Full Wave Electromagnetics for Simulating Terahertz Quantum Well Laser Diode Modulation

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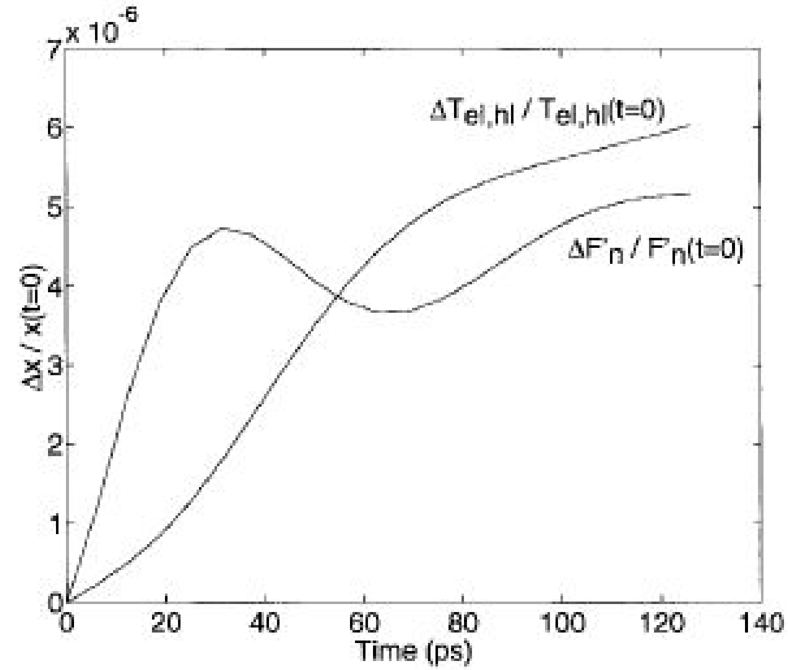
Outline

- Brief background
  - carrier heating bottleneck to direct current modulation
  - Bloch equation analysis of plasma heating by radiation
- New self-consistent simulation of plasma heating effect
  - full wave electromagnetics
  - Fermi gas thermodynamics
- Delaunay/Voronoi Surface Integration (DVSI)
  - curl operators in Ampere's and Faraday's laws
  - divergences in electrostatics, charge, and energy conservation (i.e. box integration)
- Simulate plasma heating modulation of single QW laser structure
  - electrical current pumping to achieve lasing
  - patch antenna like structure to inject high frequency radiation
- Summary

Current Injection Gain Saturation by Dual Modulation

- Both Fermi level & temperature fluctuate
  - Gorfinkel & Luryi
  - Grupen & Hess
- Quantum mechanical tunneling injection
  - decreases heating
  - decreases pumping efficiency
  - Bhattacharya & Ghosh
- Plasma heating
  - Bloch equation analysis
    - carrier density
    - energy density
    - over estimates heat capacity of degenerate Fermi gas
    - modulation depth saturation with increasing field intensity
    - Ning et al.; Li & Ning; Chow et al.
  - self-consistent EM & nonlinear charge transport
    - Maxwell's full wave vector field theory
    - Boltzmann's equation solved for a Fermi gas

M. Grupen and K. Hess, *IEEE JQE* **34** 120, 1998.



Classical Theory of Electromagnetics

electrostatic Gauss's Law

$$\nabla \cdot \varepsilon \mathbf{E} = q\left(p - n + N_D^+ - N_A^-\right)$$

magnetostatic Gauss's Law

$$\nabla \cdot \mu \mathbf{H} = 0$$

Ampere's Law

$$\nabla \times \mathbf{H} = q\left(\mathbf{J}_p - \mathbf{J}_n\right) + \frac{\partial \varepsilon \mathbf{E}}{\partial t}$$

Faraday's Law

$$\nabla \times \mathbf{E} = -\frac{\partial \mu \mathbf{H}}{\partial t}$$

electron continuity

$$-\frac{\partial n}{\partial t} = \nabla \cdot \mathbf{J}_n + U_{SRH}$$

hole continuity

$$-\frac{\partial p}{\partial t} = \nabla \cdot \mathbf{J}_p + U_{SRH}$$

electron energy conservation

$$-\frac{\partial E_n}{\partial t} = q\mathbf{E} \cdot \mathbf{J}_n + \nabla \cdot \mathbf{S}_n^{tot} + \left\langle E_n^{kin} \right\rangle U_{SRH} + n\frac{F_{3/2}}{F_{1/2}}\left(\frac{kT_n - kT_{lat}}{\tau_n}\right)$$

hole energy conservation

$$-\frac{\partial E_p}{\partial t} = -q\mathbf{E} \cdot \mathbf{J}_p + \nabla \cdot \mathbf{S}_p^{tot} + \left\langle E_p^{kin} \right\rangle U_{SRH} + p\frac{F_{3/2}}{F_{1/2}}\left(\frac{kT_p - kT_{lat}}{\tau_p}\right)$$

lattice energy conservation

$$-\rho C_p \frac{\partial T_{lat}}{\partial t} = \nabla \cdot \kappa \nabla T_{lat} - \mathbf{E}_{applied} \cdot q(\mathbf{J}_p - \mathbf{J}_n)$$

Defining Field Components

- Two vector fields and four field equations
- Decompose field flux densities into orthogonal functionals

$$\varepsilon\mathbf{E} = -\varepsilon\left(\frac{\partial\mathbf{A}}{\partial t} + \nabla\psi\right) = \varepsilon\left(\mathbf{E}_{rot} + \mathbf{E}_{irr}\right)$$

$$\nabla\times\mathbf{E} = -\nabla\times\left(\frac{\partial\mathbf{A}}{\partial t} + \nabla\psi\right) = -\nabla\times\frac{\partial\mathbf{A}}{\partial t} = \nabla\times\mathbf{E}_{rot}$$

$$\nabla\cdot\varepsilon\mathbf{E} = -\nabla\cdot\varepsilon\left(\frac{\partial\mathbf{A}}{\partial t} + \nabla\psi\right) = -\nabla\cdot\varepsilon\nabla\psi = \nabla\cdot\varepsilon\mathbf{E}_{irr}$$

→ equivalent to Coulomb gauge for $\nabla\varepsilon = 0$

from Faraday's Law and the vector potential →

$$\mu\mathbf{H} = \nabla\times\mathbf{A}$$

$$\nabla\cdot\mu\mathbf{H} = \nabla\cdot\left(\nabla\times\mathbf{A}\right) = 0$$

$$\nabla\times\mathbf{H} = \nabla\times\left(\frac{1}{\mu}\nabla\times\mathbf{A}\right) = \nabla\times\mathbf{H}_{rot}$$

Defining Charge & Energy Densities

$$n = \frac{\sqrt{2} m_n^{3/2}}{\pi^2 \hbar^3} \int_{E_C}^{\infty} \frac{\sqrt{E - E_C}}{\exp\left(\frac{E - F_n}{kT}\right) + 1} dE = \frac{\sqrt{2} m_n^{3/2}}{\pi^2 \hbar^3} (kT)^{3/2} \int_0^{\infty} \frac{\sqrt{\varepsilon}}{e^{\varepsilon - \eta_n} + 1} d\varepsilon = N_C (kT)^{3/2} F_{1/2}(\eta_n)$$

$$E_n = \frac{\sqrt{2} m_n^{3/2}}{\pi^2 \hbar^3} \int_{E_C}^{\infty} \frac{(E - E_C)^{3/2}}{\exp\left(\frac{E - F_n}{kT}\right) + 1} dE = \frac{\sqrt{2} m_n^{3/2}}{\pi^2 \hbar^3} (kT)^{5/2} \int_{E_C}^{\infty} \frac{\varepsilon^{3/2}}{e^{\varepsilon - \eta_n} + 1} d\varepsilon = N_C (kT)^{5/2} F_{3/2}(\eta_n)$$

$$F_j(\eta_n) = F_j\left(\frac{F_n - E_C}{kT_n}\right) = \int_0^{\infty} \frac{\varepsilon^j}{e^{\varepsilon - \eta_n} + 1} d\varepsilon$$

