Week 1

1.1-a for all translation groups, the group elements are $g_i = \sum_j u_{ij}\vec{a}_j$. the values of $\{u_{ij}\}$ and the structure of the basis $\{\vec{a}_j\}$ may be different, but the group elements interact in the same way; the group structure is the same. thus, there is a bijection between all translation groups (in the same dimensional space at least).

1.1-b identity (e), rotation by π (R_π) (same as inverting the bases)

1.1-c $e/R(0)$, $R(\frac{\pi}{3})$, $R(\frac{2\pi}{3})$, $R(\pi)$, $R(\frac{4\pi}{3})$, $R(\frac{5\pi}{3})$, $S(0)$, $S(\frac{\pi}{6})$, $S(\frac{\pi}{3})$, $S(\frac{\pi}{2})$, $S(\frac{2\pi}{3})$, $S(\frac{5\pi}{6})$

1.1-d rotations and reflections can be defined as unitary matrix operations on a vector space. These matrix operations generally do not commute, so then neither do the group operations.

ex: $R(\frac{\pi}{2})S(\frac{\pi}{2}) = S(\frac{3\pi}{4})$, $S(\frac{\pi}{2})R(\frac{\pi}{2}) = S(\frac{5\pi}{4})$ → do not commute!

1.2-a $\vec{T} = u_1\vec{a}_1 + u_2\vec{a}_2 + u_3\vec{a}_3$, $\vec{G} = v_1 \cdot 2\pi\left(\frac{\vec{a}_2\times\vec{a}_3}{\vec{a}_1(\vec{a}_2\times\vec{a}_3)}\right) + v_2\cdot 2\pi\left(\frac{\vec{a}_3\times\vec{a}_1}{\vec{a}_2(\vec{a}_3\times\vec{a}_1)}\right) + v_3\cdot 2\pi\left(\frac{\vec{a}_1\times\vec{a}_2}{\vec{a}_3(\vec{a}_1\times\vec{a}_2)}\right)$

↳ $\vec{T}\cdot\vec{G} = u_1v_1\cdot 2\pi - u_2v_2\cdot 2\pi + u_3v_3\cdot 2\pi = -\sum_{i=1}^{3}(-1)^i u_iv_i\cdot 2\pi$

since $u_i, v_i \in \mathbb{Z}$ and $G(\mathbb{Z}, \cdot)$ is closed:

$\vec{T}\cdot\vec{G} = -\sum_{i=1}^{3}(-1)^i n_i\cdot 2\pi$ with $n_i\in\mathbb{Z}$ → $\vec{T}\cdot\vec{G} = 2\pi N$ $(N\in\mathbb{Z})$

→ $e^{i\vec{G}\cdot\vec{T}} = e^{2\pi i N} = 1$

1.2-b $V_{rec} = \vec{b}_1 \cdot (\vec{b}_2 \times \vec{b}_3) = (2\pi)^3 \cdot \dfrac{(\vec{a}_2 \times \vec{a}_3) \cdot [(a_3 \times a_1) \times (\vec{a}_1 \times \vec{a}_2)]}{(\vec{a}_1 \cdot (\vec{a}_2 \times \vec{a}_3))^3}$

$= \dfrac{(2\pi)^3}{V^3} \cdot [(\vec{a}_2 \times \vec{a}_3) \cdot (V\vec{a}_1)]$

$= \dfrac{(2\pi)^3}{V^3} \cdot V^2 = \dfrac{(2\pi)^3}{V}$ (using vector product rules)

1.2-c multiplying $\vec{G} \cdot (P\vec{T}) = (P^{-1}\vec{G}) \cdot \vec{T}$ with P from the left gives

$(P\vec{G}) \cdot (P\vec{T}) = \vec{G} \cdot \vec{T} \rightarrow$ P is an orthogonal operator and it acts the same on both $\vec{G}$ and $\vec{T}$

1.2-d $\vec{a}_1 \cdot (\vec{a}_2 \times \vec{a}_3) = \dfrac{a^3}{8} (\hat{y}+\hat{z}) \cdot \left((\hat{z}+\hat{x}) \times (\hat{x}+\hat{y}) \right)$

$= \dfrac{a^3}{8} (\hat{y}+\hat{z}) \cdot [\hat{z} \times (\hat{x}+\hat{y}) + \hat{x} \times (\hat{x}+\hat{y})]$

$= \dfrac{a^3}{8} (\hat{y}+\hat{z}) \cdot [-\hat{x} \times \hat{z} - \hat{y} \times \hat{z} - \hat{y} \times \hat{x}]$

$= \dfrac{a^3}{8} (\hat{y}+\hat{z}) \cdot [\hat{z} \times \hat{x} + \hat{z} \times y + \hat{x} \times \hat{y}]$

$= \dfrac{a^3}{8} [\hat{y} \cdot (\hat{z} \times \hat{x}) + \hat{z} \cdot (\hat{x} \times \hat{y})] = \dfrac{a^3}{8} \cdot 2 = \left(\dfrac{a}{2}\right)^3 \cdot 2$

$\Longrightarrow \begin{cases} \vec{b}_1 = \frac{2\pi}{a}(-\hat{x}+\hat{y}+\hat{z}) \\ \vec{b}_2 = \frac{2\pi}{a}(\hat{x}-\hat{y}+\hat{z}) \\ \vec{b}_3 = \frac{2\pi}{a}(\hat{x}+\hat{y}-\hat{z}) \end{cases} \Rightarrow$ BCC lattice

1.2-e FCC lattice, as shown before the operator $P\vec{T} = \vec{G}$ is orthogonal $P\vec{G} = \vec{T} \rightarrow$ if reciprocal of [redacted] one is the other, then vice versa the same relation holds.

reciprocal of FCC $\Rightarrow$ BCC, then reciprocal of BCC $\rightarrow$ FCC

1.3-a if $\psi_{\vec{k}}(\vec{r}) = e^{i\vec{k}\cdot\vec{r}}\, u_{\vec{k}}(\vec{r}) \rightarrow \psi_{\vec{k}}(\vec{r}+\vec{T}) = e^{i\vec{k}\cdot(\vec{r}+\vec{T})}\, u_{\vec{k}}(\vec{r}+\vec{T})$

since $u_{\vec{k}}(\vec{r}+\vec{T}) = u_{\vec{k}}(\vec{r}) \rightarrow \psi_{\vec{k}}(\vec{r}+\vec{T}) = e^{i\vec{k}\cdot\vec{r}}\, e^{i\vec{k}\cdot\vec{T}}\, u_{\vec{k}}(\vec{r})$

so $\psi_{\vec{k}}(\vec{r}+\vec{T}) = e^{i\vec{k}\cdot\vec{T}} \cdot \underbrace{e^{i\vec{k}\cdot\vec{r}}\, u_{\vec{k}}(\vec{r})}_{\psi_{\vec{k}}(\vec{r})} = e^{i\vec{k}\cdot\vec{T}}\, \psi_{\vec{k}}(\vec{r})$

1.3-b 2) $\psi_{\vec{k}+\vec{G}}(\vec{r}+\vec{T}) = \underbrace{e^{i\vec{G}\cdot\vec{T}}}_{=1 \text{ as shown before (1.2 a)}}\, e^{i\vec{k}\cdot\vec{T}}\, \psi_{\vec{k}+\vec{G}}(\vec{r}) = e^{i\vec{k}\cdot\vec{T}}\, \psi_{\vec{k}+\vec{G}}(\vec{r})$

1) is trivial: $\psi_{\vec{k}+\vec{G}}(\vec{r}) = e^{i(\vec{k}+\vec{G})\vec{r}}\, u_{\vec{k}+\vec{G}}(\vec{r})$

$\psi_{\vec{k}}(\vec{r}) = e^{i\vec{k}\vec{r}}\, u_{\vec{k}}(\vec{r})$

1.4-a these are stationary states, and at relevant (low) T, these practically never get excited, only valence electrons do.

1.4-b $\underbrace{1s^2 2s^2 2p^6}_{\text{"stationary" electrons}}\, \underbrace{3s^2 3p^2}_{4 \text{ valence electrons}}$

1.4-c $\vec{k}\cdot N_i \vec{a}_i = 2\pi n_i \quad , \{n_i\} \in \mathbb{Z}$

↳ $\vec{k} = \frac{2\pi}{V}\left(\frac{n_1}{N_1}(\vec{a}_2\times\vec{a}_3) + \frac{n_2}{N_2}(\vec{a}_3\times\vec{a}_1) + \frac{n_3}{N_3}(\vec{a}_1\times\vec{a}_2)\right)$

note: [basically arb. "lattice"-vector on lattice with basis of bivectors $(\vec{a}_2\times\vec{a}_3)$, $(\vec{a}_3\times\vec{a}_1)$, $(\vec{a}_1\times\vec{a}_2)$]

1.4-d V_{1} of 1 cell: $\Delta\vec{k} = \frac{(2\pi)^3}{V^3 N_c}\left[(\vec{a}_2\times\vec{a}_3)\cdot\left[(\vec{a}_3\times\vec{a}_1)\times(\vec{a}_1\times\vec{a}_2)\right]\right]$

$= \frac{(2\pi)^3}{V^3 N_c} V^2 = \frac{(2\pi)^3}{V N_c} = \frac{(2\pi)^3}{V} \quad (V \equiv V N_c)$

↑ same as earlier

1.4-e number $= 2 \cdot \frac{V_{BZ}}{\Delta\vec{k}} = \frac{2}{(2\pi)^3} V \cdot V_{BZ} = \frac{2}{(2\pi)^3} V \cdot \frac{(2\pi)^3}{V} = 2$

(2 ← spin; V_{BZ} ← BZ volume!)

Week 2

Hilbert space product.

1 · prior: $a_\lambda|\Omega\rangle = 0$, $\frac{1}{\sqrt{\prod_\lambda n_\lambda!}} \prod_\lambda a_\lambda^\dagger |\Omega\rangle = \bigotimes_\lambda |\lambda\rangle$

Grassmann algebra: $[a_\lambda, a_\mu^\dagger]_- = \delta_{\lambda,\mu}$, $[a_\lambda, a_\mu]_- = 0$, $[a_\lambda^\dagger, a_\mu^\dagger]_- = 0$

a) $\langle \lambda_1 | \lambda_2 \rangle = \langle \Omega | a_{\lambda_1} a_{\lambda_2}^\dagger | \Omega \rangle = \langle \Omega | [a_{\lambda_2}^\dagger a_{\lambda_1} + \delta_{\lambda_1,\lambda_2}] | \Omega \rangle$

$= 0 + \langle \Omega | \delta_{\lambda_1,\lambda_2} | \Omega \rangle = \delta_{\lambda_1,\lambda_2} \langle \Omega | \Omega \rangle$

$= \delta_{\lambda_1,\lambda_2}$

b) $\langle \lambda_1, \lambda_2 | \lambda_1, \lambda_2 \rangle = \langle \Omega | a_{\lambda_2} a_{\lambda_1} a_{\lambda_1}^\dagger a_{\lambda_2}^\dagger | \Omega \rangle$

$= \langle \Omega | a_{\lambda_2} (1 + a_{\lambda_1}^\dagger a_{\lambda_1}) a_{\lambda_2}^\dagger | \Omega \rangle$ $\quad (a_{\lambda_1} a_{\lambda_2}^\dagger |\Omega\rangle = 0)$

$= \langle \Omega | a_{\lambda_2} a_{\lambda_2}^\dagger + 0 | \Omega \rangle = \langle \lambda_2 | \lambda_2 \rangle = 1$

2 a) $m_Q = \frac{1}{N} \langle \uparrow\downarrow\cdots | S_A^z - S_B^z | \uparrow\downarrow\cdots \rangle$

all same spin value $\frac{1}{2}$ on A: all $+\frac{1}{2}$ ($\frac{1}{2}N$ are on A) on B: all $-\frac{1}{2}$ ($\frac{1}{2}N$ are on B)

$= \frac{1}{N}\left[\frac{1}{2}\left(\frac{1}{2}N\right) - \frac{1}{2}\left(-\frac{1}{2}N\right)\right]$

$= \frac{1}{2}$ (depending on A/B choice of lattice, could be $-\frac{1}{2}$)

b) due to the $S_i^+ S_j^-$ and $S_i^- S_j^+$ terms, a Néel state is not an eigen state of $\mathcal{H}$, since $\mathcal{H}|\Psi_N\rangle \neq E|\Psi_N\rangle$ does not return the same state multiplied with some constant. Since it's not an eigenstate, it cannot be the groundstate!

c) $\langle \text{sing}| \mathcal{H} |\text{sing}\rangle = -\frac{J}{2} \langle \uparrow\downarrow - \downarrow\uparrow | \left[S_1^z S_2^z + \frac{1}{2}\left(S_1^+ S_2^- + S_1^- S_2^+\right)\right] | \uparrow\downarrow - \downarrow\uparrow \rangle$

$= -\frac{J}{2}\left[\frac{1}{2} + 1\right] = -\frac{3J}{4}$

(3) a) $\mathcal{H} = J\, S_1 \cdot S_2 = J\left[S_1^z S_2^z + \frac{1}{2}\left(S_1^+ S_2^- + S_1^- S_2^+\right)\right]$

(4) a) $\mathcal{H} = \begin{pmatrix} \langle R|\mathcal{H}|R\rangle & \langle R'|\mathcal{H}|R\rangle \\ \langle R|\mathcal{H}|R'\rangle & \langle R'|\mathcal{H}|R'\rangle \end{pmatrix} = \begin{pmatrix} \varepsilon & -t \\ -t & \varepsilon \end{pmatrix}$

stationary states: $\mathcal{H}|\psi_i\rangle = E_i|\psi_i\rangle$

eigenvalues of $\mathcal{H}$: $\det(\mathcal{H} - \lambda I) = 0 \rightarrow (\varepsilon-\lambda)^2 - t^2 = 0$

$\rightarrow \lambda = \frac{2\varepsilon \pm \sqrt{4\varepsilon^2 - 4(\varepsilon^2 - t^2)}}{2} = \varepsilon \pm \sqrt{t^2} = \varepsilon \pm t \quad (t \geq 0)$

eigenstates that have $\mathcal{H}|\psi\rangle = (\varepsilon \pm t)|\psi\rangle$

for $\varepsilon + t \rightarrow \begin{pmatrix} \varepsilon & -t \\ -t & \varepsilon \end{pmatrix}\begin{pmatrix} \alpha \\ \beta \end{pmatrix} = \begin{pmatrix} \varepsilon\alpha + t\alpha \\ \varepsilon\beta + t\beta \end{pmatrix} \Rightarrow \alpha = \beta = \frac{1}{\sqrt{2}}$ (since $\langle\psi|\psi\rangle = 1$)

for $\varepsilon - t \rightarrow \begin{pmatrix} \varepsilon & -t \\ -t & \varepsilon \end{pmatrix}\begin{pmatrix} \alpha \\ \beta \end{pmatrix} = \begin{pmatrix} \varepsilon\alpha - t\alpha \\ \varepsilon\beta - t\beta \end{pmatrix} \rightarrow \alpha = \beta = \frac{1}{\sqrt{2}}$ (same norm.)

