Nonequilibrium Green's Function Simulation of Quantum Cascade Laser Structures

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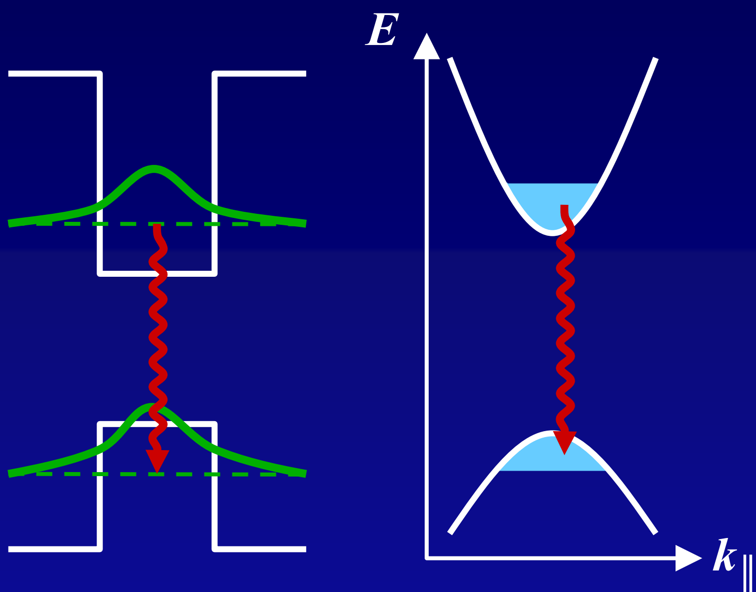
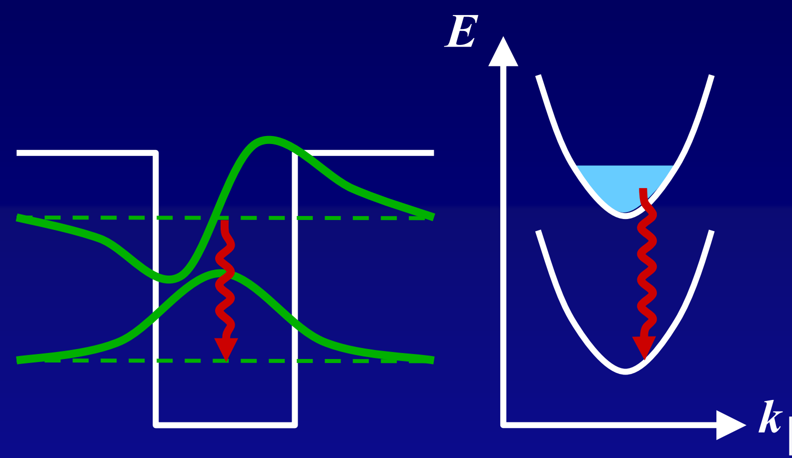
Outline

- Intersubband Optics and Quantum Cascade Lasers
- Green's function modelling of QCLs
- Numerical Illustration
- Conclusion

Interband vs. Intersubband Optics:





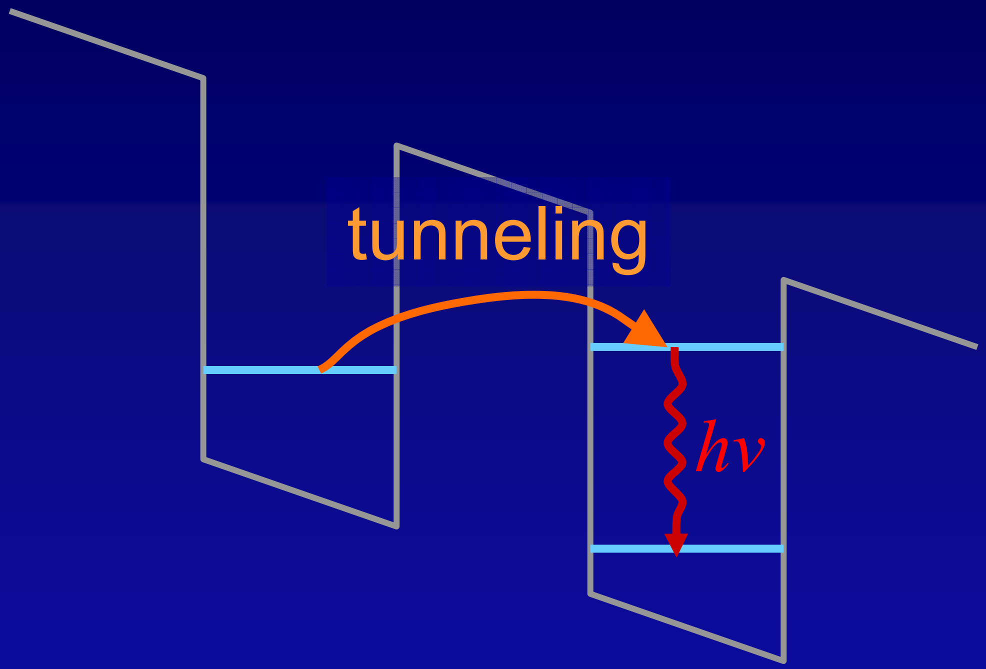
interband transition

- bipolar
- photon energy determined by bandgap energy E_{gap} of material

intersubband transition

- unipolar
- photon energy determined by well thickness, adjustable

The Challenge: Intersubband Lasing



It took 23 years to achieve this laser!

Kazarinov and Suris, 1971

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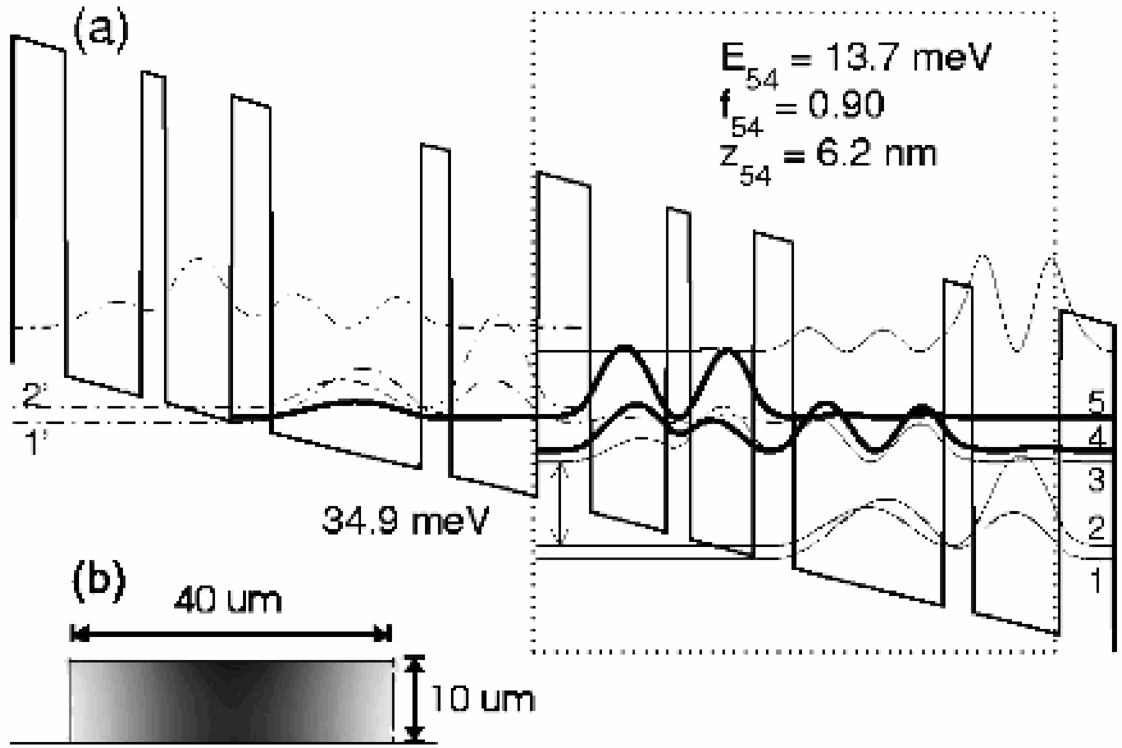
The Quantum Cascade Laser

LO-Phonon Assisted THz Design

S. Kumar et al.,

Appl. Phys. Lett., Vol. 84, No. 14, 5 April 2004



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GREEN'S FUNCTION MODELLING OF QUANTUM CASCADE LASERS

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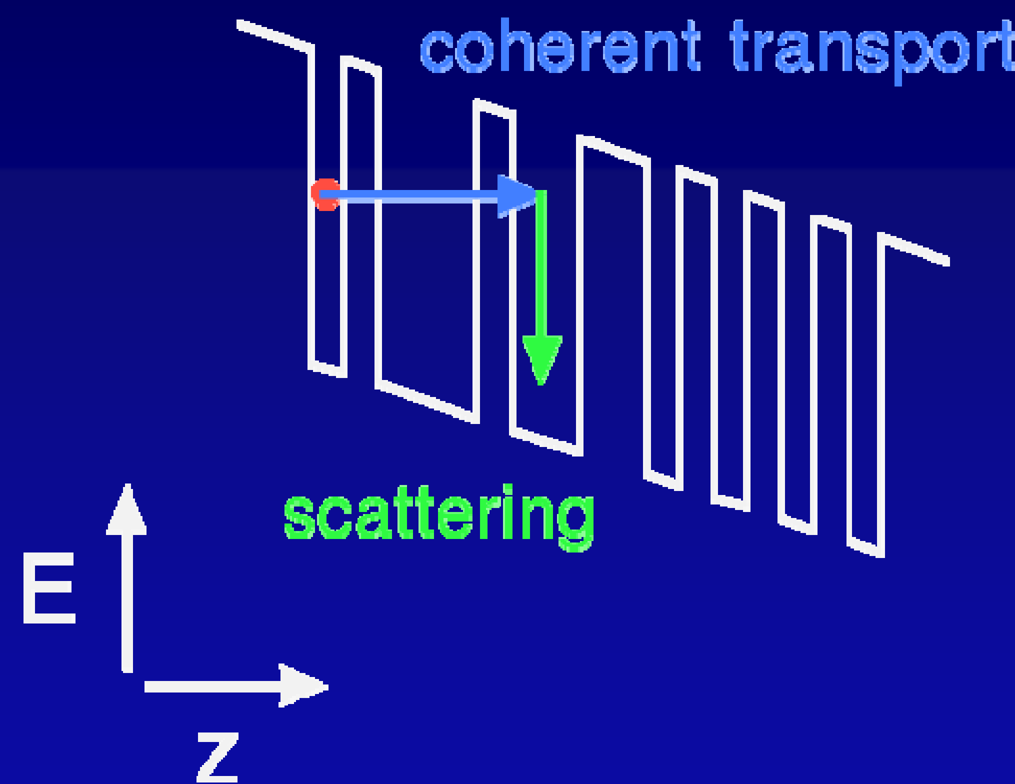
Electron transport through quantum cascade lasers is determi-ned by the balance between coherent transport and scattering:



Hamilton operator: $H = H^{(0)} + H_{\mathrm{scatt}}$

Coherent transport governed by single-particle Hamiltonian:

$$H^{(0)} = H_{\mathrm{kin}} + V_{\mathrm{SL}} + V_{\mathrm{field}}$$

Scattering through many-body interactions in H_{scatt}:

- LO-phonon scattering
- acoustic phonon scattering (currently modelled by using an artifical LO-phonon dispersion)
- impurity scattering
- interface roughness scattering
- electron-electron scattering
- radiative losses

Both coherent transport and scattering can conveniently be described on the same footing using **Green's functions**:

$$G^{<}_{\alpha\beta,\mathbf{k}}(\omega) = \int dt \left\langle \Psi^{\dagger}_{\beta,\mathbf{k}}(t)\Psi_{\alpha,\mathbf{k}}(0)\right\rangle e^{i\omega t}$$

Relation to (single particle) density matrix:

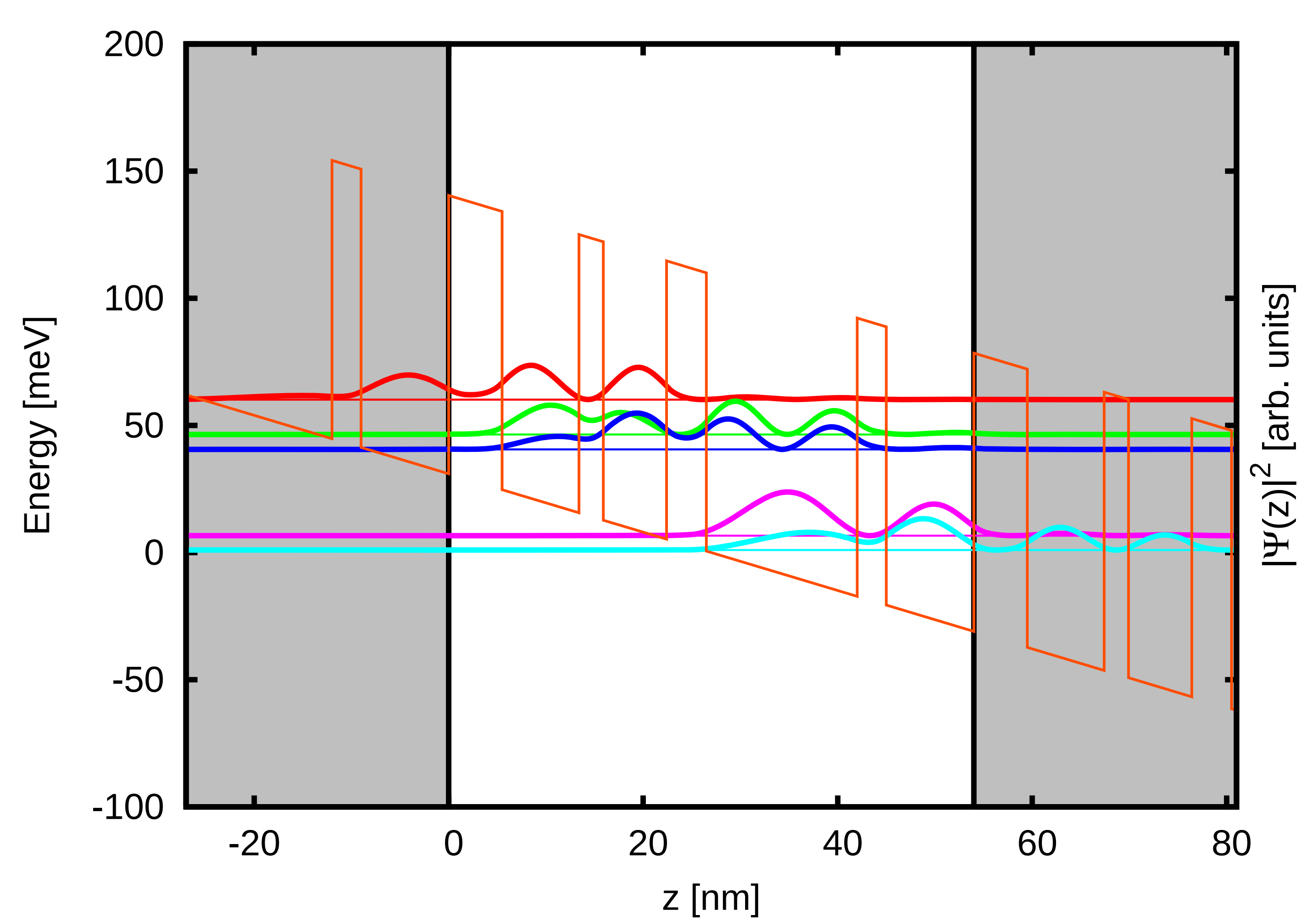
$$\rho_{\alpha\beta,\mathbf{k}} = \int d\omega\, G^{<}_{\alpha\beta,\mathbf{k}}(\omega)$$

S.-C. Lee and A. Wacker, Phys. Rev. B **66**, 245314 (2002).

S.-C. Lee, F. Banit, M. Woerner, and A. Wacker, Phys. Rev. B **73**, 245320 (2006).

α, β: Wannier-Stark states

(eigenstates of superlattice + external field)



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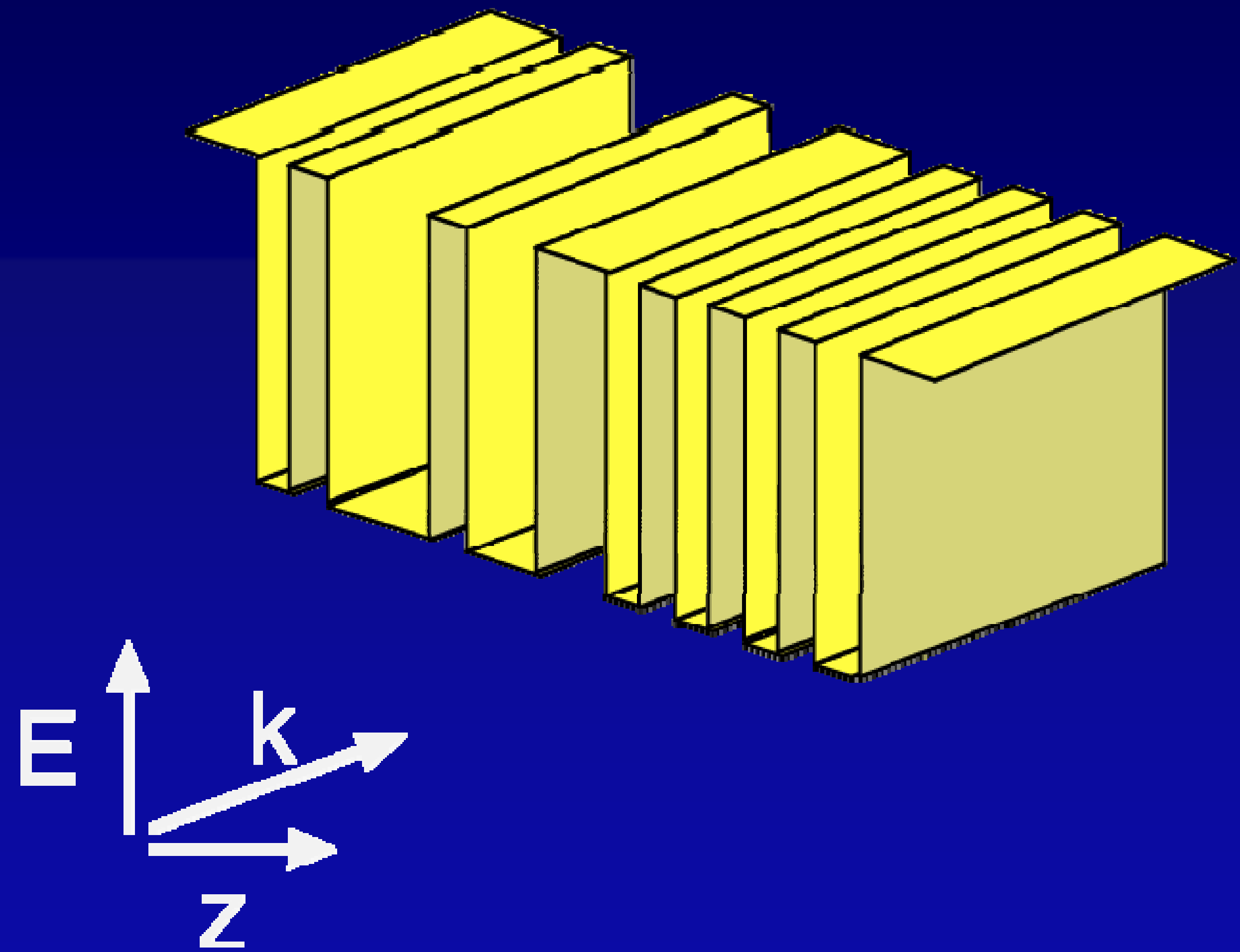
k – in-plane wavevector:



Other Green functions:

$$G^{>}_{\alpha\beta,\mathbf{k}}(\omega) = -i \int dt \, \left\langle \Psi_{\alpha,\mathbf{k}}(0)\,\Psi^{\dagger}_{\beta,\mathbf{k}}(t) \right\rangle e^{i\omega t}$$

Spectral function:

$$\hat{G}_{\alpha\beta,\mathbf{k}}(\omega) = i\,[G^{>}_{\alpha\beta,\mathbf{k}}(\omega) - G^{<}_{\alpha\beta,\mathbf{k}}(\omega)]$$

Retarded Green function (Lehmann representation):

$$G^{\mathrm{ret}}_{\alpha\beta,\mathbf{k}}(\omega) = \frac{1}{2\pi} \int d\omega' \, \frac{\hat{G}_{\alpha\beta,\mathbf{k}}(\omega')}{\omega - \omega' + i\varepsilon}$$

($\Rightarrow \hat{G}_{\alpha\beta,\mathbf{k}}(\omega) = -2\,\mathrm{Im}\,G^{\mathrm{ret}}_{\alpha\beta,\mathbf{k}}(\omega)$ if $\hat{G}$ is purely imaginary) (retarded) Dyson equation

$$G^{\rm ret}_{\alpha\beta,\mathbf{k}}(\omega) = \left((G^{\rm ret}_0)^{-1}_{\mathbf{k}}(\omega) - \Sigma^{\rm ret}_{\mathbf{k}}(\omega) \right)^{-1}_{\alpha\beta}$$

$$(G^{\rm ret}_0)^{-1}_{\alpha\beta,\mathbf{k}}(\omega) = \hbar\omega \cdot \delta_{\alpha\beta} - H^{(0)}_{\alpha\beta} + i\varepsilon\,, \quad H^{(0)} = H_{\rm kin} + V_{\rm SI.} + V_{\rm field}$$

Keldysh relation (Dyson equation for $G^{\gtrless}$)

$$G^{\gtrless}_{\alpha\beta,\mathbf{k}}(\omega) \;=\; \sum_{\alpha'\beta'} G^{\rm ret}_{\alpha\alpha',\mathbf{k}}(\omega) \cdot \Sigma^{\gtrless}_{\alpha'\beta',\mathbf{k}}(\omega) \cdot \left(G^{\rm ret}_{\beta\beta',\mathbf{k}}(\omega) \right)^{*}$$
$$+ \textit{initial condition term}$$

$\rightarrow$ G as functional of Σ!

Illustration:
only one state, constant damping $\Sigma^{\text{ret}}(\omega) = i\Gamma$

$$G_{\mathbf{k}}^{\text{ret}}(\omega) - \frac{1}{\omega - E_{\mathbf{k}} + i\Gamma}$$

Spectral function

$$\hat{G}_{\mathbf{k}}(\omega) = \frac{1}{(\hbar\omega - E_{\mathbf{k}})^2 + \Gamma^2}$$

Electron distribution in thermal equilibrium

$$G_{\mathbf{k}}^{<}(\omega) = i\, f(\hbar\omega)\, \frac{1}{(\hbar\omega - E_{\mathbf{k}})^2 + \Gamma^2}$$

LO phonon self-energy (second Born approximation)

$$\Sigma^{\gtrless}_{\alpha\beta,\mathbf{k}}(\omega) = \sum_{\substack{\alpha'\beta' \\ \mathbf{k}',q_z,\pm}} \pm b^{\gtrless}(\pm\hbar\Omega_{\mathrm{LO}}) \frac{M_{\alpha\alpha'}(-q_z)\, M_{\beta'\beta}(q_z)}{(\mathbf{k}-\mathbf{k}')^2 + q_z^2} \cdot G^{\gtrless}_{\alpha'\beta',\mathbf{k}'}(\omega \mp \Omega_{\mathrm{LO}})$$

$$M_{\alpha\beta}(q_z) = \sqrt{\frac{\hbar\Omega_{\mathrm{LO}} e^2}{4\pi}\left(\frac{1}{\varepsilon_\infty} - \frac{1}{\varepsilon_s}\right)} \int dz\, e^{-iq_z z}\, \psi^*_\alpha(z)\, \psi_\beta(z)$$

Lehmann representation for Σ:

$$\Sigma^{\mathrm{ret}}_{\alpha\beta,\mathbf{k}}(\omega) = \frac{1}{2\pi i} \int d\omega' \, \frac{\Sigma^{>}_{\alpha\beta,\mathbf{k}}(\omega') - \Sigma^{<}_{\alpha\beta,\mathbf{k}}(\omega')}{\omega - \omega' - i\varepsilon}$$

$\longrightarrow$ Σ as functional of G

$\longrightarrow$ self-consistent system of equations!

Approximation in current state-of-the-art simulator due to computational demand:

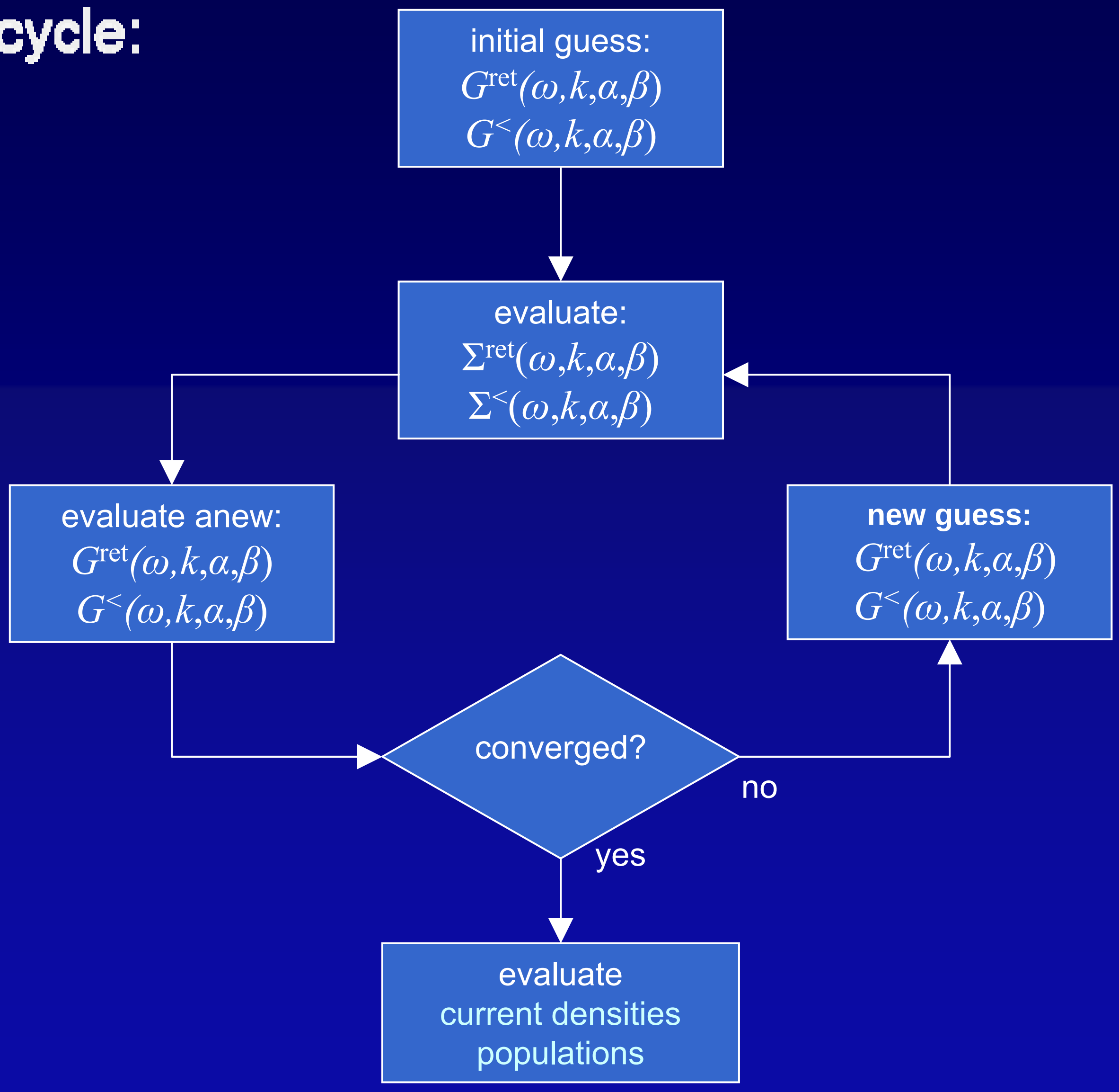
Evaluate matrix elements at 'typical wavevectors' $\mathbf{k}_{\text{typ}}$, $\mathbf{k}'_{\text{typ}}$:

$$\Sigma^{\gtrless}_{\alpha\beta}(\omega) = \sum_{\substack{\alpha'\beta' \\ \mathbf{k}', q_z, \pm}} \pm b^{\gtrless}(\pm\hbar\Omega_{\text{LO}}) \frac{M_{\alpha\alpha'}(-q_z) M_{\beta'\beta}(q_z)}{(\mathbf{k}_{\text{typ}} - \mathbf{k}'_{\text{typ}})^2 - q_z^2} \cdot G^{\gtrless}_{\alpha'\beta',\mathbf{k}'}(\omega \mp \Omega_{\text{LO}})$$

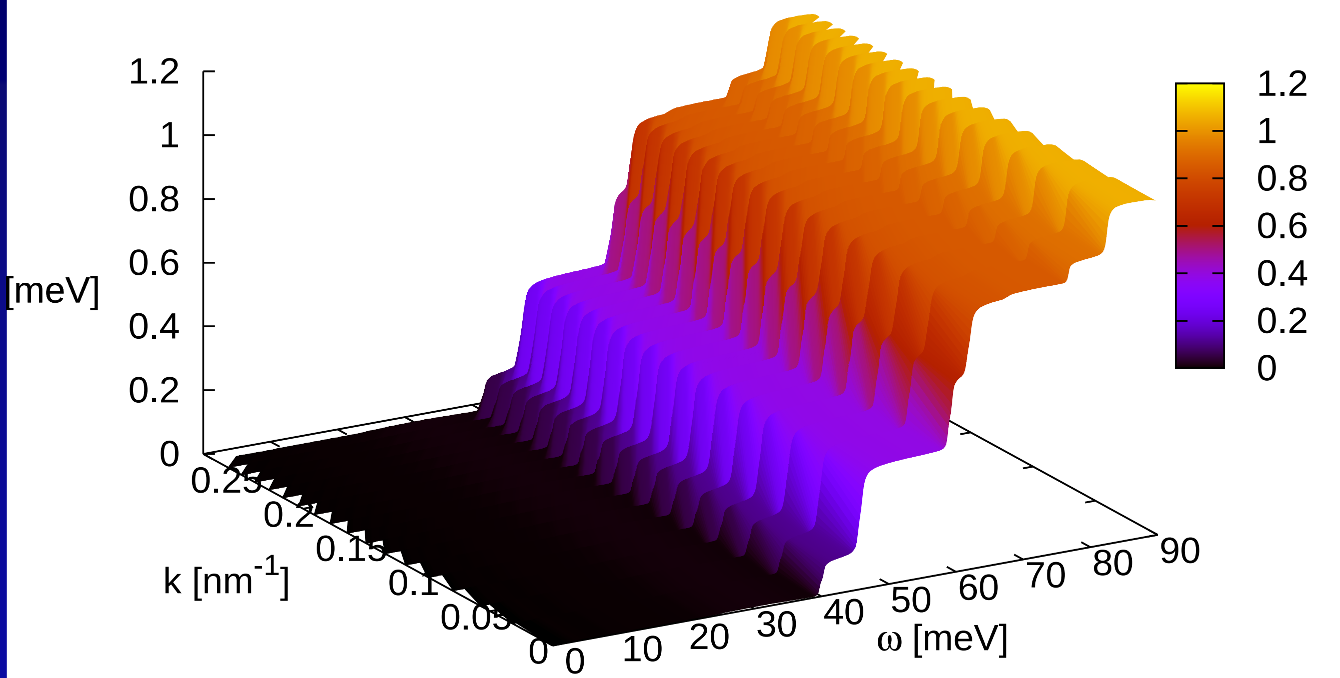
Choose $\mathbf{k}_{\text{typ}}$, $\mathbf{k}'_{\text{typ}}$ (for $\alpha = \beta$):

$$\frac{\hbar^2 \mathbf{k}^2_{\text{typ}}}{2m} = \hbar\Omega_{\text{LO}}\,, \qquad \frac{\hbar^2 \mathbf{k}'^2_{\text{typ}}}{2m} = 2\,\hbar\Omega_{\text{LO}}$$