Michele Goano, “Algorithm 745: Computation of the Complete and Incomplete Fermi-Dirac Integral,” *ACM Trans. Math. Software*, vol. 21, no. 3, Sept. 1995, pp. 221-232

Bulk Charge Fluxes: 1st Moment of Boltzmann Equation

$$\frac{1}{4\pi^3}\int_{-\infty}^{\infty}\mathbf{v}\left\{f+\tau\frac{\partial f}{\partial t}=\frac{q\tau}{\hbar}(\mathbf{E}+\mathbf{v}\times\mathbf{B})\cdot\nabla_{\mathbf{k}}f_0-\tau\mathbf{v}\cdot\nabla f_0\right\}d\mathbf{k}$$

$$\mathbf{J}+\bar{\tau}\frac{\partial\mathbf{J}}{\partial t}=-\frac{q\langle\tau\rangle}{m_n}N_C\frac{\overline{\mathbf{M}}}{1+\mu_n^2\mathbf{B}^2}\left[(kT)^{3/2}F_{1/2}\mathbf{E}+(kT)^{3/2}F_{1/2}\nabla\left(\frac{2}{3}\frac{F_{3/2}}{F_{1/2}}\frac{kT}{q}\right)+\left(\frac{2}{3}\frac{F_{3/2}}{F_{1/2}}\frac{kT}{q}\right)\nabla(kT)^{3/2}F_{1/2}\right]$$

$$\overline{\mathbf{M}}=\begin{bmatrix}1+\mu_n^2B_x^2 & -\mu_nB_z+\mu_n^2B_xB_y & \mu_nB_y+\mu_n^2B_xB_z\\ \mu_nB_z+\mu_n^2B_xB_y & 1+\mu_n^2B_y^2 & -\mu_nB_x+\mu_n^2B_yB_z\\ -\mu_nB_y+\mu_n^2B_xB_z & \mu_nB_x+\mu_n^2B_yB_z & 1+\mu_n^2B_z^2\end{bmatrix}$$

Scharfetter-Gummel discretization

$$J_{n,net}^{1\to2}+\bar{\tau}\frac{\partial J_{n,net}^{1\to2}}{\partial t}=\left(\frac{2}{3}\frac{F_{3/2}}{F_{1/2}}\frac{kT}{q}\right)_{ave}\frac{\mu_n\overline{\mathbf{M}}}{1+\mu_n^2\mathbf{B}^2}N_C\frac{1}{L}\left[B(\xi)(kT_1)^{3/2}F_{1/2}(\eta_1)-B(-\xi)(kT_2)^{3/2}F_{1/2}(\eta_2)\right]$$

$$=J_n^{1\to2}-J_n^{2\to1}$$

$$B(\xi)=\frac{\xi}{\exp(\xi)-1}$$

$$\xi=L\left(\frac{3}{2}\frac{F_{1/2}}{F_{3/2}}\frac{q}{kT}\right)_{ave}\left[E_{1\to2}+\frac{1}{L}\Delta\left(\frac{2}{3}\frac{F_{3/2}}{F_{1/2}}\frac{kT}{q}\right)\right]$$

Bulk Energy Fluxes: 3rd Moment of Boltzmann Equation

kinetic energy and chemical work

$$\frac{1}{4\pi^3}\int_{-\infty}^{\infty}\mathbf{v}E\left\{f+\tau\frac{\partial f}{\partial t}=\frac{q\tau}{\hbar}(\mathbf{E}+\mathbf{v}\times\mathbf{B})\cdot\nabla_{\mathbf{k}}f_0-\tau\mathbf{v}\cdot\nabla f_0\right\}d\mathbf{k}$$

$$\left(\mathbf{S}_n^{kin}+\mathbf{S}_n^{work}\right)+\bar{\tau}\frac{\partial\left(\mathbf{S}_n^{kin}+\mathbf{S}_n^{work}\right)}{\partial t}=-\mu_n N_C\frac{\overline{\mathbf{M}}}{1+\mu_n^2\mathbf{B}^2}\left[\frac{5}{3}(kT)^{5/2}F_{3/2}\mathbf{E}+\frac{2}{3}\nabla\frac{(kT)^{7/2}}{q}F_{5/2}\right]$$

heat capacity

$$\frac{1}{4\pi^3}\int_{-\infty}^{\infty}\mathbf{v}C_V\left\{f+\tau\frac{\partial f}{\partial t}=\frac{q\tau}{\hbar}(\mathbf{E}+\mathbf{v}\times\mathbf{B})\cdot\nabla_{\mathbf{k}}f_0-\tau\mathbf{v}\cdot\nabla f_0\right\}d\mathbf{k}$$

$$C_V\equiv(E-F_n)\frac{d}{d(kT)}$$

$$(E-F_n)\frac{df_0}{d(kT)}=\left(\frac{E-F_n}{kT}\right)^2\frac{\exp[(E-F_n)/(kT)]}{\{\exp[(E-F_n)/(kT)]+1\}^2}$$

Discretized Energy Fluxes

Scharfetter-Gummel kinetic energy & work

$$S_{kw,net}^{1\to 2} + \bar{\tau}\frac{\partial S_{kw,net}^{1\to 2}}{\partial t} = \left(\frac{2}{3}\frac{F_{5/2}}{F_{3/2}}\frac{kT}{q}\right)_{ave}\frac{\mu_n \overline{\mathbf{M}}}{1+\mu_n^2\mathbf{B}^2} N_C \frac{1}{L}\left[B(\xi)(kT_1)^{5/2}F_{3/2}(\eta_1) - B(-\xi)(kT_2)^{5/2}F_{3/2}(\eta_2)\right]$$

$$= S_{kw}^{1\to 2} - S_{kw}^{2\to 1}$$

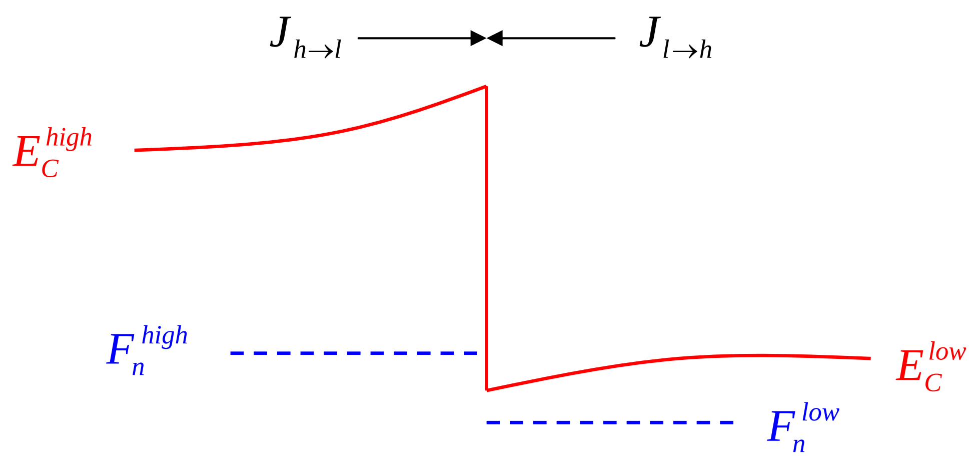
$$B(\xi) = \frac{\xi}{\exp(\xi)-1} \qquad \xi = L\left(\frac{3}{2}\frac{F_{3/2}}{F_{5/2}}\frac{q}{kT}\right)_{ave}\left[\frac{5}{3}E_{1\to 2} + \frac{1}{L}\Delta\left(\frac{2}{3}\frac{F_{5/2}}{F_{3/2}}\frac{kT}{q}\right)\right]$$

heat exchange

$$S_h^{1\to 2} - S_h^{2\to 1} = -\left[\int_{T_1}^{T_2} C_V^{1\to 2}dT - \int_{T_2}^{T_1} C_V^{2\to 1}dT\right] = -\left[\int_{T_1}^{T_2}\frac{d}{dT}\left(S_{kw}^{1\to 2} - F_{n,1}J_n^{1\to 2}\right)dT - \int_{T_2}^{T_1}\frac{d}{dT}\left(S_{kw}^{2\to 1} - F_{n,2}J_n^{2\to 1}\right)dT\right]$$

$$= \left[S_{kw}^{1\to 2} - S_{kw,T_2}^{1\to 2} - F_{n,1}\left(J_n^{1\to 2} - J_{n,T_2}^{1\to 2}\right)\right] - \left[S_{kw}^{2\to 1} - S_{kw,T_1}^{2\to 1} - F_{n,2}\left(J_n^{2\to 1} - J_{n,T_1}^{2\to 1}\right)\right]$$

