Departments of ECE and MSE, Cornell University

ECE 4070/MSE 5470: Physics of Semiconductor and Nanostructures

Spring 2015

Homework 8: Solutions

Problem 8.1 (ZigZag Carbon Nanotubes)

a) For graphene, $E(\vec{k}) = E_p \pm \hbar v \sqrt{(k_x - K_x)^2 + (k_y - K_y)^2}$

For zigzag nanotubes, $k_y = \frac{2\pi\, n}{ma}$. Suppose, $m = 3p$, then $k_y = \frac{2\pi\, n}{3pa}$. For $n = 2p$, $k_y = K_y$ and there is no bandgap. Now suppose $m = 3p \pm 1$. Then, $k_y - K_y = \frac{2\pi\, n}{(3p \pm 1)a} - \frac{4\pi}{3a}$. The smallest value of this difference will be when $n = 2p \pm 1$ and in this case,

$$k_y - K_y = \frac{2\pi\,(2p \pm 1)}{(3p \pm 1)a} - \frac{4\pi}{3a} = \mp \frac{4\pi}{3(3p \pm 1)a} = \pm \frac{2\pi}{3C} = \pm \frac{1}{3R}$$

The subband dispersions for this value of k_y are:

$$E(\vec{k}) = E_p \pm \hbar v \sqrt{(k_x - K_x)^2 + (1/3R)^2}$$

The bandgap is the difference between the energies of the conduction and valence subbands when $k_x = K_x$ and equals $2\hbar v/3R$. For a 1 nm radius nanotube, the bandgap is 0.44 eV.

b) Start from, $n = 4 \times \int_{-\infty}^{+\infty} \frac{dk_x}{2\pi} f(E(k_x) - E_f) = \frac{4}{\pi\,\hbar v} \int_{E_p + E_g/2}^{\infty} dE \frac{(E - E_p)}{\sqrt{(E - E_p)^2 - (E_g/2)^2}} f(E - E_f)$.

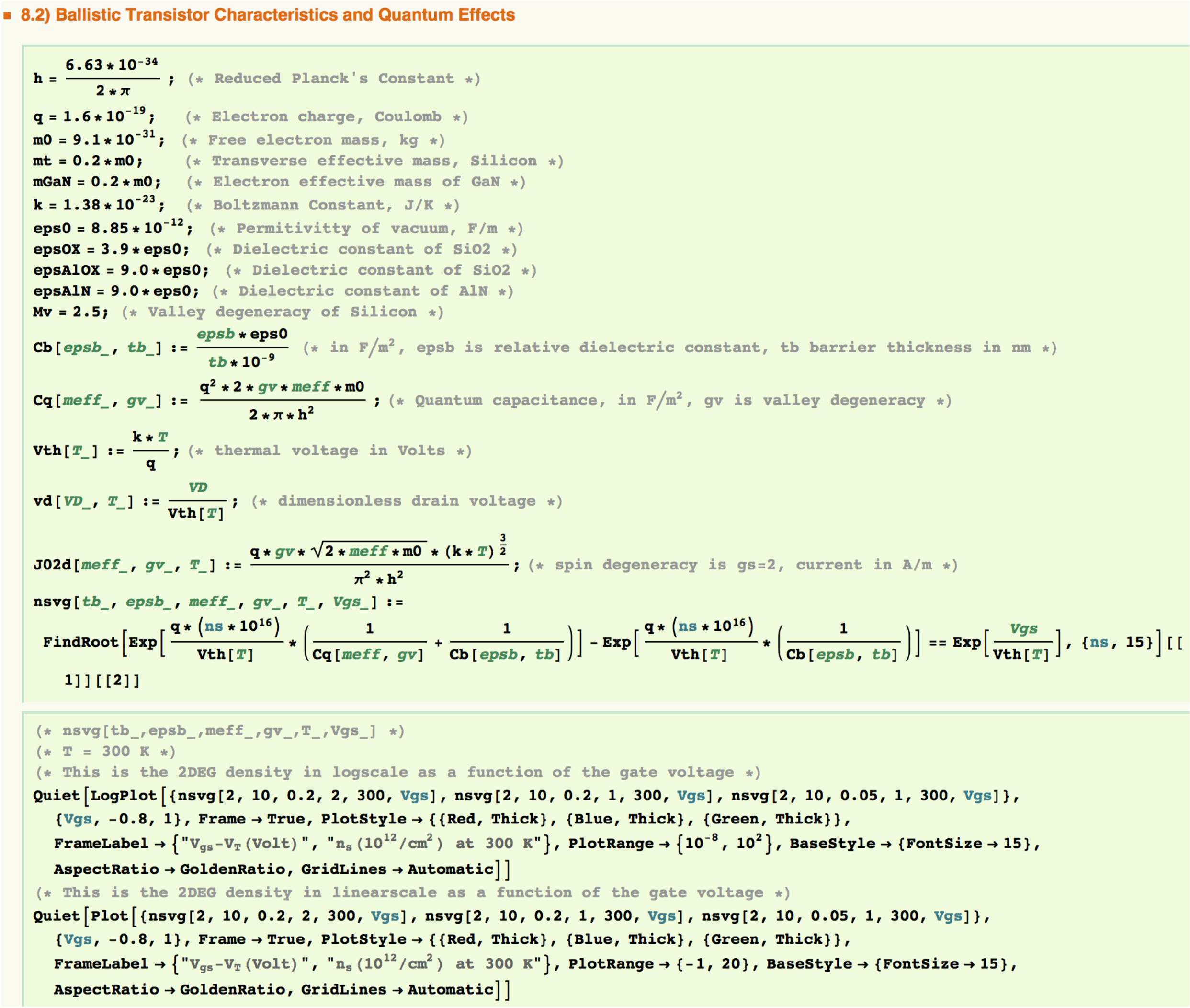
This implies, $g_{1D}(E) = \frac{4}{\pi\,\hbar v} \frac{(E - E_p)}{\sqrt{(E - E_p)^2 - (E_g/2)^2}}$.

c) At T=0K, $n = \frac{4}{\pi\,\hbar v} \int_{E_p + E_g/2}^{E_F} dE \frac{(E - E_p)}{\sqrt{(E - E_p)^2 - (E_g/2)^2}} = \frac{4}{\pi\,\hbar v} \sqrt{(E_F - E_p)^2 - (E_g/2)^2}$

d) Start from: $E(\vec{k}) = E_p \pm \hbar v \sqrt{(k_x - K_x)^2 + (1/3R)^2}$ and perform a Taylor expansion for small values of $(k_x - K_x)$ to get, $E(\vec{k}) \approx E_p \pm \frac{\hbar v}{3R}\left(1 + \frac{(k_x - K_x)^2}{2(1/3R)^2}\right) = E_p \pm \frac{\hbar v}{3R} \pm \hbar v \frac{(k_x - K_x)^2}{2(1/3R)}$. This implies, $m_e = m_h = \hbar/3Rv$. So the effective masses get smaller with increase in radius (or decrease in bandgap). This relation between bandgaps and effective masses is a common property of almost all semiconductor systems in 1D, 2D, and 3D.

