Solution problem set #2 EE 230 Spring 02

1. a) The restoring force due to the electron se is $4\pi r^2 E = -\frac{3}{4\pi R^3}\cdot\frac{4\pi r^3}{3}\left(\frac{e}{\epsilon_0}\right)$ from Gaus law

$$\therefore \quad E = -\frac{e}{4\pi R^3 \epsilon_0} r.$$

The force is $F = eE = \frac{e^2}{4\pi R^3 \epsilon_0} r = M\omega^2$

$$\omega = \left(\frac{e^2}{4\pi M R^3 \epsilon_0}\right)^{1/2} \quad \text{in MKS}$$

$$= \left(\frac{e^2}{M R^3}\right)^{1/2} \quad \text{in CGS}$$

b) For Na, $M \cong 4\times10^{-23}$ g, $R \simeq 2\times10^{-8}$ cm.

Hence $\omega_0 \cong 3\times10^{13}$ rad/sec

$$\lambda = \frac{c}{\nu} = \frac{2\pi c}{\omega} = 62.8\ \mu m$$

c) The maximum phonon wavevector magnitude is about the size of the first Brillouin zone which is on the order of $1\,\text{Å}^{-1} = 10^8$ cm^{-1}. If we suppose ω_0 is relate to the maximum wavevector.

$$v_s = \omega_0 / k_{max} \simeq 3\times10^5 \text{ cm/sec.}$$

From literature $\longrightarrow$ At room temp, $v_s \cong 3.3\times10^5$ cm/s.

Ref: H. Kamioka, J. Phys. Soc. Japan 52, 2433 (1983).

2. Lattice vibration energy is given by

$$U_{acoustic} + U_{optic}$$

$$U_{acoustic} = 9Nk_B T\left(\frac{T}{T_D}\right)^3 \int_0^{x_D} dx \frac{x^3}{e^x - 1}$$

with $x_D = T_D/T$.

$$U_{optic} = 3N \frac{\hbar\omega_0}{e^{\hbar\omega_0/k_BT} - 1}$$

$N = n/2 = 4.42\times10^{22}/2 = 2.21\times10^{22}$ atoms/c

$T_D = 393\,K$ from 3.

$9Nk_B \cdot (1K) = 2.75\ J$

$3N\hbar\omega_0 = 382.4\ J$

At $T = 77\,K$ $\quad x_D = 393/77 = 5.1$

$\hbar\omega_0/k_BT = 5.43$

$$U_L = 2.75 \times 77 \times \left(\frac{1}{5.1}\right)^3 \times (4.98)$$

$$+ 382.4 \times \frac{1}{e^{5.43} - 1}$$

$$= 9.63\ J/cm^3$$

at $T = 300K$ $\quad x_D = \frac{393}{300} = 1.31$

$\hbar\omega_0 / k_B T = 1.39$

$$U_L = 2.75 \times 300 \times \left(\frac{1}{1.31}\right)^3 \times 0.444$$

$$+ 382.4 \times \frac{1}{e^{1.39} - 1}$$

$$= 289.8 \ J/cm^3$$

at $T = 1000K$ $\quad x_D = \frac{393}{1000} = 0.393$

$\frac{\hbar\omega_0}{k_B T} = 0.418$

$$U_L = 2.75 \times 1000 \times \left(\frac{1}{0.393}\right)^3 \times 0.0174$$

$$+ 382.4 \times \frac{1}{e^{0.418} - 1}$$

$$= 1525.24 \ J/cm^3$$

cf. $(2N)\left(\frac{3}{2} k_B T\right) \cdot 2 = 6 N k_B T$

$\cong 1831. \ J/cm^3$

Binding energy is (4 bonds/atom)

$U_B = n(1eV) \times 4 \times 1/2$ ← accounts for double counting

$= 14.2 \ kJ/cm^3$

(3) 100 fs duration laser pulse irradiates gold film 1000 Å thick and instantaneously heats the electrons. On a scale of few picoseconds, the electrons cool by transferring energy to the lattice

a) pulse absorbed uniformly through the thickness (1 mJ energy, 1 cm^2 spot size)
neglect reflection and use free-electron heat capacity C_e to find peak electron temperature

$$C_e = \frac{\partial U}{\partial T} = \frac{\pi^2}{2} N k \frac{T}{T_F} \qquad T_F = \frac{\hbar^2}{2m}\frac{1}{k}\left(3\pi^2 \frac{N}{V}\right)^{2/3} \text{ Fermi temperature}$$

for gold. $\frac{N}{V} = \left(6.02\times10^{23}\frac{1}{mol}\right)\left(\frac{19.3\,g/cm^3}{197\,g/mol}\right) = 5.9\times10^{22}\ cm^{-3}$