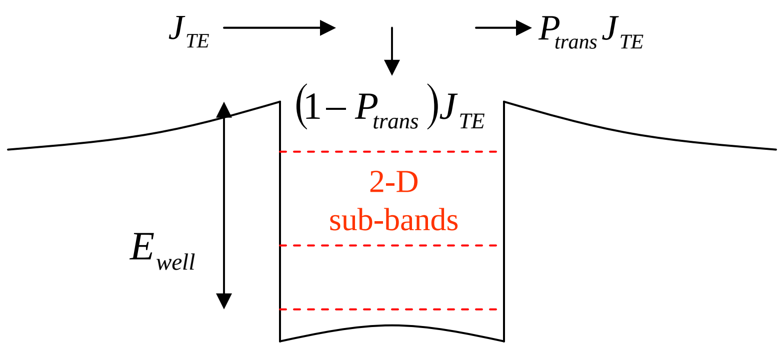
Heterojunction Flux



thermionic emission

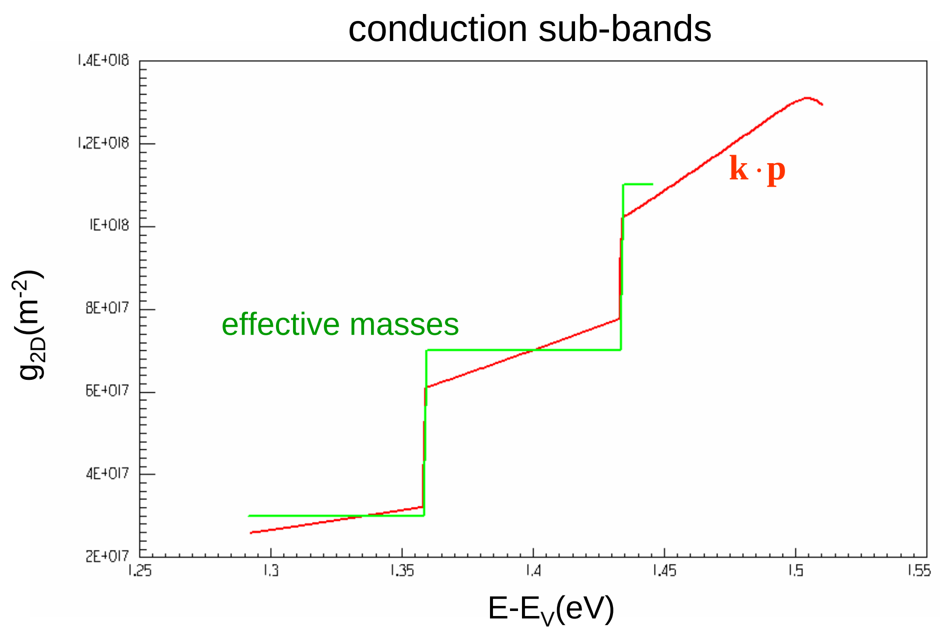
$$J_{net} = J_{h \to l} - J_{l \to h} = \frac{1}{2\pi^2} \frac{m}{\hbar^3} \left[\left(kT_n^{high} \right)^2 F_1\left(\frac{F_n^{high} - E_C^{high}}{kT_n^{high}} \right) - \left(kT_n^{low} \right)^2 F_1\left(\frac{F_n^{low} - E_C^{high}}{kT_n^{low}} \right) \right]$$

Quantum Well



$$P_{trans} = e^{-L_{QW}/L_{mean}}$$

$$L_{mean} = \tau_{scat}\sqrt{2E_{well}/m^*}$$



$$n_{2D} = \sum_j \frac{m_j^*}{\pi\hbar^2} \int_{E_j}^{\infty} \frac{1}{\exp\left(\frac{E-F_n}{T_n}\right)+1} dE$$

$$= \sum_j N_j^{(2D)} T_n F_0\left(\frac{F_n - E_j}{T_n}\right)$$

Optical Photon Emission

$$U_{spon} = \sum_m B_{c\to v} g_m^{spon} g_{red} f_c (1-f_v) \Delta E_m \qquad U_{stim} = \sum_m B_{c\to v} S_m g_m^{stim} g_{red} [f_c(1-f_v) - f_v(1-f_c)] \Delta E_m$$

$$g_{red} = \sum_i \frac{1}{\pi\hbar^2} \left(\frac{2m_{c,i}^* m_{v,i}^*}{m_{c,i}^* + m_{v,i}^*} \right) \qquad B_{c\to v} = \left(\frac{\pi q^2}{m_0^2 \varepsilon_0 \omega n^2} \right) |\mathbf{M}|^2 \qquad |\mathbf{M}|^2 = \begin{cases} \dfrac{m_0^2 E_G}{12 m_c^*} \dfrac{1+\Delta/E_G}{1+2\Delta/3E_G} = |\mathbf{M}_b|^2 & \text{bulk} \\ \left\langle |\hat{e}\cdot\mathbf{M}_{c-hh}|^2 \right\rangle + \left\langle |\hat{e}\cdot\mathbf{M}_{c-lh}|^2 \right\rangle = 2|\mathbf{M}_b|^2 & \text{QW} \end{cases}$$

$$\frac{dS_m}{dt} = \int \left(U_m^{spon} + U_m^{stim} \right) dV - \frac{S_m}{\tau_m}$$

$$\nabla_t^2 \phi + \left(\varepsilon_\omega \omega^2 - \beta^2 \right) \phi = 0$$

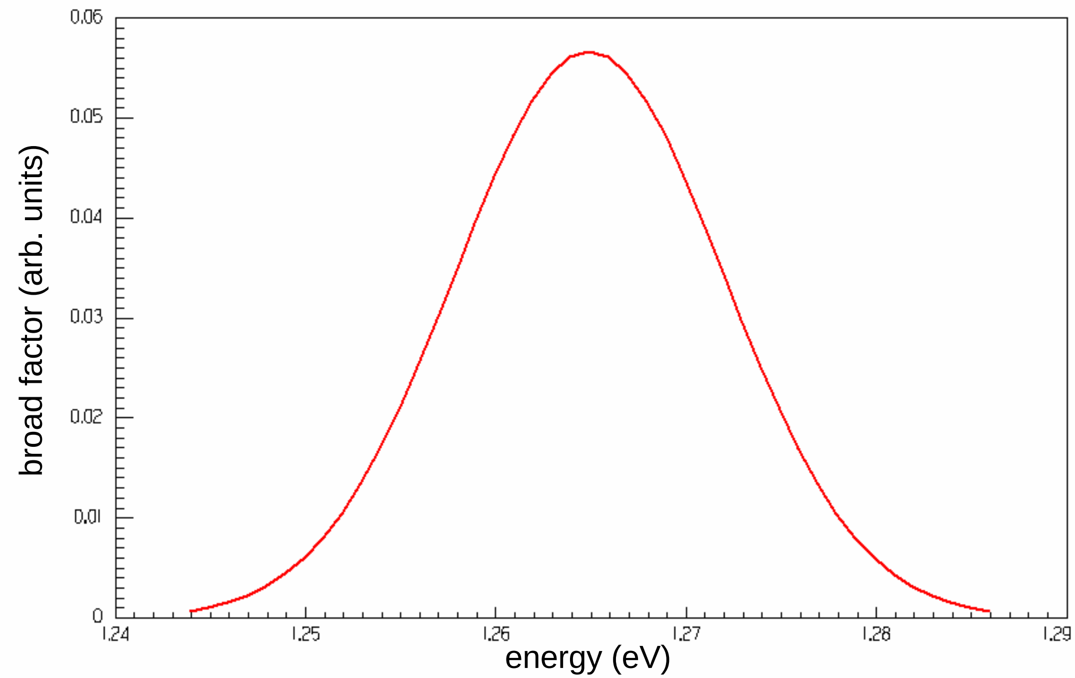
$$g_m^{stim} \Delta E_m = \frac{\phi^2}{\int \phi^2 dV}$$

$$g_m^{spon} \Delta E_m = \begin{cases} \dfrac{E_m^2}{\pi^2 c^3 \hbar^3} \Delta E_m & \text{Planck density over estimate} \\ g_m^{stim} \Delta E_m & \text{coherent density under estimate} \end{cases}$$