Problem 8.2 (Ballistic Transistor Characteristics and Quantum Effects)

(a) Here is the Mathematica code:

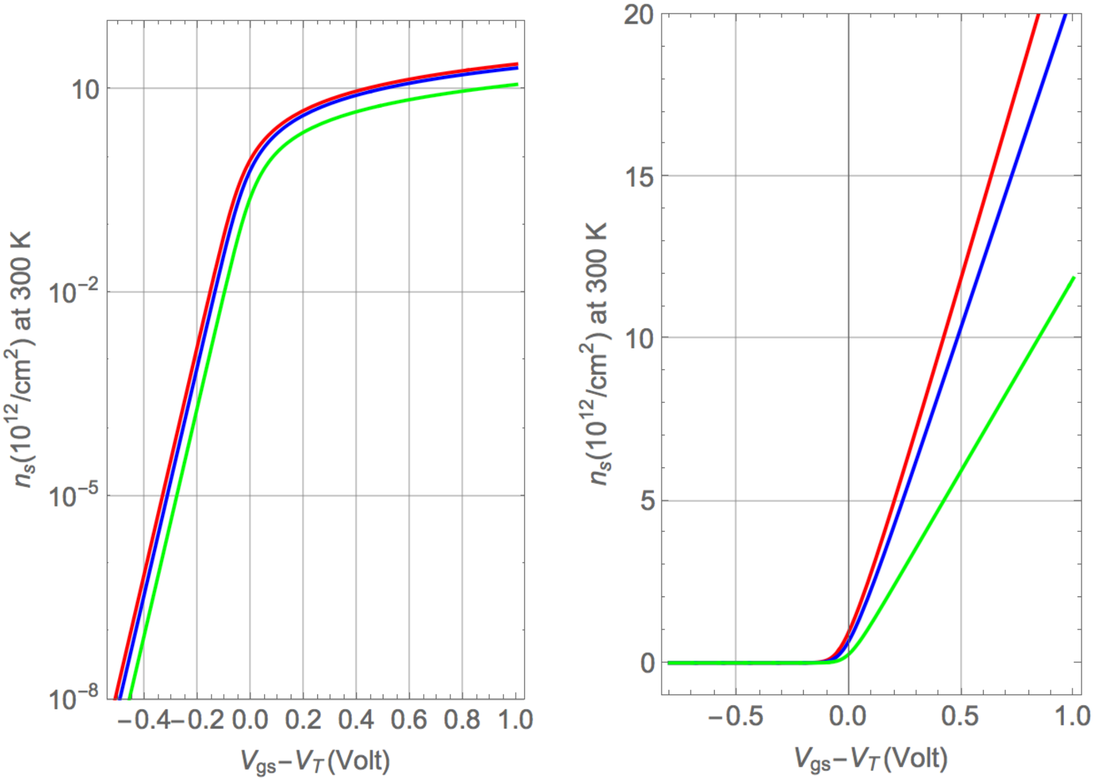


▪ 8.2) Ballistic Transistor Characteristics and Quantum Effects

```
h = (6.63*10^-34)/(2*π); (* Reduced Planck's Constant *)
q = 1.6*10^-19;    (* Electron charge, Coulomb *)
m0 = 9.1*10^-31;  (* Free electron mass, kg *)
mt = 0.2*m0;     (* Transverse effective mass, Silicon *)
mGaN = 0.2*m0;   (* Electron effective mass of GaN *)
k = 1.38*10^-23;   (* Boltzmann Constant, J/K *)
eps0 = 8.85*10^-12;  (* Permitivitty of vacuum, F/m *)
epsOX = 3.9*eps0;  (* Dielectric constant of SiO2 *)
epsAlOX = 9.0*eps0;  (* Dielectric constant of SiO2 *)
epsAlN = 9.0*eps0; (* Dielectric constant of AlN *)
Mv = 2.5; (* Valley degeneracy of Silicon *)
Cb[epsb_, tb_] := (epsb*eps0)/(tb*10^-9)  (* in F/m^2, epsb is relative dielectric constant, tb barrier thickness in nm *)
Cq[meff_, gv_] := (q^2*2*gv*meff*m0)/(2*π*h^2) ; (* Quantum capacitance, in F/m^2, gv is valley degeneracy *)
Vth[T_] := (k*T)/q; (* thermal voltage in Volts *)
vd[VD_, T_] := VD/Vth[T]; (* dimensionless drain voltage *)
J02d[meff_, gv_, T_] := (q*gv*Sqrt[2*meff*m0]*(k*T)^(3/2))/(π^2*h^2); (* spin degeneracy is gs=2, current in A/m *)
nsvg[tb_, epsb_, meff_, gv_, T_, Vgs_] :=
 FindRoot[Exp[(q*(ns*10^16))/Vth[T]*(1/Cq[meff, gv] + 1/Cb[epsb, tb])] - Exp[(q*(ns*10^16))/Vth[T]*(1/Cb[epsb, tb])] == Exp[Vgs/Vth[T]], {ns, 15}][[
   1]][[2]]
```

```
(* nsvg[tb_,epsb_,meff_,gv_,T_,Vgs_] *)
(* T = 300 K *)
(* This is the 2DEG density in logscale as a function of the gate voltage *)
Quiet[LogPlot[{nsvg[2, 10, 0.2, 2, 300, Vgs], nsvg[2, 10, 0.2, 1, 300, Vgs], nsvg[2, 10, 0.05, 1, 300, Vgs]},
  {Vgs, -0.8, 1}, Frame → True, PlotStyle → {{Red, Thick}, {Blue, Thick}, {Green, Thick}},
  FrameLabel → {"V_gs-V_T (Volt)", "n_s (10^12/cm^2) at 300 K"}, PlotRange → {10^-8, 10^2}, BaseStyle → {FontSize → 15},
  AspectRatio → GoldenRatio, GridLines → Automatic]]
(* This is the 2DEG density in linearscale as a function of the gate voltage *)
Quiet[Plot[{nsvg[2, 10, 0.2, 2, 300, Vgs], nsvg[2, 10, 0.2, 1, 300, Vgs], nsvg[2, 10, 0.05, 1, 300, Vgs]},
  {Vgs, -0.8, 1}, Frame → True, PlotStyle → {{Red, Thick}, {Blue, Thick}, {Green, Thick}},
  FrameLabel → {"V_gs-V_T (Volt)", "n_s (10^12/cm^2) at 300 K"}, PlotRange → {-1, 20}, BaseStyle → {FontSize → 15},
  AspectRatio → GoldenRatio, GridLines → Automatic]]
```

