Departments of ECE and MSE, Cornell University

ECE 4070/MSE 5470: Physics of Semiconductor and Nanostructures

Spring 2015

Homework 9: Solutions

Problem 9.1 (Electron velocity saturation at high fields in semiconductors)

(Problem 9.1)

(A) – $\boxed{\underbrace{\frac{dE}{dt}}_{\text{change}} = \underbrace{eFv}_{\text{gain from electric field}} - \underbrace{\frac{\hbar\omega_{op}}{\tau_E}}_{\text{loss to phonons.}}}$ Rate of change of electron energy

(B) – $\boxed{\underbrace{\frac{dp}{dt}}_{\text{change}} = \underbrace{eF}_{\text{increase due to electric force}} - \underbrace{\frac{p}{\tau_m}}_{\text{momentum scattering.}}}$ Rate of change of electron momentum

@ steady state, $\frac{d}{dt}(\ldots) = 0$. (A) gives $eFv = \frac{\hbar\omega_{op}}{\tau_E}$

$(p = m^* v)$ (B) gives $eF = \frac{m^* v}{\tau_m}$

Divide to get

$$v^2 = \frac{\hbar\omega_{op}}{m^*}\frac{\tau_m}{\tau_E} \Rightarrow \boxed{v = \sqrt{\frac{\hbar\omega_{op}}{m^*}} \cdot \sqrt{\frac{\tau_m}{\tau_E}}}$$

Problem 9.2 (Electron Scattering and Mobility)

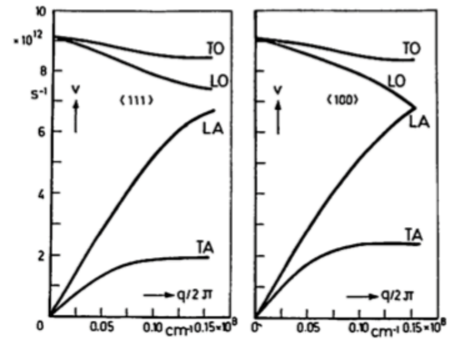
(a) Acoustic phonon scattering:

Phonons in Semiconductors

$$
\begin{aligned}
u_s(x,t) &= u_0 e^{i(\beta x-\omega t)} + u_0 e^{-i(\beta x-\omega t)} \\
|u_s|^2 &= 4u_0^2\cos(\beta x-\omega t) \\
\mathrm{KE} = \frac{1}{2}M\left(\frac{du_s}{dt}\right)^2 &= 2M\omega^2 u_0^2 \sin^2(\beta x-\omega t) \\
\mathrm{PE} = \frac{1}{2}K u_s^2 &= 2K u_0^2 \cos^2(\beta x-\omega t) \\
\text{but}\ldots \omega^2 &= \frac{K}{M} \rightarrow \\
\mathrm{KE} + \mathrm{PE} = 2M\omega^2 u_0^2 &= N_\omega \cdot \hbar\omega \rightarrow \\
\text{since}\ldots M &= \rho V,
\end{aligned}
$$

$$
\boxed{u_0^2 = \frac{\hbar}{2\omega\rho V}\cdot N_\omega}
$$

$$
\boxed{N_\omega(T) = \frac{1}{e^{\frac{\hbar\omega}{kT}} - 1}}
$$



Typical phonon spectra of semiconductors

Vibration amplitude as a function of the temperature: Quantum-Classical connection of the phonon harmonic oscillator

The above is the way you can find the amplitude of phonon vibrations at a temperature T for feeding into the golden rule calculation of the scattering rates.

Electron-Def. Pot. Acoustic Phonon interaction

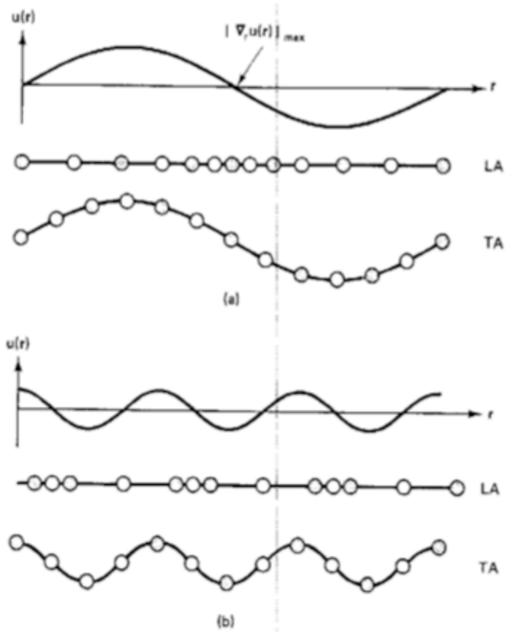


Figure 6.2 Displacements of a diatomic chain for LA and TA phonons at (a) the center and (b) the edge of the Brillouin zone. The lighter mass atoms are indicated by open circles. For zone edge acoustic phonons only the heavier atoms are displaced.