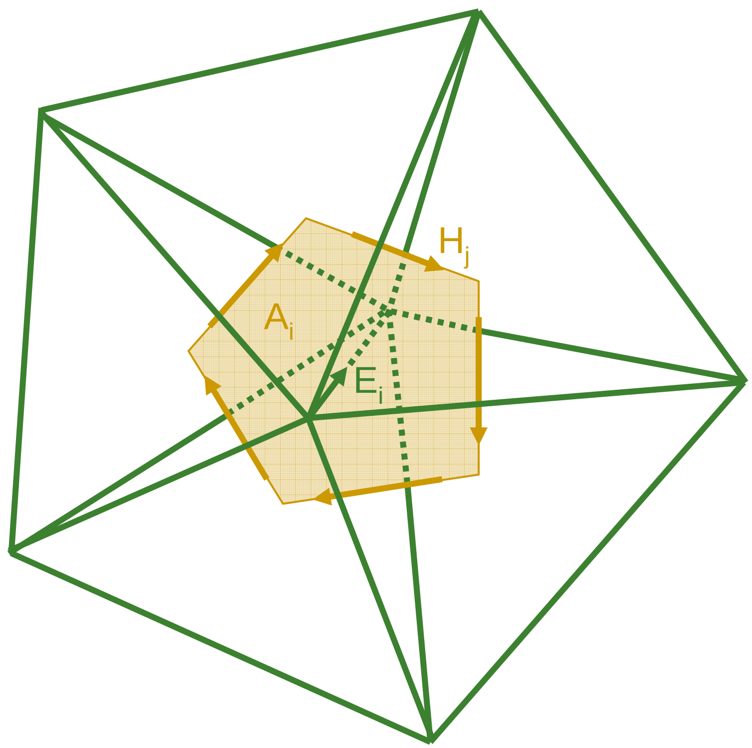
Collision Broadening

$$U_m^{stim} = S_m \sum_i \rho_i B_{c\to v} g_i^{stim} g_{red} \left[f_c (1 - f_v) - f_v (1 - f_c) \right] \Delta E_i$$

$$\rho_i \propto \exp\left[-\frac{(E_m - E_{c,i} - E_{v,i})^2}{E_{broad}^2} \right]$$



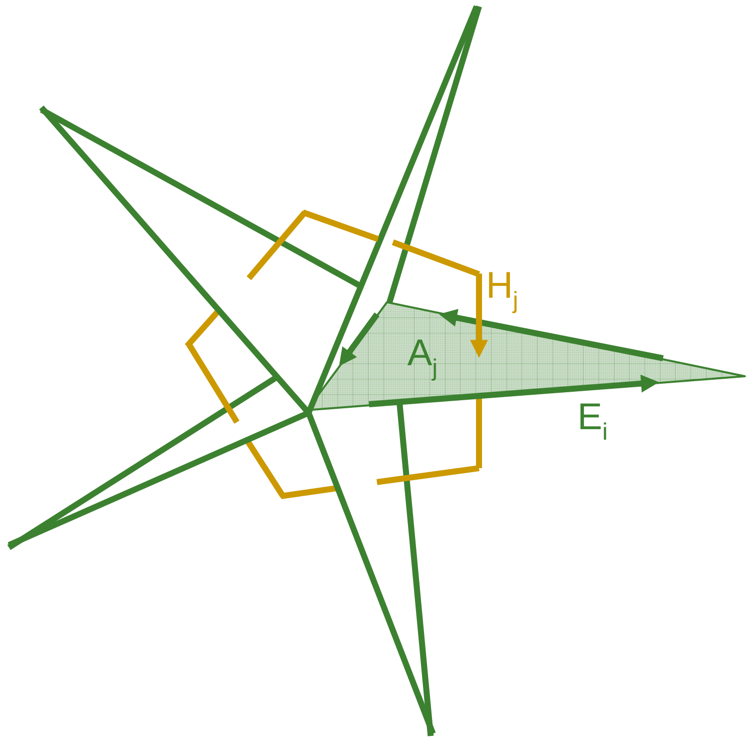
Delaunay/Voronoi Surface Integration (DVSI): Ampere's Law



$$\mathbf{J} + \frac{\partial(\varepsilon \mathbf{E})}{\partial t} = \nabla \times \mathbf{H}$$

$$J_i A_i + \frac{\partial(\varepsilon E_i)}{\partial t} A_i = \sum_j H_j L_j$$

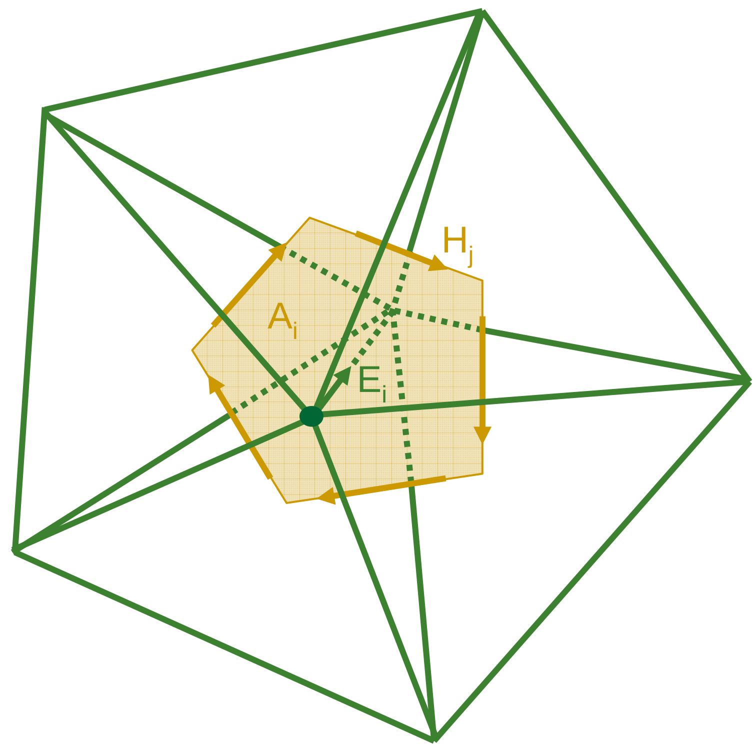
Delaunay/Voronoi Surface Integration (DVSI): Faraday's Law