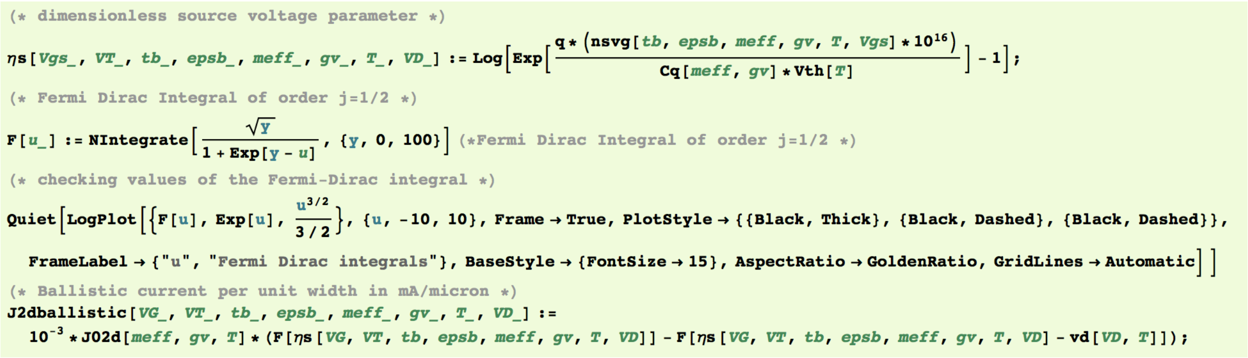
The plots are in the next page:



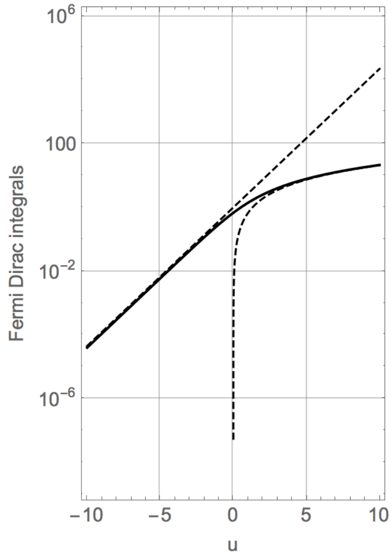
Plots for Problem 8.2 (a): Logscale and Linear plots of the 2DEG density vs the gate voltage. The colors: Red is for $m^*=0.2m_0$, $g_s=2$, $g_v=2$, Blue for $m^*=0.2m_0$, $g_s=2$, $g_v=1$, and Green for $m^*=0.05m_0$, $g_s=2$, $g_v=1$. As the net DOS increases with higher effective mass or number of valleys, a smaller gate voltage generates more 2DEG charge.

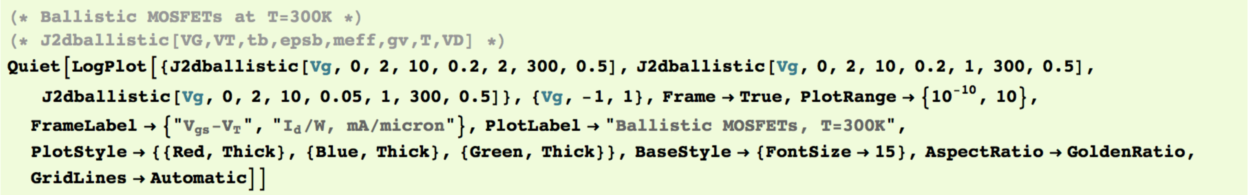
(b) This follows directly from the definition of the 3D band edge DOS N_C and the formulae derived in class and notes for the ballistic FET.

(c) Here is the Mathematica code:

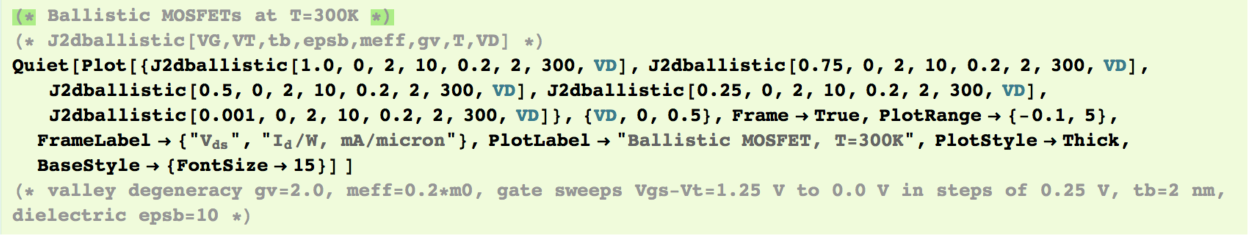


```
(* dimensionless source voltage parameter *)
ηs[Vgs_, VT_, tb_, epsb_, meff_, gv_, T_, VD_] := Log[Exp[(q * (nsvg[tb, epsb, meff, gv, T, Vgs] * 10^16))/(Cq[meff, gv] * Vth[T])] - 1];
(* Fermi Dirac Integral of order j=1/2 *)
F[u_] := NIntegrate[Sqrt[y]/(1 + Exp[y - u]), {y, 0, 100}] (*Fermi Dirac Integral of order j=1/2 *)
(* checking values of the Fermi-Dirac integral *)
Quiet[LogPlot[{F[u], Exp[u], u^(3/2)/(3 / 2)}, {u, -10, 10}, Frame → True, PlotStyle → {{Black, Thick}, {Black, Dashed}, {Black, Dashed}},
  FrameLabel → {"u", "Fermi Dirac integrals"}, BaseStyle → {FontSize → 15}, AspectRatio → GoldenRatio, GridLines → Automatic] ]
(* Ballistic current per unit width in mA/micron *)
J2dballistic[VG_, VT_, tb_, epsb_, meff_, gv_, T_, VD_] :=
  10^-3 * J02d[meff, gv, T] * (F[ηs[VG, VT, tb, epsb, meff, gv, T, VD]] - F[ηs[VG, VT, tb, epsb, meff, gv, T, VD] - vd[VD, T]]);
```