Deformation Potential Acoustic Phonon Scattering Potential

$$\mathbf{u}(\mathbf{r}, t) = \mathbf{a}u(\mathbf{r}, t) \tag{6.4}$$

where

$$u(\mathbf{r}, t) = u \exp[i(\mathbf{q}_s \cdot \mathbf{r} - \omega_s t)] \tag{6.5}$$

In these equations $\mathbf{a}$ is the displacement direction, and u is the amplitude. The strain associated with the displacement is

$$\nabla \cdot \mathbf{u}(\mathbf{r}, t) = \mathbf{a} \cdot \nabla u(\mathbf{r}, t) \tag{6.6}$$

$$\nabla \cdot \mathbf{u}(\mathbf{r}, t) = i\mathbf{q}_s \cdot \mathbf{a}u(\mathbf{r}, t) \tag{6.7}$$

Equation (6.7) indicates that for the transverse components of a phonon where the displacement and the wavevector are orthogonal, $\mathbf{q}_s \cdot \mathbf{a} = 0$, and no strain is produced. The scattering potential for the longitudinal component is, therefore,

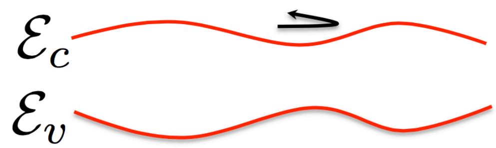
$$\boxed{\Delta U(\mathbf{r}, t) = \mathscr{E}_A \nabla \cdot \mathbf{u}(\mathbf{r}, t)} \tag{6.8}$$

where the *deformation potential*, $\mathscr{E}_A$, in units of energy, is defined as the proportionality constant between the scattering potential (units of energy) and the strain.

This is how the deformation potential scattering potential is found.

Electron-Acoustic Phonon interaction: Mobility

Acoustic phonon scattering



$$\delta \boldsymbol{r} = A_l \exp[\pm \mathrm{i}(\boldsymbol{q}_l \cdot \boldsymbol{r})],$$

$$|H_{k'k}| = \frac{\varepsilon_{ac} q_l A_l}{V} \left|\int \exp[\mathrm{i}(\boldsymbol{k} - \boldsymbol{k}' \pm \boldsymbol{q}_l)\cdot \boldsymbol{r}]\, d^3r\right|$$

$$\boldsymbol{k}' = \boldsymbol{k} \pm \boldsymbol{q}_l$$

$$2M\omega^2 u_0^2 \approx N_{ph} \times \hbar\omega$$

$$|H_{k'k}| = \varepsilon_{ac} q_l A_l .$$

$$\boxed{A_l \to \left|\int \psi^*_{N\pm 1}\, x\, \psi_N\, d^3r\right| = \begin{cases} (N\hbar/2M\omega_l)^{1/2} & \text{for } N \to N-1 \\ ((N+1)\hbar/2M\omega_l)^{1/2} & \text{for } N \to N+1 \end{cases}.}$$

SHO: |amplitude|^2 ~ number of phonons

$$\boxed{N \to N_q = [\exp(\hbar\omega_l/k_B T) - 1]}$$

$$S \approx \frac{2\pi}{\hbar} |H_{k'k}|^2 [\delta(\varepsilon(\boldsymbol{k}') - \varepsilon(\boldsymbol{k}) + \hbar\omega_l) + \delta(\varepsilon(\boldsymbol{k}') - \varepsilon(\boldsymbol{k}) - \hbar\omega_l)]$$

$$\approx 2\frac{2\pi}{\hbar} |H_{k'k}|^2 \delta[\varepsilon(\boldsymbol{k}') - \varepsilon(\boldsymbol{k})] .$$

absorption~emission

$$|H_{k\pm q,k}| = \varepsilon_{ac} q_l [(N_q + 1/2 \mp 1/2)\hbar/2\varrho V\omega_l]^{1/2} .$$

$$c_l = \rho v_s^2$$

$$|H_{k'k}| = \varepsilon_{ac} q_l [k_B T/2\varrho V\omega_l^2]^{1/2} = \varepsilon_{ac} [k_B T/2Vc_l]^{1/2}$$

