HW4

22 March 2022 14:59

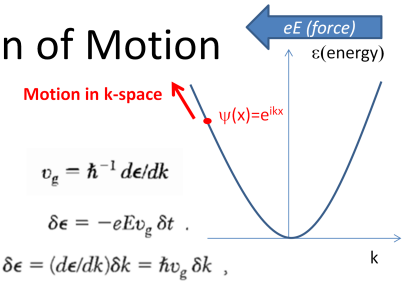
1. Argue that scattering and external biases are perturbations to the atomic potentials in the crystal.

Ans:

Scattering:
The scattering changes the momentum and energy of the particles. Due to scattering, the electrons are thrown to the states outside the Fermi sphere in the k space. The collisions result in the transfer of momentum which results in the change in wave vector. Because of non-zero change in momentum , the probabilities of occupancy of a state as governed by the fermi Dirac principles, are now no longer the same as equilibrium. This mechanism, therefore, perturbs the system from the equilibrium state.
(Answer courtesy: Omkar's group)

2. Show that under electric field, k-vector changes versus time. This defines the dynamics of the electron in k-space. Check your model with simulations from SSS package ziman. Go through the presets and write 1-2 sentence explanation of the observations. Note the anisotropy of bands.

Equation of Motion



1. Force e*E*
2. Particle velocity
3. Work done
4. Using 2 & 3
5. Force changes k (i.e. momentum p/ ħ)

$$v_g = \hbar^{-1}\, d\epsilon/dk$$

$$\delta\epsilon = -eEv_g\,\delta t\ .$$

$$\delta\epsilon = (d\epsilon/dk)\delta k = \hbar v_g\,\delta k\ ,$$

$$\delta k = -(eE/\hbar)\delta t$$

$$\hbar\frac{d\mathbf{k}}{dt} = \mathbf{F}$$

k vector changes in time with the application for force e*E*

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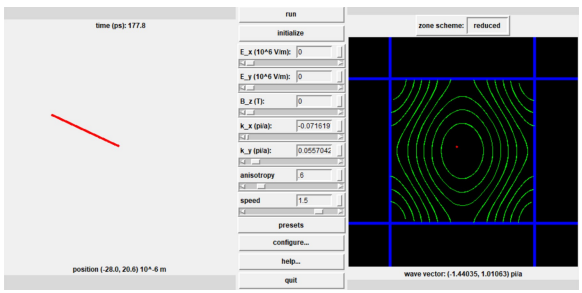
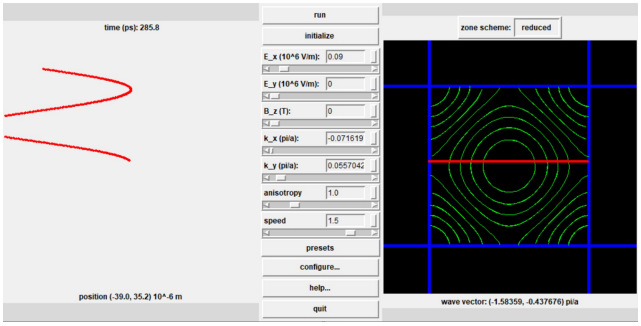
Ziman

1. E=0:



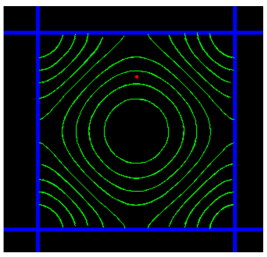
2. Ex is applied --> wave vector moves along x

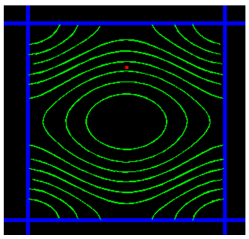


Anisotropy: Diff. mass in x and y direction. Same applied field in X and Y direction will Have different impact on the rate of change of velocity along with the directions.

Effective mass : Anisotropy

- Draw E(k) diagram in k_x and k_y directions.
- Comment on effective mass magnitude in x- vs y-directions?
- Left: isotropic; right: Anisotropic: $m_y < m_x$
- Why are BZ and iso-energy lines orthogonal?
- Across BZ, $dE/dk = 0$;
- This is why we choose specific direction for nMOS and pMOS to maximize mobility





3. Prove that effective mass of electron is given as: ; m*= 2d2E/dk2 ;
==>

Mass of the particle

1. Group Velocity
2. Differentiate
3. Substitute force
4. Get F=ma form
5. Mass

$$v_g = \hbar^{-1}\, d\epsilon/dk$$

$$\frac{dv_g}{dt} = \hbar^{-1}\frac{d^2\epsilon}{dk\,dt} = \hbar^{-1}\left(\frac{d^2\epsilon}{dk^2}\frac{dk}{dt}\right)$$

$$\hbar\frac{d\mathbf{k}}{dt} = \mathbf{F}$$

$$\frac{dv_g}{dt} = \left(\frac{1}{\hbar^2}\frac{d^2\epsilon}{dk^2}\right)F \;; \qquad \text{or} \qquad F = \frac{\hbar^2}{d^2\epsilon/dk^2}\frac{dv_g}{dt}\;.$$

1/mass term

$$\frac{1}{m^*} = \frac{1}{\hbar^2}\frac{d^2\epsilon}{dk^2}$$

The wave packet has a mass like property (effective mass) which relates force to acceleration (F=ma) or energy to momentum (E=p²/2m)
The mass depends upon the local "shape" of the E-k diagram (not on actual electron mass)

5. The band diagram is for a square 2D crystal with is atomic spacing is done in class. The k-space has i.e. for a nanosheet () where . What happens to the E-k diagram when we have a nanoribbon i.e. . Please draw the states in space. If you add the energy in the 3rd dimension , how does this diagram look for nanoribbon?

==> let $L_x = L_y \gg a$ i.e. large 2D crystal. What happens to the k_x, k_y space for $L_x \gg L_y = 10a$

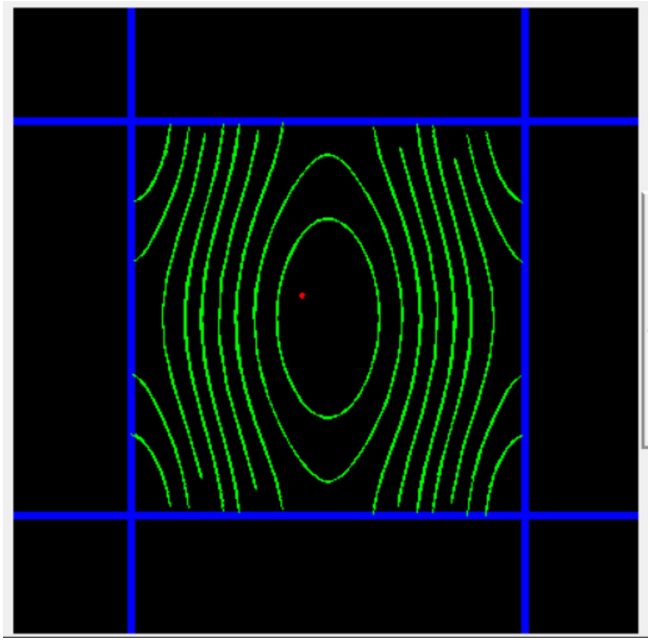
Let -> Lx = 10Ly and Ly= 10a

Kx= n$\frac{\pi}{10a}$

Ky= n$\frac{\pi}{100a}$

==> ky = Kx/10

==> Highly anisotrpic x and y dimensions



6. Derive expression relating Fermi energy of a free electron gas to the electron density per unit volume. This is a reasonable model for a metal.

==> https://unlcms.unl.edu/cas/physics/tsymbal/teaching/SSP-927/Section%2007_Free_Electron_Model.pdf

7. In a free electron gas, the E(k) diagram is parabolic. Given that an electron density is present, if a constant electric field is applied, how will the position, k value and velocity change (a) with scattering (b) without scattering (long timescale). Test your guesses with SSS simulations program sommer. Note the average as well as individual electron trajectory with time in real and k-space

==> With scattering

a. Due to electric field==> there is a net shift in center of electron cloud.
b. Net velocity is in direction of Electric field
c. Collisions due to scattering ==> Leads to sudden shifts in momentum with time

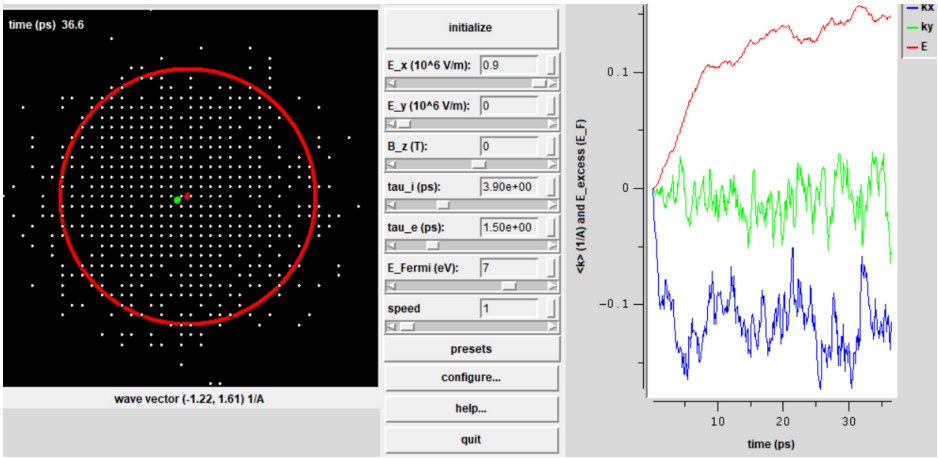


Fig. Mild scattering time scale with E-field

D. If the scattering rate is very high (lower tau)==> There will be no net displacement in the Kx space

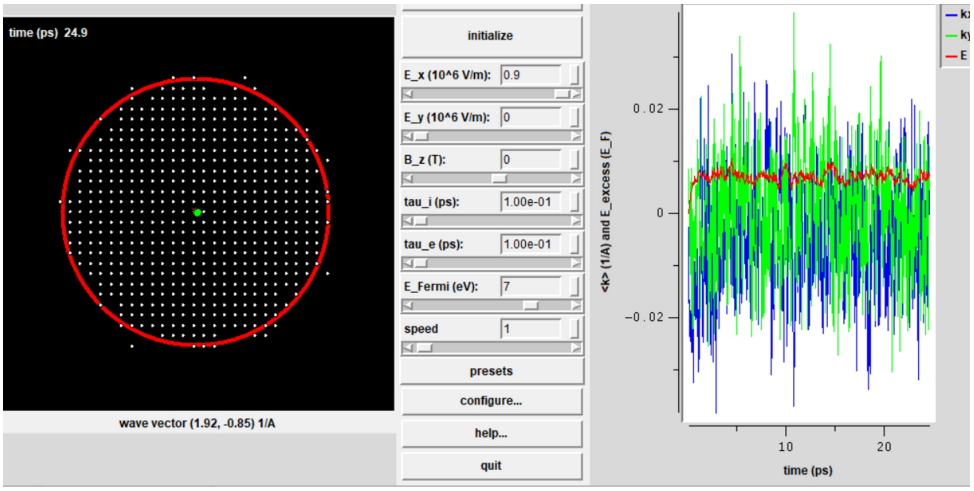


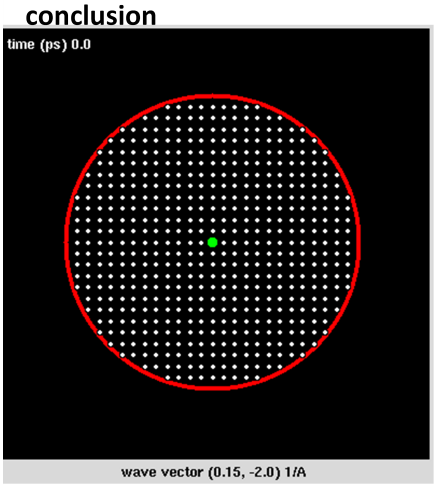
Fig: Higher scattering time case

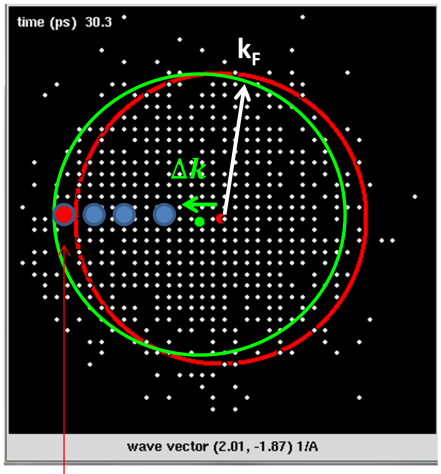
Scattering enables ==> Net velocity in direction of E-field.

Program: sommer

Scattering simplification (Free electron)

Case 2: Electrons in k-space (with pauli's exclusion and Fermi surface) leads to same conclusion





Approximate k displacement for each state

$$\Delta k = \frac{F}{\hbar}\tau$$

Hence we assume that the Fermi sphere is shifted.
This is a small compared to k_F i.e. Fermi k-vector.

Average velocity change for each state

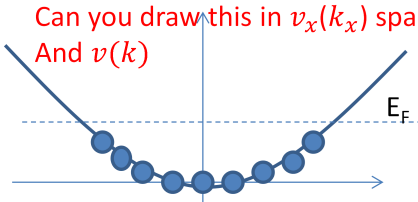
$$\Delta v = \frac{\hbar \Delta k}{m*} = \frac{e\tau}{m*}E$$

μ

This is final velocity of each state as net initial velocity is zero

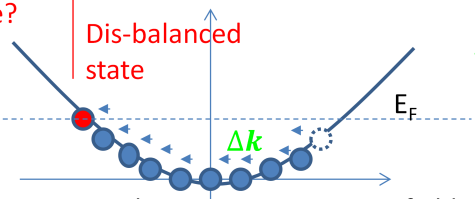
Thus J=nqΔv

Can you draw this in $v_x(k_x)$ space?
And $v(k)$



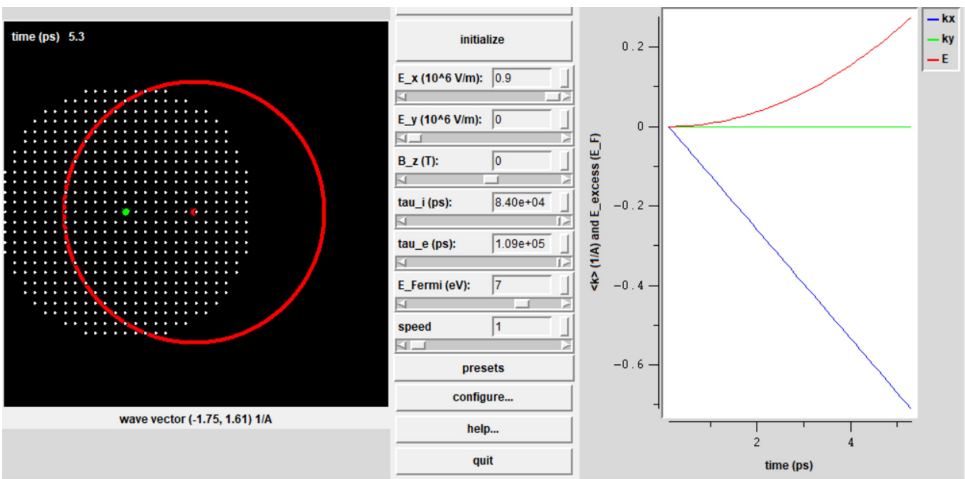
Net velocity is zero as bands is filled symmetrically

Dis-balanced state



Net velocity is non-zero as E field makes e-distribution asymmetric

No scattering: There is almost a linear change in center of e-cloud . But, such case is not suitable for current conduction. Net velocity is zero.



Also,
(Answer courtesy: Omkar's group)

$$\vec{F} = q\vec{E} = \hbar\frac{d\vec{k}}{dt} \quad (\text{from relation } p = \hbar k)$$

$$\Rightarrow \frac{d\vec{k}}{dt} = \frac{q\vec{E}}{\hbar}$$

$$\Rightarrow k = \frac{q}{\hbar}\int \vec{E}\, dt \Rightarrow \boxed{\vec{k} = \frac{q\vec{E}t}{\hbar}}$$

Considering $\vec{E}$ remains constant w.r.t time.

Hence, $\vec{k}$ is the linear f^n of time

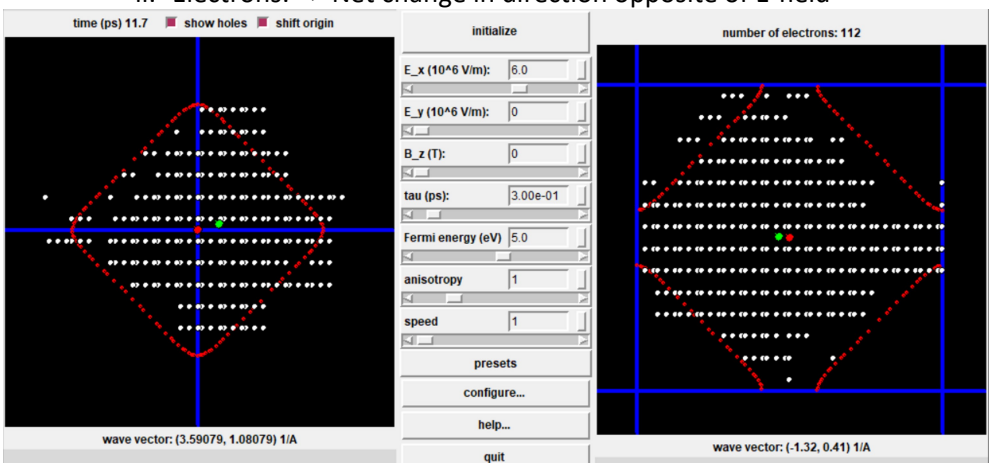
K linear relationship can be seen in above figure.

8. For nearly free electron gas, the band may be (a) partly filled (b) fully filled to the BZ. E(k) diagram maybe approximated as a sinusoid. For the above cases, how will the position, k value and velocity change (a) with scattering (b) without scattering (long timescale). Test your guesses with SSS simulations program peierls. Note the average as well as individual electron trajectory with time in real and k-space

Though scattering does seem to be the origin of resistance, it seems that scattering maybe essential to get a current out of devices. This idea is not foreign - a classical and approximate analog is that without friction, people will not be able to walk!

==> Scattering

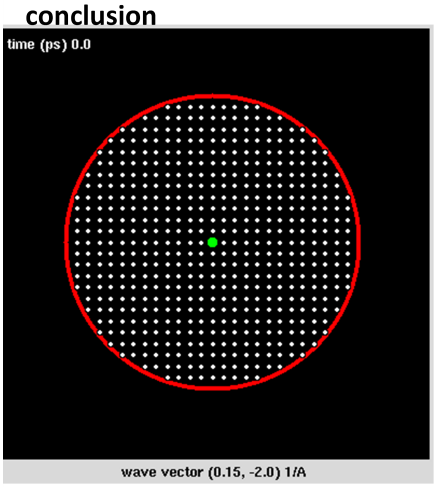
A. Net change in velocity==> on the application of force
   i. Holes: => Net change in direction of E-field
   ii. Electrons: => Net change in direction opposite of E-field

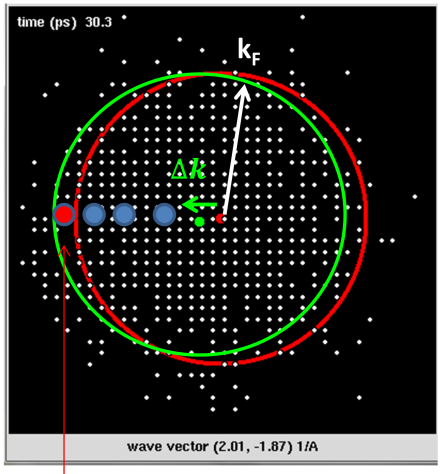


Scattering will enable the current conduction: (For visualization, image is shown below)

Scattering simplification (Free electron)

Case 2: Electrons in k-space (with pauli's exclusion and Fermi surface) leads to same conclusion





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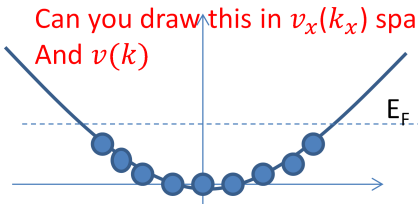

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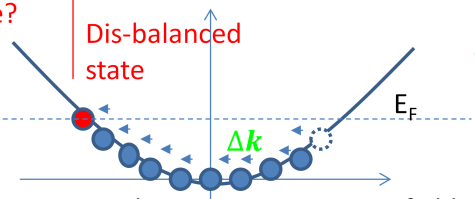

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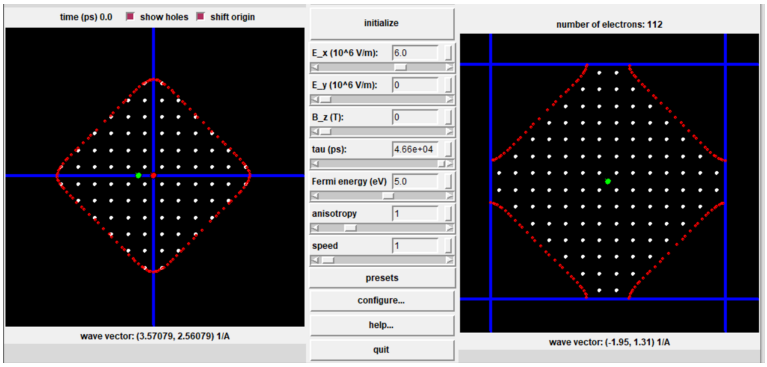
This is final velocity of each state as net initial velocity is zero

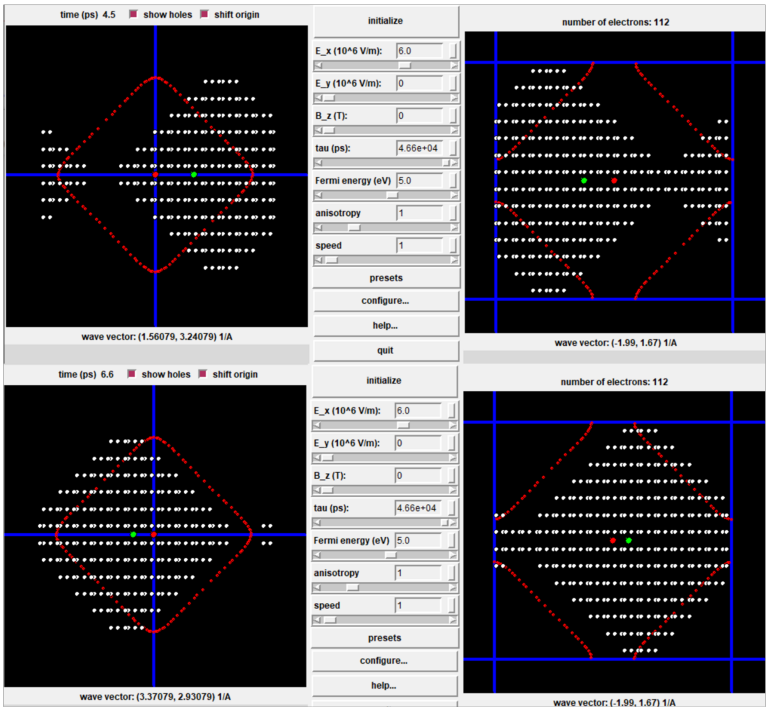
Thus J=nqΔv

Without scattering:

Initial



No scattering



No scattering: a. No net velocity

b. With time: center of charge clouds shifts from left to right