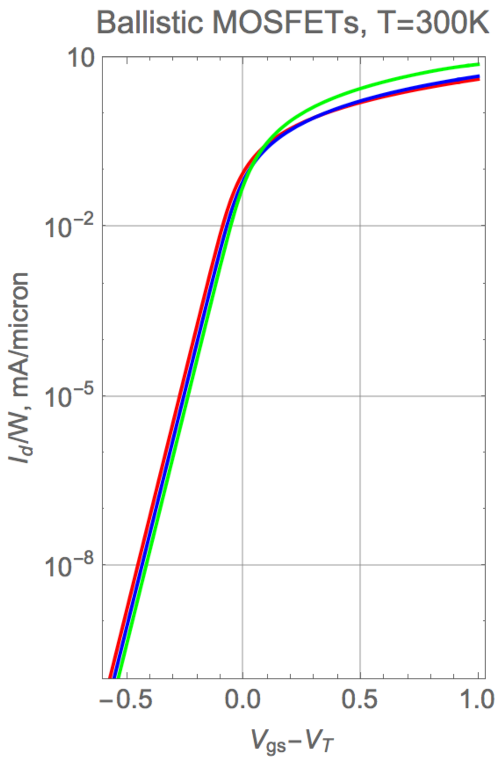


```
(* Ballistic MOSFETs at T=300K *)
(* J2dballistic[VG,VT,tb,epsb,meff,gv,T,VD] *)
Quiet[LogPlot[{J2dballistic[Vg, 0, 2, 10, 0.2, 2, 300, 0.5], J2dballistic[Vg, 0, 2, 10, 0.2, 1, 300, 0.5],
   J2dballistic[Vg, 0, 2, 10, 0.05, 1, 300, 0.5]}, {Vg, -1, 1}, Frame → True, PlotRange → {10^-10, 10},
  FrameLabel → {"Vgs-VT", "Id/W, mA/micron"}, PlotLabel → "Ballistic MOSFETs, T=300K",
  PlotStyle → {{Red, Thick}, {Blue, Thick}, {Green, Thick}}, BaseStyle → {FontSize → 15}, AspectRatio → GoldenRatio,
  GridLines → Automatic]]
```

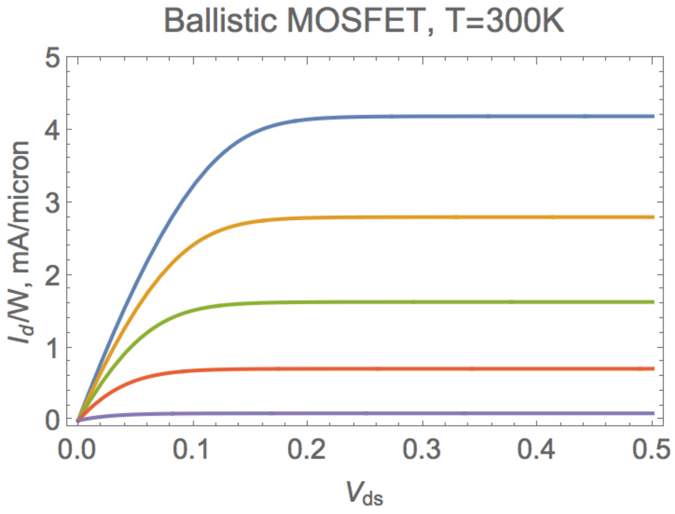


```
(* Ballistic MOSFETs at T=300K *)
(* J2dballistic[VG,VT,tb,epsb,meff,gv,T,VD] *)
Quiet[Plot[{J2dballistic[1.0, 0, 2, 10, 0.2, 2, 300, VD], J2dballistic[0.75, 0, 2, 10, 0.2, 2, 300, VD],
   J2dballistic[0.5, 0, 2, 10, 0.2, 2, 300, VD], J2dballistic[0.25, 0, 2, 10, 0.2, 2, 300, VD],
   J2dballistic[0.001, 0, 2, 10, 0.2, 2, 300, VD]}, {VD, 0, 0.5}, Frame → True, PlotRange → {-0.1, 5},
  FrameLabel → {"Vds", "Id/W, mA/micron"}, PlotLabel → "Ballistic MOSFET, T=300K", PlotStyle → Thick,
  BaseStyle → {FontSize → 15}] ]
(* valley degeneracy gv=2.0, meff=0.2*m0, gate sweeps Vgs-Vt=1.25 V to 0.0 V in steps of 0.25 V, tb=2 nm,
dielectric epsb=10 *)
```

And the ballistic FET plots are in the next page:



Plots for Problem 8.3: Logscale and Linear plots of the Ballistic FET characteristics. The colors: Red is for $m^*=0.2m_0$, $g_s=2$, $g_v=2$, Blue for $m^*=0.2m_0$, $g_s=2$, $g_v=1$, and Green for $m^*=0.05m_0$, $g_s=2$, $g_v=1$. As the net DOS increases with higher effective mass or number of valleys, a smaller gate voltage generates more 2DEG charge, but the group velocity of the low effective mass semiconductor lets it drive more on current, and slightly lower off current. In the Id-Vds curves below, the current saturates, which is an important characteristic of any transistor that has gain.



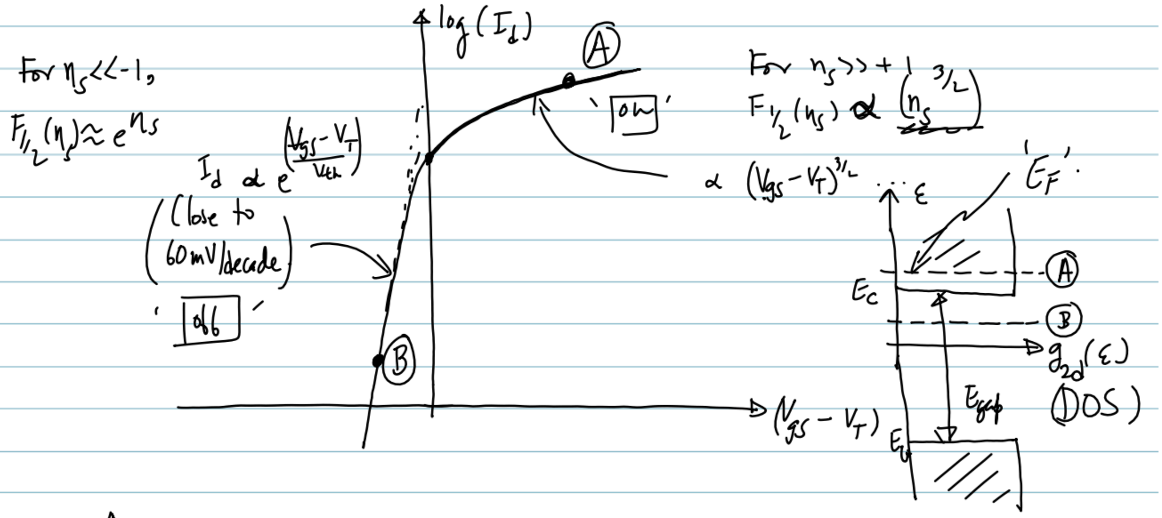
(d) The qualitative features of a 1D channel FET will not be much different from the 2D channel. The maximum conductance will however be limited by the quantum of conductance for the 1D channel. See Problem 8.3 (b), where this is derived for a topological edge state – but this is universal, and does not depend on the bandstructure details. Also look at the notes on quantum transport, where this is derived.