so: $\frac{1}{\sqrt{2}}\left[|R\rangle \pm |R'\rangle\right]$ are eigenstates!

$$\mathcal{H}\left[\frac{1}{\sqrt{2}}\left(|R\rangle \mp |R'\rangle\right)\right] = (\varepsilon \pm t)\left[\frac{1}{\sqrt{2}}\left(|R\rangle \mp |R'\rangle\right)\right]$$

b) probability of both is R:

$$P(R_1, R_2) = \left|\langle R_1 R_2 | \tfrac{1}{2}\left(|R\rangle_1|R\rangle_2 + |R\rangle_1|R'\rangle_2 + |R'\rangle_1|R\rangle_2 + |R'\rangle_1|R'\rangle_2\right)\right|^2$$

$$= \left|\tfrac{1}{2}\right|^2 = \tfrac{1}{4}$$

both in $R' \rightarrow P(R'_1, R'_2) = \left|\frac{1}{2}\right|^2 = \frac{1}{4}$ (same method)

so $P(R_1 R_2 \text{ or } R'_1 R'_2) = P(R_1, R_2) + P(R'_1 R'_2) = \frac{1}{4} + \frac{1}{4} = \frac{1}{2}$

c)) product of independent ground states:

$$|\Psi\rangle_1 |\Psi\rangle_2 = \frac{1}{2}\left[(|R\rangle_1 \pm |R'\rangle_1)(|R\rangle_2 + |R'\rangle_2)\right]$$

$$= \underbrace{\frac{1}{2}|R\rangle_1|R\rangle_2}_{\Phi_1} + \underbrace{\frac{1}{2}|R'\rangle_1|R'\rangle_2}_{\Phi_2} + \underbrace{\frac{1}{2}\left(\frac{1}{\sqrt{2}}(|R\rangle_1|R'\rangle_2 + |R'\rangle_1|R\rangle_2)\right)}_{\Phi_0}$$

$$= \frac{1}{2}\Phi_1 + \frac{1}{2}\Phi_2 + \frac{1}{\sqrt{2}}\Phi_0 = \frac{1}{\sqrt{2}}\Phi_0 + \frac{1}{2}(\Phi_1 + \Phi_2)$$

d)) eigenvalues of the matrix:

$$(2\varepsilon-\lambda)(2\varepsilon+u-\lambda)^2 - 4t^2(2\varepsilon+u-\lambda) = 0$$

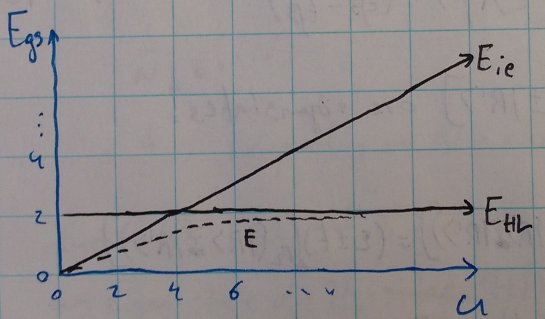
$$\rightarrow 2\varepsilon+u=\lambda \quad \vee \quad \lambda^2 + (-4\varepsilon-u)\lambda + (4\varepsilon^2 - 4t^2 + 2\varepsilon u) = 0$$

$$\lambda = 2\varepsilon+u \quad \vee \quad \lambda = \frac{4\varepsilon+u \pm \sqrt{(u^2+16t^2)}}{2}$$

$$\lambda = 2\varepsilon+u \quad \vee \quad \lambda = 2\varepsilon + \frac{1}{2}u \pm \sqrt{\frac{1}{4}u^2 + 4t^2}$$

lowest energy: $\lambda = 2\varepsilon + \frac{1}{2}u - \sqrt{\frac{1}{4}u^2+4t^2}$ → ground state energy.

$\varepsilon = t = 1$



~~E_HL good~~

$u \ll t$ → interactions much larger than tunnel prob.:
practically similar to 2 independent atoms:
total gs-energy sum of independent gs ● (HL)

$u \gg t$ → interactions much smaller than tunnel prob.:
independent electrons → gs from independent electron approx (ie)

$u \sim t$ → both (HL) and (ie) fairly poor

Week 3

3.1 $v_i = \frac{1}{\hbar}\frac{\partial E}{\partial k_i} \rightarrow \dot{v}_i = \frac{1}{\hbar}\frac{\partial}{\partial t}\left(\frac{\partial E}{\partial k_i}\right) = \frac{1}{\hbar}\sum_j \frac{\partial k_j}{\partial t}\frac{\partial^2 E}{\partial k_i \partial k_j}$

$\frac{\partial k_j}{\partial t} = -\frac{e}{\hbar}\mathcal{E}_j \rightarrow \dot{v}_i = -\sum_j \frac{1}{\hbar^2}\frac{\partial^2 E}{\partial k_i \partial k_j} e\mathcal{E}_j = -\sum_j \left(\frac{1}{m^*}\right)_{ij} e\mathcal{E}_j$

so $\dot{v}_i = -\sum_j \left(\frac{1}{m^*}\right)_{ij} e\mathcal{E}_j$ with $\left(\frac{1}{m^*}\right)_{ij} = \frac{\partial^2 E}{\partial k_i \partial k_j}$

3.2 $E(\vec{k}) = E_0 - \frac{\hbar^2 k^2}{2|m_n^*|} \rightarrow \nabla_{\vec{k}}^2 E(\vec{k}) = -\frac{\hbar^2}{|m_n^*|}$

$\vec{v} = \frac{1}{\hbar}\nabla_{\vec{k}} E(\vec{k}) \rightarrow \dot{\vec{v}} = \frac{1}{\hbar}\nabla_{\vec{k}}^2 E(\vec{k})\cdot\dot{\vec{k}} = \frac{1}{\hbar}\cdot -\frac{\hbar^2}{|m_n^*|}\cdot\frac{-e\vec{\mathcal{E}}}{\hbar}$

$\rightarrow \dot{\vec{v}} = \frac{e}{|m_n^*|}\vec{\mathcal{E}}$

3.3 $(1-f_0(k))W_{kk'}f_0(k') = \frac{e^{E(k)-E_F/kT}}{e^{E(k)-E_F/kT}+1} \cdot W_{k'k} e^{-E(k)+E(k')/kT} \cdot \frac{1}{e^{E(k')-E_F/kT}+1}$

$= \frac{1}{e^{E(k)-E_F/kT}+1} W_{k'k} \frac{e^{E(k')-E_F/kT}}{e^{E(k')-E_F/kT}+1}$

$= f_0(k) W_{k'k} (1-f_0(k'))$

so both the gain and the loss term are equal here: $\left(\frac{\partial f}{\partial t}\right)_{scatt} = \frac{V}{(2\pi)^3}\int \dot{o}\, d\vec{k}' = \emptyset$

↳ no total contribution due to scattering.

$\int o\, d\vec{k}' = 0 \rightarrow \left(\frac{\partial f}{\partial t}\right)_{scatt} = 0$

3.4 $\vec{\vec{\sigma}} = -\frac{e^2}{4\pi^3}\int \vec{v}\tau\vec{v}\frac{\partial f_0}{\partial E} d\vec{k}$

spherical coord. $\rightarrow = -\frac{e^2}{4\pi^3}\left[\int_0^\infty \frac{4}{3}\pi\tau v^2 \frac{\partial f_0}{\partial E} k^2 dk\right]\cdot\vec{\vec{I}}$

$= -\frac{e^2}{3\pi^3}\int_0^\infty \tau v^2 \frac{\partial f_0}{\partial E} k^2 dk \cdot \vec{\vec{I}}$

$\sigma = -\frac{e^2}{3\pi^3}\int_0^\infty k^2 dk\, v^2(k)\tau(k)\frac{\partial f_0}{\partial E}$

3.4 b

~~$kT \ll E_F \rightarrow f_0 = \frac{1}{e^{(E-E_F)/kT}+1} \approx \frac{1}{e^{E(k)/kT}+1}$~~

if $kT \ll E_F \rightarrow f_0(E) \approx \begin{cases} \frac{1}{e^{-\infty}+1} = 1 & E < E_F \\ \frac{1}{e^{\infty}+1} = 0 & E > E_F \end{cases}$

this is a deformed theaviside step function $\Theta(E_F - E)$

of which the derivative is $\frac{\partial \Theta(E_F-E)}{\partial E} = \delta(E_F - E) \cdot -1$

$= -\delta(E - E_F)$ ~~symmetric~~ $\delta(E-E_F) = \delta(E_F - E)$

so $\frac{\partial f_0(E)}{\partial E} \approx \frac{\partial \Theta(E_F-E)}{\partial E} = -\delta(E-E_F)$ (since $\delta(a) = \delta(-a)$)

when $kT \ll E_F$

c ~~the~~ the number of particles in the fermi-sphere can be calculated by saying:

$N = \underbrace{2}_{\text{spin}} \cdot \underbrace{\left(\frac{4}{3}\pi k_F^3\right)}_{\text{k-vol of fermi sphere}} \cdot \underbrace{\frac{V}{(2\pi)^3}}_{\text{reciprocal of volume per k-point}}$

$\hookrightarrow \frac{N}{V} = \frac{8\pi k_F^3}{3 \cdot 8\pi^3} = \frac{k_F^3}{3\pi^2}$ simple argument, done before

$\rightarrow n = \frac{k_F^3}{3\pi^2}$

d $\sigma = -\frac{e^2}{3\pi^2}\int_0^\infty k^2 dk\, v^2 \tau \frac{\partial f_0}{\partial E} = -\frac{e^2}{3\pi^2}\int_0^\infty k^2 dk \frac{\hbar^2 k^2}{m^{*2}} \tau \frac{\partial f_0}{\partial E}$

$\approx \frac{e^2}{3\pi^2}\int_0^\infty k^2 dk \frac{\hbar^2 k^2}{m^{*2}} \tau\, \delta(E - E_F)$

$= \frac{e^2}{3\pi^2}\int_0^\infty dk \cdot \frac{k^3}{m^*} \tau\, \delta(k - k_F)$

$\delta(E-E_F)\frac{dE}{dk} = \delta(k-k_F)$

$\delta(E-E_F) = \frac{m^*}{\hbar^2 k}\delta(k-k_F)$

$= \frac{e^2}{3\pi^2} \cdot \frac{k_F^3}{m^*}\tau_F = \frac{e^2 \tau_F}{m^*} n \rightarrow \sigma \approx \frac{e^2 \tau_F}{m^*} n$

(assuming • $kT \ll E_F$ • metallic free electron gas)

3.5 (a) $j_x = -\frac{e}{4\pi^3}\int \vec{v}\, f_0\, d\vec{k} - \frac{e}{4\pi^3}\int \vec{v}\cdot\vec{\mathcal{E}}\cdot\frac{e}{\hbar}\tau\frac{\partial f_0}{\partial E}\frac{\partial E}{\partial \vec{k}}\cdot d\vec{k} + \frac{e}{4\pi^3}\int |\vec{v}|^2\tau\frac{\partial f_0}{\partial T}\frac{\partial T}{\partial \vec{x}}d\vec{k}$

($\int \vec{v}\, f_0\, d\vec{k} = 0$)

$= -\frac{e^2}{4\pi^3}\cdot\frac{4}{3}\pi\int k^2 v_x^2 \mathcal{E}_x \tau\frac{\partial f_0}{\partial E}dk + \frac{e}{4\pi^3}\int |\vec{v}|^2\tau\frac{\partial f_0}{\partial T}d\vec{k}\frac{\partial T}{\partial x}$

(coord. transform; $\frac{\partial E}{\partial k} = \hbar v_x$; independent of k)

$= \sigma\left[\mathcal{E}_x + \left[\frac{e}{4\pi^3\sigma}\int |\vec{v}|^2\tau\frac{\partial f_0}{\partial T}d\vec{k}\right]\frac{\partial T}{\partial x}\right] = \sigma\left[\mathcal{E}_x + K\frac{\partial T}{\partial x}\right]$

$\longrightarrow K = \frac{e}{4\pi^3\sigma}\int |\vec{v}|^2\tau\frac{\partial f_0}{\partial T}d\vec{k}$

(b) in general: $g(\vec{k})\,d\vec{k} = D(E)\,dE$

$D(E) = \frac{2}{(2\pi)^3}\cdot 4\pi k^2\left(\frac{\partial E}{\partial k}\right)^{-1} \longrightarrow D(E)\,dE = \frac{k^2}{\pi^2}\frac{d\vec{k}}{dE}dE$

then for some function $F(E) = F(E(\vec{k}))$

$\longrightarrow \int d\vec{k}\, F(E(\vec{k})) = \int 4\pi k^2 dk\, F(E(\vec{k})) = \int 4\pi k^2\frac{dk}{dE}F(E)\,dE$

$= \int \frac{\pi^2}{k^2}4\pi k^2 F(E)D(E)dE = 4\pi^3\int F(E)D(E)\,dE$

(c) using $F(E) = \tau(E(\vec{k}))v_x^2(E(\vec{k}))\frac{\partial f_0}{\partial T}$ (only 1 of 3 dimensions)

$\hookrightarrow K = \frac{e}{4\pi^3\sigma}\cdot\int d\vec{k}\, F(E(\vec{k})) = \frac{1}{3}\frac{e}{4\pi^3\sigma}\cdot 4\pi^3\int dE\, F(E)D(E)$

$= \frac{e}{3\sigma}\int dE\,\tau(E)v^2(E)D(E)\frac{\partial f_0}{\partial T}$

(d) $\frac{\partial f_0}{\partial T} = \frac{\partial}{\partial T}\left[\left(\exp\left(\frac{E-E_F}{kT}\right)+1\right)^{-1}\right] = -\frac{1}{\left(e^{E-E_F/kT}+1\right)^2}\cdot e^{E-E_F/kT}\cdot\frac{E-E_F}{k}\cdot -\frac{1}{T^2}$

$= \frac{e^{E-E_F/kT}}{\left(e^{E-E_F/kT}+1\right)^2}\left(\frac{E-E_F}{kT}\right)\frac{1}{T}$

(e) using $\eta = \frac{E-E_F}{kT}$

$$\rightarrow K = \frac{e}{3\sigma}\int dE\left[\tau_F v_F^2 \underbrace{(E-E_F)}_{=0} D(E_F) + (E-E_F)D'(E_F)\right)\cdot \frac{\eta e^\eta}{(e^\eta+1)^2 T}\Big]$$

$$= \frac{e\tau_F v_F^2 k_B D'(E_F)}{3\sigma}\int dE \frac{\eta^2 e^\eta}{(e^\eta+1)^2} = \frac{e\tau_F v_F^2 k_B^2 D(E_F) T}{3\sigma}\underbrace{\int d\eta \frac{\eta^2 e^\eta}{(e^\eta+1)^2}}_{\text{standard integral} \rightarrow = \pi^2/3}$$

$$\hookrightarrow K = \frac{\pi^2 e \tau_F v_F^2 k_B^2 T D'(E_F)}{9\sigma}$$

(f) when the DOS is constant around E_F, an applied temperature gradient will not change the density of charge carriers and thus no current will be generated.