$V = \text{thickness}\cdot\text{spot size} = (1000\times10^{-8}\,cm \times 1\,cm^2) = 10^{-5}\,cm$

$$U = \int_{T_0}^{T_{MAX}} \frac{\partial U}{\partial T}\, dT = \int_{T_0}^{T_{MAX}} \frac{\pi^2}{2}\frac{Nk}{T_F}\, T\, dT = \frac{\pi^2}{4}\frac{Nk}{T_F}\left(T_{MAX}^2 - T_0^2\right)$$

$U = 1\,mJ$, $T_0 = 300K$ (initial temperature)

$$T_F = \frac{(1.055\times10^{-34}\,J\cdot s)^2\,(3\pi^2\times5.9\times10^{28}\,m^{-3})^{7/3}}{2\,(9.11\times10^{-31}\,kg)(1.38\times10^{-23}\,J/K)} = 6.42$$

$$T_{MAX} = \left(\frac{4UT_F}{\pi^2 Nk} + T_0^2\right)^{1/2} = \left(\frac{4(10^{-3}\,J)(6.42\times10^4\,K)}{\pi^2(5.9\times10^{17})(1.38\times10^{-23}\,J/K)} + 300^2\right)^{1/2}$$

$$\boxed{T_{MAX} = 1813\ K}$$

b) use Debye model for phonons to calculate peak lattice temperature rise after electrons equilibriate with phonons
assume no lateral heat diffusion
electron and phonon temperatures are governed by:

$$(1)\quad C_e(T_e)\frac{\partial T_e}{\partial t} = \kappa\nabla^2 T_e - g(T_e - T_p)$$
$$(2)\quad C_p(T_p)\frac{\partial T_p}{\partial t} = g(T_e - T_p)$$

κ - electronic thermal conductivity
g - electron-phonon coupling constant

note: Actually to do this correctly, we should consider the laser heating of the electrons and the energy transfer to the phonons simultaneously by including a term $A(\vec{r},t)$ in equation (1) that represents energy input to the electrons from the laser. Since we're only interested in estimates of $(T_e)_{MAX}$ and $(T_p)_{MAX}$ we assume $A(\vec{r},t)$ can be treated separately as in part a).

Neglect first term on RHS of eq. (1) which represents diffusion of electrons. There's no such term in eq. (2) because heat diffusion through phonons is much slower than through electrons.

combine (1) and (2): $\quad -C_e(T_e)\,dT_e = C_p(T_p)\,dT_p$

and integrate: $\int_{T_{e\,MAX}}^{T_{P\,MAX}} -C_e(T_e)\,dT_e = \int_{T_0}^{T_{P\,MAX}} C_p(T_p)\,dT_p$ $\quad T_{P\,MAX}$ - equilibri temperu

$$C_e(T_e) = \frac{\pi^2}{2} Nk \frac{T_e}{T_F}$$

$$C_p(T_p) = 9Nk\left(\frac{T}{\theta_D}\right)\int_0^{x_D} \frac{x^4 e^x}{(e^x-1)^2}\,dx$$ Debye model

$x = \frac{\hbar\omega}{kT}$, $x_D = \frac{\theta_D}{T}$

The phonon heat capacity approaches the classical limit $3Nk$ when $T/\theta_D \geq 2$. Since $T_{PMAX} \geq T_P \geq T_0 = 300K$ and $\theta_D = 165K$ for gold (from Kittel), to a good approximation the phonon heat capacity is

$$C_p(T_p) \approx 3Nk$$

$$\Rightarrow \int_{T_{eMAX}}^{T_{PMAX}} -\frac{\pi^2}{2} Nk \frac{T_e}{T_F}\,dT_e = \int_{T_0}^{T_{PMAX}} 3Nk\,dT_p$$

$$-\frac{\pi^2}{4T_F} \cancel{Nk}\left(T_{PMAX}^2 - T_{eMAX}^2\right) = 3\cancel{Nk}\left(T_{PMAX} - T_0\right)$$