Problem 8.3 (Topological Insulator Field-Effect Transistors)

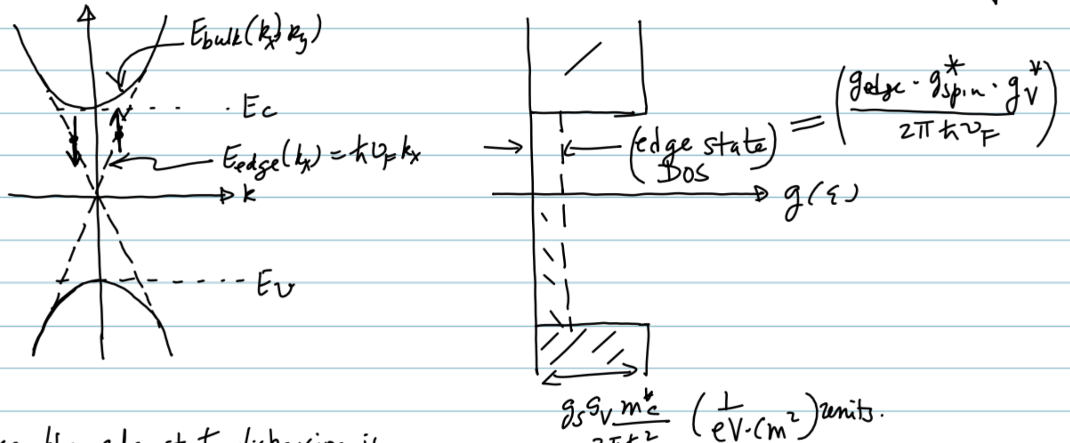
8.3) Topological insulator Field-Effect Transistors

(a) For a normal ballistic 2D-channel FET, the current is

$$I_d = J_d * W = (J^0_{2d}\cdot W)\cdot\{F_{1/2}(\eta_s) - F_{1/2}(\eta_s - v_d)\}$$



(b)



Since the edge-state dispersion is

$E_{edge}(k_x) = \hbar v_F k_x$,

$$\frac{dE_{edge}(k_x)}{dk_x} = \hbar v_F, \quad \left(\overset{\text{\# of edge states}}{g_{edge}} * \overset{\text{spin deg. of edge states}}{g^*_{spin}} * \overset{\text{valley deg. of edge states}}{g^*_v}\right)\cdot\frac{dk}{2\pi} = g_{edge}(\varepsilon)\cdot d\varepsilon$$

$\Downarrow$

$\boxed{\text{Group velocity of all TI states} = v_F}$

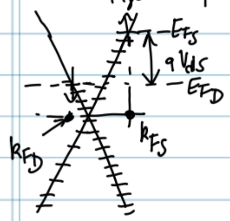
$$\Rightarrow \boxed{g_{edge}(\varepsilon) = \frac{g_{edge} * g^*_{spin} * g^*_v}{2\pi\hbar v_F}}$$

Constant DOS for the topological edge states.

8.3 (b) contd...

Thus, the current due to the TI edge states is:

$$I_{edge} = q \cdot \frac{g_s^* g_v^*}{L} \cdot \int \frac{dk}{\left(\frac{2\pi}{L}\right)} \cdot v_F = q \cdot \frac{g_s^* g_v^*}{2\pi} \cdot v_F \cdot \left(\overset{\frac{E_{FS}}{\hbar v_F}}{k_{F_S}} - \overset{\frac{E_{FD}}{\hbar v_F}}{k_{F_D}}\right)$$



$$\Rightarrow \quad I_{edge} = q \cdot \frac{g_s^* g_v^*}{2\pi} \cdot \cancel{v_F} \cdot \frac{\overbrace{E_{F_S} - E_{F_D}}^{qV_{ds}}}{\hbar \cancel{v_F}}$$

$$I_{edge} = \frac{q^2}{h} \cdot g_s^* g_v^* \cdot V_{ds}.$$

$$\Rightarrow \quad \frac{I_{edge}}{V_{ds}} = (g_s^* g_v^*) \frac{q^2}{h}$$ for each edge channel.

But $g_s^* = 1$ & $g_v^* = 1$ for a TI edge state!

$$\Rightarrow \quad \boxed{\frac{I_{edge}}{V_{ds}} = G_0 = \frac{q^2}{h}}$$ for each edge channel in a TI.

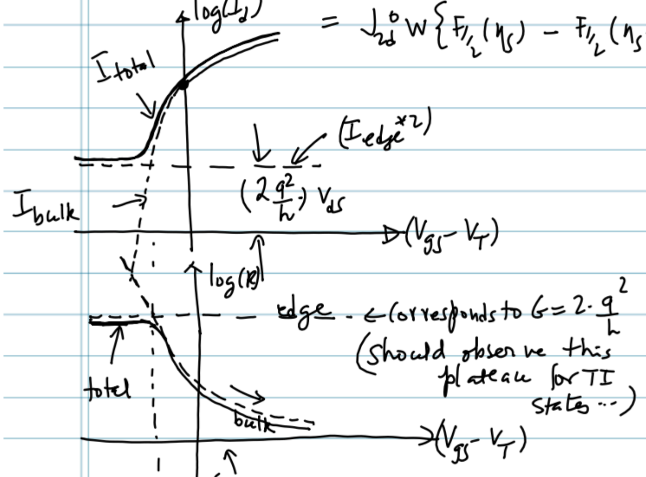
This clearly differs from a non-TI edge state by the spin degeneracy being 1 instead of 2, and the valley degeneracy being unity.

8.3 (c). $\boxed{G = 2 * \frac{q^2}{h}}$ for 2 parallel edge states:

8.3 (d) Now

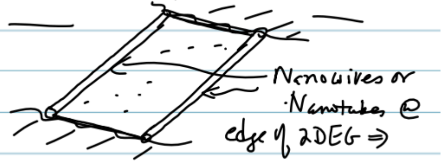
$$I_d = \overbrace{J_{2d}^0 \cdot W \cdot \{F_{1/2}(\eta_s) - F_{1/2}(\eta_s - v_d)\}}^{I_{bulk}} + \overset{\text{(2 edge states)}}{(I_{edge} * 2)}$$

$$= J_{2d}^0 W \{F_{1/2}(\eta_s) - F_{1/2}(\eta_s - v_d)\} + \underbrace{\left(2 \cdot \frac{q^2}{h}\right) \cdot V_{ds}}_{\text{Sets a min floor, no matter where } E_F \text{ is ...}}.$$



(Compare with 2007 paper ...)

