi\alpha^{3/2}\int_{-\infty}^{+\infty} a_1(\phi_y)\mathrm{d}\phi_y} \tag{61}$$

Now using fourier representation of $f(\phi_x,\phi_y)$ and $f_0(\phi_y)$ (equations 41, 42) we can rewrite Boltzmann equation (23) like this

$$\sum_{(n)}\left\{\frac{\partial a_n}{\partial t}\cos(n\phi_x)+\frac{\partial b_n}{\partial t}\sin(n\phi_x) = a_n^{(0)}\cos(n\phi_x) - a_n\cos(n\phi_x) - b_n\sin(n\phi_x) + \right.$$
$$\left. n(\tilde{E}+\tilde{B}\phi_y)(a_n\sin(n\phi_x) - b_n\cos(n\phi_x)) + \tilde{B}\frac{\partial a_n}{\partial\phi_y}\sin(\phi_x)\cos(n\phi_x) + \tilde{B}\frac{\partial b_n}{\partial\phi_y}\sin(\phi_x)\sin(n\phi_x)\right\} \tag{62}$$

In absence of magnetic field there is no mixing of different harmonic, however when $\tilde{B}$ is not 0 then harmonics will be come mixed due to presence of $\sin(\phi_x)\cos(n\phi_x)$ and $\sin(\phi_x)\sin(n\phi_x)$, since

$$\sin(\phi_x)\cos(n\phi_x) = \{\sin((n+1)\phi_x) - \sin((n-1)\phi_x)\}/2 \tag{63}$$

$$\sin(\phi_x)\sin(n\phi_x) = \{\cos((n-1)\phi_x) - \cos((n+1)\phi_x)\}/2 \tag{64}$$

And using this equations, after some manipultion of symbols, combining elements with the same harmonics, and noting special treatment of b_1 we get

$$\frac{\partial a_n}{\partial t} =a_n^{(0)} - a_n - n(\tilde{E}+\tilde{B}\phi_y)b_n + \tilde{B}\left(\frac{\partial b_{n+1}}{\partial\phi_y} - \frac{\partial b_{n-1}}{\partial\phi_y}\right) \tag{65}$$

$$\frac{\partial b_n}{\partial t} = -b_n - n(\tilde{E}+\tilde{B}\phi_y)a_n + \tilde{B}\left(\chi(n)\frac{\partial a_{n-1}}{\partial\phi_y} - \frac{\partial a_{n+1}}{\partial\phi_y}\right) \tag{66}$$

where

$$\chi(n) = \begin{cases} 2 & : n = 1 \\ 1 & : n \neq 1 \end{cases} \tag{67}$$

The quantity we are most intersted is absorption defined like this

2 Numerical solution

Straightforward application of method of finite differences to (65) and (66) leads to either unstable or difficult, i.e. computationally intensive, equations. To combat this problem I am using several methods at once. First, we are going to discretize a_n and b_n along time and ϕ_y axes.

$$a_{n,m \leftarrow \phi_y\text{lattice step}}^{t \leftarrow \text{time step}} \tag{68}$$

and n is "harmonic number".