Iterative cycle:



Self-Energy $\Sigma(\omega,k,\alpha,\beta)$



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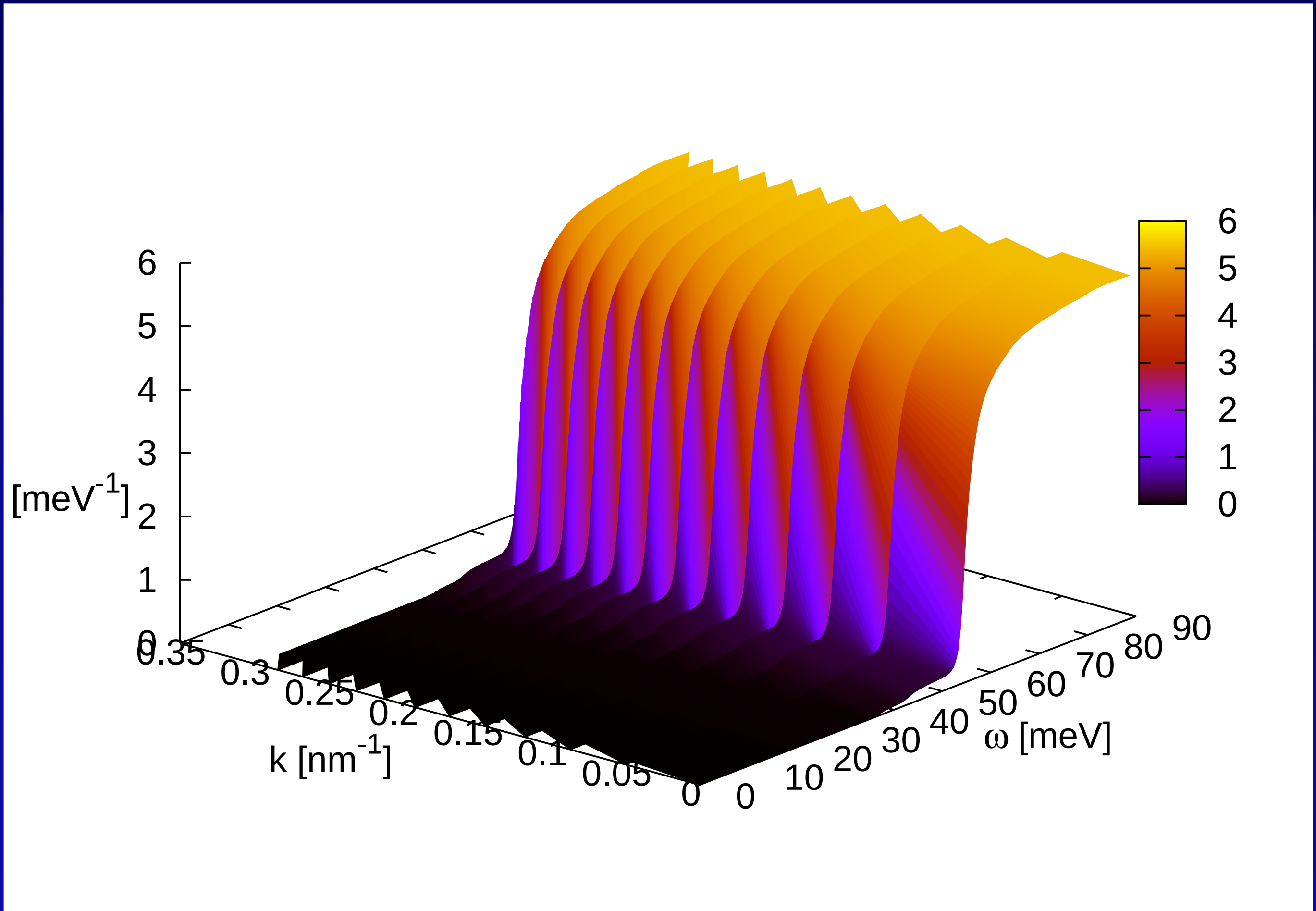
Self-Energy Σ(ω,k,5,5)