$$T_{PMAX}^2 - T_{eMAX}^2 = \frac{-12T_F}{\pi^2}\left(T_{PMAX} - T_0\right)$$

$$T_{PMAX}^2 + \frac{12T_F}{\pi^2} T_{PMAX} - \frac{12T_F T_0}{\pi^2} - T_{eMAX}^2 = 0$$

$$T_{PMAX}^2 = \frac{-6T_F}{\pi^2} \pm \sqrt{\frac{36T_F^2}{\pi^4} + \frac{12T_F T_0}{\pi^2} + T_{eMAX}^2}$$

$$T_{PMAX} = \frac{-6(6.42\times10^4)}{\pi^2} + \sqrt{\frac{36}{\pi^4}(6.42\times10^4)^2 + \frac{12}{\pi^2}(6.42\times10^4)(300) + (1813)^2}\ K$$

$$\boxed{T_{PMAX} = 340.6\ K}$$

4.

a) $[a, a^\dagger] = 1$.

(solution) $[a, a^\dagger] = \left[\frac{\alpha}{\sqrt{2}} x + \frac{i}{\sqrt{2}\hbar\alpha} p_x, \frac{\alpha}{\sqrt{2}} x - \frac{i}{\sqrt{2}\hbar\alpha} p_x \right]$

$\alpha = \left(\frac{m\omega}{\hbar}\right)^{1/2}$ $\quad = -\frac{i}{2\hbar}[x, p_x] + \frac{i}{2\hbar}[p_x, x]$

$[p_x, x] = -i\hbar \Rightarrow \quad = \frac{2i}{2\hbar}[p_x, x] = \frac{2i}{2\hbar}(-i\hbar) = 1$

b) $H = \frac{p_x^2}{2m} + \frac{1}{2}Kx^2 = \frac{p_x^2}{2m} + \frac{m\omega^2}{2}x^2$

$= \frac{1}{2m}\left(\frac{-\hbar^2\alpha^2}{2}\right)(a^\dagger - a)(a^\dagger - a)$

$+ \frac{m\omega^2}{2}\left(\frac{1}{2\alpha^2}\right)(a^\dagger + a)(a^\dagger + a)$

$= -\frac{\hbar\omega}{4}(a^\dagger a^\dagger - a^\dagger a - aa^\dagger + aa - a^\dagger a^\dagger - aa$
$- aa^\dagger - a^\dagger a)$

$= \frac{\hbar\omega}{2}(a^\dagger a + aa^\dagger)$

$= \frac{\hbar\omega}{2}(a^\dagger a + a^\dagger a + 1) \Leftarrow aa^\dagger - a^\dagger a = 1$

$= \hbar\omega(N + 1/2)$ with $N = a^\dagger a$

c) Note that $N = a^\dagger a$ is a Hermitian operator.
Hence its eigenvalue is real. i.e.
$N|n\rangle = n|n\rangle$ with $n \in R$.

$\therefore a^\dagger a|n\rangle = n|n\rangle$ and $\langle n|a^\dagger a = n|n\rangle$

$\therefore \langle n'|(a^\dagger a|n\rangle) = n\langle n'|n\rangle$ ... ①

$(\langle n'|a^\dagger a)|n\rangle = n'\langle n'|n\rangle$ ... ②

① = ② gives you $(n-n')\langle n'|n\rangle = 0$

If $n' \neq n$, this leads to $\langle n'|n\rangle = 0$.

$\langle \alpha|\alpha\rangle = 0$ iff $|\alpha\rangle \equiv$ null vector.

Hence by choosing proper normalization for a nontrivial vector $|n\rangle$, we can make

$$\langle n|n\rangle = 1.$$

Hence, $\langle n'|n\rangle = \delta_{n'n}$.

d) $N a^\dagger|n\rangle = a^\dagger(a a^\dagger|n\rangle) = a^\dagger(a^\dagger a + 1)|n\rangle$

$= a^\dagger(n+1)|n\rangle = (n+1)a^\dagger|n\rangle$

e) Because $N(a^\dagger|n\rangle) = (n+1)(a^\dagger|n\rangle)$,

$a^\dagger|n\rangle$ is an eigenvector of N. with eigenvalue $n+1$. Hence. $a^\dagger|n\rangle = \eta|n+1\rangle$

$(\langle n|a)(a^\dagger|n\rangle) = \langle n|aa^\dagger|n\rangle = \langle n|a^\dagger a+1|n\rangle$

$= n+1$

$(\langle n|a)(a^\dagger|n\rangle) = \eta^2\langle n+1|n+1\rangle = \eta^2$

$\therefore \eta^2 = n+1 \qquad \eta = \pm\sqrt{n+1}$.

Choosing sign is a matter of phase between $|n\rangle$ and $|n+1\rangle$ which we can choose at our freedom. $\eta = \sqrt{n+1}$

$\therefore a^\dagger|n\rangle = \sqrt{n+1}\,|n+1\rangle$

(5) density of states in lower dimensionalities

a) non-interacting particles in a 2D box of size $L_x \times L_y$ (quantum well)

allowed k-values: $k_x = \frac{2\pi}{L_x} n_x \qquad n_x = 0, \pm 1, \pm 2, \ldots$

$k_y = \frac{2\pi}{L_y} n_y \qquad n_y = 0, \pm 1, \pm 2, \ldots$

number of states per unit area with k-values less than k:

$$N = \underset{\text{spin}}{2} \frac{1}{L_x L_y} \frac{\pi k^2}{\left(\frac{2\pi}{L_x}\right)\left(\frac{2\pi}{L_y}\right)} = \frac{k^2}{2\pi} \qquad k^2 = k_x^2 + k_y^2$$

$$E = \frac{\hbar^2 k^2}{2m} \rightarrow k^2 = \frac{2mE}{\hbar^2}$$

$$= \frac{2mE}{2\pi\hbar^2} = \frac{m}{\pi\hbar^2} E$$

density of states: $\boxed{\mathcal{D}(E) = \frac{dN}{dE} = \frac{m}{\pi\hbar^2}}$

b) 1D case (quantum wire of length L)

k-values: $k = \frac{2\pi}{L} n \qquad n = 0, \pm 1, \pm 2, \ldots$

number of states per unit length with $|k|$ less than k:

$$N = \underset{\text{spin}}{2} \frac{1}{L} \frac{2k}{(2\pi/L)} = \frac{2k}{\pi} = \frac{2}{\pi}\sqrt{\frac{2mE}{\hbar^2}} \qquad k = \sqrt{\frac{2mE}{\hbar^2}}$$

density of states: $\mathcal{D}(E) = \frac{dN}{dE} = \frac{1}{\pi}\sqrt{\frac{2m}{\hbar^2}}\frac{1}{\sqrt{E}} = \boxed{\frac{1}{\pi}\sqrt{\frac{2m}{\hbar^2 E}}}$

assume density of states mass $m^* = 0.067\, m_0$ for GaAs

3D case: $\mathcal{D}(E) = \frac{\sqrt{2}\, m^{3/2}}{\pi^2 \hbar^3} \sqrt{E}$

c) plot density of electron states in GaAs in units of $eV^{-1} cm^{-D}$, where D is the dimensionality

3D: $\mathcal{D}(E) = \frac{\sqrt{2}\, m^{*3/2}}{\pi^2 \hbar^3} \sqrt{E} =$

$$= \frac{\sqrt{2}\,(0.067 \times 9.11 \times 10^{-31}\, kg)^{3/2} (1.6 \times 10^{-19}\, J/eV)^{3/2} \sqrt{E(eV)}}{\pi^2 (1.055 \times 10^{-34}\, J \cdot s)^3\, 10^6\, cm^3/m^3}$$

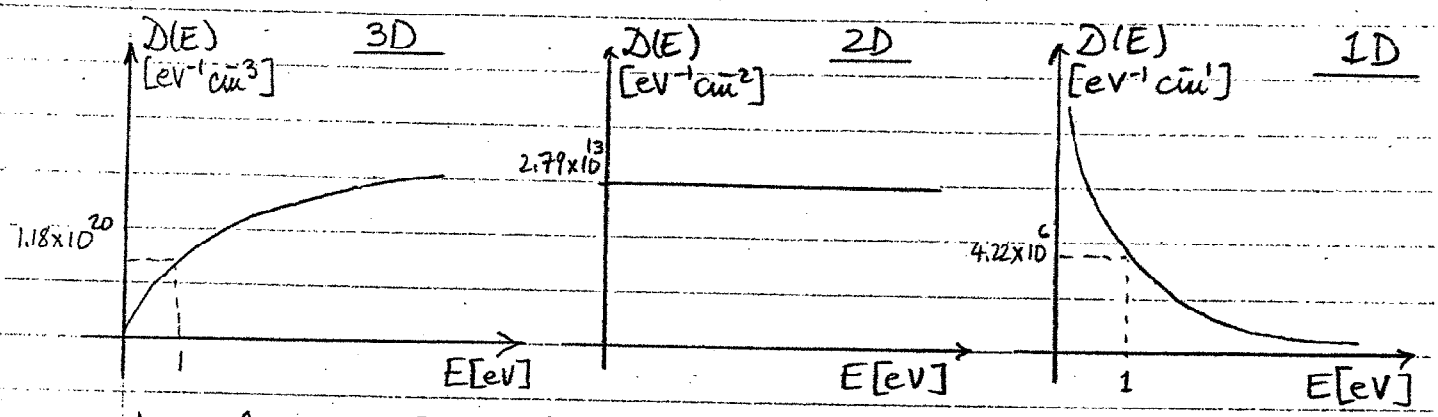
$$= 1.18 \times 10^{20} \sqrt{E} \quad eV^{-1} cm^{-3} \qquad E \text{ in } eV$$

2D: $\mathcal{D}(E) = \frac{m^*}{\pi\hbar^2} = \frac{(0.067\times 9.11\times 10^{-31}\,kg)(1.6\times 10^{-19}\,J/eV)}{\pi(1.055\times 10^{-34}\,J\cdot s)^2\,10^4\,cm^2/m^2}$

$= 2.79\times 10^{13}\,eV^{-1}cm^{-2}$

1D: $\mathcal{D}(E) = \frac{1}{\pi}\frac{\sqrt{2m^*}}{\hbar}\frac{1}{\sqrt{E}} = \frac{\sqrt{2}}{\pi}\frac{(0.067\times 9.11\times 10^{-31}\,kg)^{1/2}(1.6\times 10^{-19}\,J/eV)^{1/}}{(1.055\times 10^{-34}\,J\cdot s)\sqrt{E(eV)}(10^2\,cm}$

$= 4.22\times 10^6\frac{1}{\sqrt{E}}\,eV^{-1}cm^{-1}$



d) value of Fermi level at T=0K for electron concentration

3D: $n = 10^{18}\,cm^{-3}$

electron state density: $n = 2\frac{1}{L^3}\frac{4\pi k^3}{3}\frac{1}{(2\pi/L)^3} = \frac{k^3}{3\pi^2} = \frac{1}{3\pi^2}\left(\frac{2m^*E}{\hbar^2}\right)^{3/}$

Fermi level: $E_f = \frac{\hbar^2}{2m^*}(3\pi^2 n)^{2/3}$

$= \frac{(1.055\times 10^{-34}\,J\cdot s)^2}{2(0.067\times 9.11\times 10^{-31})}\left(3\pi^2\times 10^{18}\,cm^{-3}\times 10^6\frac{cm^{-3}}{m^3}\right)^{2/3}\frac{eV}{1.6\times 10^{-}}$

$\boxed{E_f = 0.0545\,eV}$

2D: $n = 10^{12}\,cm^{-2}$ $\qquad n = \frac{m^*E}{\pi\hbar^2}$

Fermi level: $E_f = \frac{\pi\hbar^2}{m^*}n$

$= \frac{\pi(1.055\times 10^{-34}\,J\cdot s)^2(10^{12}\,cm^{-2}\times 10^4\frac{cm^2}{m^2})}{(0.067\times 9.11\times 10^{-31}\,kg)(1.6\times 10^{-19}\,J/eV)}$

$\boxed{E_f = 0.0358\,eV}$

1D: $n = 10^6\ cm^{-1}$ $\qquad n = \frac{2}{\pi}\sqrt{\frac{2m^*E}{\hbar^2}}$

$$E_f = \frac{\hbar^2}{2m^*}\left(\frac{\pi}{2}n\right)^2 = \frac{(1.055\times10^{-34}\,J\cdot s)^2\,\pi^2\,(10^6\,cm^{-1}\,10^2\,\frac{cm}{m})^2}{8\,(0.067\times9.11\times10^{-31}\,kg)(1.6\times10^{-19}\,J/eV)} = \boxed{0.0141\ eV}$$

e) plot the function $f(E)D(E)$ versus energy E at $T = 300K$.