TODO: Complete this section

3 Results

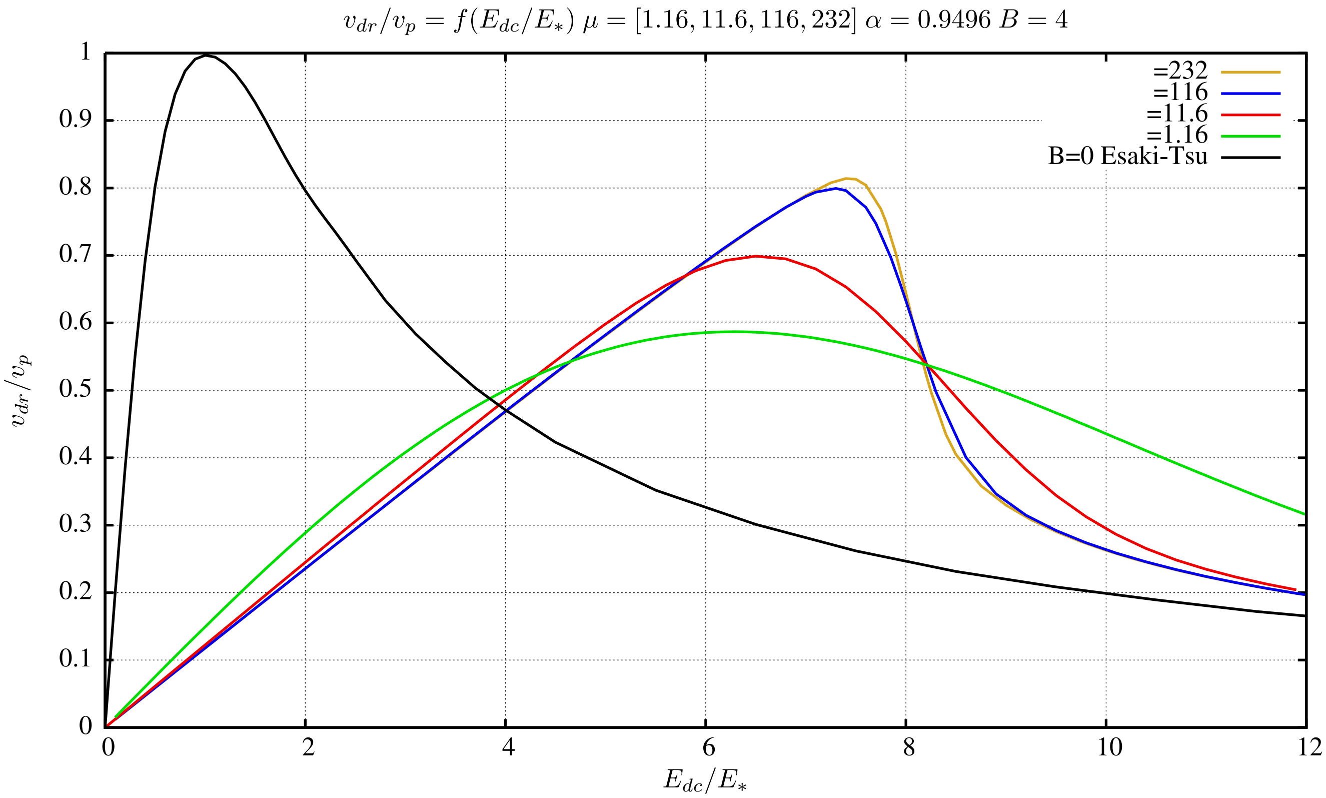


Figure 1:

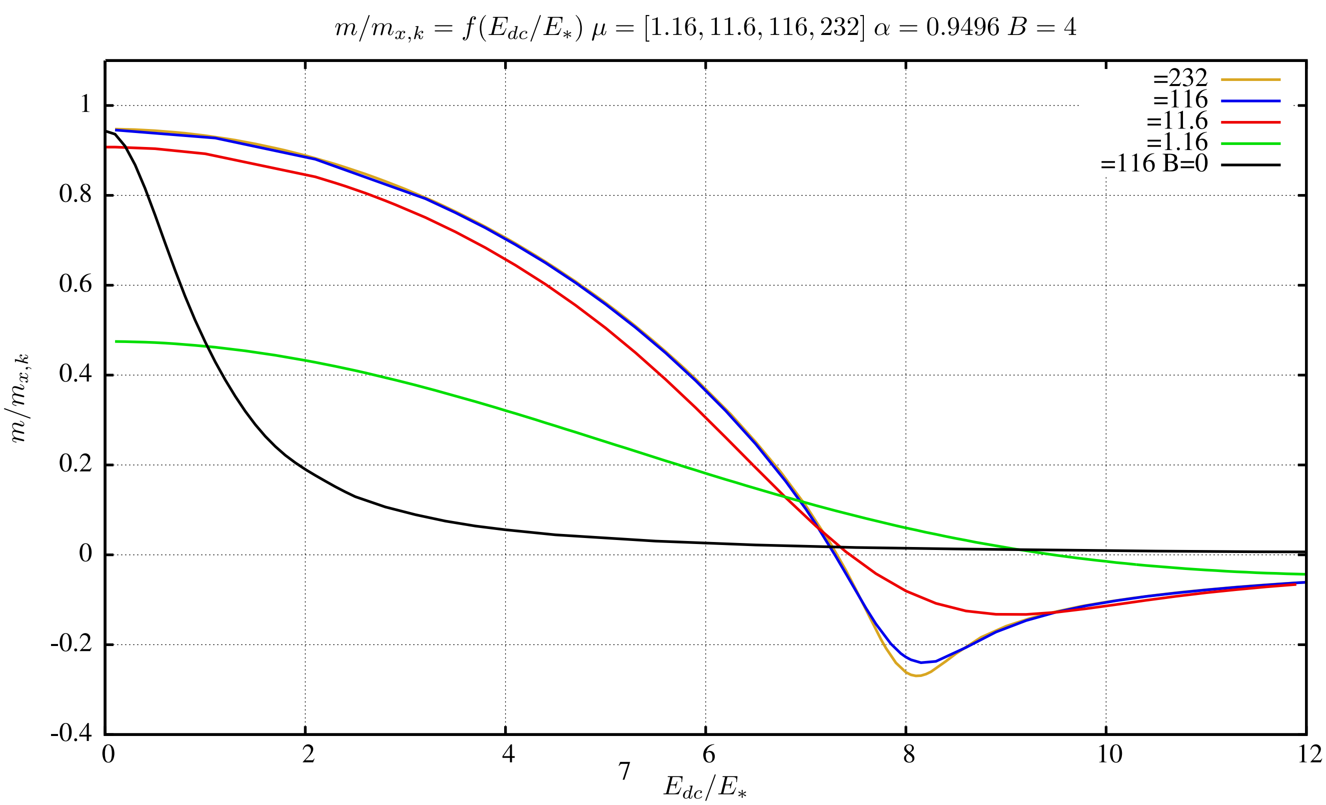


Figure 2:

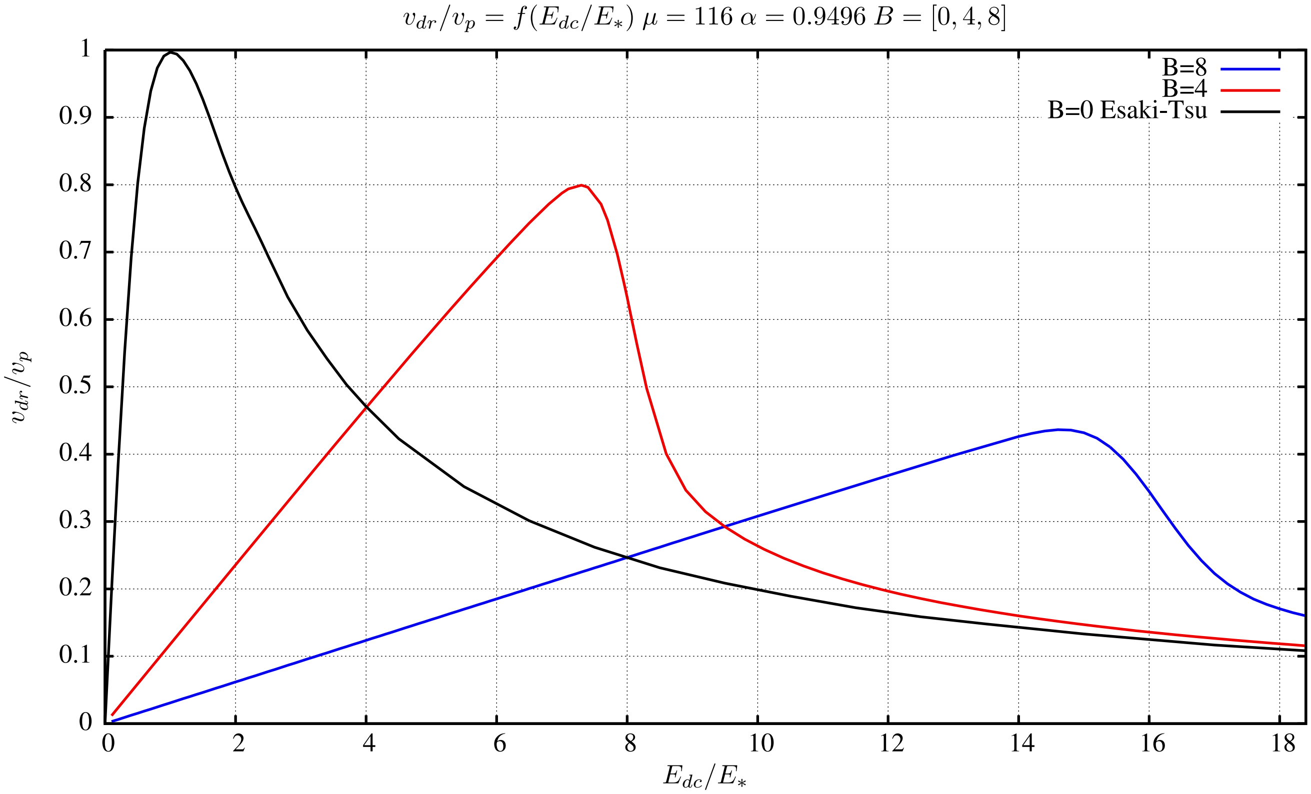


Figure 3:

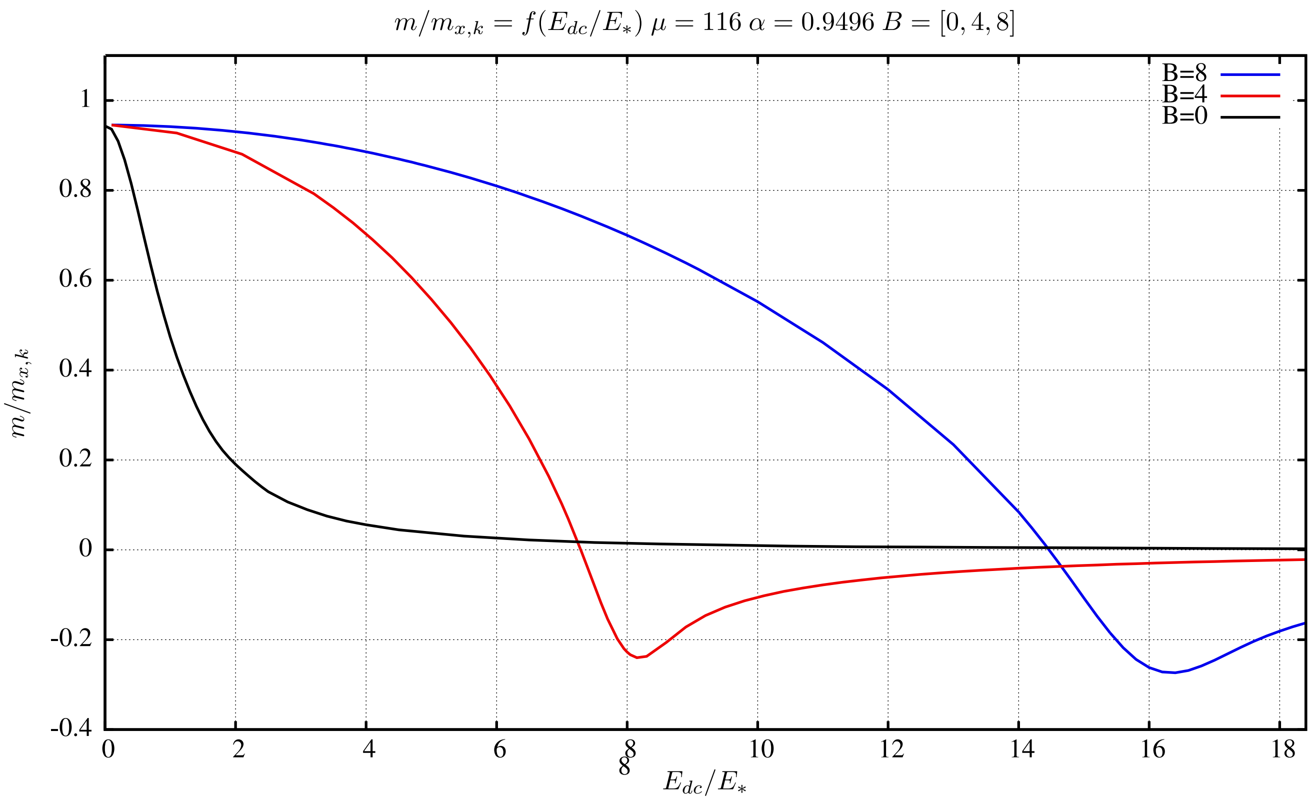
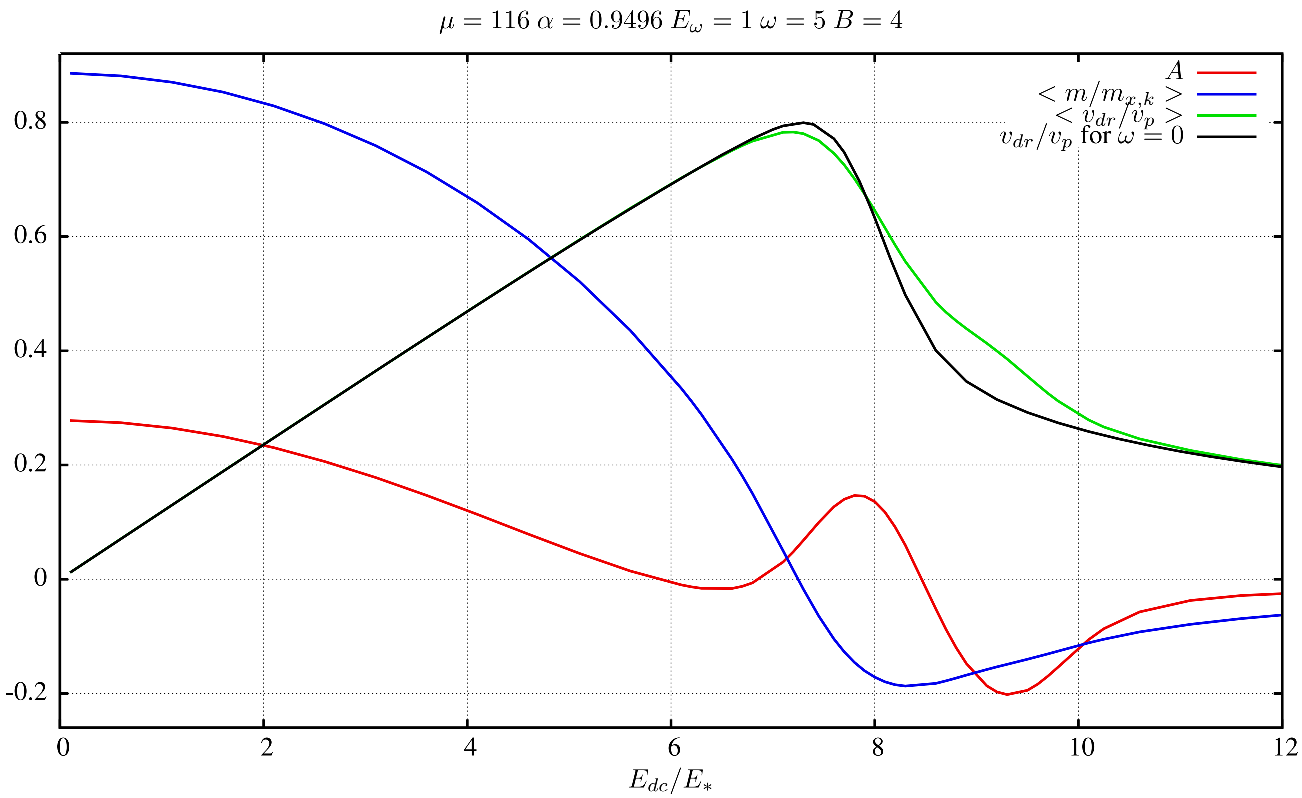


Figure 4:



$\mu = 116$ $\alpha = 0.9496$ $E_\omega = 1$ $\omega = 5$ $B = 4$
A
$< m/m_{x,k} >$
$< v_{dr}/v_p >$
v_{dr}/v_p for $\omega = 0$
0.8
0.6
0.4
0.2
0
-0.2
0
2
4
6
8
10
12
E_{dc}/E_*

Figure 5: