Software: http://pages.physics.cornell.edu/sss/

EE724: QM to Semi-classical Picture

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Chapter 6: Free Electron Gas

Outline

- Electron in solid: simplifying the QM problem
- Perfect Crystal
  - Wave packet is a Particle
  - Particle motion
  - Effective Mass
  - Electronic Structure
- Scattering
- Electron Transport by E-field

Goal

- Set up the mechanics of electrons

  OR

- How does an electron move under force? (Need speed for a good transistor)

Formulating the Exact QM Solution

- To understand motion of electron in a solid, we require the solution of eigen energies of the electrons in the solid by solving the Hamiltonian.
- There are many electrons ➔ but we cannot solve for more than 1 electron (e.g. H atom) ➔ need independent electron approximation
- Thus we need to find all the states in the solid discounting electron-electron interaction

$$i\hbar \frac{\partial \Psi}{\partial t} = -\frac{\hbar^2}{2m} \frac{\partial^2 \Psi}{\partial x^2} + V\Psi.$$

Question

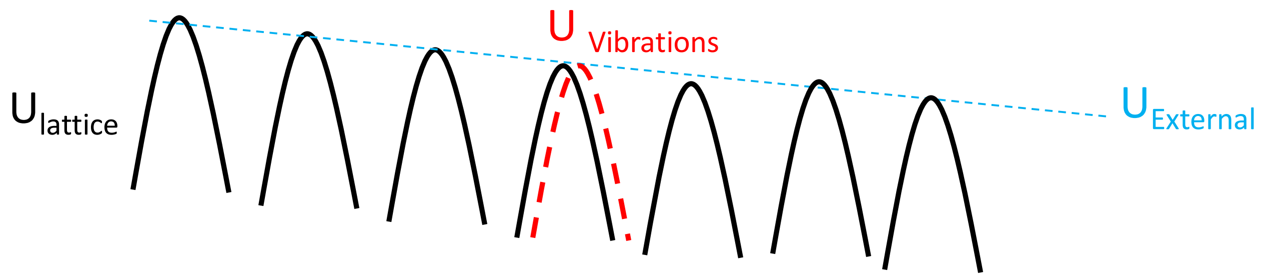
- What are the influences on the independent electron in a solid that need to be considered

$$i\hbar \frac{\partial \Psi}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2 \Psi}{\partial x^2} + V\Psi.$$

Think: What are the relevant interactions that electron sees in a solid?
Pair: Estimate the extent of the interactions (property and order of magnitude) – whatever you can?
Share: Have you considered particle like interactions or wave like?

What is the environment of an electron in a solid?

Potential profile $U_{total}(x,t) = U_{lattice} + U_{Vibrations} + U_{External}$



<u>3 source of potential</u>

1. Atomic potential of perfectly periodic lattice **(~10 eV** periodic boundary conditions electrons move fast frequency 10^{15}Hz)– high spatial frequency (~few Å) ➔ DC $\mathbf{U_{lattice}}$

2. Lattice vibrations that are time dependent & random – (atoms move slightly a/10 where a= atomic distance) high spatial frequency; low amplitude+ AC (fast- 10^{12}Hz ~ energy **hν~10 meV** given Planck's constant h=4.15x10^{-15}eV.s): $\mathbf{U_{Vibrations}}$

3. External field – low spatial frequency AC or DC (10^9 Hz) $\mathbf{U_{External}}$
   - Electric Field 10MV/cm i.e. 10^7 V/cm
   - atomic spacing is 1Å i.e. 10^{-8}cm
   - Max Voltage drop in 1 atomic distance ~ **0.1V per atom**

Options: (a) Solve everything simultaneously or
(b) perturbation approach as $U_{lattice} \gg U_{Vibrations}, U_{external}$ **(thankfully available & preferred)**

Perfect Crystal

Question:

1. Can we simplify the QM and treat the electron like a classical objects with quantum corrected physical parameters?

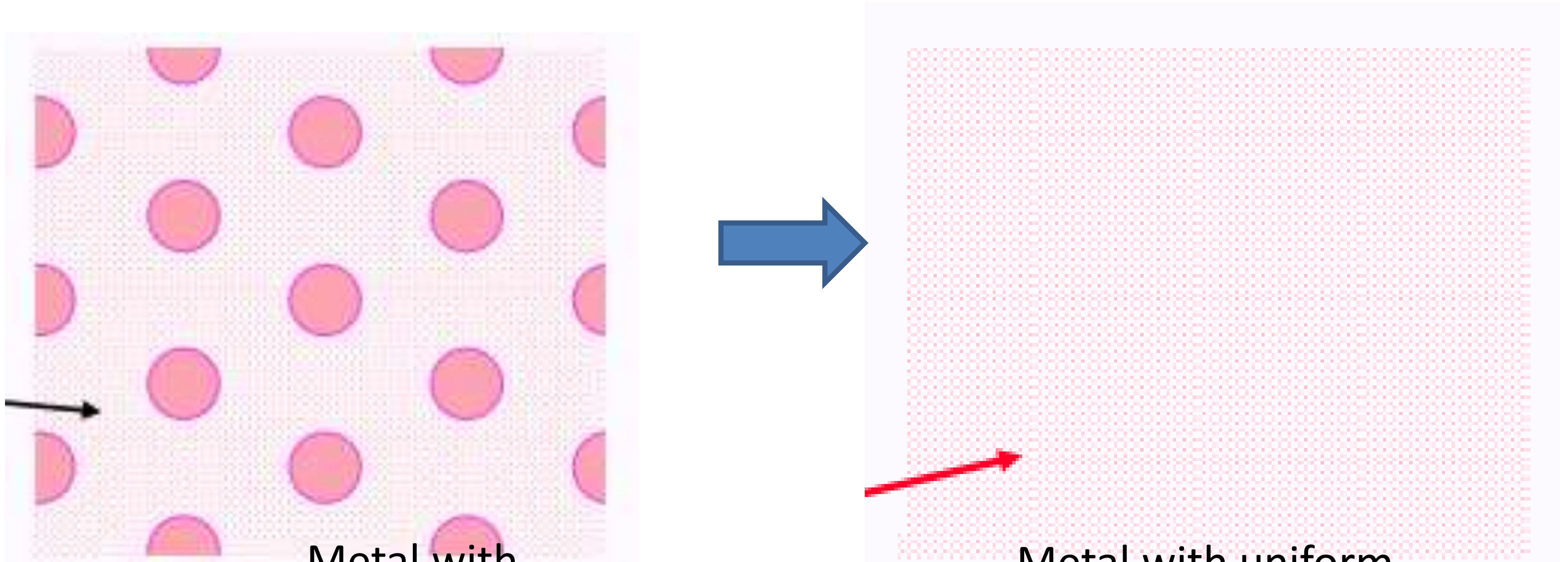
Method

1. Wave ➔ particle: Free electron gas
2. Effect of Periodic Lattice
   - Nearly Free electron gas
   - Tight binding

http://www.physics.smu.edu/scalise/P5337fa11/notes/ch06/chapter6.pdf

Free Electron Gas (Metals)

- The nuclear charge is uniform (not periodic)
- Can be treated as Particle in the box



Metal with ionic cores

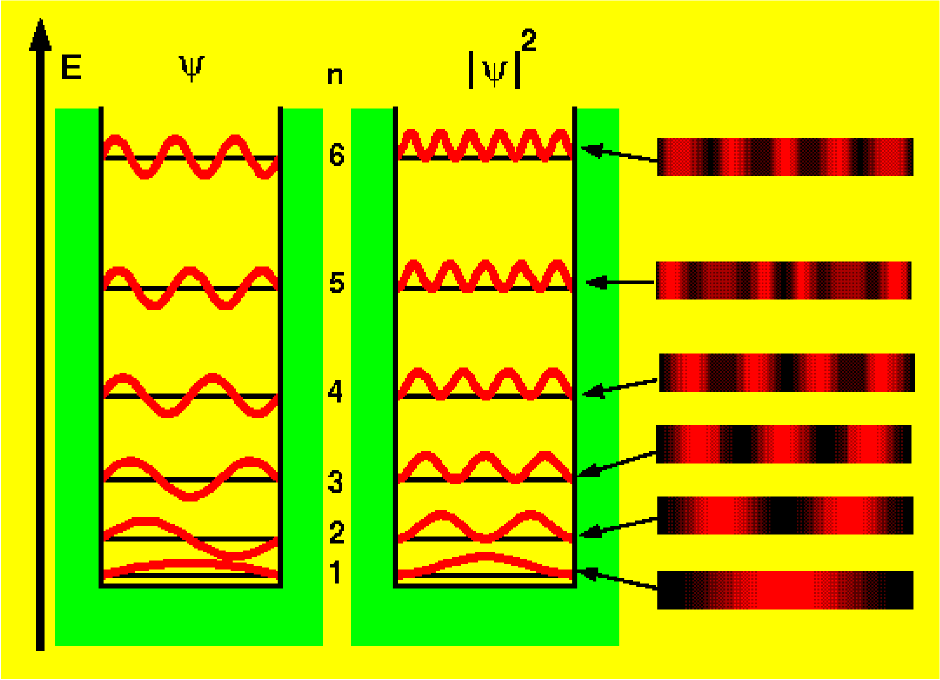
Metal with uniform ionic charge

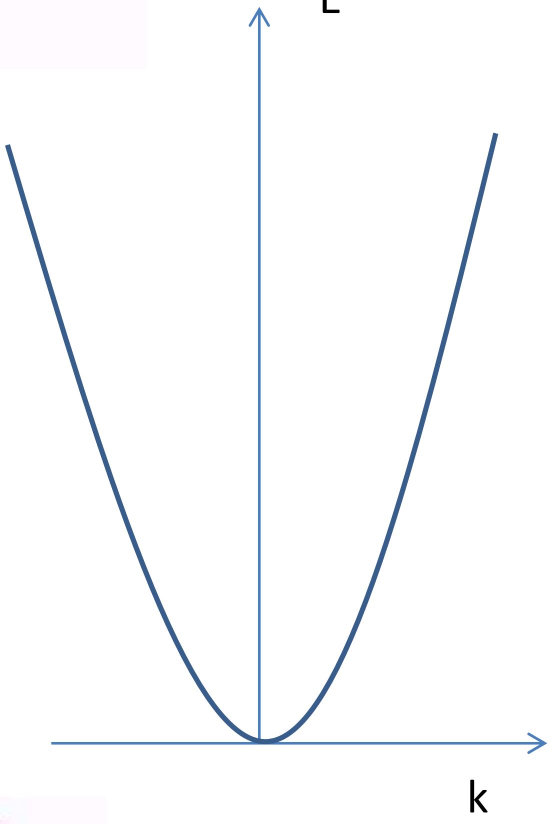
Wave Functions & Dispersion Relationship (E-k)

- Schrodinger Eq. In 1D with V = 0

  $- (\hbar^2/2m)\, d^2/dx^2\, \Psi(x) = E\, \Psi(x)$

http://www.chem.ufl.edu/~itl/4412_aa/partinbox.html





- Solution with $\Psi(x) = 0$ at $x = 0, L$ ← Boundary Condition

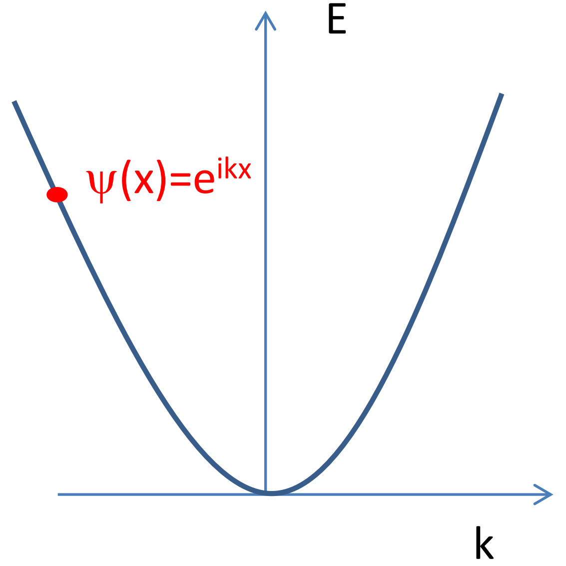
  $\Psi(x) = 2^{1/2} L^{-1/2} \sin(kx)$, $k = n\pi/L$, $n = 1,2, \ldots$