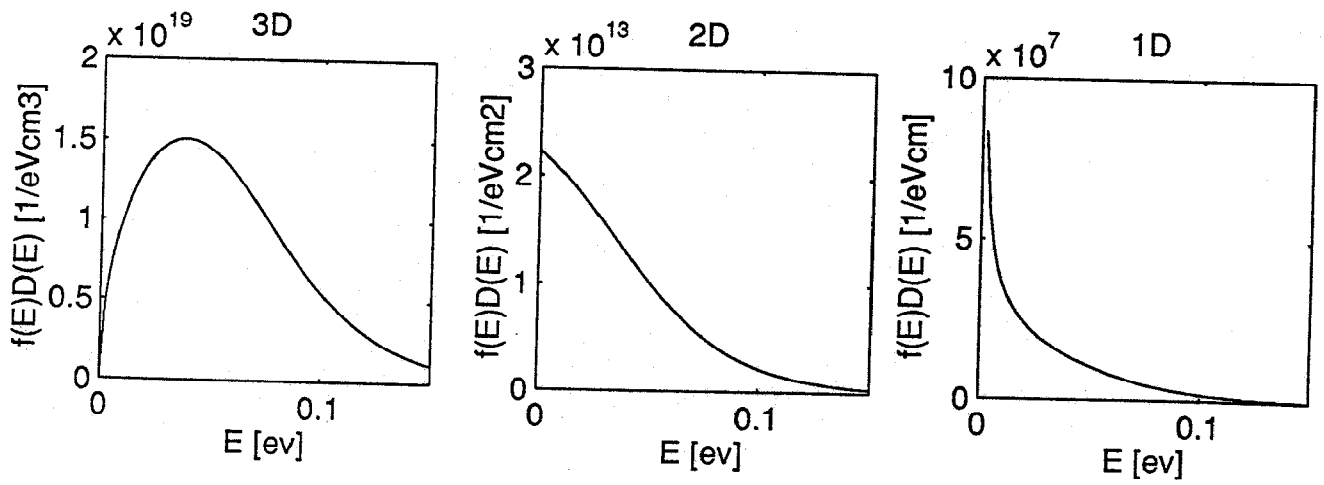
3D: $f(E)D(E) = \frac{\sqrt{2}\,m^{*3/2}}{\pi^2\hbar^3}\frac{\sqrt{E}}{(e^{(E-E_f)/kT}+1)}$

2D: $f(E)D(E) = \frac{m^*}{\pi\hbar^2}\frac{1}{(e^{(E-E_f)/kT}+1)}$

1D: $f(E)D(E) = \frac{\sqrt{2m^*}}{\pi\hbar}\frac{1}{\sqrt{E}\,(e^{(E-E_f)/kT}+1)}$

at $T = 300K$
$kT = (8.62\times10^{-5}\,eV/K)(300$
$= 0.0259\,eV$

using results of parts c) and d):



From the plots, it is apparent that as the dimensionality is reduced, $f(E)D(E)$ at the band edge ($E=0$) gets larger and has a narrower width. For semiconductor lasers this means a narrower laser linewidth and higher gain.

6) energies within bandgap → states with complex k-value

nearly-free electron model with

$$V(x) = -2u\cos\left(\frac{2\pi x}{a}\right) = -u\left(e^{\frac{i2\pi x}{a}} + e^{-\frac{i2\pi x}{a}}\right)$$

same form as: $V(x) = \sum u_n e^{iGx}$ here: $G = \pm 2\pi/a$

$u_n = -u$

nearly-free electron model: $V(x) = \sum_G u_G e^{iGx}$

$$\rightarrow \quad \psi(x) = u_k(x) e^{ikx} = \sum_k c(k) e^{ikx}$$

Central equation: $(\varepsilon_k - E)c(k) + \sum_G u_G c(k-G) = 0$

$\varepsilon_k = \frac{\hbar^2 k^2}{2m}$ $\qquad (\varepsilon_k - E)c(k) + u_G c(k-G) = 0$