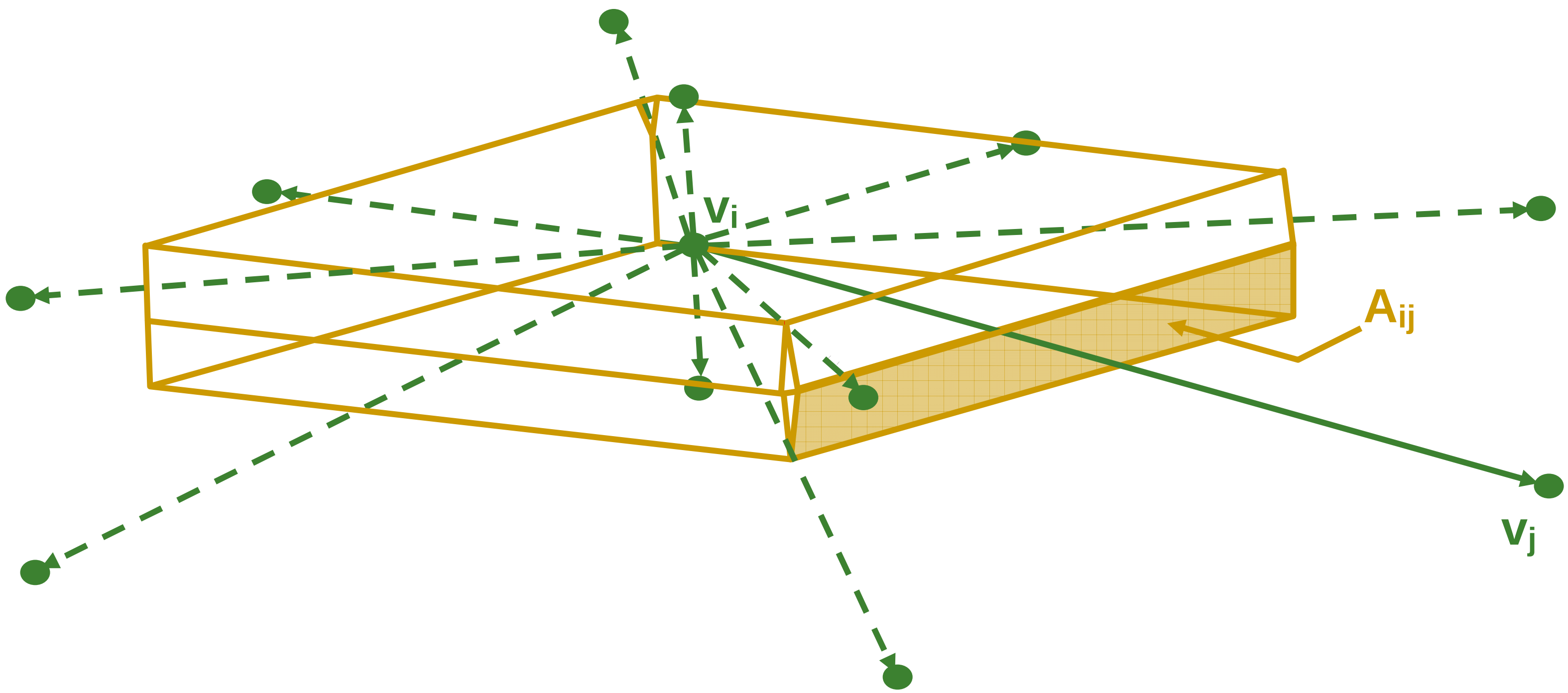
$$-\frac{\partial(\mu \mathbf{H})}{\partial t} = \nabla \times \mathbf{E}$$

$$-\frac{\partial(\mu H_j)}{\partial t} A_j = \sum_i E_i L_i$$

DVSI: Compatible with Box Integration Method



Divergences: Electrostatics & Charge Conservation



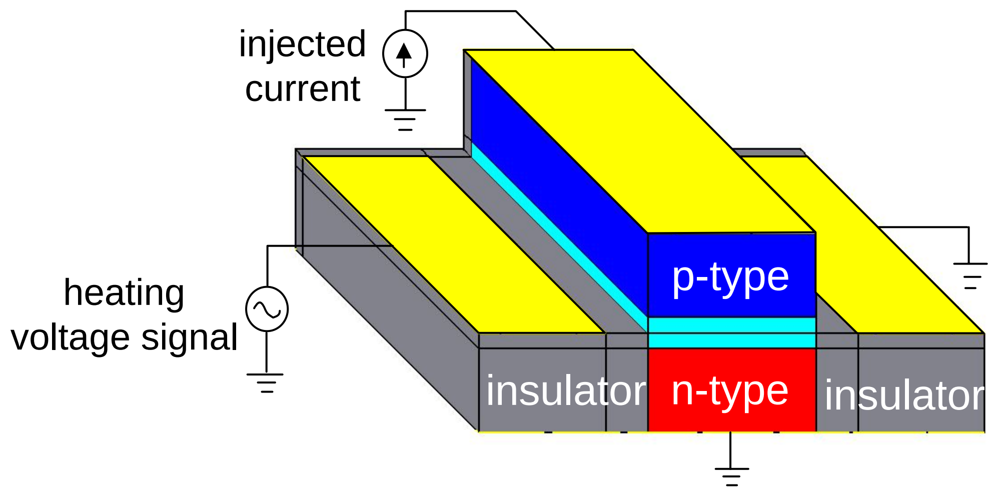
divergence theorem

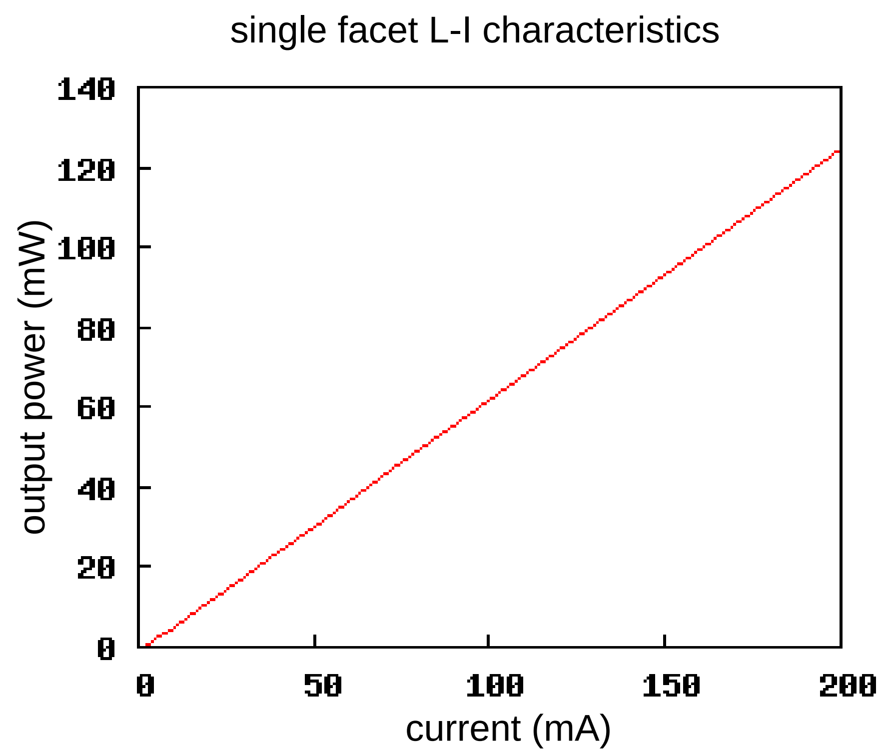
$$\int_{V_i} \nabla \cdot \mathbf{D} dV = \oint_{S_i} \mathbf{D} \cdot d\mathbf{S} = \sum_j D_{ij} A_{ij}$$