Deformation potential

$$\Delta U(\mathbf{r}, t) = \mathscr{E}_A \nabla\cdot\mathbf{u}(\mathbf{r}, t)$$

$$\mu = \frac{2\sqrt{2\pi}}{3} \frac{e\hbar^4 c_l}{m^{5/2}(k_B)^{3/2}\varepsilon_{ac}^2} T^{-3/2}$$

which in units of $cm^2/V\,s$ is given by

$$\mu = 3.06 \times 10^4 \frac{c_l/10^{12}\ \mathrm{dyn\ cm^{-2}}}{(m/m_0)^{5/2}(T/100\ \mathrm{K})^{3/2}(\varepsilon_{ac}/\mathrm{eV})^2} \propto T^{-3/2} .$$

$$\boxed{K^2 = \frac{e_{pz}^2/c_l}{\varkappa\varkappa_0 + e_{pz}^2/c_l} .}$$

Coupling K ~10^{-3}

Piezoelectric

$$\Delta U(\mathbf{r}, t) = \frac{iqe_{pz}}{\epsilon(0)q_s} \nabla\cdot\mathbf{u}(\mathbf{r}, t)$$

$$\mu = \frac{16\sqrt{2\pi}}{3} \frac{\hbar^2 \varkappa\varkappa_0}{m^{3/2} e K^2 (k_B T)^{1/2}} \propto T^{-1/2}$$

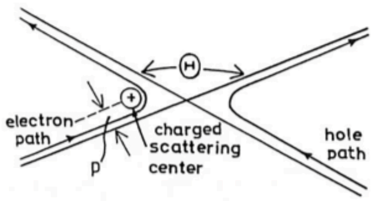
and in units of $cm^2/V\,s$

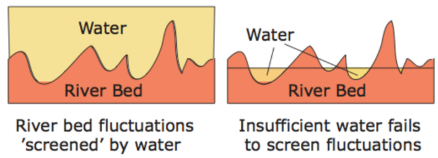
$$\mu = 2.6 \frac{\varkappa}{(m/m_0)^{3/2} K^2 (T/100\ \mathrm{K})^{1/2}} .$$

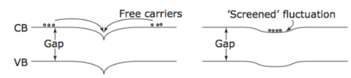
The left method is how the scattering rate is found from the scattering potential.

(b) Ionized impurity scattering rate:

Scattering by charged impurities







Screened coulomb scattering potential

$$\boxed{V(r) = -(Z|e|/4\pi\varkappa\varkappa_0 r)\exp(-r/L_D)}$$

$$\begin{aligned} H_{k'k} &= -\frac{Z e^2}{V\varkappa\varkappa_0 |\boldsymbol{k}-\boldsymbol{k}'|}\int_0^\infty \exp(-r/L_D)\sin(|\boldsymbol{k}-\boldsymbol{k}'|\,r)\,dr \\ &= -\frac{Z e^2}{V\varkappa\varkappa_0}\frac{1}{|\boldsymbol{k}-\boldsymbol{k}'|^2 + L_D^{-2}} \approx -\frac{Z e^2}{V\varkappa\varkappa_0 4k^2}\frac{1}{\sin^2(\theta/2)+(2kL_D)^{-2}}, \end{aligned} \qquad (6.3.13)$$

$$|\boldsymbol{k}-\boldsymbol{k}'| \approx 2k\sin(\theta/2)$$

$$\boxed{\beta_{BH} = 2\frac{m}{\hbar}\left(\frac{2}{m}3k_BT\right)^{1/2} L_D}$$

$$\beta_{BH} = \left(\frac{\varkappa}{16}\right)^{1/2}\frac{T}{100\ \text{K}}\left(\frac{m}{m_0}\right)^{1/2}\left(\frac{2.08\times10^{18}\ \text{cm}^{-3}}{n}\right)^{1/2}$$