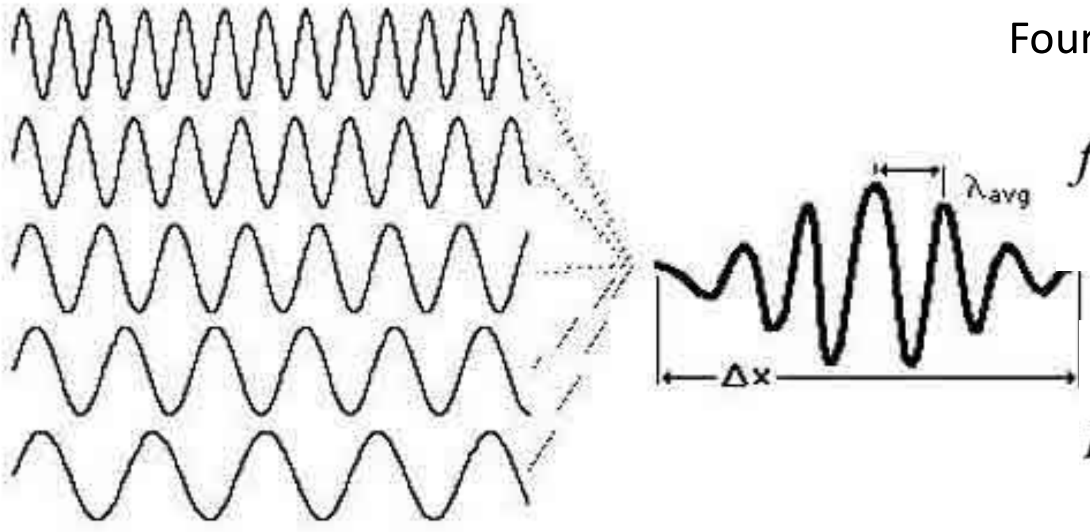
  (Note similarity to vibration waves)

- $E(k) = (\hbar^2/2m)\, k^2$

Free particle Dispersion Relationship

- Wave-function is traveling wave spread all over solid (not very particle like)
- How can we proceed to convert these waves into particle? ➔ Create wave packet around a k-value





Fourier transforms

$$f(x)=\frac{1}{\sqrt{2\pi}}\int_{-\infty}^{+\infty}F(k)e^{ikx}\,dk$$

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Wave Packet is confined in x and k ➔ particle like

Phase Velocity of the traveling wave

- Velocity of a wave at a fixed phase (crest or trough) $x \pm vt = \text{constant}$

$$\psi(x,t)=e^{i(kx-\omega t)}$$

- Comparing with exponent $v=\omega/k$ (phase velocity)

Velocity of wave packet/particle: Group Velocity

- Assume $\phi(k)$ as a narrow distribution at k_o

$$\Psi(x,t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} \phi(k) e^{i(kx-\omega t)}\, dk.$$

- Use a Taylor expansion

$$\omega(k) \cong \omega_0 + \omega_0'(k-k_0),$$

- Change variables

$$k \text{ to } s \equiv k - k_0,$$

- To get

$$\Psi(x,t) \cong \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} \phi(k_0+s) e^{i[(k_0+s)x-(\omega_0+\omega_0' s)t]}\, ds.$$

- At t=0

$$\Psi(x,0) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} \phi(k_0+s) e^{i(k_0+s)x}\, ds,$$

- At t=t

$$\Psi(x,t) \cong \frac{1}{\sqrt{2\pi}} e^{i(-\omega_0 t+k_0\omega_0' t)} \int_{-\infty}^{+\infty} \phi(k_0+s) e^{i(k_0+s)(x-\omega_0' t)}\, ds.$$

Time dependent phase shift → does not affect $|\Psi|^2$

Integral where x shifted to x-ω_o't after time t → wave packet is traveling at <u>group</u> velocity ω_o'

Based on group velocity, the particle velocity and momentum can be determined

- Need to show that

$$(k_o + s)x - (\omega_0 + \omega_0' s)t = (k_o + s)(x - vt) + P$$

If $\omega_0' = v$ then

$$-\omega_0 t + k_o \omega_0' t = P$$

This is a purely t-dependent phase term that does not affect amplitude.

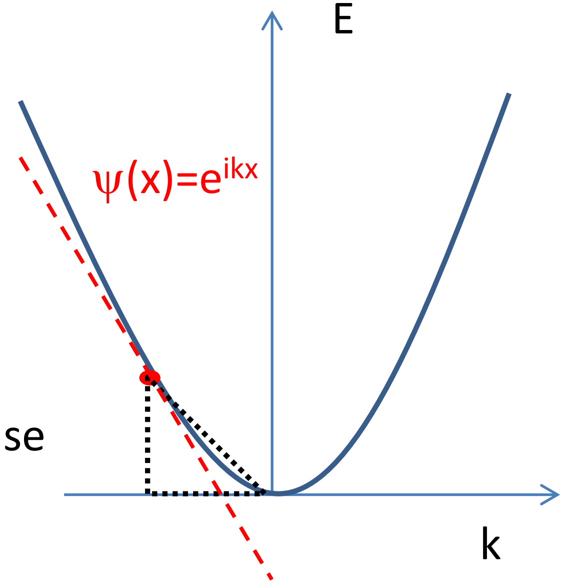
The s dependent part shows the time-dependent shift in the $\phi(k_o + s)$

Demos

- See wikipedia demo on group velocity and phase velocity http://en.wikipedia.org/wiki/Group_velocity

- Does group and phase velocity need to be correlated to each other (how?)