Solving the Discretized Equations with Newton Method

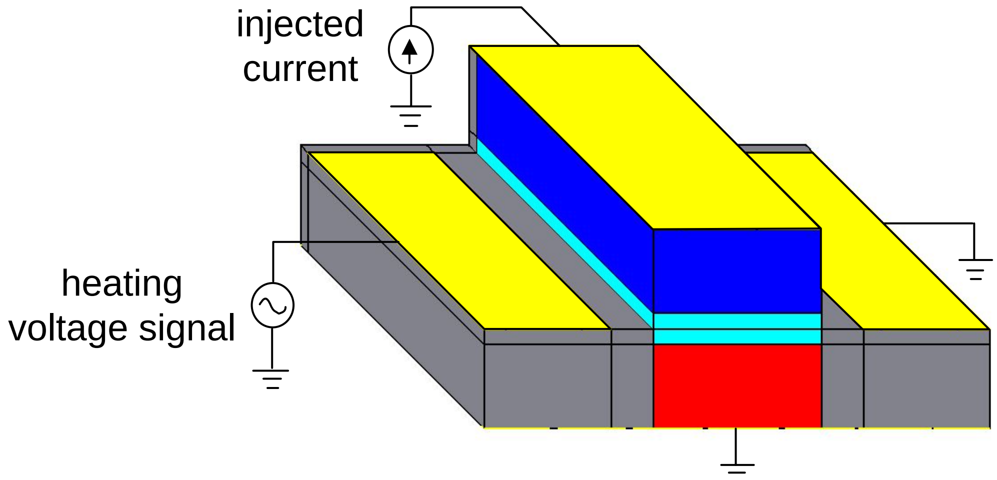
$$
\begin{bmatrix}
\frac{\partial \mathrm{Gauss_D}}{\partial \psi} & 0 & 0 & \frac{\partial \mathrm{Gauss_D}}{\partial F_n} & \frac{\partial \mathrm{Gauss_D}}{\partial F_p} & \frac{\partial \mathrm{Gauss_D}}{\partial T_n} & \frac{\partial \mathrm{Gauss_D}}{\partial T_p} & 0 \\
\frac{\partial \mathrm{Amp}}{\partial \psi} & \frac{\partial \mathrm{Amp}}{\partial E_{rot}} & \frac{\partial \mathrm{Amp}}{\partial H_{rot}} & \frac{\partial \mathrm{Amp}}{\partial F_n} & \frac{\partial \mathrm{Amp}}{\partial F_p} & \frac{\partial \mathrm{Amp}}{\partial T_n} & \frac{\partial \mathrm{Amp}}{\partial T_p} & \frac{\partial \mathrm{Amp}}{\partial T_l} \\
0 & \frac{\partial \mathrm{Far}}{\partial E_{rot}} & \frac{\partial \mathrm{Far}}{\partial H_{rot}} & 0 & 0 & 0 & 0 & 0 \\
\frac{\partial \mathrm{cont}_n}{\partial \psi} & \frac{\partial \mathrm{cont}_n}{\partial E_{rot}} & \frac{\partial \mathrm{cont}_n}{\partial H_{rot}} & \frac{\partial \mathrm{cont}_n}{\partial F_n} & \frac{\partial \mathrm{cont}_n}{\partial F_p} & \frac{\partial \mathrm{cont}_n}{\partial T_n} & \frac{\partial \mathrm{cont}_n}{\partial T_p} & \frac{\partial \mathrm{cont}_n}{\partial T_l} \\
\frac{\partial \mathrm{cont}_p}{\partial \psi} & \frac{\partial \mathrm{cont}_p}{\partial E_{rot}} & \frac{\partial \mathrm{cont}_p}{\partial H_{rot}} & \frac{\partial \mathrm{cont}_p}{\partial F_n} & \frac{\partial \mathrm{cont}_p}{\partial F_p} & \frac{\partial \mathrm{cont}_p}{\partial T_n} & \frac{\partial \mathrm{cont}_p}{\partial T_p} & \frac{\partial \mathrm{cont}_p}{\partial T_l} \\
\frac{\partial \mathrm{energy}_n}{\partial \psi} & \frac{\partial \mathrm{energy}_n}{\partial E_{rot}} & \frac{\partial \mathrm{energy}_n}{\partial H_{rot}} & \frac{\partial \mathrm{energy}_n}{\partial F_n} & \frac{\partial \mathrm{energy}_n}{\partial F_p} & \frac{\partial \mathrm{energy}_n}{\partial T_n} & \frac{\partial \mathrm{energy}_n}{\partial T_p} & \frac{\partial \mathrm{energy}_n}{\partial T_l} \\
\frac{\partial \mathrm{energy}_p}{\partial \psi} & \frac{\partial \mathrm{energy}_p}{\partial E_{rot}} & \frac{\partial \mathrm{energy}_p}{\partial H_{rot}} & \frac{\partial \mathrm{energy}_p}{\partial F_n} & \frac{\partial \mathrm{energy}_p}{\partial F_p} & \frac{\partial \mathrm{energy}_p}{\partial T_n} & \frac{\partial \mathrm{energy}_p}{\partial T_p} & \frac{\partial \mathrm{energy}_p}{\partial T_l} \\
\frac{\partial \mathrm{energy}_l}{\partial \psi} & \frac{\partial \mathrm{energy}_l}{\partial E_{rot}} & \frac{\partial \mathrm{energy}_l}{\partial H_{rot}} & \frac{\partial \mathrm{energy}_l}{\partial F_n} & \frac{\partial \mathrm{energy}_l}{\partial F_p} & \frac{\partial \mathrm{energy}_l}{\partial T_n} & \frac{\partial \mathrm{energy}_l}{\partial T_p} & \frac{\partial \mathrm{energy}_l}{\partial T_l}
\end{bmatrix}
\begin{bmatrix}
\Delta \psi \\ \Delta E_{rot} \\ \Delta H_{rot} \\ \Delta F_n \\ \Delta F_p \\ \Delta T_n \\ \Delta T_p \\ \Delta T_l
\end{bmatrix}
= -
\begin{bmatrix}
\mathrm{R}_{\mathrm{Gauss}} \\ \mathrm{R}_{\mathrm{Amp}} \\ \mathrm{R}_{\mathrm{Far}} \\ \mathrm{R}_{\mathrm{cont}_n} \\ \mathrm{R}_{\mathrm{cont}_p} \\ \mathrm{R}_{\mathrm{energy}_n} \\ \mathrm{R}_{\mathrm{energy}_p} \\ \mathrm{R}_{\mathrm{energy}_l}
\end{bmatrix}
$$