E-eigenvalues $\qquad (\varepsilon_{k-G} - E)c(k-G) + u_G c(k) = 0$

rewrite
$$\begin{bmatrix} \varepsilon_k - E & u_G \\ u_G & \varepsilon_{k-G} - E \end{bmatrix} \begin{bmatrix} c(k) \\ c(k-G) \end{bmatrix} = 0$$

solutions exist when
$$\begin{vmatrix} \varepsilon_k - E & u_G \\ u_G & \varepsilon_{k-G} - E \end{vmatrix} = 0$$

$$(\varepsilon_k - E)(\varepsilon_{k-G} - E) - u_G^2 = 0$$
$$E^2 - (\varepsilon_k + \varepsilon_{k-G})E + \varepsilon_k \varepsilon_{k-G} - u_G^2 = 0$$

$$E = \frac{1}{2}(\varepsilon_k + \varepsilon_{k-G}) \pm \sqrt{\frac{\varepsilon_k^2 + 2\varepsilon_k\varepsilon_{k-G} + \varepsilon_{k-G}^2}{4} - \varepsilon_k\varepsilon_{k-G} + u_G^2}$$

$$E = \frac{1}{2}(\varepsilon_k + \varepsilon_{k-G}) \pm \sqrt{\left(\frac{\varepsilon_k - \varepsilon_{k-G}}{2}\right)^2 + u_G^2}$$ energy eigenvalues

k is complex: $k = k_R + ik_I$ where $k_I = \mathrm{Im}\, k$ (Im k small at the boundary of the first Brillouin zone:

$k_R = \frac{G}{2} \quad \Longrightarrow \quad k = \frac{G}{2} + ik_I$

$k - G = -\frac{G}{2} + ik_I$

$$\varepsilon_k = \frac{\hbar^2}{2m}k^2 = \frac{\hbar^2}{2m}\left(\left(\frac{G}{2}\right)^2 + iGk_I - k_I^2\right)$$
$$\varepsilon_{k-G} = \frac{\hbar^2}{2m}\left(\left(\frac{-G}{2}\right)^2 - iGk_I - k_I^2\right)$$

$$\frac{\varepsilon_k + \varepsilon_{k-G}}{2} = \frac{\hbar^2}{2m}\left(\frac{G^2}{4} - k_I^2\right) \qquad \frac{\varepsilon_k - \varepsilon_{k-G}}{2} = \frac{i\hbar^2}{2m}Gk_I$$

energy eigenvalues: $E = \frac{\hbar^2}{2m}\left(\frac{G^2}{4} - k_I^2\right) \pm \sqrt{\left(\frac{\hbar^2}{2m}Gk_I\right)^2 + u_G^2}$

at midgap: $\sqrt{u_G^2 - \left(\frac{\hbar^2 G k_I}{2m}\right)^2} = 0$

$$u_G^2 = \left(\frac{\hbar^2 G k_I}{2m}\right)^2$$

$$k_I^2 = \left(\frac{2m}{\hbar^2}\frac{u_G}{G}\right)^2 = \boxed{\left(\frac{2m}{\hbar^2}\frac{u}{G}\right)^2 = (\mathrm{Im}\, k)^2}$$

physical interpretation:

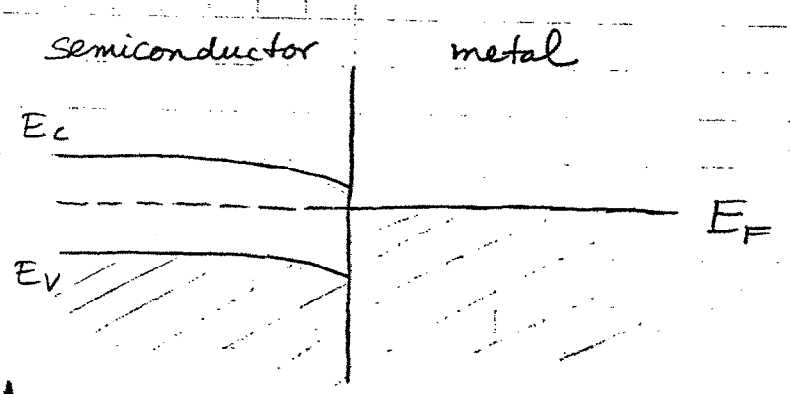
electron wavefunction $\psi(x) = \sum_k C(k) e^{ikx}$

k complex: $k = k_R + i k_I \Rightarrow \psi(x) = \sum_k C(k) e^{ik_R x} e^{-k_I x}$

The imaginary part of the k-vector is responsible for exponential decay of the wavefunction (evanescent waves) while purely real k-vectors correspond to periodic solutions (standing waves). Real k-vectors are allowed in the bulk material while complex k-vectors (with $\mathrm{Im}\, k > 0$) are allowed within bandgaps.

metal/semiconductor interface:

standing wave solutions within metal (no bandgaps)
decaying exponential solutions within semiconductor (within bandgap)



band diagram
- depends on electron affinities of specific metal/semiconductor