3.7 (a) $E = \frac{\hbar}{2m^*}\left(\frac{1}{L^2} + k_z^2\right)$

lowest subband: $\left(\frac{\pi}{L}\right)^2 + \left(\frac{\pi}{L}\right)^2 = k_F^2 \rightarrow L = \left(\frac{2\pi^2}{k_F^2}\right)$

first higher subband: $\left(\frac{\pi}{L}\right)^2 + \left(\frac{2\pi}{L}\right)^2 = k_F^2 \rightarrow L = \frac{5\pi^2}{k_F^2}$

so $\frac{2\pi^2}{k_F^2} < L < \frac{5\pi^2}{k_F^2}$ only first subband occupied

since $k_F = \sqrt[3]{3\pi^2 n} \rightarrow k_F^2 = (3\pi^2 n)^{2/3}$

$$\hookrightarrow 2\left(\frac{\pi}{3n}\right)^{2/3} < L < 5\left(\frac{\pi}{3n}\right)^{2/3}$$

(b) $\left(\frac{\pi}{3n}\right)^{2/3} = \left(\frac{\pi}{3\cdot 10^{29}}\right)^{2/3} \approx 4{,}78\cdot 10^{-20}\ m = 4{,}78\cdot 10^{-17}\ nm$

$\hookrightarrow 9{,}6\cdot 10^{-11}\ nm < L < 7{,}4\cdot 10^{-10}\ nm$ very small... probably wrong

3.8 Since in the QPC conductor part, collisions are very rare, the heat as a result of the resistance is not generated in the conductor. However, collisions are not rare in the contacts (electrodes), and as such, this is where the heat is generated as a result of the resistance. it is the only place in the system where energy can be transferred to the outside.

Week 4

1a for some vector field $\vec{F}$: $\Delta\vec{F} = \nabla(\nabla\cdot\vec{F}) - \nabla\times(\nabla\times\vec{F})$

then for $\vec{B}$:

$$\Delta\vec{B} = \nabla\underbrace{(\nabla\cdot\vec{B})}_{=0} - \nabla\times(\nabla\times\vec{B}) \overset{\text{Maxwell}}{=} -\nabla\times(\mu_0\vec{j}_s)$$

$$= -\mu_0\nabla\times\vec{j}_s \overset{\text{London}}{=} \frac{\mu_0}{\lambda_L}\vec{B}$$

so then $\Delta\vec{B} = \frac{\mu_0}{\lambda_L}\vec{B} \Rightarrow \boxed{\Delta\vec{B} - \frac{\mu_0}{\lambda_L}\vec{B} = 0}$

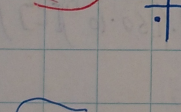
and for $\vec{j}_s$:

$$\Delta\vec{j}_s = \nabla\underbrace{(\nabla\cdot\vec{j}_s)}_{=0} - \nabla\times(\nabla\times\vec{j}_s) \overset{\text{London}}{=} -\nabla\times\left(-\frac{1}{\lambda_L}\vec{B}\right)$$

$$= \frac{1}{\lambda_L}\nabla\times\vec{B} \overset{\text{Maxwell}}{=} \frac{\mu_0}{\lambda_L}\vec{j}_s$$

so then $\Delta\vec{j}_s = \frac{\mu_0}{\lambda_L}\vec{j}_s \Rightarrow \boxed{\Delta\vec{j}_s - \frac{\mu_0}{\lambda_L}\vec{j}_s = 0}$

1b



$\vec{B}(z) = B_x(z)\vec{e}_x$

$\vec{B} = B_x^0\vec{e}_x$

$$\nabla\times\vec{B} = \left(0, \frac{\partial B_x(z)}{\partial z}, 0\right) = \frac{\partial B_x(z)}{\partial z}\vec{e}_y$$

$$\hookrightarrow \vec{j}_s = \frac{1}{\mu_0}\frac{\partial B_x(z)}{\partial z}\vec{e}_y$$ only has y-component

$$\rightarrow B_x(z) = \begin{cases} B_x(z) & \forall\ z \geq 0 \\ B_x^0 = 0 & \forall\ z \leq 0 \end{cases} \Rightarrow j_{sy}(z) = \begin{cases} \frac{1}{\mu_0}\partial_z B_x(z) & \forall\ z \geq 0 \\ 0 & \forall\ 0 \geq z \end{cases}$$

so: $\vec{j}_s = \Theta(z)\cdot\frac{1}{\mu_0}\frac{\partial B_x(z)}{\partial z}\vec{e}_y$ with Θ Heaviside's step function

1c for given IC's + BC's

as proven earlier $\rightarrow \nabla^2 B_x = \frac{\mu_0}{\lambda_L} B_x \rightarrow \frac{\partial^2 B_x}{\partial z^2} = \frac{\mu_0}{\lambda_L} B_x \rightarrow B_x = B_x^0 e^{-\sqrt{\frac{\mu_0}{\lambda_L}} z}$

$\hookrightarrow \nabla^2 j_{sy} = \frac{\mu_0}{\lambda_L} j_{sy} \rightarrow \partial_z^2 j_{sy} = \frac{\mu_0}{\lambda_L} j_{sy} \rightarrow j_{sy} = j_{sy}^0 e^{-\sqrt{\frac{\mu_0}{\lambda_L}} z}$

or: $\frac{B_x(z)}{B_x^0} = \frac{j_{sy}(z)}{j_{sy}^0} = \exp\left[-\left(\frac{\mu_0}{\lambda_L}\right)^{1/2} z\right]$

using $\left(\frac{\mu_0}{\lambda_L}\right)^{1/2} = \left(\frac{\mu_0 n_s e^2}{m}\right)^{1/2} \equiv \Lambda_L^{-1} \qquad \left(\lambda_L \equiv \frac{m}{n_s e^2}\right)$

$\hookrightarrow \begin{cases} B_x(z) = B_x^0 \exp(-z/\Lambda_L) \\ j_{sy}(z) = j_{sy}^0 \exp(-z/\Lambda_L) \end{cases}$

1d $j_{sy}(z) = j_{sy}^0 e^{-z/\Lambda_L} \rightarrow \frac{1}{\mu_0}\frac{\partial B_x(z)}{\partial z} = -\frac{1}{\mu_0 \Lambda_L} B_x^0 e^{-z/\Lambda_L}$

$\hookrightarrow \underline{j_{sy}^0 = -\frac{B_x^0}{\mu_0 \Lambda_L}}$

1e $\Lambda_L = \left(\frac{m}{\mu_0 n_s e^2}\right)^{1/2} \approx \left(\frac{9.1010^{-31}\ [kg]}{1.257 \cdot 10^{-6}\ [NA^{-2}] \cdot 10^{29}\ [m^{-3}] \cdot (1.60 \cdot 10^{-19})^2\ [C^2]}\right)^{1/2}$

[illegible] [m]

$\approx 1.68 \cdot 10^{-6}\ [m] \equiv \underline{1.68\ \mu m}$

2a using $\vec{r}_1 - \vec{r}_2 \equiv \vec{r}$ (no individual $\vec{r}_1, \vec{r}_2$ dependence, only difference)

$$-\frac{\hbar^2}{2m}\left(\nabla_1^2 + \nabla_2^2\right)\psi(\vec{r}) + V(\vec{r})\psi(\vec{r}) = (\varepsilon + 2E_F)\psi(\vec{r})$$

$\Rightarrow$ insert $\psi(\vec{r}) = \frac{1}{2V}\sum_{\vec{k}} g(\vec{k})\left[e^{i\vec{k}\cdot\vec{r}} + e^{-i\vec{k}\cdot\vec{r}}\right]$

then $(\nabla_1^2 + \nabla_2^2)\psi(\vec{r}) = -2k^2\psi(\vec{r})$ (work only on exponentials)

$$\rightarrow \frac{\hbar^2 k^2}{2mV}\sum_{\vec{k}} g(\vec{k})\left[e^{i\vec{k}\cdot\vec{r}} + e^{-i\vec{k}\cdot\vec{r}}\right] + \frac{V(\vec{r})}{2V}\sum_{\vec{k}} g(\vec{k})\left[e^{i\vec{k}\cdot\vec{r}} + e^{-i\vec{k}\cdot\vec{r}}\right] = \frac{\varepsilon + 2E_F}{2V}\sum_{\vec{k}} g(\vec{k})\left[e^{i\vec{k}\cdot\vec{r}} + e^{-i\vec{k}\cdot\vec{r}}\right]$$

take fourier transform of full eq. $\mathcal{F}[\ldots]$

$$\frac{\hbar^2 k^2}{2mV}\int \sum_{\vec{k}'} g(\vec{k}')\left[e^{-i(\vec{k}-\vec{k}')\cdot\vec{r}} + e^{-i(\vec{k}+\vec{k}')\cdot\vec{r}}\right]d\vec{r} + \frac{1}{2V}\int V(\vec{r})\sum_{\vec{k}'} g(\vec{k}')\left[e^{-i(\vec{k}-\vec{k}')\cdot\vec{r}} + e^{-i(\vec{k}+\vec{k}')\cdot\vec{r}}\right]d\vec{r}$$

$$= \frac{\varepsilon + 2E_F}{2V}\int \sum_{\vec{k}'} g(\vec{k}')\left[e^{-i(\vec{k}-\vec{k}')\cdot\vec{r}} + e^{-i(\vec{k}+\vec{k}')\cdot\vec{r}}\right]d\vec{r}$$

separate calculations:

- (1)
$$\int \sum_{\vec{k}'} g(\vec{k}')\left[e^{-i(\vec{k}-\vec{k}')\cdot\vec{r}} + e^{-i(\vec{k}+\vec{k}')\cdot\vec{r}}\right]d\vec{r} = \mathcal{F}\left[\mathcal{F}^{-1}[g(\vec{k})] + \mathcal{F}^{-1}[g(-\vec{k})]\right]$$
$$= g(\vec{k}) + g(-\vec{k}) = 2g(\vec{k}) \quad \left[g(\vec{k}) \text{ symmetric function}\right]$$

- (2)
since $V_{\vec{k}\vec{k}'} = \int V(\vec{r}) e^{-i(\vec{k}-\vec{k}')\cdot\vec{r}}\, d\vec{r} \rightarrow V(\vec{r}) = \frac{1}{V}\sum_{\vec{k}} e^{i\vec{k}\cdot\vec{r}} V_{\vec{k}\vec{k}'}$

$$\hookrightarrow \int V(\vec{r})\sum_{\vec{k}'} g(\vec{k}')\left[e^{-i(\vec{k}-\vec{k}')\cdot\vec{r}} + e^{-i(\vec{k}+\vec{k}')\cdot\vec{r}}\right]d\vec{r} = \frac{1}{V}\int \sum_{\vec{k}'} V_{\vec{k}\vec{k}'} g(\vec{k}')\left[e^{-i(\vec{k}-\vec{k}')\cdot\vec{r}} + e^{-i(\vec{k}+\vec{k}')\cdot\vec{r}}\right]d\vec{r}$$
$$= \mathcal{F}\left[\mathcal{F}^{-1}\left[\sum_{\vec{k}'} V_{\vec{k}\vec{k}'} g(\vec{k}')\right] + \mathcal{F}^{-1}\left[\sum_{\vec{k}'} V_{\vec{k}-\vec{k}'} g(-\vec{k}')\right]\right]$$
$$= \sum_{\vec{k}'}\left[V_{\vec{k}\vec{k}'} g(\vec{k}') + V_{\vec{k}-\vec{k}'} g(-\vec{k}')\right] = 2\sum_{\vec{k}'} V_{\vec{k}\vec{k}'} g(\vec{k}') \quad \left(\text{symmetry of both } g(\vec{k}) \text{ and } V_{\vec{k}\vec{k}'}\right)$$

fill back in: $\frac{\hbar^2 k^2}{mV} g(\vec{k}) + \frac{1}{V^2}\sum_{\vec{k}'} V_{\vec{k}\vec{k}'} g(\vec{k}') = \frac{\varepsilon + 2E_F}{V} g(\vec{k})$

$$\hookrightarrow \frac{\hbar^2 k^2}{m} g(\vec{k}) + \frac{1}{V}\sum_{\vec{k}'} V_{\vec{k}\vec{k}'} g(\vec{k}') = (\varepsilon + 2E_F) g(\vec{k})$$

where the summations condition $|\vec{k}'| > k_F$ is of course carried over from the initial filled in condition (4)

2b $g(\vec{k}) = \frac{V_0}{V}\frac{\sum_{\vec{k}'} g(\vec{k}')}{2E_{\vec{k}} - \varepsilon} \Longrightarrow \frac{g(\vec{k})}{\sum_{\vec{k}'} g(\vec{k}')} = \frac{V_0}{V(2E_{\vec{k}} - \varepsilon)}$

summing LHS over $\vec{k}$ gives: $\sum_{\vec{k}} \frac{g(\vec{k})}{\sum_{\vec{k}'} g(\vec{k}')} = \frac{\sum_{\vec{k}} g(\vec{k})}{\sum_{\vec{k}'} g(\vec{k}')} = 1$

$\sum_{\vec{k}'} g(\vec{k}')$ independent of $\vec{k}$

same summation but different "dummy" index

so summing full equation over $\vec{k}$ gives

$$1 = \frac{V_0}{V}\sum_{\vec{k}} \frac{1}{2E_{\vec{k}} - \varepsilon}$$ (since $\frac{V_0}{V}$ also independent of $\vec{k}$

where "$\sum_{\vec{k}'}$" is assumed over $|\vec{k}| > k_F$ such that summation spaces of $\vec{k}$ and $\vec{k}'$ match and $\sum_{\vec{k}} g(\vec{k}) = \sum_{\vec{k}'} g(\vec{k}')$ is valid.