1. Can they have different magnitudes? Yes/No
2. Can they have different signs? Yes/No



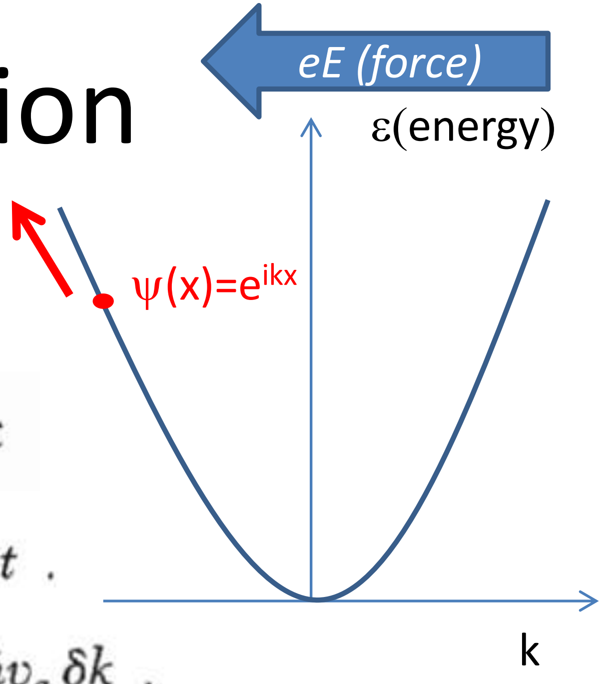
Slope dω/dk is group velocity

Ratio ω/k is phase velocity

Group velocity is <u>the</u> critical parameter determining particle velocity

For parabolic $E(k)$ diagram, calculate the ratio of group to phase velocity

Equation of Motion



1. Force e*E*
2. Particle velocity

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

3. Work done

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

4. Using 2 & 3

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

5. Force changes k (i.e. momentum p/ ħ)

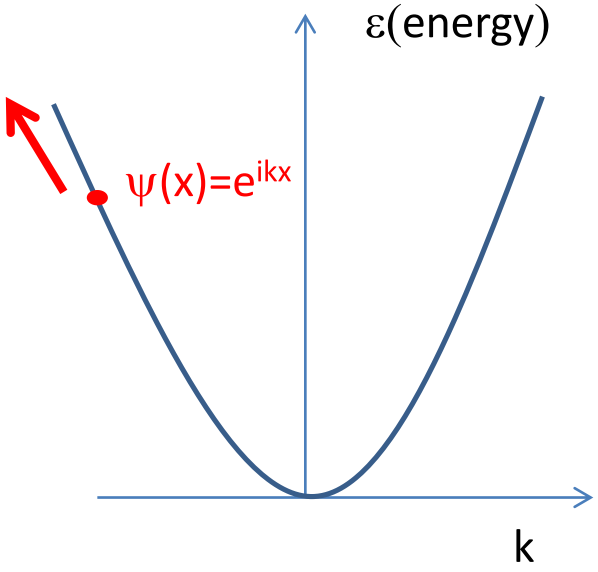
$$\delta k = -(eE/\hbar)\delta t$$

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

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

Exercise: Motion in real space from E(k) space

- What is the motion when there is no force?
- Given $E(k)$ space, motion due to force F=0 is given by $k = k_o$ as $\frac{dk}{dt} = \frac{F}{\hbar} = 0$
- In real space, constant velocity $v_g(k_o)$ is observed
- What is the motion when there is Force=F?
- Then constant force causes uniform k increase i.e. $k(t) = k_o + \frac{F}{\hbar}t$
- In real space, velocity $v_g(k)$changes as k evolves ; hence $x = \int v_g(k)dt + x_0$



See drude model in sss software

Note: In k-space, effect of applied F is simple;
No force produces static k even when in real space x is evolving (uniform velocity);
When F is applied, we know how it changes

Use Drude model without scattering ($\tau \to \infty$)

- Show how force causes evolution of position of electron in real space in 2D.
- For (a) Force F=0 (b) $F = F\hat{x}$
  - Relate the position of k-space coordinates with velocity
  - Relate velocity to real space position evolution

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 ($E=p^2/2m$)