8.3 (e) —



$$\& \; I_{edge} = \underset{\substack{\uparrow \\ \text{\# of wires} \\ \text{or tubes}}}{2} * \underset{\substack{\uparrow \\ 2}}{g_s} * \underset{\substack{\uparrow \\ 1 \text{ or } 2}}{g_v} * \frac{q^2}{h}$$

$$\left.\begin{aligned} &= 4\frac{q^2}{h} \text{ for } g_v = 1 \\ &= 8\frac{q^2}{h} \text{ for } g_v = 2 \end{aligned}\right\} \neq \left(\frac{2q^2}{h}!\right).$$

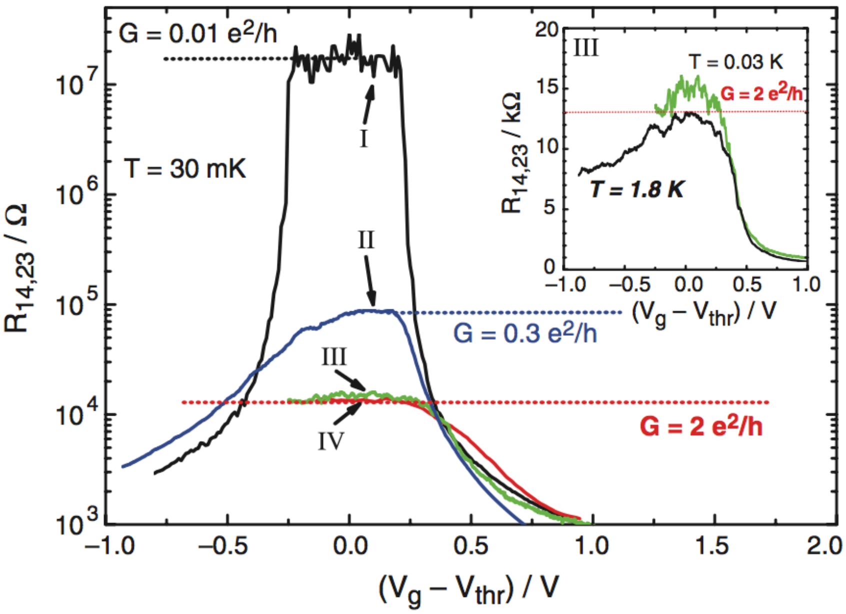


Fig. 4. The longitudinal four-terminal resistance, $R_{14,23}$, of various normal (d = 5.5 nm) (I) and inverted (d = 7.3 nm) (II, III, and IV) QW structures as a function of the gate voltage measured for B = 0 T at T = 30 mK. The device sizes are (20.0 × 13.3) μm^2 for devices I and II, (1.0 × 1.0) μm^2 for device III, and (1.0 × 0.5) μm^2 for device IV. The inset shows $R_{14,23}(V_g)$ of two samples from the same wafer, having the same device size (III) at 30 mK (green) and 1.8 K (black) on a linear scale.

Figure from “Quantum Spin Hall Insulator State in HgTe Quantum Wells”, Markus Konig et al., Science vol 318, pg 766, 2007.

8.3(f) This is a research problem. If you are interested in working on it, please talk to me!

Problem 8.4 (Boltzmann Transport in d-dimensions)

(8.4)

$$f(k) \approx f_0(k) + \tau(k)\left(-\frac{\partial f_0(k)}{\partial E(k)}\right)\vec{v}_k\cdot\underset{\text{force } = -q\underset{\text{electric field.}}{\vec{E}}}{\vec{F}}$$

$$\approx f_0(k) + q\tau(k)\left(+\frac{\partial f_0(k)}{\partial E(k)}\right)\cdot\vec{v}_k\cdot\vec{E} \leftarrow \text{electric field.}$$

Carrier density: $n = \frac{\overset{\text{spin}}{g_s}\,\overset{\text{valley}}{g_v}}{L^d}\sum_k f(k) = \frac{g_s g_v}{L^d}\cdot\int\frac{d^dk}{\left(\frac{2\pi}{L}\right)^d}\,f(k)$

$\Rightarrow$

$$n = \frac{g_s g_v}{(2\pi)^d}\int d^dk\; f_0(k)$$

$$f(k) \rightarrow \underbrace{f_0(k)}_{\text{even.}} + \underbrace{q\tau(k)\left(\frac{\partial f_0}{\partial E}\right)\vec{v}_k\cdot\vec{E}}_{\text{odd} \rightarrow 0!}$$

Volume of a d-dimensional sphere in k-space: $\boxed{V_d = \frac{\pi^{d/2}k^d}{\Gamma\left(\frac{d}{2}+1\right)}}$

Check:
$d=2 \Rightarrow \pi k^2$
$d=3 \Rightarrow \frac{4}{3}\pi k^3 \ldots$

"Surface" of a d-dimensional sphere in k-space:

$$\boxed{S_d = \nabla_k V_d = \frac{d\,\pi^{d/2}k^{d-1}}{\Gamma\left(d/2+1\right)}}$$

Check:
$d=2 \Rightarrow 2\pi k$
$d=3 \Rightarrow 4\pi k^2 \ldots$

$\Rightarrow$ Carrier density in d-dimensions is.

$$n = \frac{g_s g_v}{(2\pi)^d}\int\frac{d\cdot\pi^{d/2}k^{d-1}\,dk}{\Gamma\left(\frac{d}{2}+1\right)}\cdot f_0(k)$$

$$E = E_c + \overbrace{\frac{\hbar^2k^2}{2m^*}}^{\mathcal{E}_k}$$

$$= \frac{g_s g_v\cdot d\cdot\pi^{d/2}}{(2\pi)^d\,\Gamma\left(\frac{d}{2}+1\right)}\int k^{d-1}\,dk\cdot f_0(k)$$

$$\Rightarrow k^{d-1}dk = \frac{2m^*}{2\cdot\hbar^2}\left\{\frac{2m^*}{\hbar^2}\underbrace{(E-E_c)}_{\mathcal{E}}\right\}^{\frac{d}{2}-1} dE$$

$$n = \frac{g_s g_v\; d\cdot\pi^{d/2}}{(2\pi)^d\,\Gamma\left(\frac{d}{2}+1\right)}\cdot\frac{1}{2}\cdot\left(\frac{2m^*}{\hbar^2}\right)^{d/2}\int d\mathcal{E}\cdot\mathcal{E}^{\frac{d}{2}-1}\,f_0(\mathcal{E})$$

$$\boxed{k^{d-1}dk \quad \frac{1}{2}\left(\frac{2m^*}{\hbar^2}\right)^{d/2}\mathcal{E}^{\frac{d}{2}-1}}$$

$$\boxed{n = \int g_d(\mathcal{E})\,f_0(\mathcal{E})\,d\mathcal{E},} \text{ where } \underbrace{\boxed{g_d(\mathcal{E}) = \frac{g_s g_v}{2^{d-2}\pi^{d/2}\Gamma\left(\frac{d}{2}\right)}\left(\frac{2m^*}{\hbar^2}\right)^{d/2}\mathcal{E}^{\frac{d}{2}-1}}}_{\text{generalized d-dimensional DOS.}}$$

Similarly, $\vec{J} = q\cdot \frac{g_s g_v}{L^d} \sum_k f(k)\, \vec{v}_k$

Let the electric field point along a fixed direction $\vec{E}$, say $\hat{x}$.