2c $$1 = \frac{V_0}{V}\sum_{|\vec{k}|>k_F} \frac{1}{2E_{\vec{k}} - \varepsilon} \approx \frac{V_0}{(2\pi)^3}\int_{k_F}^{\infty} d^3k \frac{1}{2E_{\vec{k}} - \varepsilon} = \frac{1}{2}V_0 \int_{E_F}^{\infty} dE\, D(E)\frac{1}{2E(E) - \varepsilon}$$

$$= \frac{1}{2}V_0 \int_0^{\infty} d\xi\, D(\xi + E_F)\frac{1}{2\xi - \varepsilon} \approx \frac{1}{2}V_0 \int_0^{\hbar\omega_D} d\xi\, D(E_F)\frac{1}{2\xi - \varepsilon}$$

$\uparrow$ $\begin{cases} E_F \gg \hbar\omega_D \\ \xi \in [-\hbar\omega_D, \hbar\omega_D] \text{ from phonon theory} \end{cases}$

$$1 = V_0 Z(E_F)\int_0^{\hbar\omega_D} d\xi \frac{1}{2\xi - \varepsilon} \quad \text{with } Z(E_F) = \frac{1}{2}D(E_F)$$

2d $$\int_0^{\hbar\omega_D} \frac{1}{2\xi - \varepsilon} d\xi = \left[\frac{1}{2}\ln(2\xi - \varepsilon)\right]_0^{\hbar\omega_D} = \frac{1}{2}\ln\left(\frac{2\hbar\omega_D - \varepsilon}{-\varepsilon}\right) = \frac{1}{2}\ln\left(1 - \frac{2\hbar\omega_D}{\varepsilon}\right)$$

$$\rightarrow \frac{1}{2}\ln\left(1 - \frac{2\hbar\omega_D}{\varepsilon}\right) = \frac{1}{V_0 Z(E_F)} \rightarrow \frac{2\hbar\omega_D}{\varepsilon} = 1 - \exp\left(2/V_0 Z(E_F)\right)$$

$$\rightarrow \varepsilon = \frac{2\hbar\omega_D}{1 - \exp\left(2/V_0 Z(E_F)\right)}$$

2e $\psi(\vec{r}) \propto \frac{1}{V}\sum_{\vec{k}}\sum_{\vec{k}'}\frac{g(\vec{k}')}{2\xi_{\vec{k}}-\varepsilon}\cos(\vec{k}'\cdot\vec{r}) \propto \frac{1}{V}\sum_{\vec{k}}\frac{\cos(\vec{k}\cdot\vec{r})}{2\xi_k-\varepsilon}$

($\sum_{\vec{k}'} g(\vec{k}')$ is independent of the sum constant w.r.t. $\vec{k}$.)

$$\psi(\vec{r}) \sim \frac{1}{V}\int_{|k|\geq k_F} d\vec{k}\,\frac{\cos(\vec{k}\cdot\vec{r})}{2\xi_k-\varepsilon} = \frac{1}{V}\int_{k_F}^{\infty}\int d\Omega\, dk\cdot k^2\frac{\cos(kr\cos\Omega)}{2\xi_k-\varepsilon}$$

$$\psi(\vec{r}) \propto \int\int d\Omega\, dk\cdot k^2\frac{\cos(kr\cdot\cos\Omega))}{2\xi_k-\varepsilon} \propto \int_{k_F}^{\infty} dk\,\frac{k^2}{kr}\frac{\sin(kr)}{2\xi_k-\varepsilon}$$

$$\hookrightarrow \psi(r) \propto \frac{1}{r}\int_{k_F}^{\infty} dk\,\frac{k}{2\xi_k-\varepsilon}\sin(kr)$$

• through spherical coordinate integration

3a $W_{BCS} = 2\sum_k v_k^2\xi_k - \frac{V_0}{V}\sum_k\sum_{k'} v_k u_k v_{k'} u_{k'}$

$v_k = \cos\theta_k$, $u_k = \sin\theta_k$

$$\hookrightarrow W_{BCS} = 2\sum_k \cos^2\theta_k\cdot\xi_k - \frac{V_0}{V}\sum_k\sum_{k'}\cos\theta_k\sin\theta_k\cos\theta_{k'}\sin\theta_{k'}$$

$\cos\theta\cdot\sin\theta = \frac{1}{2}\sin(2\theta)$ [trig identity]

$$\hookrightarrow W_{BCS} = 2\sum_k \cos^2\theta_k\,\xi_k - \frac{1}{4}\frac{V_0}{V}\sum_k\sum_{k'}\sin(2\theta_k)\sin(2\theta_{k'})$$

3b take $\frac{\partial W_{BCS}}{\partial\theta_k} = 0$ for finding minimum

$$\hookrightarrow \frac{\partial W_{BCS}}{\partial\theta_k} = 4\cos\theta_k\sin\theta_k\,\xi_k - \frac{V_0}{V}\cdot\cos(2\theta_k)\sum_{k'}\sin(2\theta_{k'}) = 0$$

$$\hookrightarrow 2\frac{\sin(2\theta_k)}{\cos(2\theta_k)}\cdot\xi_k = -\frac{V_0}{V}\sum_{k'}\sin(2\theta_{k'})$$

$$\hookrightarrow \tan(2\theta_k)\cdot\xi_k = -\frac{1}{2}\frac{V_0}{V}\sum_{k'}\sin(2\theta_{k'})$$

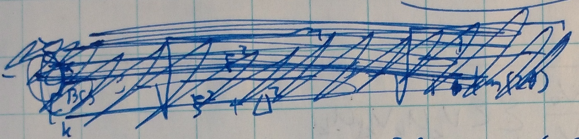
$$\hookrightarrow \xi_k\tan(2\theta_k) = -\frac{1}{2}\frac{V_0}{V}\sum_{k'}\sin(2\theta_{k'})$$

3c (14.a) using $\Delta = -\frac{1}{2}\frac{V_0}{V}\sum_k \sin(2\theta_k) = \frac{1}{2}\frac{V_0}{V}\sum_{k'} \sin(2\theta_{k'})$ (just change in name of index.)

↳ (12) becomes $\xi_k \tan(2\theta_k) = -\Delta \rightarrow \tan(2\theta_k) = -\Delta/\xi_k$

(14.b) $$\frac{\Delta}{E_k^{BCS}} = \sqrt{\frac{\Delta^2}{\xi^2+\Delta^2}} = \sqrt{\frac{1}{\frac{1}{\tan^2 2\theta}+1}} = \sqrt{\frac{1}{\frac{\cos^2 2\theta}{\sin^2 2\theta}+\frac{\sin^2 2\theta}{\sin^2 2\theta}}} = \sqrt{\frac{1}{\left(\frac{1}{\sin^2(2\theta)}\right)}}$$

$$= \sqrt{\sin^2(2\theta_k)} = \sin(2\theta_k)$$

(14.c) 

$$V_k^2 - U_k^2 = \cos^2\theta_k - \sin^2\theta_k = \cos(2\theta_k) = \frac{\sin(2\theta_k)}{\tan(2\theta_k)}$$

$$= \frac{\Delta/E_k^{BCS}}{-\Delta/\xi_k} = -\xi_k/E_k^{BCS}$$

3d $$W_k \equiv V_k^2 = \frac{1}{2}\left(V_k^2 + V_k^2 + U_k^2 - U_k^2\right) = \frac{1}{2}\left(\overbrace{V_k^2+U_k^2}^{=1} + \overbrace{V_k^2-U_k^2}^{=-\xi_k/E_k^{BCS}}\right)$$

$$= \frac{1}{2}\left(1 - \frac{\xi_k}{E_k^{BCS}}\right) = \frac{1}{2}\left(1 - \frac{\xi_k}{\sqrt{\xi_k^2+\Delta^2}}\right)$$

3f if $V_k^2 = \frac{1}{2}\left(1 - \frac{\xi_k}{E_k^{BCS}}\right) \rightarrow U_k^2 = 1 - V_k^2 = \frac{1}{2}\left(\frac{\xi_k}{E_k^{BCS}} + 1\right)$

so then $$\Delta = \frac{V_0}{V}\sum_k \left[\frac{1}{4}\left(1 - \frac{\xi_k}{E_k^{BCS}}\right)\left(1 + \frac{\xi_k}{E_k^{BCS}}\right)\right]^{1/2}$$

$$\Delta = \frac{1}{2}\frac{V_0}{V}\sum_k \left[1 - \left(\frac{\xi_k}{E_k^{BCS}}\right)^2\right]^{1/2}$$

$$\Delta = \frac{1}{2}\frac{V_0}{V}\sum_k \left[\frac{E_{BCS}^2 - \xi_k^2}{(E_k^{BCS})^2}\right]^{1/2} = \frac{1}{2}\frac{V_0}{V}\sum_k \left[\frac{\Delta^2}{E_k^{BCS\,2}}\right]^{1/2}$$

$$\Delta = \frac{1}{2}\frac{V_0}{V}\sum_k \frac{\Delta}{\sqrt{\xi_k^2+\Delta^2}}$$

3g $\Delta = \frac{1}{2}\frac{V_0}{V}\sum_k \frac{\Delta}{\sqrt{\xi_k^2+\Delta^2}} = \frac{1}{2}\frac{V_0}{(2\pi)^3}\int_0^\infty d\vec{k}\ \frac{\Delta}{\sqrt{\xi_k^2+\Delta^2}}$

$= \frac{1}{4}V_0\int_0^\infty d\epsilon\, D(\epsilon)\frac{\Delta}{\sqrt{\xi_k^2+\Delta^2}} = \frac{1}{4}V_0\int_{-E_F}^\infty d\xi\, D(\xi+E_F)\frac{\Delta}{\sqrt{\xi_k^2+\Delta^2}}$

$E_F \gg \hbar\omega_D$, $\xi \in [-\hbar\omega_D, \hbar\omega_D]$

$\approx \frac{1}{4}V_0\int_{-\hbar\omega_D}^{\hbar\omega_D} d\xi\, D(E_F)\frac{\Delta}{\sqrt{\xi^2+\Delta^2}} = V_0 Z(E_F)\frac{1}{2}\int_{-\hbar\omega_D}^{\hbar\omega_D}\frac{\Delta}{\sqrt{\xi^2+\Delta^2}}d\xi$

3h $\int_{-\hbar\omega_D}^{\hbar\omega_D}\frac{\Delta}{\sqrt{\xi^2+\Delta^2}}d\xi = \Delta\ln\left(\frac{\sqrt{(\hbar\omega_D)^2+\Delta^2}+\hbar\omega_D}{\sqrt{(\hbar\omega_D)^2+\Delta^2}-\hbar\omega_D}\right) = \frac{2\Delta}{V_0 Z}$

$\ln\left(\sqrt{\left(\frac{\hbar\omega_D}{\Delta}\right)^2+1}+\frac{\hbar\omega_D}{\Delta}\right) - \ln\left(\sqrt{\left(\frac{\hbar\omega_D}{\Delta}\right)^2+1}-\frac{\hbar\omega_D}{\Delta}\right) = \frac{2}{V_0 Z}$

using mathematica: correct!

$\Delta = \frac{\hbar\omega_D}{\sinh(1/V_0 Z)}$

4a

$$W_{BCS} = 2\sum_{\vec{k}} \xi_{\vec{k}} \cos^2\theta_{\vec{k}} - \underbrace{\left[\frac{1}{2}\frac{V_0}{V}\sum_{\vec{k}} \sin(2\theta_{\vec{k}})\right]}_{\Delta}\underbrace{\left[\frac{V}{V_0}\left[\frac{1}{2}\frac{V_0}{V}\sum_{\vec{k}'} \sin(2\theta_{\vec{k}'})\right]\right]}_{\Delta}$$

$\cos^2\theta_{\vec{k}} = V_{\vec{k}}^2 = \frac{1}{2}\left(1 - \frac{\xi_{\vec{k}}}{E_{\vec{k}}^{BCS}}\right)$ as in Rk. 3D

$$\hookrightarrow W_{BCS}^0 = \sum_{\vec{k}} \xi_{\vec{k}}\left(1 - \frac{\xi_{\vec{k}}}{E_{\vec{k}}^{BCS}}\right) - \frac{V}{V_0}\Delta^2$$

4b

$$W_{BCS}^0 = 2\sum_{\vec{k}} \xi_{\vec{k}} V_{\vec{k}}^2 - \frac{V}{V_0}\Delta^2 = 2\sum_{|\vec{k}|<k_F} \xi_{\vec{k}} V_{\vec{k}}^2 + 2\sum_{|\vec{k}|>k_F} \xi_{\vec{k}} V_{\vec{k}}^2 - \frac{V}{V_0}\Delta^2$$

($V_{\vec{k}}^2 = 1 - U_{\vec{k}}^2$)

$$= 2\sum_{|\vec{k}|<k_F} \xi_{\vec{k}}(1 - U_{\vec{k}}^2) + 2\sum_{|\vec{k}|>k_F} \xi_{\vec{k}} V_{\vec{k}}^2 - \frac{V}{V_0}\Delta^2$$

$$= 2\sum_{|\vec{k}|<k_F} \xi_{\vec{k}} - 2\sum_{|\vec{k}|<k_F} \xi_{\vec{k}} U_{\vec{k}}^2 + 2\sum_{|\vec{k}|>k_F} \xi_{\vec{k}} V_{\vec{k}}^2 - \frac{V}{V_0}\Delta^2$$

5a

$$\Delta = V_0 Z(E_F)\int_0^{\hbar\omega_D} \frac{\Delta}{\sqrt{\xi^2+\Delta^2}}\left[1 - 2f_0\left(\sqrt{\xi^2+\Delta^2} + E_F, T\right)\right] d\xi$$

$$= V_0 Z(E_F)\int_0^{\hbar\omega_D} \frac{\Delta}{\sqrt{\xi^2+\Delta^2}}\left[1 - \frac{2}{\exp\left(\frac{\sqrt{\xi^2+\Delta^2}}{k_BT}\right)+1}\right] d\xi$$

$$= V_0 Z(E_F)\int_0^{\hbar\omega_D} \frac{\Delta}{\sqrt{\xi^2+\Delta^2}}\left[\frac{\exp\left(\frac{\sqrt{\xi^2+\Delta^2}}{kT}\right) - 1}{\exp\left(\frac{\sqrt{\xi^2+\Delta^2}}{kT}\right)+1}\right] d\xi$$

$$= V_0 Z(E_F)\int_0^{\hbar\omega_D} \Delta \frac{1}{\sqrt{\xi^2+\Delta^2}} \tanh\left(\frac{1}{2}\frac{\sqrt{\xi^2+\Delta^2}}{kT}\right) d\xi$$

since Δ independent of ξ, take outside of $\int$ and divide out:

$$1 = V_0 Z(E_F)\int_0^{\hbar\omega_D} \frac{\tanh\left(\frac{1}{2}\sqrt{\xi^2+\Delta^2}/k_BT\right)}{\sqrt{\xi^2+\Delta^2}} d\xi$$