The mass depends upon the local “shape” of the E-k diagram (not on actual electron mass)

Discussion

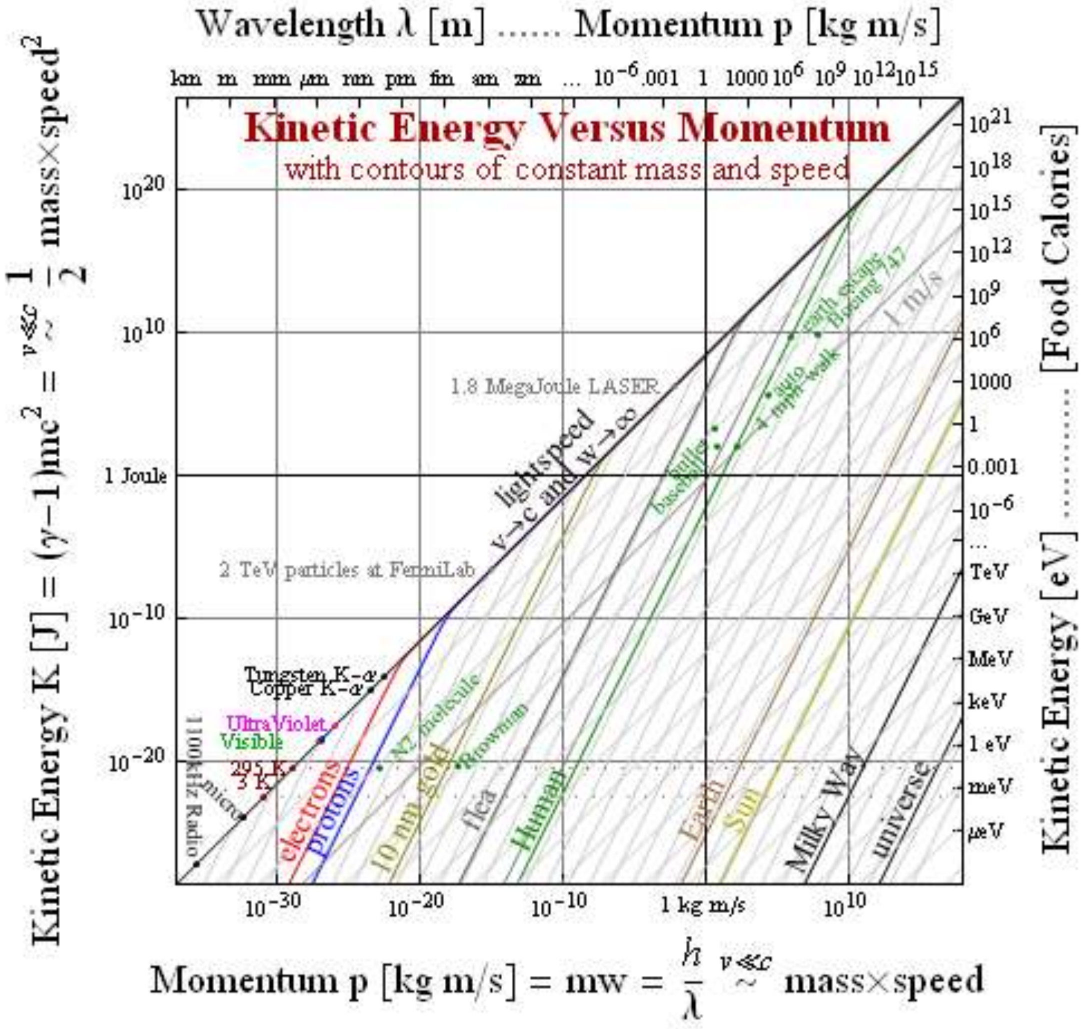
- Mass is the fundamental property that relates acceleration caused by a force or velocity due to energy imparted.

- Higher velocity (for same force) of electrons may imply higher current and faster circuits

- Questions: How can we increase electron velocity? Reduce mass but by how much
    - Can we get electron with zero mass?
        - 2D materials have zero electron mass

Typical E-k relations

- $\omega = p^2/2m\hbar$ (quadratic dispersion → massive particle free space)
- $\omega = ck$ (linear dispersion → photons mass-less)
- Can mass be engineered in a crystal?



Summary

- For a free-electron-gas, the E-k diagram has been derived as parabolic
- Velocity of a wave packet is group velocity
- Mass is defined for E-k diagram curvature → which is electron rest mass

- Next we will study the effect of electrons in a crystal to obtain effective mass