Brooks-Herring dimensionless factor

The mobility $\mu = (e/m)\langle\tau_m\rangle$ is given by

$$\boxed{\mu = \frac{2^{7/2}(4\pi\varkappa\varkappa_0)^2(k_BT)^{3/2}}{\pi^{3/2}Z^2e^3m^{1/2}N_I\left[\ln(1+\beta_{BH}^2) - \beta_{BH}^2/(1+\beta_{BH}^2)\right]}}$$

which in units of cm²/V s is

$$\mu = \frac{3.68\times10^{20}\ \text{cm}^{-3}}{N_I}\frac{1}{Z^2}\left(\frac{\varkappa}{16}\right)^2\left(\frac{T}{100\ \text{K}}\right)^{1.5} \cdot \frac{1}{(m/m_0)^{1/2}\left[\log(1+\beta_{BH}^2) - 0.434\,\beta_{BH}^2/(1+\beta_{BH}^2)\right]}$$

and the log is to the base 10.

Problem 9.3 (Optical absorption in graphene)

a+b) Use the expression from the handouts except that integration is now over 2D k-space and an extra factor of two comes in because of the two pockets in the FBZ:

$$R_{\uparrow} = \frac{2\pi}{\hbar}\left(\frac{eA_o}{2m}\right)^2 \left\langle \left|\vec{P}_{cv} \, . \, \hat{n}\right|^2 \right\rangle \; 4\times\int \frac{d^2\vec{k}}{(2\pi)^2} \;\; \delta\left(E_c\left(\vec{k}\right) - E_v\left(\vec{k}\right) - \hbar\omega\right)$$

$$= \frac{2\pi}{\hbar}\left(\frac{e}{2m}\right)^2 \left(\frac{2\eta_o I_{inc}}{\omega^2}\right) \left\langle \left|\vec{P}_{cv} \, . \, \hat{n}\right|^2 \right\rangle \; 4\times\int \frac{d^2\vec{k}}{(2\pi)^2} \;\; \delta\left(E_c\left(\vec{k}\right) - E_v\left(\vec{k}\right) - \hbar\omega\right)$$

$$= \frac{2\pi}{\hbar}\left(\frac{e}{2m}\right)^2 \left(\frac{2\eta_o I_{inc}}{\omega^2}\right) \frac{m^2 v^2}{2} \; 4\times\int_0^{\infty} \frac{k\,dk}{(2\pi)} \delta(2\hbar v k - \hbar\omega)$$

$$= \frac{e^2}{4\hbar}\eta_o\left(\frac{I_{inc}}{\hbar\omega}\right)$$

c) Incident photon flux per unit area is, $I_{inc}/\hbar\omega$. The photon absorption rate per unit area is $R_{\uparrow}$. Therefore, the fraction of incident photons absorbed in the graphene sheet is,

$\hbar\omega\, R_{\uparrow} \big/ I_{inc} = \left(e^2/4\hbar\right)\eta_o \approx .023$.

It follows that ~2.3% of the incident photons are absorbed by graphene through interband transitions (irrespective of the wavelength!).

Problem 9.4 (Population inversion, optical gain, and lasing)

(a)

$$E_c(\mathbf{k}) = E_g + \frac{\hbar^2 k^2}{2m_e^\star}$$

$$E_v(\mathbf{k}) = -\frac{\hbar^2 k^2}{2m_h^\star}$$

$$E_c(\mathbf{k}) - E_v(\mathbf{k}) = E_g + \frac{\hbar^2 k^2}{2m_r^\star}$$

$$\frac{1}{m_r^\star} = \frac{1}{m_e^\star} + \frac{1}{m_h^\star}$$

first assume $f_v(k)=1$, $f_c(k)=0$

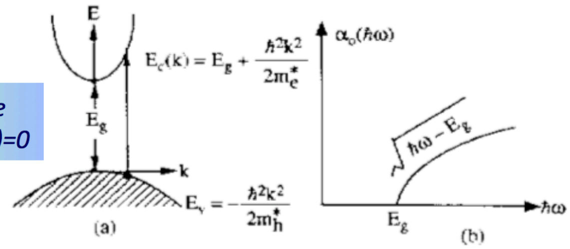


Figure 9.5 (a) Optical absorption in a direct-band-gap semiconductor. (b) The absorption spectrum due to the interband transitions.