5b $\Delta=0 \rightarrow 1 = V_0 Z(E_F) \int_0^{\hbar\omega_0} \frac{\tanh(\xi/2kT)}{\xi} d\xi$

$$1 = V_0 Z(E_F) \int_0^{\hbar\omega_0/2kT} \frac{\tanh(x)}{x} dx$$

$$1 = V_0 Z(E_F) \left[\underbrace{\int_0^N \frac{\tanh(x)}{x} dx}_{\text{solve numerically for Large } N < \hbar\omega_0/2kT \rightarrow \text{can do b.c. for } X \gtrsim 10 : \tanh(x) \simeq 1 \text{ call A}} + \int_N^{\hbar\omega_0/2kT} \frac{dx}{x} \right]$$

$$1 = V_0 Z(E_F) \left[\underbrace{A}_{\text{call B for simplicity}} - \ln(N) + \ln\left(\frac{\hbar\omega_B}{2kT}\right) \right]$$

$$\hookrightarrow \ln\left(\frac{\hbar\omega_D}{2kT}\right) = \frac{1}{V_0 Z(E_F)} - B \rightarrow k_B T = \frac{\hbar\omega_D}{2 \exp\left(\frac{1}{V_0 Z(E_F)} - B\right)}$$

so then $k_B T_c = \frac{1}{2} e^B \hbar\omega_D e^{-1/V_0 Z(E_F)}$

where $\frac{1}{2} e^B = \frac{1}{2} \exp\left[\int_0^N \frac{\tanh(x)}{x} dx - \ln(N)\right]$

mathematica: $\frac{1}{2} e^B \approx 1.1338\ldots$ for $N \approx 10$

$$\hookrightarrow k_B T_c \simeq 1.14 \cdot \hbar\omega_D \exp\left(-\frac{1}{V_0 Z(E_F)}\right)$$

6a $\iint_\Sigma \nabla \times \vec{H} \cdot d\vec{S} = \oint_{\partial\Sigma} \vec{H} \cdot d\vec{r} = \iint_\Sigma \vec{j} \cdot d\vec{S}$

for wire with radius R and Σ = cross-section of the wire

$\rightarrow \oint_{\partial\Sigma} \vec{H} \cdot d\vec{r} = 2\pi R \cdot H$ and $\iint_\Sigma \vec{j} \cdot d\vec{S} = \iint_{\text{cross section}} \vec{j} \cdot d\vec{S}$

so then $H = \frac{1}{2\pi R} \iint_{\text{cross section}} \vec{j}_s \cdot d\vec{S}$ (where $\vec{j} = \vec{j}_s$ for semiconductor)

$= \frac{V}{R} \cdot -\Lambda_L \left[(\Lambda_L + z) e^{-\frac{z}{\Lambda_L}} \right]$

since $R \gg \Lambda_L$ generally

(6b) $H = \frac{1}{2\pi R} \iint_S \vec{j}_s \cdot d\vec{S} \approx \frac{2\pi}{2\pi R} \int_{-\Lambda_L}^{0} j^\circ e^{-z/\Lambda_L} \cdot R\, dz$

$= j^\circ \cdot -\Lambda_L \left[e^{-z/\Lambda_L} \right]_{-\Lambda_L}^{0} = -j^\circ \Lambda_L \left[1 - e \right]$

$= j^\circ \Lambda_L \left[e^1 - 1 \right] \approx j^\circ \Lambda_L$

(6c) $H = \Lambda_L j^\circ = \sqrt{\frac{m}{\mu_0 n_s e^2}} \cdot \frac{n_s e \sqrt{\Delta}}{\sqrt{2m}} = \sqrt{\frac{m n_s^2 e^2 \Delta}{2 m n_s e^2 \mu_0}} = \sqrt{\frac{n_s \Delta}{2\mu_0}}$

$= \frac{1}{\sqrt{2\mu_0}} \sqrt{n_s \Delta}$

Week 5

5.1 (1) a)

$$\begin{cases} E = \dfrac{\hbar^2 k^2}{2m} \rightarrow \dfrac{dE}{dk} = \dfrac{\hbar^2 k}{m} \\ k = \sqrt{\dfrac{2mE}{\hbar^2}} \rightarrow dk = \sqrt{\dfrac{m}{2\hbar^2 E}}\, dE \end{cases}$$

$$\Rightarrow \underline{g(\vec{k})\, d\vec{k} = D(E)\, dE}$$

3D: $g(\vec{k})\, d\vec{k} = \frac{1}{\pi^2} k^2 dk \rightarrow g(E)dE = \frac{1}{\pi^2} k^2 dk = \frac{1}{\pi^2} \cdot \frac{2mE}{\hbar^2} dk$

$$g(E)_{3D} = \frac{1}{\pi^2} \frac{2mE}{\hbar^2} \frac{dk}{dE} = \frac{1}{\pi^2} \frac{2mE}{\hbar^2} \sqrt{\frac{m}{2\hbar^2 E}} = \frac{1}{2\pi^2} \left(\frac{2m}{\hbar^2}\right)^{3/2} \sqrt{E}$$

2D: $g(\vec{k})\, d\vec{k} = \frac{2}{(2\pi)^2} \cdot 2\pi k\, dk = \frac{1}{\pi} \sqrt{\frac{2mE}{\hbar^2}} \cdot dk$

$$g(E)dE = g(\vec{k})\, d\vec{k} = \frac{1}{\pi} \sqrt{\frac{2mE}{\hbar^2}}\, dk \rightarrow g(E) = \frac{1}{\pi} \sqrt{\frac{2mE}{\hbar^2}} \frac{dk}{dE}$$

$$\rightarrow g(E)_{2D} = \frac{1}{\pi} \sqrt{\frac{2mE}{\hbar^2}} \cdot \sqrt{\frac{m}{2\hbar^2 E}} = \frac{1}{\pi} \cdot \frac{m}{\hbar^2} = \underline{\frac{m}{\pi\hbar^2}}$$

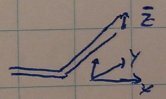
1D $g(\vec{k})\, d\vec{k} = g(E)\, dE = \frac{2}{2\pi} dk = \frac{2}{2\pi} \sqrt{\frac{m}{2\hbar^2 E}}\, dE$

$$\hookrightarrow g(E)_{1D} = \sqrt{\frac{m}{2\hbar^2 \pi^2}} \cdot E^{-1/2}$$

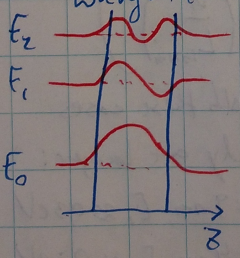
b)

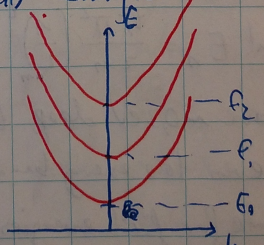
assume infinitely deep quantum well

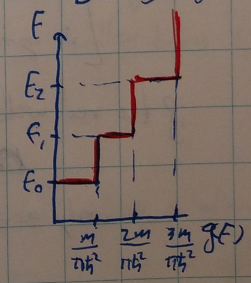
for **2D**: system wedged between 2 surfaces



wavefunctions (in 2D well) | energies | DOS $g(E)_{2D}$







Standard Well-type Ψ's

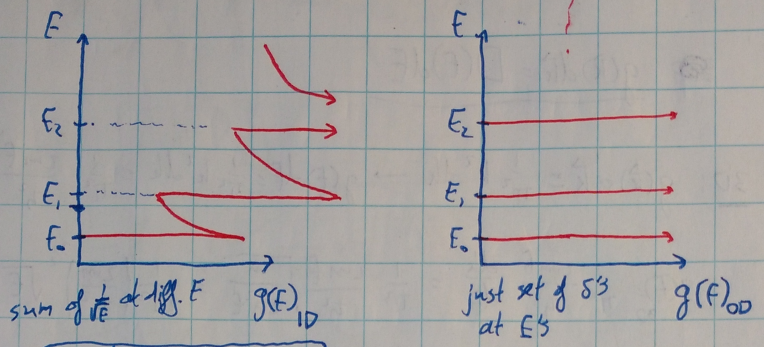
free electrons basically ↳ parabolic dispersions, multiple discrete ones due to discretization

DOS is $\frac{m}{\pi\hbar^2}$ per band. at higher energies: multiple bands so $\frac{m}{\pi\hbar^2}$ multiple times

! $E_2 - E_1$ is larger than $E_1 - E_0$, might not be clear from drawing...

1) C) 1D DOS is $g(E) \propto \frac{1}{\sqrt{E}}$

0D DOS is $g(E) \propto \delta(E)$



basically $g(E) = \sum_n g(E_n)$

total $\begin{cases} g_{1D}(E) = N \sum_n (E - E_n)^{-1/2} & \text{for all } E_n < E \\ g_{0D}(E) = N \sum_n \delta(E - E_n) \end{cases}$

d) $E_n = \frac{\hbar^2}{2m} k_n^2$ with L = width of well, $k_n = \frac{\pi}{L} n$

↳ $E_0 = 0$, $E_1 = \frac{\hbar^2}{2m}\left(\frac{\pi}{L}\right)^2$, $E_2 = \frac{\hbar^2}{2m}\left(\frac{2\pi}{L}\right)^2$ ... $E_n = \frac{\hbar^2}{2m}\left(\frac{n\pi}{L}\right)^2$

$L = 9\,nm \rightarrow$ $E_0 = 0\,eV$, $E_1 \approx 0{,}07\,eV$, $E_2 \approx 0{,}28\,eV$

$L = 4\,nm \rightarrow$ $E_0 = 0\,eV$, $E_1 \approx 0{,}35\,eV$, $E_2 \approx 1{,}4\,eV$

$\left[\text{in general } E_n = \frac{\hbar^2 \pi^2}{2m}\left(\frac{n}{L}\right)^2_{nm} \approx 5{,}61\left(\frac{n}{L_{in\,nm}}\right)^2\right]$

if the real wells are $\sim 0{,}3\,eV$ deep, then in both these cases even low energy bands already are larger:

only accurate for first energies (at $L = 9\,nm$, $E_2 \approx 0{,}3\,eV$; at $L = 4\,nm$, $E_1 \approx 0{,}3\,eV$)

not that accurate

e) energies of these holes follows same eq. $E_n = \frac{\hbar^2}{2m^*}\left(\frac{n\pi}{L}\right)^2$ but different masses.

		E_0	E_1	E_2
$L = 9$ nm	m_{hh}:	0 eV	9 meV	37 meV
	m_{Lh}:	0 eV	57 meV	0,23 eV
$L = 4$ nm	m_{hh}:	0 eV	47 meV	0,19 eV
	m_{Lh}:	0 eV	0,29 eV	1,15 eV

for these holes, all energies on the first 2 energy levels are lower for the heavy holes (except $L = 4$ nm, $E_2 \approx 0,2$ eV). however, for the light holes, energies are outside the 0,2 eV real quick as well (like for electrons). So the infinitely deep well model is only valid for low energy levels (only a few levels before continuum conditions are reached).

---

2) a) for the 9 nm well, a photon with $\lambda = 790$ nm $\leftrightarrow E = \frac{1,2398}{0,79} = 1,57$ eV is emitted. Assuming the exciton binding energy is approx.

$R^* = \frac{R}{m_0 \varepsilon_r^2}\left(\frac{1}{m_e^*} + \frac{1}{m_h^*}\right) \approx$ 5 meV.

Looking at the energy difference between electron and hole, plus the exciton binding energy, the predicted energy would be $70 + 9 + 5 = 84$ meV which is much smaller than 1,57 eV. (for the lowest bandgap).

So not a very good approx.

b) the peak at (e) could be the result of a photon emission from a higher energy level within a band. Instead of emmission by recombination in the first energy band, it could happen from the second. It could also be a decay to the split-off band, rather than the valence band.

(3) a)

$$V_T = \frac{V_b}{e} - \frac{eN_d d(d+2c)}{2\varepsilon_0 \varepsilon_b}$$

$V_b = 0{,}7\,eV$, $N_D = 1{,}35 \cdot 10^{24}\,m^{-3}$, $n_{2DEG} = 3 \cdot 10^{15}\,m^{-2}$, $V_g = 0{,}2\,V$

$\varepsilon_b = 13{,}2$ for GaAs

$$V_T = 0{,}7 - \frac{1{,}6 \cdot 10^{-19} \cdot 1{,}35 \cdot 10^{24} \cdot 10(30) \cdot 10^{-9} \cdot 10^{-3}}{2 \cdot 13{,}2 \cdot 8{,}85 \cdot 10^{-12}}$$

$$\approx 0{,}7 - 0{,}28 = 0{,}42\,V$$

so the threshold voltage will be around ~0,4V

b) $$n_{2D} = \frac{\varepsilon_0 \varepsilon_b}{e} \frac{-V_T}{c+d+s+\frac{1}{4}a_b+h} = \frac{-V_T C_G}{e}$$

using $h \sim 8{,}5\,nm$ ↳ $$C_G = \frac{\varepsilon_0 \varepsilon_b}{c+d+s+\frac{1}{4}a_b+h} = \frac{13{,}2 \cdot 10^{-12} \cdot 8{,}85}{10^{-3}(10+10+10+\frac{1}{4} \cdot 10 + 7{,}5)}$$

$$= 2{,}9\,mF$$

so then $$n_{2D} = \frac{0{,}9 \cdot 2{,}9 \cdot 10^{-3}}{1{,}6 \cdot 10^{-19}} \approx 7{,}7 \cdot 10^{15}\,m^{-2}$$

c) the fraction that left to the 2DEG $= \frac{n_{2D} - n_{2DEG}}{N_D} = \frac{4{,}7 \cdot 10^{15}}{1{,}35 \cdot 10^{24}}$

$$= 3{,}5 \cdot 10^{-9}$$

5.2 (1) a) $\frac{1}{2} m C_{rms}^2 = k_B T$, $\bar{c} = \sqrt{\frac{16 k_B T}{3\pi m}}$

$n = \frac{P}{k_B T} \rightarrow F = \frac{1}{4} n \bar{c}$

↳ $F = \sqrt{\frac{P^2}{3\pi m k_B T}} = \frac{1}{\xi A_{molecule} t_{bg}} \rightarrow t_{bg} = \frac{1}{\xi A_{molecule} F}$

↳ $t_{bg} = \frac{1}{\xi A_{molecule}} \sqrt{\frac{3\pi m k_B T}{P^2}} \approx \frac{1}{(100 \cdot 10^{-12})^2} \sqrt{\frac{3 \cdot \pi \cdot 3{,}3 \cdot 10^{-27} \cdot 4 \cdot 10^{-21}}{(5 \cdot 10^{-11})^2}}$

$\approx 3 \cdot 10^0$ s

b) in this case $n = \frac{P}{k_B T} \approx 3 \cdot 10^{13}$ m^{-2} in the cell,

and $\bar{c} = \sqrt{\frac{P}{3\pi}} \cdot \sqrt{\frac{3 k_B T}{m}} \approx$ 599 ms^{-1}

so then the average flux is $F_{av} = \frac{1}{4} \bar{c} n = 4{,}6 \cdot 10^{15}$

$\rightarrow F_{GA} = 2 F_{av} \approx 9{,}24 \cdot 10^{15}$

↳ $t_{ML} = \frac{1}{A_{molecule} F} = \frac{1}{(210 \cdot 10^{-12})^2 \cdot 9{,}24 \cdot 10^{15}} = 2453$ s

$t_{1\mu m} = t_{ML} \cdot \frac{1\mu m}{a} = t_{ML} \cdot \frac{10000 \text{ Å}}{5{,}65 \text{ Å}} = 4{,}3 \cdot 10^6$ s

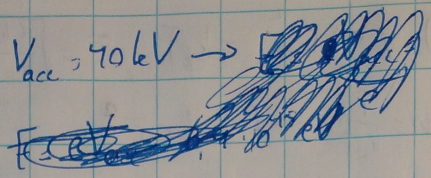
c) $\frac{t_{ML}}{t_{bg}} = \frac{2453}{3 \cdot 10^{10}} \approx 8 \cdot 10^{-8}$

d) $L = \frac{1}{\pi d^2 n}$

$L_{bg} = \frac{1{,}38 \cdot 10^{-23} \cdot 293}{\pi (100 \cdot 10^{-12})^2 \cdot 5 \cdot 10^{-14}} = 2{,}57 \cdot 10^{12}$ m

$L_{ML} = \frac{1{,}38 \cdot 10^{-23} \cdot 1193}{\pi (210 \cdot 10^{-12})^2 \cdot 5 \cdot 10^{-7}} = 2{,}3 \cdot 10^5$ m

both much larger than 200 mm...