Then, $$f(\vec{k}) \simeq f_0(\vec{k}) + q\tau(\vec{k})\left(+\frac{\partial f_0}{\partial \varepsilon_k}\right) \vec{v}_k \cdot \vec{E}$$

$$\Rightarrow \quad \vec{J} = q\cdot \frac{g_s g_v}{L^d} \cdot \int \frac{d^d k}{\left(\frac{2\pi}{L}\right)^d}\, \vec{v}_k \cdot \left[\cancelto{0}{f_0(\vec{k})} + q\tau(\vec{k})\left(-\frac{\partial f_0(\vec{k})}{\partial \varepsilon_k}\right) \cdot \vec{v}_k \cdot \vec{E}\right]$$

$$= q^2 \cdot \frac{g_s g_v}{(2\pi)^d} \int d^d k \; \underbrace{\vec{v}_k\left(\vec{v}_k \cdot \vec{E}\right)}_{?} \cdot \tau(\vec{k}) \left(-\frac{\partial f_0(\vec{k})}{\partial \varepsilon_k}\right)$$

Now $\vec{v}_k(\vec{v}_k \cdot \vec{E}) = \vec{v}_k\, v_{kx} E = \vec{v}_k\, v_k \cos\theta_k E$

& $$J_x = \left\{ q^2 \cdot \frac{g_s g_v}{(2\pi)^d} \cdot \int d^d k \; v_k^2 \cos^2\theta_k\, \tau(\vec{k}) \left(-\frac{\partial f_0(\vec{k})}{\partial \varepsilon_k}\right) \right\} * E$$

$$\frac{J_x}{n} = q^2 \; \frac{\int d_k V_d \; v_k^2 \cos^2\theta_k \; \tau(\vec{k}) \left(-\frac{\partial f_0}{\partial \varepsilon_k}\right)}{\int d_k V_d \cdot f_0(\vec{k})}$$

$v_k^2 = \frac{2\varepsilon_k}{m^*}$

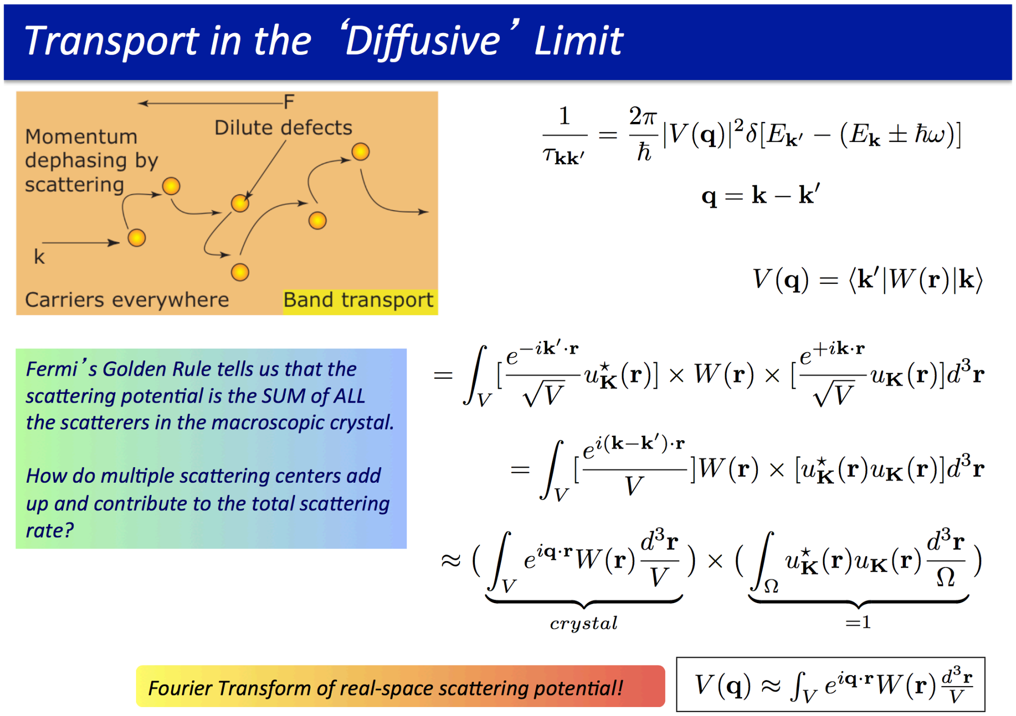
$$\boxed{\langle \cos^2\theta_k \rangle = \frac{1}{d}}$$

↑ Note!

$$\Rightarrow \quad J_x = \frac{n\cdot q^2}{m^*} \cdot \left\{ \underbrace{\frac{2}{d} \cdot \frac{\int d\varepsilon_k \; \varepsilon_k^{d/2}\, \tau(\varepsilon_k) \left(-\frac{\partial f_0}{\partial \varepsilon_k}\right)}{\int d\varepsilon_k \cdot \varepsilon_k^{d/2 - 1}\, f_0(\varepsilon_k)}} \right\}$$

$$\Rightarrow \quad \boxed{J_x = \frac{n\cdot q^2}{m^*} \langle \tau \rangle}$$

Problem 8.5 (Scattering from uncorrelated events)



Transport in the 'Diffusive' Limit

$$\frac{1}{\tau_{\mathbf{kk}'}} = \frac{2\pi}{\hbar}|V(\mathbf{q})|^2\delta[E_{\mathbf{k}'} - (E_{\mathbf{k}} \pm \hbar\omega)]$$

$$\mathbf{q} = \mathbf{k} - \mathbf{k}'$$

$$V(\mathbf{q}) = \langle \mathbf{k}'|W(\mathbf{r})|\mathbf{k}\rangle$$

Fermi's Golden Rule tells us that the scattering potential is the SUM of ALL the scatterers in the macroscopic crystal.

How do multiple scattering centers add up and contribute to the total scattering rate?