$$\alpha_0(\hbar\omega) = C_0|\hat{e}\cdot\mathbf{p_{cv}}|^2 \times (g_s g_v) \times \int_{\mathbf{k}} \frac{d^3\mathbf{k}}{(2\pi)^3}\delta[E_c(\mathbf{k}) - (E_v(\mathbf{k}) + \hbar\omega)]$$

$$\boxed{\begin{aligned} \alpha_0(\hbar\omega) &= C_0|\hat{e}\cdot\mathbf{p_{cv}}|^2 \cdot \rho_r(\hbar\omega - E_g) \\ \rho_r(u) &= g_s g_v \cdot \frac{1}{(2\pi)^2}\cdot\left(\frac{2m_r^\star}{\hbar^2}\right)^{\frac{3}{2}}\cdot\sqrt{u} \\ C_0 &= \frac{\pi e^2}{n_r c\varepsilon_0 m_0^2\omega} \end{aligned}}$$

Optical absorption coeff. of bulk semiconductor (general form applicable to quantum wells, etc…)

"Joint" density of states of (VB,CB)

This and next few slides: From: S. L. Chuang's textbook

The above shows the equilibrium absorption coefficient of a 3D semiconductor.

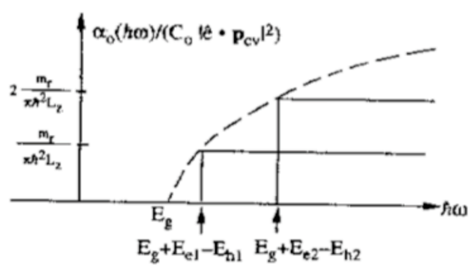


Figure 9.7. The stepwise absorption spectrum for a quantum-well structure.

$$\frac{\alpha_0(\hbar\omega)}{C_0|\hat{e}\cdot\mathbf{p}_{cv}|^2} = \begin{cases} \dfrac{m_r}{\pi\hbar^2 L_z} & \text{for } E_{h1}^{e1} < \hbar\omega < E_{h2}^{e2} \\ 2\dfrac{m_r}{\pi\hbar^2 L_z} & \text{for } E_{h2}^{e2} < \hbar\omega < E_{h3}^{e3} \\ 3\dfrac{m_r}{\pi\hbar^2 L_z} & \text{for } E_{h3}^{e3} < \hbar\omega < E_{h4}^{e4} \\ \text{etc.} & \end{cases}$$

Equilibrium absorption coefficient in QW is proportional to the joint DOS and has 2D subband features

$$\alpha(\hbar\omega) = \alpha_0(\hbar\omega)[f_v^m(E_t = \hbar\omega - E_{hm}^{en}) - f_c^n(E_t = \hbar\omega - E_{hm}^{en})]$$

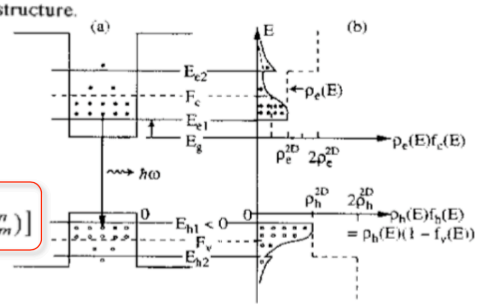
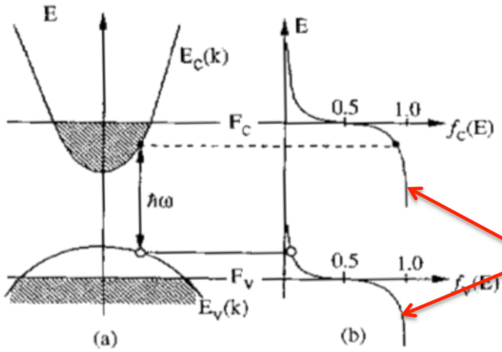


Figure 9.8. (a) Population inversion in a quantum well such that $F_c - F_v > \hbar\omega > E_g + E_{e1} - E_{h1}$. Here F_c is measured from the valence band edge where the energy level is chosen to be zero. (b) The products of the density of states and the occupation probability for electrons in the conduction band $\rho_e(E)f_c(E)$ and holes in the valence band $\rho_h(E)f_h(E) = \rho_h(E)[1 - f_v(E)]$ are plotted vs. the energy E in the vertical scale.

The above is the absorption spectrum of a 2D quantum well. Because of the quantization, and the constant 2D DOS, the joint optical DOS is in steps for every subband of the quantum well.