(2) a) $\lambda = \frac{h}{p}$ $V_{acc} = 40\,kV \rightarrow$  $E = 40\,keV$

$\lambda = \frac{hc}{E}$

$\lambda = 3 \cdot 10^{-11}\,m = 0{,}03\,nm = 0{,}3\,Å$

c) both techniques do give surface information, as it is dependant on the structure on the surface rather then the bulk properties.

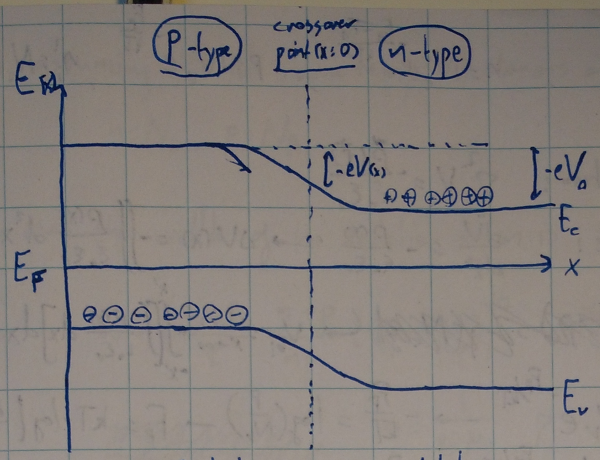
(3) the unit cell consists of the $-3\vec{a} + \vec{b}$ and $4\vec{a} + 6\vec{b}$

$\hookrightarrow \begin{pmatrix} -3 & x \\ 3 & \end{pmatrix}$

this is obtained by just counting the unit vectors in either direction.

week 61

excercise 1a)



excess of electrons | excess of holes

↓

electrons diffuse from p → n

due to electron/hole density difference in the depletion region, a charge density in this region is created, giving rise to an E-field. this causes an electron current from n → p.

under forward bias, the energy difference between the p- and n-type sides decreases (and so does the depletion region) due to the applied voltage. this increases the particle flow towards the depletion region (since drift due to the ~~field~~ energy difference decreases, favoring diffusion) where electrons and holes recombine.

under reverse bias, the energy difference between the materials increases due to the applied voltage. because of this, diffusion is damped due to the high energy necessary to cross the depletion region.

this means that under forward bias, current through the junction increases, while it is heavily suppressed in reverse bias. this means they are very suitable for transistors, since this directionality is exactly what transistors are required to do.

a typical I-V curve looks as follows:



1b)

$eV_{bi} = F_n - F_p$, $n = N_c e^{-\frac{E_g - F_n}{kT}}$, $p = N_v e^{-\frac{F_p}{kT}}$, $n_i^2 = N_c N_v e^{-\frac{E_g}{kT}}$

poisson's equation: $\nabla^2 V = -\frac{\rho(\vec{r})}{\varepsilon_0 \varepsilon_r}$

1D device: $\frac{d^2V}{dx^2} = -\frac{\rho(x)}{\varepsilon_0 \varepsilon_r} \rightarrow \Delta V(x) = -\iint \frac{\rho(x)}{\varepsilon_0 \varepsilon_r} d^2x$

$\hookrightarrow V_{bi} = \lim_{x' \to \infty} -\int_{-x'}^{x'} \left[\int \frac{\rho(x)}{\varepsilon_0 \varepsilon_r} dx \right] dx$

using $p = N_v e^{-F_p/kT} \rightarrow -\frac{F_p}{kT} = \log\left(\frac{p}{N_v}\right) \rightarrow F_p = kT \cdot \log\left(\frac{N_v}{p}\right)$

also, $\frac{n}{n_i^2} = \frac{1}{N_v} e^{F_n/kT} \rightarrow \frac{F_n}{kT} = \log\left(N_v \frac{n}{n_i^2}\right) \rightarrow F_n = kT \log\left(N_v \frac{n}{n_i^2}\right)$

such that $eV_{bi} = F_n - F_p = kT\left[\log\left(N_v \frac{n}{n_i^2}\right) - \log\left(\frac{N_v}{p}\right)\right]$

$= kT\left[\log\left(N_v \frac{n}{n_i^2} \cdot \frac{p}{N_v}\right)\right] = kT\left[\log\left(\frac{np}{n_i^2}\right)\right]$

$\rightarrow V_{bi} = \frac{kT}{e} \log\left(\frac{np}{n_i^2}\right)$

[illegible]

in bulk for silicon: resistivity $= 2{,}3 \cdot 10^3\ \Omega m$ (at room temp)

↳ (Wikipedia) and $\rho^{-1} = \sigma = ne\mu_n$ V $\sigma = pe\mu_p$

then $n = \frac{1}{e\rho\mu_n}$, $p = \frac{1}{e\rho\mu_p} = \frac{3.1}{e\rho\mu_n}$

such that $V_{bi} = \frac{kT}{e} \log\left(\frac{1}{e^2\rho^2\mu_n\mu_p n_i^2}\right) = \frac{kT}{e} \log\left(\frac{3.1}{e^2\rho^2\mu_n^2 n_i^2}\right)$

filling in gives $\frac{1{,}38 \cdot 10^{-23} \cdot 293{,}15}{1{,}60 \cdot 10^{-19}} \ln\left[\frac{3.1}{(1.60 \cdot 10^{-19} \cdot 2{,}3 \cdot 10^3 \cdot 1{,}4 \cdot 10^{-1} \cdot 1{,}05 \cdot 10^{15})^2}\right]$

↳ $V_{bi} \simeq 0{,}05967\ldots V \approx 0{,}06\ V$

(using a bulk resistivity for silicon at 20°C of $\rho_{Si} = 2{,}3 \cdot 10^3\ \Omega m$)

c) assuming that at room temp, all donors and acceptors are ionized:

$n = N_D$, $p = N_A$

then the width of the depletion region is

$$W = \left(\frac{2 \varepsilon_0 \varepsilon_{Si}}{q} \frac{n+p}{np} (V_{bi} - V_{app}) \right)^{1/2}$$ with V_{app} the applied voltage.

~~$\frac{n+p}{np}$~~ $n = \frac{1}{e \rho \mu_n}$, $p = \frac{3,1}{e \rho \mu_n}$

$$\Rightarrow W(V) = \left(\frac{2 \varepsilon_0 \varepsilon_{Si}}{q} \cdot e \rho \mu_n \frac{4,1}{3,1} \cdot (V_{bi} - V) \right)^{1/2}$$

for all previous values

$$W(V) \approx \left(\frac{2 \cdot 8,854 \cdot 10^{-12} \cdot 11,9}{1,6 \cdot 10^{-19}} \cdot 1,6 \cdot 10^{-19} \cdot 2,3 \cdot 10^{3} \cdot 1,4 \cdot 10^{-1} \cdot \frac{4,1}{3,1} (0,06 - V) \right)^{1/2}$$

$$\approx \left(8,97 \cdot 10^{-8} \cdot (0,06 - V) \right)^{1/2}$$

$\rightarrow$ $W(-10V) \approx 9,5 \cdot 10^{-4}$ m

$W(+0,3V) \approx 1,47 \cdot 10^{-4}\, i$ m complex!!!! (pure imaginary actually...)

---

d) Capacity follows $C = \frac{\varepsilon_0 \varepsilon_{Si} S}{4 \pi W}$

for the real-valued distance:

$$C(-10V) \approx \frac{8,854 \cdot 10^{-12} \cdot 11,9 \cdot 0,1 \cdot 10^{-4}}{4 \cdot 3,1415 \cdot 9,5 \cdot 10^{-4}} \approx 8,8 \cdot 10^{-14} \text{ F}$$

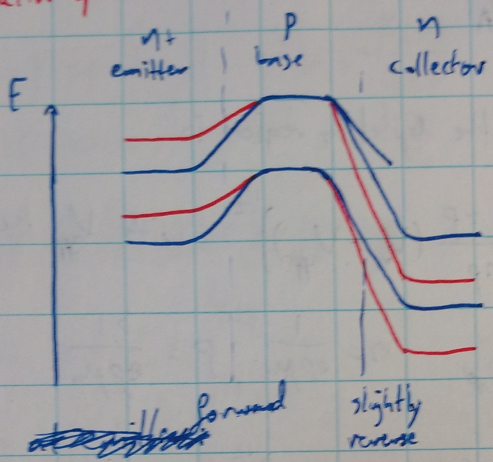
---

e) $j_S = 1,66 \text{ mA} \cdot e^{-\frac{eV}{kT}} \approx 4,4 \mu A$

---

2 a

blue: thermal equilibrium
red: active operation



b

$$n_B = \frac{n_i^2}{N_B} e^{\left(\frac{eV_{EB}}{kT}\right)}$$

$N_E = 5 \cdot 10^{18}\ cm^{-3}$, $N_B = 10^{16}\ cm^{-3}$, $N_C = 10^{15}\ cm^{-3}$

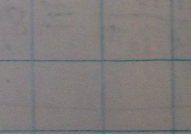
$V_{EB} = 0{,}5\ V$, $V_{CB} = 5\ V$ (reverse)

$T = 293{,}15\ K$ base width $\delta_B = 1.0\ \mu m$

built in potentials are

$$V_{bi,EB} = \frac{kT}{e} \ln\left(\frac{N_E N_B}{n_i^2}\right)$$

$$V_{bi,CB} = \frac{kT}{e} \ln\left(\frac{N_B N_C}{n_i^2}\right)$$





Week 6

6.1 (3) a) As explained, the scale of the Coulomb blockade is $\sim O\left(\frac{e^2}{C}\right)$, and is dependent on the difference in energy of the consecutive states in the "island".

b) Capacitance is $C = \frac{Q}{\Delta V}$.

$$\Delta V = \frac{Q}{4\pi\varepsilon_0}\int_r^\infty \frac{1}{r^2}dr = \frac{Q}{4\pi\varepsilon_0 r}$$

$$C = 4\pi\varepsilon_0 r \approx 1{,}1\cdot 10^{-19}\ \text{F} \quad \text{for } r = 1\text{nm}$$

so then the relevant energy scale is $\frac{e^2}{C} \approx 2{,}3\cdot 10^{-19}$ J

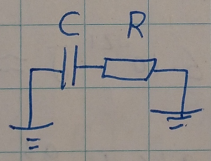
or $\frac{e}{C} \approx 1{,}43$ eV

at $T = 293$ K $\rightarrow k_B T \approx 25{,}7$ meV

at $T = 50$ mK $\rightarrow k_B T \approx 4{,}3$ μeV

so in <u>both</u> cases this energy E_c is much larger than $k_B T$

c)



using KVL $\rightarrow V_a = i(t)R + \frac{1}{C}\int_{t_0}^{t} i(\tau)d\tau$

$\hookrightarrow RC\frac{di}{dt} + i(t) = 0$

the time constant of such a system is <u>R · C</u>

$\hookrightarrow$ KVL $\rightarrow V_{ci} = i(t)R + \frac{1}{C}\int_{t_0}^{t} i(\tau)d\tau$

$\hookrightarrow RC\frac{di}{dt} + i(t) = 0 \rightarrow i \propto e^{-t/RC}$

d) $\delta E \cdot \delta t \geq \hbar/2 \rightarrow \delta E \geq \frac{\hbar}{2\delta t}$

for time scale $RC \rightarrow \delta E \geq \frac{\hbar}{2RC} \rightarrow$ <u>$\delta E \geq \frac{\hbar}{2RC}$</u>

so the uncertainty in energy is at least $\frac{\hbar}{2RC}$, if not more

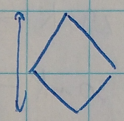
e) if the energy uncertainty is larger than the charging energy, electrons with different energies can still enter the system and no blockade will be observed: Blockade only if $E_c \gg \delta E$

$\rightarrow \delta E \ll E_c$

f) $\frac{t_h}{2RC} \ll E_c \rightarrow \frac{t_h}{2RC} \ll \frac{e^2}{C} \rightarrow R \gg \frac{t_h}{2e^2}$

~~Tunneling resistance~~ this does not depend on C

this is actually the inverse of the conductance quantum:
R should be much larger than the resistivity quantum! (QPC)

g) vertical difference in diamond  is $2\frac{e^2}{C}$

this is in the image: approx 150 mV

$\rightarrow C = \frac{2e}{150\,mV} = 2,1 \cdot 10^{-18}\,F$

then charging energy is $\frac{e^2}{2C} = 6 \cdot 10^{-21}\,J \approx 37,5\,eV$

h) $\frac{C_g}{C_{tot}} = \frac{1}{\frac{1}{\alpha}+\frac{1}{\beta}+\frac{1}{\gamma}}$, $\beta \approx \frac{75\,mV}{0,25\,V} \approx 0,3$, $\gamma = \frac{75\,mV}{0,33,5} \approx 0,5$

$\alpha \approx \frac{3}{2}$ by eyeballing slopes and height/width ratio

$\rightarrow \frac{C_g}{C_{tot}} = \frac{1}{\frac{2}{3}+0,5+0,3} = \frac{1}{\frac{22}{15}} = \frac{15}{22} \approx 0,68$

since $\beta = C_g/(C_g+C_D) \rightarrow C_D = C_g\left(\frac{1}{\beta}-1\right)$