Microwave Heating Structure

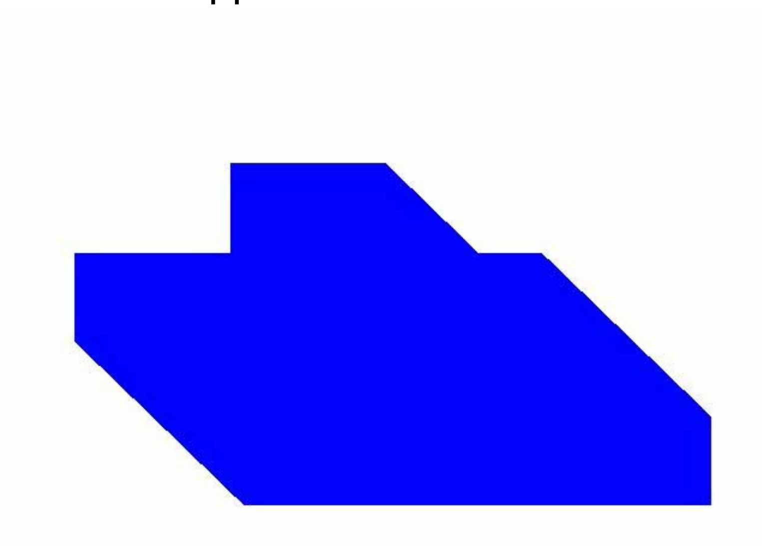




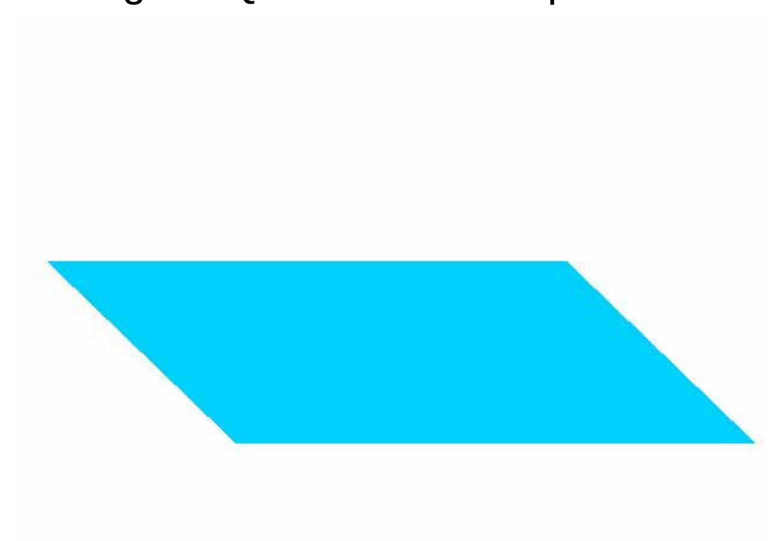
200 mA Bias, 0.5 V Heating Voltage Step



applied electric field



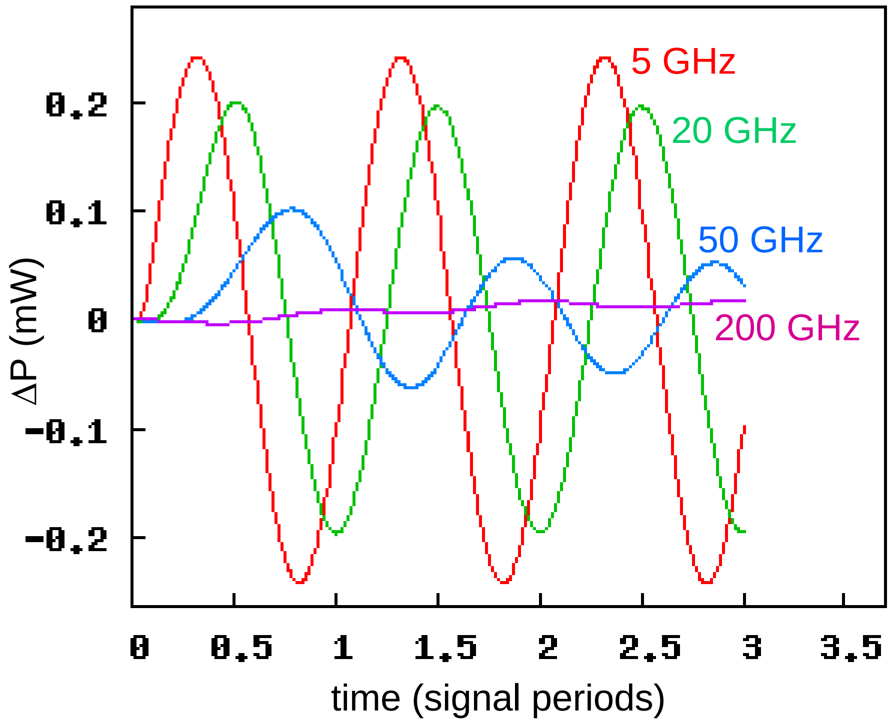
change in QW electron temperature



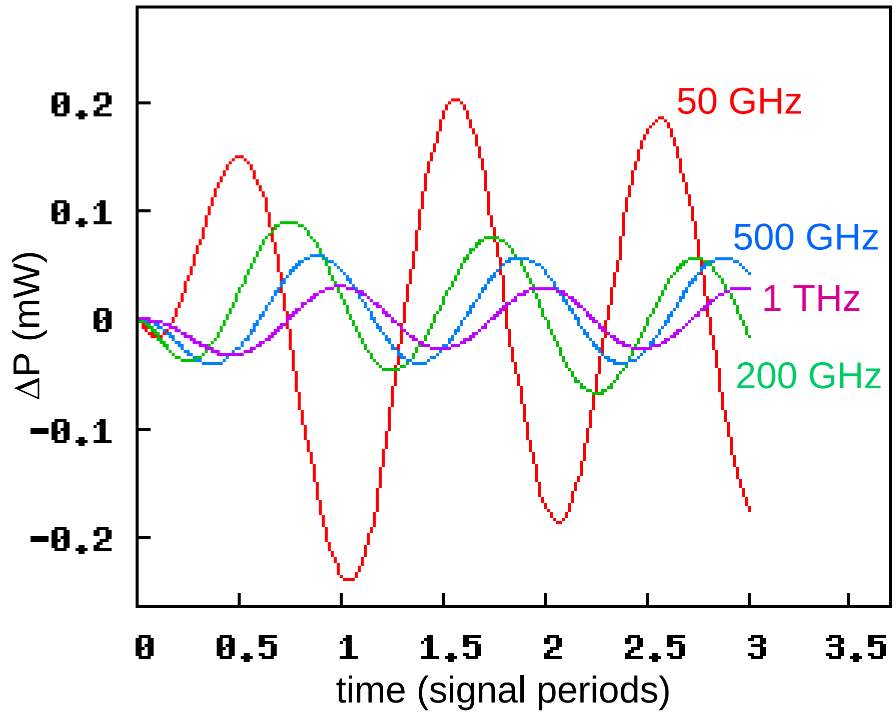
Current & Plasma Heating Modulation Schemes