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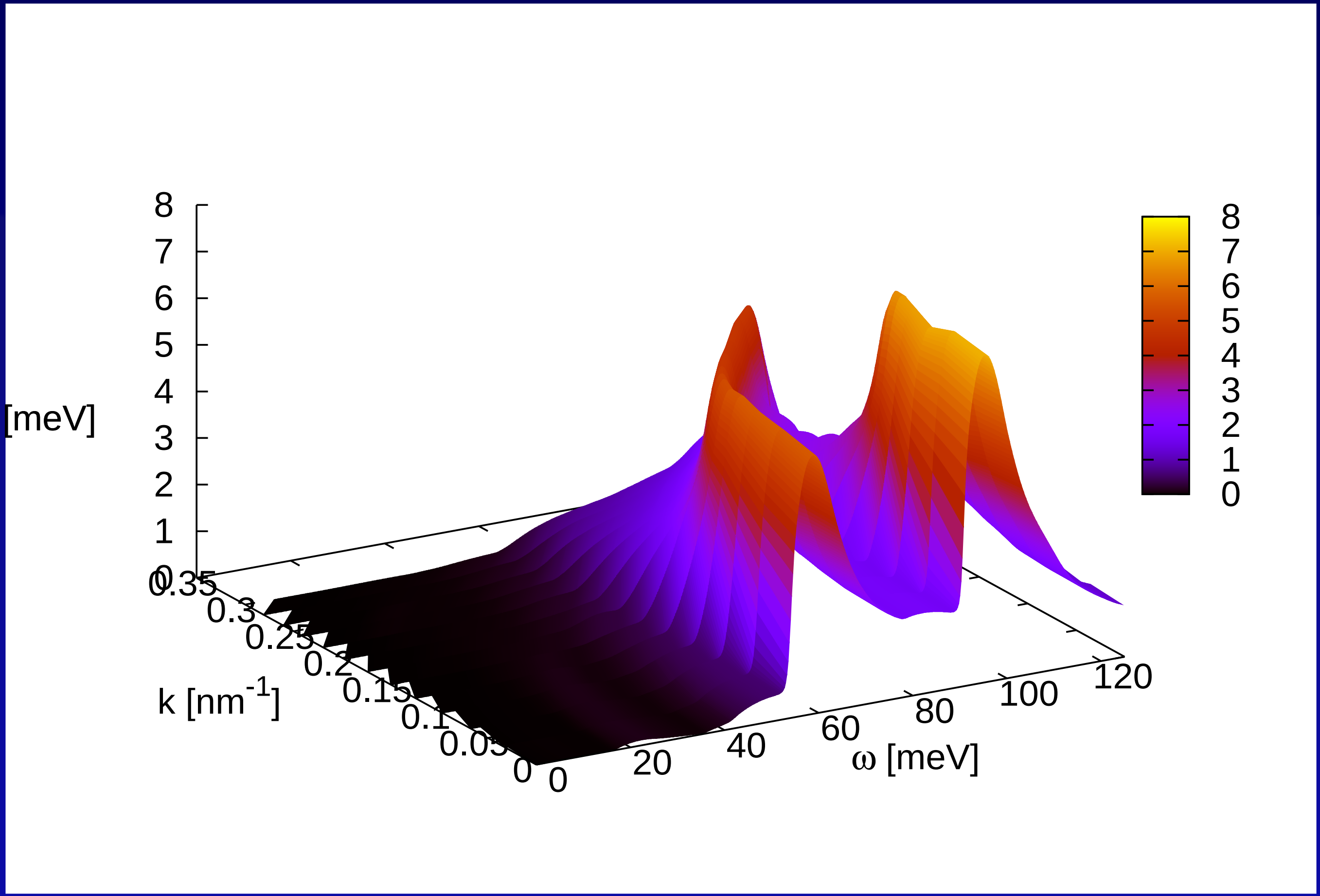
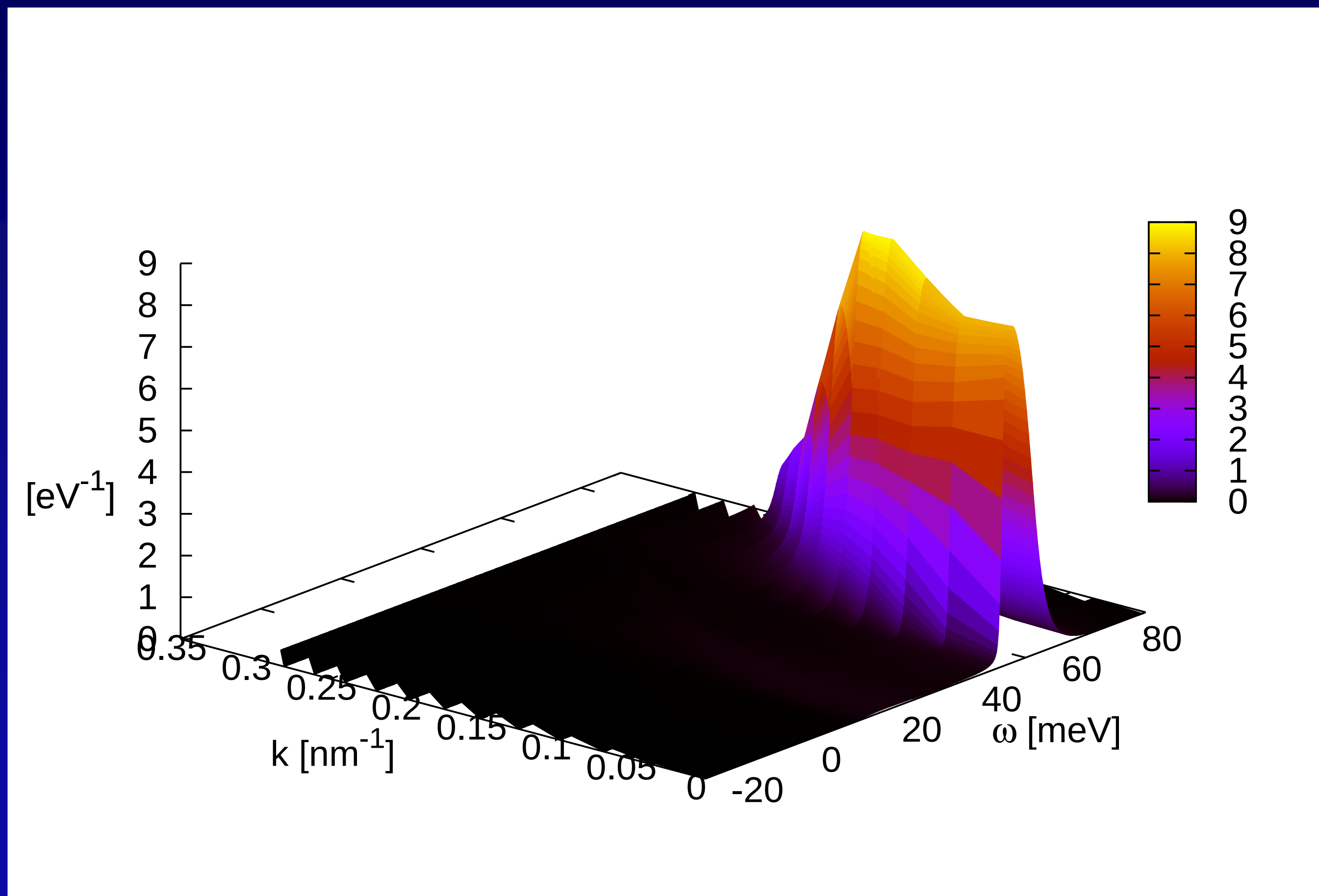
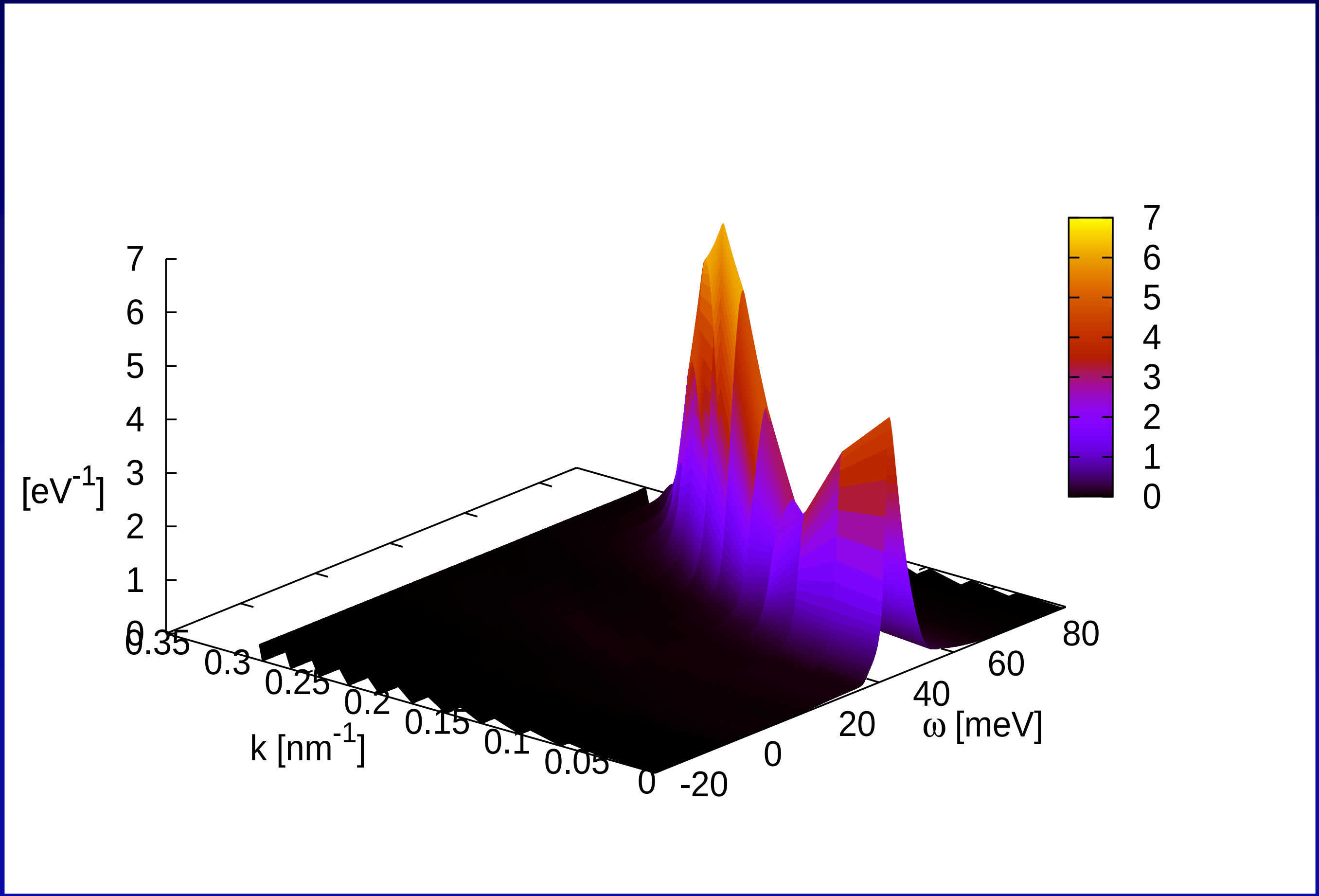
Self-Energy Σ(*ω*,*k*,*5*,*5*)