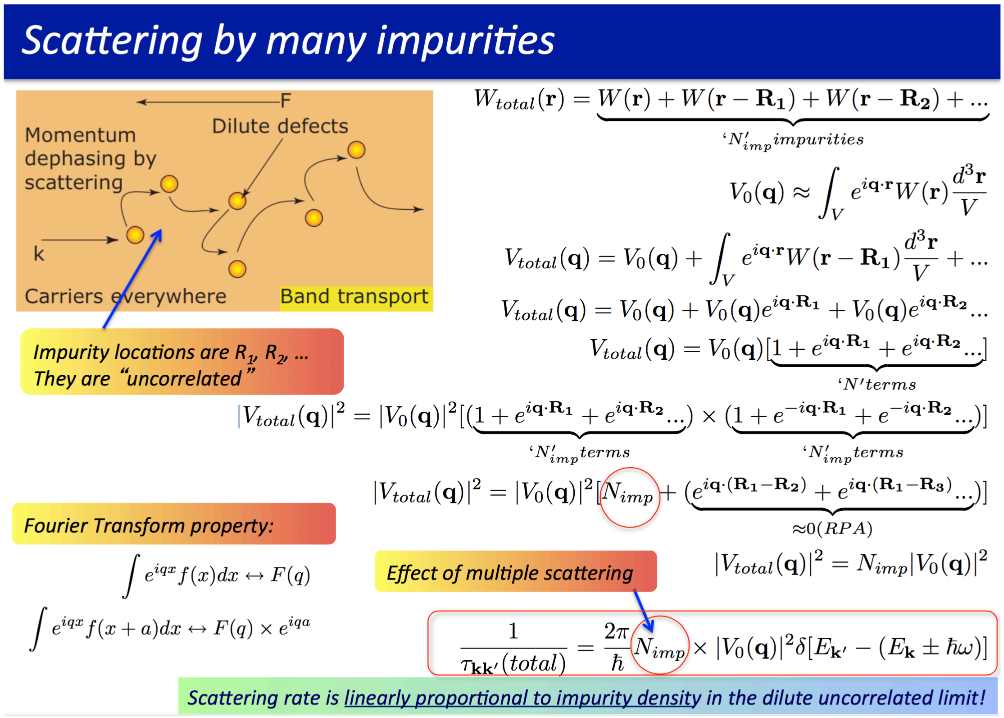
$$= \int_V \left[\frac{e^{-i\mathbf{k}'\cdot\mathbf{r}}}{\sqrt{V}} u^\star_{\mathbf{K}}(\mathbf{r})\right] \times W(\mathbf{r}) \times \left[\frac{e^{+i\mathbf{k}\cdot\mathbf{r}}}{\sqrt{V}} u_{\mathbf{K}}(\mathbf{r})\right] d^3\mathbf{r}$$

$$= \int_V \left[\frac{e^{i(\mathbf{k}-\mathbf{k}')\cdot\mathbf{r}}}{V}\right] W(\mathbf{r}) \times \left[u^\star_{\mathbf{K}}(\mathbf{r}) u_{\mathbf{K}}(\mathbf{r})\right] d^3\mathbf{r}$$

$$\approx \underbrace{\left(\int_V e^{i\mathbf{q}\cdot\mathbf{r}} W(\mathbf{r})\frac{d^3\mathbf{r}}{V}\right)}_{crystal} \times \underbrace{\left(\int_\Omega u^\star_{\mathbf{K}}(\mathbf{r})u_{\mathbf{K}}(\mathbf{r})\frac{d^3\mathbf{r}}{\Omega}\right)}_{=1}$$

Fourier Transform of real-space scattering potential!

$$\boxed{V(\mathbf{q}) \approx \int_V e^{i\mathbf{q}\cdot\mathbf{r}}W(\mathbf{r})\frac{d^3\mathbf{r}}{V}}$$



Scattering by many impurities

$$W_{total}(\mathbf{r}) = \underbrace{W(\mathbf{r}) + W(\mathbf{r}-\mathbf{R_1}) + W(\mathbf{r}-\mathbf{R_2}) + \ldots}_{'N'_{imp}impurities}$$

$$V_0(\mathbf{q}) \approx \int_V e^{i\mathbf{q}\cdot\mathbf{r}}W(\mathbf{r})\frac{d^3\mathbf{r}}{V}$$

$$V_{total}(\mathbf{q}) = V_0(\mathbf{q}) + \int_V e^{i\mathbf{q}\cdot\mathbf{r}}W(\mathbf{r}-\mathbf{R_1})\frac{d^3\mathbf{r}}{V} + \ldots$$

$$V_{total}(\mathbf{q}) = V_0(\mathbf{q}) + V_0(\mathbf{q})e^{i\mathbf{q}\cdot\mathbf{R_1}} + V_0(\mathbf{q})e^{i\mathbf{q}\cdot\mathbf{R_2}}\ldots$$

$$V_{total}(\mathbf{q}) = V_0(\mathbf{q})[\underbrace{1 + e^{i\mathbf{q}\cdot\mathbf{R_1}} + e^{i\mathbf{q}\cdot\mathbf{R_2}}\ldots}_{'N'terms}]$$

Impurity locations are R_1, R_2, ...
They are "uncorrelated"

$$|V_{total}(\mathbf{q})|^2 = |V_0(\mathbf{q})|^2[(\underbrace{1 + e^{i\mathbf{q}\cdot\mathbf{R_1}} + e^{i\mathbf{q}\cdot\mathbf{R_2}}\ldots}_{'N'_{imp}terms}) \times (\underbrace{1 + e^{-i\mathbf{q}\cdot\mathbf{R_1}} + e^{-i\mathbf{q}\cdot\mathbf{R_2}}\ldots}_{'N'_{imp}terms})]$$

$$|V_{total}(\mathbf{q})|^2 = |V_0(\mathbf{q})|^2[N_{imp} + (\underbrace{e^{i\mathbf{q}\cdot(\mathbf{R_1}-\mathbf{R_2})} + e^{i\mathbf{q}\cdot(\mathbf{R_1}-\mathbf{R_3})}\ldots}_{\approx 0(RPA)})]$$

Fourier Transform property:

$$\int e^{iqx}f(x)dx \leftrightarrow F(q)$$

$$\int e^{iqx}f(x+a)dx \leftrightarrow F(q) \times e^{iqa}$$

Effect of multiple scattering

$$|V_{total}(\mathbf{q})|^2 = N_{imp}|V_0(\mathbf{q})|^2$$

$$\boxed{\frac{1}{\tau_{\mathbf{kk}'}(total)} = \frac{2\pi}{\hbar}N_{imp} \times |V_0(\mathbf{q})|^2\delta[E_{\mathbf{k}'} - (E_{\mathbf{k}} \pm \hbar\omega)]}$$

Scattering rate is linearly proportional to impurity density in the dilute uncorrelated limit!