200 mA quiescent bias current

0.2 mA sinusoidal current signal

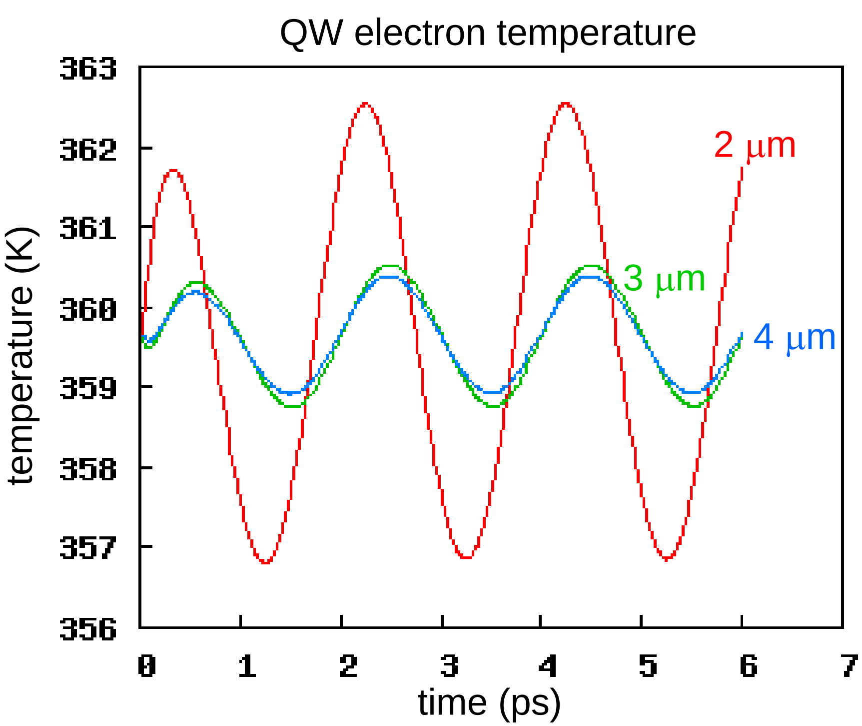


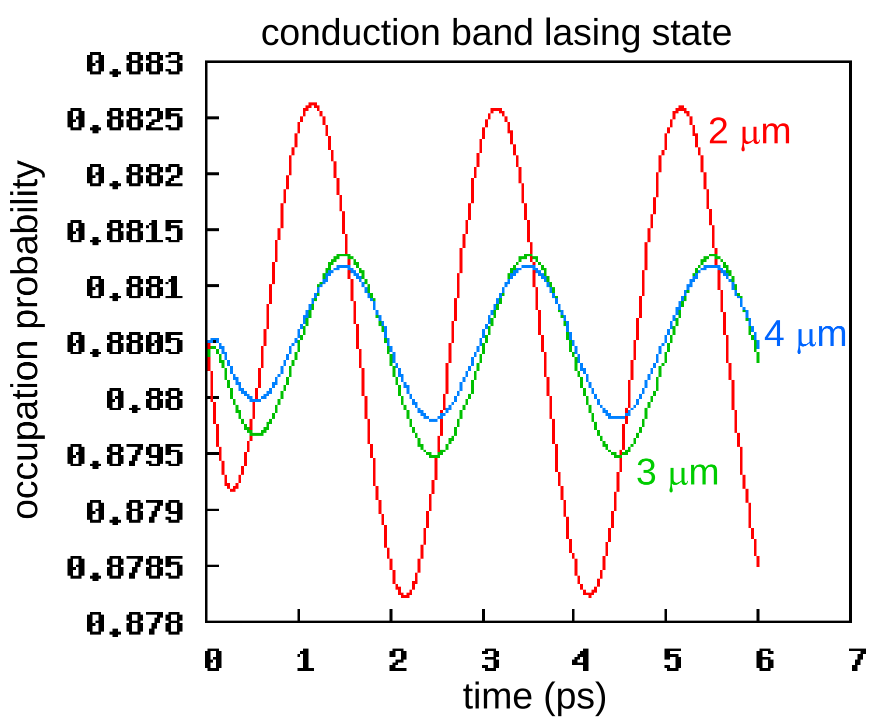
1 V sinusoidal voltage heating signal



QW Carrier Temperature Variations Affect Optical Gain

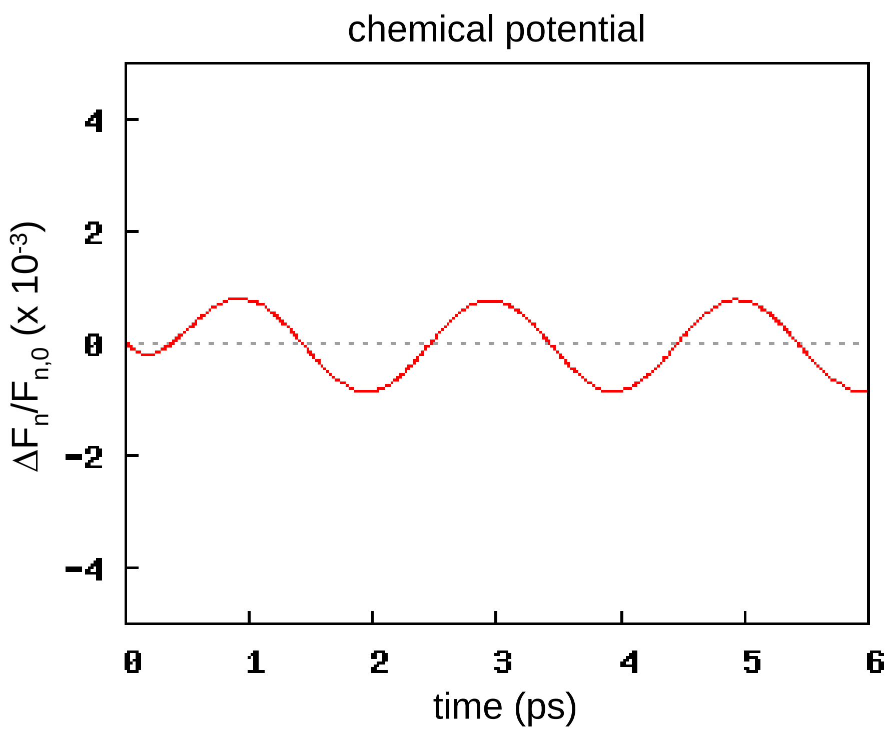
- 200 mA dc current bias
- 2 V amplitude, 500 GHz heating signal
- distance measured from the injected radiation boundary

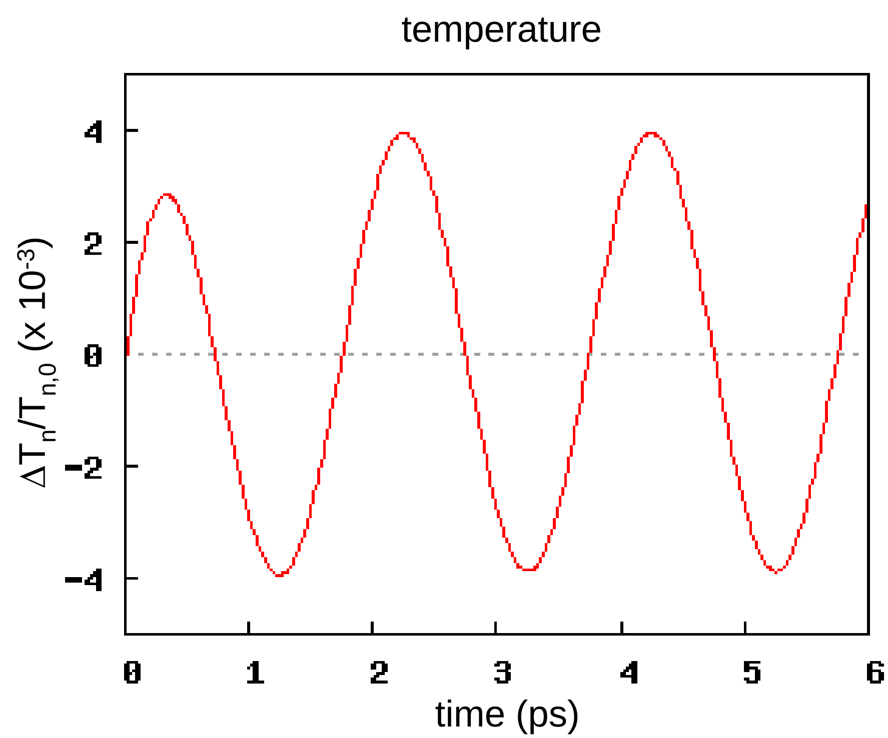




Relative Variations in QW Electron Gas

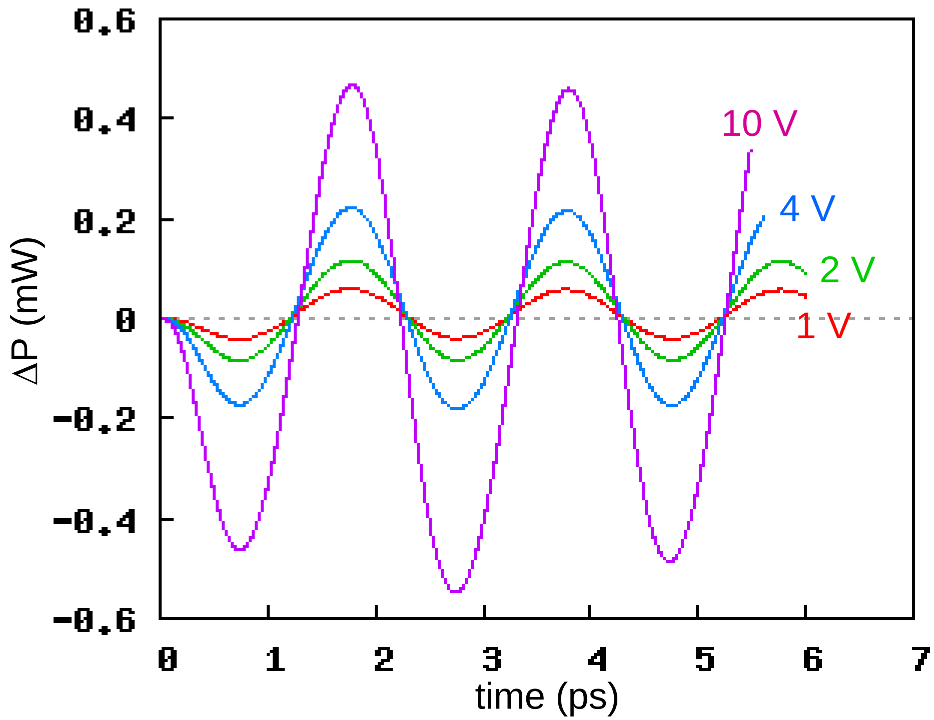
- 200 mA dc current bias
- 1 V amplitude, 500 GHz heating signal





Approximately Linear Scaling with Heating Voltage

- 200 mA dc current bias
- 500 GHz voltage heating signal



- radiation energy goes as square of field strength
- linear scaling may be due to coupling efficiency

Summary

- Gain saturation from carrier heating limits laser diode current modulation
  - increasing injected current raises QW chemical potential
  - dissipating injected carriers' excess energies increases QW temperature
  - gain increase from chemical potential offset by temperature increase
- New simulation techniques used to study dual modulation effect
  - full wave electromagnetics
  - Fermi gas dynamics with full thermal effects
  - new treatment of heat flow using heat capacity of Fermi gases
  - new vector field discretization scheme allows self-consistent solutions
- Terahertz modulation through QW carrier heating by injected radiation
  - appears permissible by Maxwell's vector field theory and kinetic theory of Fermi gases
  - practical laser diode structures
    - will exhibit significant lattice heating
    - likely adversely affect this high frequency modulation scheme

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