$\gamma = C_g/C_s \rightarrow C_s = \frac{C_g}{\gamma}$

$\rightarrow C_g = 0,68\,C_{tot}$

$C_D = \left(\frac{1}{0,3}-1\right) 0,68\,C_{tot}$

$C_s = \frac{0,68}{0,5} C_{tot}$

$\rightarrow \begin{cases} C_g = 0,68\,C_{tot} \\ C_D = 1,59\,C_{tot} \\ C_s = 1,36\,C_{tot} \end{cases}$

6.2 1) a) $I = \sqrt{E-E_g}\, e^{-E/kT}$

max at $\frac{dI}{dE} = 0 \Rightarrow e^{-E/kT}\left[\frac{1}{2(E-E_g)^{1/2}} - \frac{(E-E_g)^{1/2}}{kT}\right] = 0$

$\rightarrow \frac{1}{2(E-E_g)^{1/2}} = \frac{(E-E_g)^{1/2}}{kT} \Rightarrow E - E_g = \frac{kT}{2}$

so: maximum at $E = \frac{kT}{2} + E_g$

FWHM is $|E_1 - E_2|$ where $I(E_{1,2}) = \frac{1}{2} I\left(E_g + \frac{kT}{2}\right)$

$\rightarrow (E-E_g)^{1/2} e^{-E/kT} = \frac{1}{2}\left(\frac{kT}{2}\right)^{1/2} e^{-\left[\frac{E_g}{kT} + \frac{1}{2}\right]}$

no analytical simple solution

with Mathematica: $E_1 \approx 1{,}84632\, kT + E_g$

$E_2 \approx 0{,}0509142\, kT + E_g$

$\rightarrow$ FWHM $= |E_1 - E_2| \approx 1{,}79541\, k_B T$

b) $E \mapsto \lambda$ is $E = \frac{hc}{\lambda} \rightarrow \lambda = \frac{hc}{E}$

$\hookrightarrow \left(\frac{hc}{\lambda} - E_g\right)^{1/2} e^{-hc/\lambda kT} = \frac{1}{2}\left(\frac{kT}{2}\right)^{1/2} e^{-\left[\frac{E_g}{kT} + \frac{1}{2}\right]}$

$\hookrightarrow$ $\lambda_1 \approx \frac{2hc}{0{,}101828kT + 2E_g}$, $\lambda_2 \approx \frac{2hc}{3{,}69263kT + 2E_g}$ $\Big\}$ FWHM $\approx \frac{19{,}0993\, hc k_B T}{(k_B T)^2 + 20{,}1826\, k_B T E_g + 10{,}6379 E_g^2}$

at room temp: $k_B T \approx 4{,}11 \cdot 10^{-21}$ J

max at $E = \frac{hc}{\lambda_{max}} = \frac{kT}{2} + E_g$

$\rightarrow E_g = \frac{hc}{\lambda_{max}} - \frac{kT}{2} \approx \frac{1{,}9864 \cdot 10^{-25}\,\text{Jm}}{0{,}555 \cdot 10^{-6}\,\text{m}} - \frac{4{,}11 \cdot 10^{-21}}{2} \approx 3{,}5585 \cdot 10^{-19}$ J

$\rightarrow$ FWHM $\approx \frac{19{,}0993 \cdot 1{,}9864 \cdot 10^{-25} \cdot 4{,}11 \cdot 10^{-21}}{(4{,}11 \cdot 10^{-21})^2 + 20{,}1826 \cdot 4{,}11 \cdot 10^{-21} \cdot 3{,}5585 \cdot 10^{-19} + 10{,}6379 \cdot (3{,}5585 \cdot 10^{-19})^2}$

FWHM $\approx 1{,}133 \cdot 10^{-8}$ m $\approx 11{,}33$ nm

FWHM of wavelength

c) $f = \frac{1}{2\pi\tau}$, $\frac{1}{\tau} = \frac{1}{\tau_{nr}} + \frac{1}{\tau_r} = \frac{10^{19}}{10^9} + \frac{1}{10^{-7}} = 10^{10} + 10^7$

$\hookrightarrow \tau = \frac{1}{10^{10}+10^7} = 9{,}99 \cdot 10^{-11}\ s$

$\rightarrow f = \frac{1}{2\cdot\pi\cdot 9{,}99\cdot 10^{-11}} \simeq 1{,}6\cdot 10^9\ Hz \simeq 1{,}6\ GHz$

---

2 a) $\left.\begin{array}{l}\lambda = 1{,}3\cdot 10^{-6}\ m \\ L = 300\cdot 10^{-6}\ m \\ n_{av} = 3{,}4\end{array}\right\} \Delta\lambda = \frac{\lambda^2}{2Ln_{av}} = \frac{1{,}3^2}{600\cdot 3{,}4}\cdot 10^{-6} \simeq 0{,}83\ nm$

b) $n = n_0 + \frac{dn}{d\lambda}(\lambda - \lambda_0)$

$\hookrightarrow \Delta\lambda = \frac{\lambda^2}{2L\left(n_0 + \frac{dn}{d\lambda}(\lambda-\lambda_0)\right)} = \frac{\lambda^2}{2\cdot 3\cdot 10^{-4}\cdot\left(3{,}58 + 2{,}58\cdot 10^6(\lambda - 0{,}89\cdot 10^{-6})\right)}$

which depends on λ and increases with increasing λ.

$\Delta\lambda \approx \frac{6{,}5\cdot 10^{-4}\cdot\lambda^2}{\lambda + 4{,}98\cdot 10^{-7}}$ / $\Delta\lambda \approx \frac{\lambda^2}{1548\lambda + 7{,}7\cdot 10^{-4}}$

c) $g = \alpha + \frac{1}{L}\ln\left(\frac{1}{R}\right)$

if $\alpha = 10\ cm^{-1} = 1000\ m^{-1}$, $L = 300\ \mu m = 3\cdot 10^{-4}\ m$, $R = 0{,}9$

$\hookrightarrow g = 1000 + \frac{1}{3\cdot 10^{-4}}\cdot\ln\left(\frac{1}{0{,}9}\right) \approx 1351{,}2\ m^{-1}$

so a gain of $g = 13{,}51\ cm^{-1}$ is the minimum gain for lasing to occur.

---

3 a) $J_{sc} = \frac{I_{sc}}{A} = \frac{95\ mA}{2\ cm^2} = \frac{95\cdot 10^{-3}\ A}{2\cdot 10^{-4}\ m^2} = 475\ A/m^2$

$J_0 = eA\left(\sqrt{\frac{D_p}{\tau_p}}\frac{n_i^2}{N_D} + \sqrt{\frac{D_n}{\tau_n}}\frac{n_i^2}{N_A}\right)$

$\hookrightarrow \frac{J_{sc}}{J_0} = \frac{I_{sc}}{e}\left(\sqrt{\frac{D_p}{\tau_p}}\cdot\frac{n_i^2}{N_D} + \sqrt{\frac{D_n}{\tau_n}}\frac{n_i^2}{N_A}\right)^{-1}$

$\hookrightarrow V_{oc} \approx \frac{kT_c}{e}\left[\ln\left(\frac{I_{sc}}{e}\right) - \ln\left(\sqrt{\frac{D_p}{\tau_p}}\frac{n_i^2}{N_D} + \sqrt{\frac{D_n}{\tau_n}}\frac{n_i^2}{N_A}\right)\right]$

3a) cont.)

$n_i = \sqrt{N_c N_v}\, e^{-E_g/kT} \approx 10^{10}\ cm^{-3}$ for Si $\rightarrow n_i = 10^{16}\ m^{-3}$

$N_A = 1{,}7 \cdot 10^{16}\ cm^{-3} = 1{,}7 \cdot 10^{22}\ m^{-3}$

$N_D = 5 \cdot 10^{19}\ cm^{-3} = 5 \cdot 10^{25}\ m^{-3}$

$\tau_n = 10\,\mu s = 10^{-5}\ s$

$\tau_p = 0{,}5\,\mu s = 5 \cdot 10^{-7}\ s$

$D_n = 9{,}3\ cm^2/s = 9{,}3 \cdot 10^{-4}\ m^2/s$

$D_p = 2{,}5\ cm^2/s = 2{,}5 \cdot 10^{-4}\ m^2/s$

$T \approx 300\ K$

$$J_0 = 1{,}6 \cdot 10^{-19} \cdot 2 \cdot 10^{-4} \left(\sqrt{\frac{2{,}5 \cdot 10^{-4}}{5 \cdot 10^{-7}}}\ \frac{10^{32}}{5 \cdot 10^{25}} + \sqrt{\frac{9{,}3 \cdot 10^{-4}}{10^{-5}}}\ \frac{10^{32}}{1{,}7 \cdot 10^{22}} \right)$$

$\approx 1{,}8 \cdot 10^{-12}\ A/m^2$

$\hookrightarrow \ln\left(\frac{J_{sc}}{J_0} + 1\right) \approx 33{,}2$

$$\rightarrow V_{oc} = \frac{kT_c}{q} \ln\left(\frac{J_{sc}}{J_0} + 1\right) \approx \frac{1{,}38 \cdot 10^{-23} \cdot 300}{1{,}6 \cdot 10^{-19}} \cdot 33{,}2 \approx 0{,}859\ V$$

$$V_{max} = V_{oc} - \frac{kT}{e} \ln\left(1 + \frac{eV_{max}}{kT}\right)$$

with previously used values, in Mathematica: $V_{max} \approx 0{,}77\ V$

$P = V_{max} \cdot J_{sc} \approx 0{,}77 \cdot 475 \approx 367\ W/m^2$

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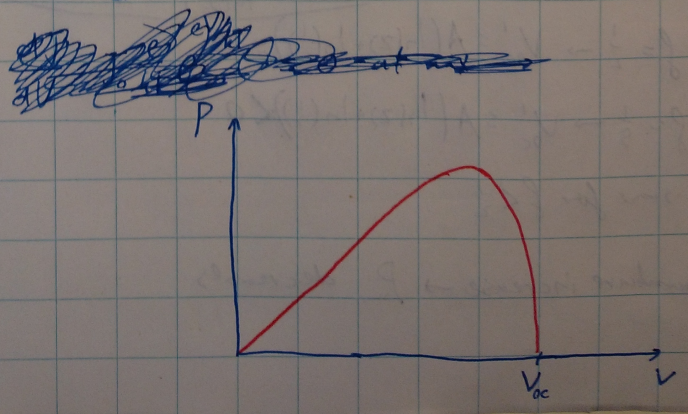
b) $J = -J_0\left[e^{eV/kT} - 1\right] + J_{sc} \rightarrow P = JV = V\left[J_{sc} - J_0\left[e^{eV/kT} - 1\right]\right]$



P_{max} at $\frac{\partial P}{\partial V} = 0 \rightarrow [J_{sc} - J_0[e^{eV/kT} - 1]] - V J_0$

if P_{max} is calculated, then fill factor $FF = \frac{P_{max}}{V_{oc} \cdot J_{sc}} = \frac{P_{max}}{3 \cdot 0,6}$

$FF = \frac{P_{max}}{1,8}$

c) Changing the light intensity will change the J_{sc} and V_{oc}.

J_{sc} depends linearly on light intensity, and thus would decrease by a factor of $\frac{1}{1,5} = \frac{2}{3} \rightarrow J_{sc}' = \frac{2}{3} J_{sc}^{init}$

V_{oc} would decrease a little bit, ~~$V_{oc} \propto \ln(\frac{J_{sc}}{J_0}) \propto \ln(J_{sc})$~~ since the IV curve slides down is I, but as the drop near V_{oc} is so steep, not much changes.

~~because~~ because of this I and V behaviour, P_{max} also decreases.

d) ~~Since $V_{oc} \propto \ln(\frac{J_{sc}}{J_0})$, if $J_{sc}' = f J_{sc}$~~

~~$\rightarrow V_{oc}' \propto \ln(\frac{f J_{sc}}{J_0}) \propto V_{oc} + \ln(\frac{f}{J_0})$~~

Since $V_{oc} \propto \ln(J_{sc})$, if $J_{sc}' = f J_{sc}$

then $V_{oc}' \propto \ln(J_{sc}) + \ln(f)$

if $V_{oc} = 0,5V$, $J_{sc} = 2A \rightarrow V_{oc} = A \ln(J_{sc})$

$\rightarrow A = \frac{V_{oc}}{\ln(J_{sc})} \approx 0,72135$

if $f = \frac{1}{2} \rightarrow V_{oc}' = A(\ln(2) + \ln(\frac{1}{2})) = 0$

if $f = \frac{1}{5} \rightarrow V_{oc}' = A(\ln(2) + \ln(\frac{1}{5})) < 0$

same for $f < \frac{1}{2}$

e) Temperature increase $\rightarrow$ P_{max} decreases

Week 7

2a)

$$|\psi\rangle = \sum_{\vec{R}\in G} e^{i\vec{k}\cdot\vec{R}}\left[b_1|\phi_1\rangle + b_2|\phi_2\rangle\right]$$

$$\hookrightarrow \langle\phi_j|\psi\rangle = \sum_{\vec{R}\in G} e^{i\vec{k}\cdot\vec{R}} b_j$$

$$\hat{\mathcal{H}}|\phi_j\rangle = \Delta\hat{U}_j|\phi_j\rangle$$

$$\hookrightarrow \hat{\mathcal{H}}|\psi\rangle = \sum_{\vec{R}\in G} e^{i\vec{k}\cdot\vec{R}}\left[b_1\hat{\mathcal{H}}|\phi_1\rangle + b_2\hat{\mathcal{H}}|\phi_2\rangle\right]$$

$$= \sum_{\vec{R}\in G} e^{i\vec{k}\cdot\vec{R}}\left[b_1\Delta\hat{U}_1|\phi_1\rangle + b_2\Delta\hat{U}_2|\phi_2\rangle\right]$$

$\rightarrow$ $\langle\phi_j|\hat{\mathcal{H}}|\psi\rangle =$ [redacted] $\langle\phi_j|\Delta\hat{U}_j|\psi\rangle$ (only ΔU_j contribution from $\mathcal{H}$ projected on $|\phi_j\rangle$)

but [redacted] $\hat{\mathcal{H}}|\psi\rangle = E(\vec{k})|\psi\rangle \rightarrow \langle\phi_j|\hat{\mathcal{H}}|\psi\rangle = E(\vec{k})\langle\phi_j|\psi\rangle$

so: $E(\vec{k})\langle\phi_j|\psi\rangle = \langle\phi_j|\Delta\hat{U}_j|\psi\rangle = \langle\phi_j|\hat{\mathcal{H}}|\psi\rangle$