(b, c, d):



Non-equilibrium Fermi-Dirac functions with electron quasi-Fermi levels (note: not necessary to talk about holes here)
F_c: Conduction Band quasi-Fermi level
F_v: Valence Band quasi-Fermi level

$$f_v(\mathbf{k}) = \frac{1}{1 + e^{(E_v(\mathbf{k}) - F_v)/k_B T}}$$

$$f_c(\mathbf{k}) = \frac{1}{1 + e^{(E_c(\mathbf{k}) - F_c)/k_B T}}$$

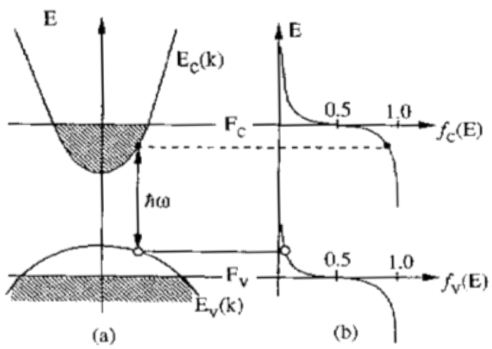
$$\alpha(\hbar\omega) = C_0 |\hat{e} \cdot \mathbf{p_{cv}}|^2 \times (g_s g_v) \times \int_{\mathbf{k}} \frac{d^3\mathbf{k}}{(2\pi)^3} \delta[E_g + \frac{\hbar^2 k^2}{2m_r^\star} - \hbar\omega] \times [f_v(\mathbf{k}) - f_c(\mathbf{k})]$$

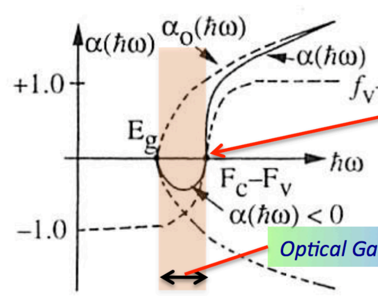
Non-equilibrium absorption coefficient

$$\boxed{\alpha(\hbar\omega) = \alpha_0(\hbar\omega) \times [f_v(k_0) - f_c(k_0)]}$$

$$k_0 = \sqrt{\frac{2m_r^\star}{\hbar^2}(\hbar\omega - E_g)}$$

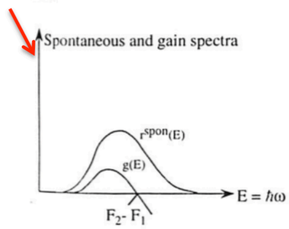
Fundamental result for understanding LEDs and LASERs





Optical transparency!!

Optical Gain!!



$$\boxed{\alpha(\hbar\omega) = \alpha_0(\hbar\omega) \times [f_v(k_0) - f_c(k_0)]} \quad k_0 = \sqrt{\frac{2m_r^\star}{\hbar^2}(\hbar\omega - E_g)}$$

$$f_v(k_0) - f_c(k_0) = \frac{\exp\left(\frac{E_c - F_c}{kT}\right) - \exp\left(\frac{E_v - F_v}{kT}\right)}{[1 + \exp\left(\frac{E_v - F_v}{kT}\right)][1 + \exp\left(\frac{E_c - F_c}{kT}\right)]} < 0 \rightarrow$$

$$\exp\left(\frac{E_c - F_c}{kT}\right) < \exp\left(\frac{E_v - F_v}{kT}\right)$$

$$\boxed{F_c - F_v > E_c - E_v = \hbar\omega}$$

Bernard-Duraffourg inversion condition

The inversion conditions can be achieved by
- *Optical pumping (gas lasers), or*
- *Electrical pumping (semiconductor LEDs & Lasers)*

A laser requires a light emitter to be placed in a high-finesse (hi-Q) optical cavity to amplify a specific mode.

(e) One can achieve population inversion in a quantum well with a lower threshold current than in a bulk semiconductor because the DOS in a QW is lower, so filling them with less carriers raises their Fermi-levels more.

Problem 9.5 (Superconductivity)

The microscopic (BCS) theory of superconductivity turned out to essentially non-perturbative, because the Schrodinger equation solution of the Cooper pair problem needs an exact solution for the "ground state" of the system. The bound state energy of the Cooper pair problem is of the form $\Delta \sim \hbar\omega_D \cdot \exp[-\frac{1}{V_0 g(E_F)}]$, where $\hbar\omega_D$ is the Debye energy of the crystal, $g(E_F)$ is the DOS at the Fermi energy, and V_0 is the weak attractive perturbation potential. This is of the functional form $f(x) = \exp[-\frac{1}{x}]$: this function does not have a Taylor series expansion. In that sense it is non-perturbative.