2b) $\langle\phi_j$[redacted]$|\psi\rangle = \langle\phi_j(\vec{x})|\sum_{\vec{R}\in G} e^{i\vec{k}\cdot\vec{R}}\left[b_1|\phi_1(\vec{x}-\vec{R})\rangle + b_2|\phi_2(\vec{x}-\vec{R})\rangle\right]$

only nearest neighbours: for (lattice) state 1: [redacted] $\vec{R}\in\{\vec{0}, -\vec{a}_1, -\vec{a}_2\}$ overlaps

for Lattice 2: $\vec{R}\in\{\vec{0}, \vec{a}_1, \vec{a}_2\}$ overlaps

$$\rightarrow \langle\phi_1|\psi\rangle = \langle\phi_1(\vec{x})|\left[b_1|\phi_1(\vec{x})\rangle + b_2\left(|\phi_2(\vec{x})\rangle + e^{-i\vec{k}\cdot\vec{a}_1}|\phi_2(\vec{x}-\vec{a}_1)\rangle + e^{-i\vec{k}\cdot\vec{a}_2}|\phi_2(\vec{x}-\vec{a}_2)\rangle\right)\right.$$

$$= b_1 + b_2\left(\int\phi_1^*\phi_2(\vec{x}) + \int\phi_1^*\phi_2(\vec{x}-\vec{a}_1)e^{-i\vec{k}\cdot\vec{a}_1} + \int\phi_1^*\phi_2(\vec{x}-\vec{a}_2)e^{-i\vec{k}\cdot\vec{a}_2}\right)$$

overlaps all the same: $\langle\phi_1|\psi\rangle = b_1 + b_2\left(\int\phi_1^*\phi_2\right)\left(1 + e^{-i\vec{k}\cdot\vec{a}_1} + e^{-i\vec{k}\cdot\vec{a}_2}\right)$

same method for $\langle\phi_2|\psi\rangle = b_2 + b_1\left(\int\phi_2^*\phi_1\right)\left(1 + e^{+i\vec{k}\cdot\vec{a}_1} + e^{+i\vec{k}\cdot\vec{a}_2}\right)$

first contributions due to projection on state itself, second contributions due to Φ-overlap with nearest neighbours

2c) determinante $=0$

$$\rightarrow E^2(k) - |\alpha|^2\left[\gamma_0^2 E^2(k) + \gamma_1^2 - 2\gamma_0\gamma_1 E(k)\right] = 0$$

$$\rightarrow (1-|\alpha|^2\gamma_0^2)E^2(k) + 2\gamma_0\gamma_1|\alpha|^2 E(k) - |\alpha|^2\gamma_1^2 = 0$$

$$\rightarrow E(k) = \frac{-2\gamma_0\gamma_1|\alpha|^2 \pm \sqrt{4\gamma_0^2\gamma_1^2|\alpha|^4 + 4|\alpha|^2\gamma_1^2(1-|\alpha|^2\gamma_0^2)}}{2(1-|\alpha|^2\gamma_0^2)}$$

$$= \frac{-2\gamma_0\gamma_1|\alpha|^2 \pm \sqrt{4|\alpha|^2\gamma_1^2}}{2(1-|\alpha|^2\gamma_0^2)} \leq \frac{-2\gamma_0\gamma_1|\alpha|^2 \pm 2|\alpha|\gamma_1}{2(1-|\alpha|^2\gamma_0^2)}$$

$$= |\alpha|\gamma_1\left[\frac{-|\alpha|\gamma_0 \pm 1}{1-|\alpha|^2\gamma_0^2}\right] = |\alpha|\gamma_1\left[\frac{-|\alpha|\gamma_0 \pm 1}{(1+|\alpha|\gamma_0)(1-|\alpha|\gamma_0)}\right]$$

- since $|\alpha| \sim \mathcal{O}(1)$ and $\gamma_0 \ll 1$ is assumed, we can say $|\alpha|\gamma_0 \ll 1$

$$\hookrightarrow E(k) \approx \lim_{|\alpha|\gamma_0 \to 0} |\alpha|\gamma_1\left[\frac{-|\alpha|\gamma_0 \pm 1}{1-|\alpha|^2\gamma_0^2}\right] = |\alpha|\gamma_1\left[\frac{0 \pm 1}{1-0}\right] = \pm|\alpha(k)|\gamma_1$$

$\frac{0\pm1}{1-0} = \pm 1$

2d) $|\alpha| = \sqrt{\alpha^*\alpha} = \Big[1 + e^{-i\vec{k}\cdot\vec{a}_1} + e^{-i\vec{k}\cdot\vec{a}_2} + e^{i\vec{k}\cdot\vec{a}_1} + e^{i\vec{k}\cdot\vec{a}_2} + e^{i\vec{k}(\vec{a}_1-\vec{a}_2)} + e^{i\vec{k}(\vec{a}_2-\vec{a}_1)} + e^{i\vec{k}\cdot(\vec{a}_1-\vec{a}_2)} + e^{i\vec{k}\cdot(\vec{a}_2-\vec{a}_1)}\Big]^{1/2}$

$$= \Big[1 + 2\cos(\vec{k}\cdot\vec{a}_1) + 2\cos(\vec{k}\cdot\vec{a}_2) + 1 + 1 + 2\cos(\vec{k}\cdot(\vec{a}_2-\vec{a}_1))\Big]^{1/2}$$

$$= \sqrt{3 + 2\left[\cos(\vec{k}\cdot\vec{a}_1) + \cos(\vec{k}\cdot\vec{a}_2) + \cos(\vec{k}\cdot(\vec{a}_2-\vec{a}_1))\right]}$$

such that $E(\vec{k}) = \pm\gamma_1\sqrt{3 + 2\left[\cos(\vec{k}\cdot\vec{a}_1) + \cos(\vec{k}\cdot\vec{a}_2) + \cos(\vec{k}\cdot(\vec{a}_2-\vec{a}_1))\right]}$

(2e) $\vec{k}\cdot\vec{a}_1 = a_0\sqrt{3}\left(\frac{k_x}{2} + \frac{\sqrt{3}k_y}{2}\right)$

$\vec{k}\cdot\vec{a}_2 = a_0\sqrt{3}\left(-\frac{k_x}{2} + \frac{\sqrt{3}k_y}{2}\right)$

$\vec{k}\cdot(\vec{a}_2 - \vec{a}_1) = a_0\sqrt{3}\cdot -k_x = -a_0\sqrt{3}k_x$

will $\frac{a_0\sqrt{3}}{2} \equiv \eta$

$\vec{k}\cdot\vec{a}_1 = \eta k_x + \sqrt{3}\eta k_y$

$\vec{k}\cdot\vec{a}_2 = -\eta k_x + \sqrt{3}\eta k_y$

$\vec{k}\cdot\Delta\vec{a} = -2\eta k_x$

using identities: $\cos(\theta-\varphi) + \cos(\theta+\varphi) = 2\cos\theta\cos\varphi$

$\cos(2\theta) = 2\cos^2\theta - 1$

(using $\frac{a_0\sqrt{3}}{2} = \eta$) we write: $\cos(\vec{k}\cdot\vec{a}_1) + \cos(\vec{k}\cdot\vec{a}_2) + \cos(\vec{k}\cdot(\vec{a}_2 - \vec{a}_1))$ (symmetry: $= \cos(2\eta k_x)$)

$= \cos(\sqrt{3}\eta k_y + \eta k_x) + \cos(\sqrt{3}\eta k_y - \eta k_x) + \cos(-2\eta k_x)$

$= 2\cos(\eta k_x)\cos(\sqrt{3}\eta k_y) + 2\cos^2(\eta k_x) - 1$

so then $E(\vec{k}) = \pm\gamma_1\sqrt{3 + 4\cos\left(\frac{ak_x}{2}\right)\cos\left(\frac{\sqrt{3}ak_y}{2}\right) + 4\cos^2\left(\frac{ak_x}{2}\right) - 2}$

[since $a = \frac{\eta}{2}$]

so $E(\vec{k}) = \pm\gamma_1\sqrt{1 + 4\cos\left(\frac{ak_x}{2}\right)\cos\left(\frac{\sqrt{3}ak_y}{2}\right) + 4\cos^2\left(\frac{ak_x}{2}\right)}$

(2f) the plot is really already given in the text

(2g) graphene cannot really be characterized as either a semiconductor or a metal, since it does not have a bandgap (not a semiconductor) but the valence "band" is fully filled (it can still be considered a band since the energy is zero between the two "bands"), so it is also not a metal. it is neither and therefore is fairly unique (maybe call it "semimetal"?)

(2h) the fermi energy is right at the point where the two "bands" touch. this is, in this case, the reference energy $E_F = 0$

3a this is already done in "Figure 3" ...

3b $\vec{a}_i \cdot \vec{b}_j = 2\pi \delta_{ij}$, $a_1 = \left(\frac{\sqrt{3}a_0}{2}, \frac{3a_0}{2}\right)$, $a_2 = \left(-\frac{\sqrt{3}a_0}{2}, \frac{3a_0}{2}\right)$

$a_1 \cdot b_1 = 2\pi \rightarrow \frac{\sqrt{3}a_0}{2}\left(b_{1x} + \sqrt{3} b_{1y}\right) = 2\pi$

$a_1 \cdot b_2 = 0 \rightarrow \frac{\sqrt{3}a_0}{2}\left(-b_{1x} + \sqrt{3} b_{1y}\right) = 0 \rightarrow b_{1x} = \sqrt{3} b_{1y}$

$\hookrightarrow \frac{\sqrt{3}a_0}{2} \cdot 2\sqrt{3} b_{1y} = 2\pi \rightarrow b_{1y} = \frac{2\pi}{3a_0} \rightarrow b_{1x} = \frac{2\pi}{\sqrt{3}a_0}$

$\rightarrow |\vec{b}_1| = \sqrt{\frac{4\pi^2}{9a_0^2} + \frac{4\pi^2}{3a_0^2}} = \frac{2\pi}{a_0}\sqrt{\frac{1}{9} + \frac{3}{9}} = \frac{2\pi}{a_0} \cdot \frac{2}{3} = \underline{\frac{4\pi}{3a_0}}$

$a_1 \cdot b_2 = 0 \rightarrow \frac{\sqrt{3}a_0}{2}\left(b_{2x} + \sqrt{3} b_{2y}\right) = 0 \rightarrow b_{2x} = -\sqrt{3} b_{2y}$

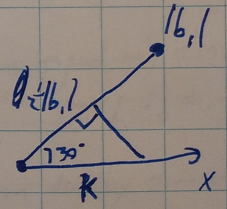
$a_2 \cdot b_2 = 2\pi \rightarrow \frac{\sqrt{3}a_0}{2}\left(-b_{2x} + \sqrt{3} b_{2y}\right) = 2\pi$

$\hookrightarrow b_{2y} = \frac{2\pi}{\sqrt{3}a_0} \rightarrow b_{2x} = -\frac{2\pi}{\sqrt{3}a_0}$

$\rightarrow |\vec{b}_2| = \sqrt{\frac{4\pi^2}{9a_0} + \frac{4\pi^2}{3a_0}} = \frac{4\pi}{3a_0}$ (same term under $\sqrt{}$)

$\hookrightarrow \underline{|\vec{b}_{1,2}| = \frac{4\pi}{3a_0}}$

3c geometric argument:



$\hookrightarrow |\vec{K}| = \frac{\frac{1}{2}|\vec{b}_1|}{\cos(30^\circ)} = \frac{\frac{1}{2}\cdot\frac{4\pi}{3a_0}}{\frac{1}{2}\sqrt{3}}$

$= \frac{4\pi}{3\sqrt{3}a_0}$. since $\vec{K} \parallel \vec{e}_x \rightarrow \vec{K} = |\vec{K}|\vec{e}_x$

$\rightarrow \vec{K} = |\vec{K}|\vec{e}_x = \frac{4\pi}{3\sqrt{3}a_0}\vec{e}_x$

(3d) dispersion is given by

$$E(\vec{k}) = \pm\gamma_1\sqrt{1+4\cos\left(\frac{3a_0k_y}{2}\right)\cos\left(\frac{\sqrt{3}a_0k_x}{2}\right)+4\cos^2\left(\frac{\sqrt{3}a_0k_x}{2}\right)}$$

so for $(k_x, k_y) \mapsto \left(\frac{4\pi}{3\sqrt{3}a_0}, 0\right)$

$$\hookrightarrow E(\vec{K}) = \pm\gamma_1\sqrt{1+4\cos\left(\frac{4\pi}{3}\right)+4\cos^2\left(\frac{4\pi}{3}\right)}$$

$$= \pm\gamma_1\sqrt{1-4\cdot\frac{1}{2}+4\cdot\frac{1}{4}} = \pm\gamma_1\sqrt{1-2+1} = \pm 0$$

so for $\vec{K}$, dispersion is $\emptyset$: $E(\vec{K}) = 0$

(3e) same as before [it's still undoped graphene after all] : $E_F = 0$

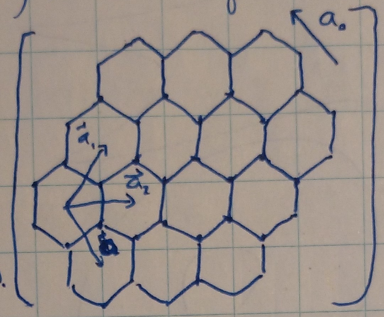
(3g) Eigenvalue is $\emptyset$ for all K-points $\{K_i\}_{i=1}^{6}$: $E(K_i)\big|_{i=1}^{6} = 0$

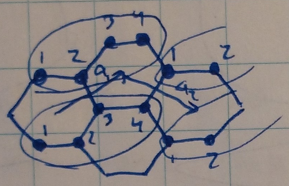
with $\vec{K}_i = \left(\frac{4\pi}{3\sqrt{3}a_0}\right)\left(\cos\left(\frac{2\pi i}{6}\right)\vec{e}_x + \sin\left(\frac{2\pi i}{6}\right)\vec{e}_y\right)$

CM@Nano
week 3

4a) the lattice constant of an armchair nanotube would be exactly that of the graphene it consists of, since its 1D periodicity is this graphene LC.

4b) if the wrapping vector is defined as $\vec{w} = N(\vec{a}_1 + \vec{a}_2)$, then there would be $4 \cdot N$ atoms per 1D unit cell, when using $(\vec{a}_1, \vec{a}_2)$ as shown.





per N there's 4 atoms: $4N$ valence electrons!

4c) the first BZ for an armchair nanotube is simply of length $\frac{2\pi}{a_0}$ since the 1D lattice "vector" is $\vec{a}_1 = a_0 \vec{e}_x \rightarrow \vec{a}_1 \cdot \vec{b}_1 = 2\pi$

$\therefore b_x = \frac{2\pi}{a_x} = \frac{2\pi}{a_0}$

4d) figure drawn in the exercises file already (figure 5).
this figure can be obtained by substituting eq. (25) into eq. (18) for $m \in \{\mathbb{Z}, -N \leq m \leq N\}$.

4e) since $n - m = 0$ is a multiple of 3, this is a metallic nanotube. there is no bandgap present.