$G<(\omega,k,5,5)$


[eV^-1]
9
8
7
6
5
4
3
2
1
0
0.35
0.3
0.25
0.2
0.15
0.1
0.05
0
k [nm^-1]
-20
0
20
40
60
80
ω [meV]

G<(ω,k,4,4)



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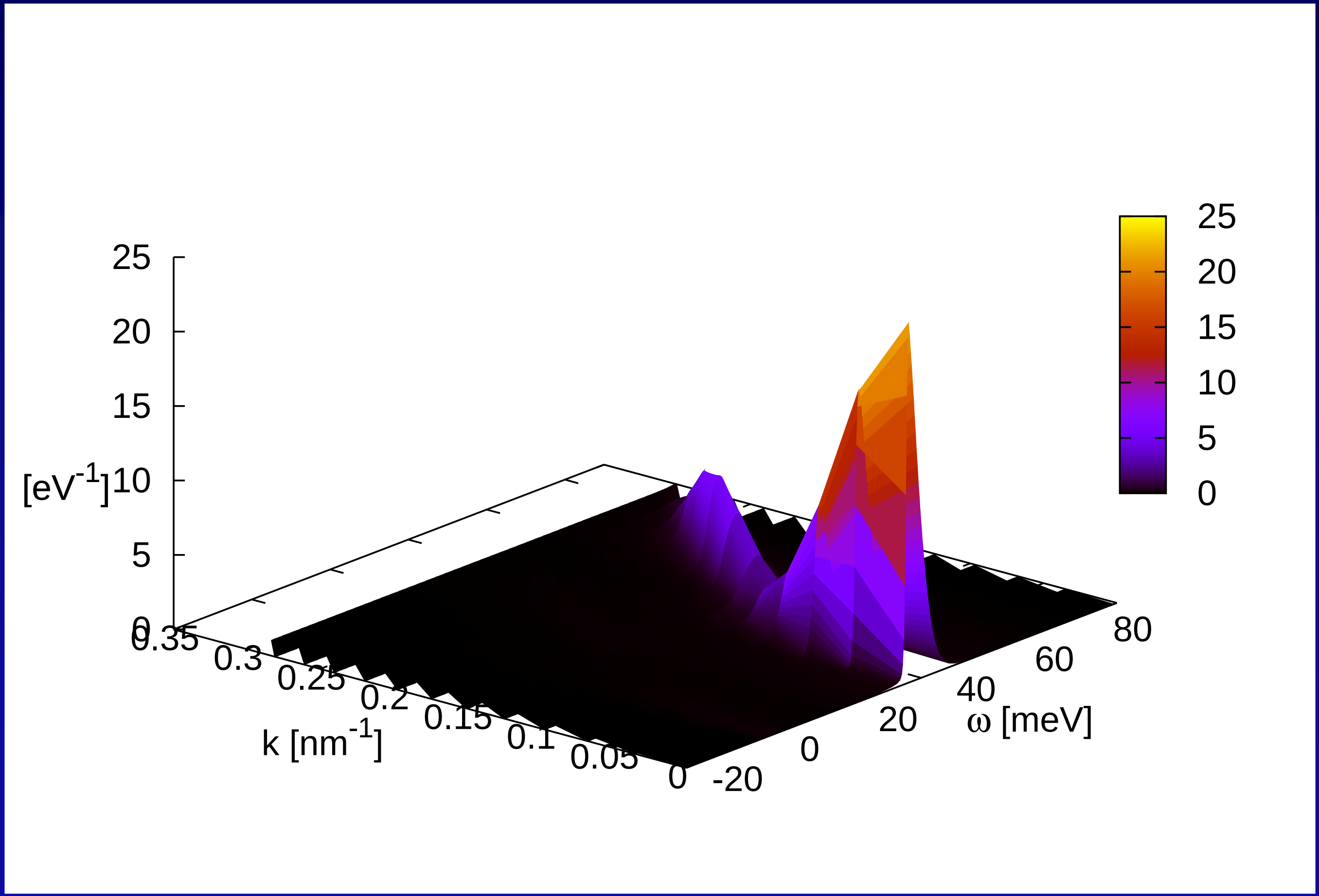
G<(ω,k,3,3)



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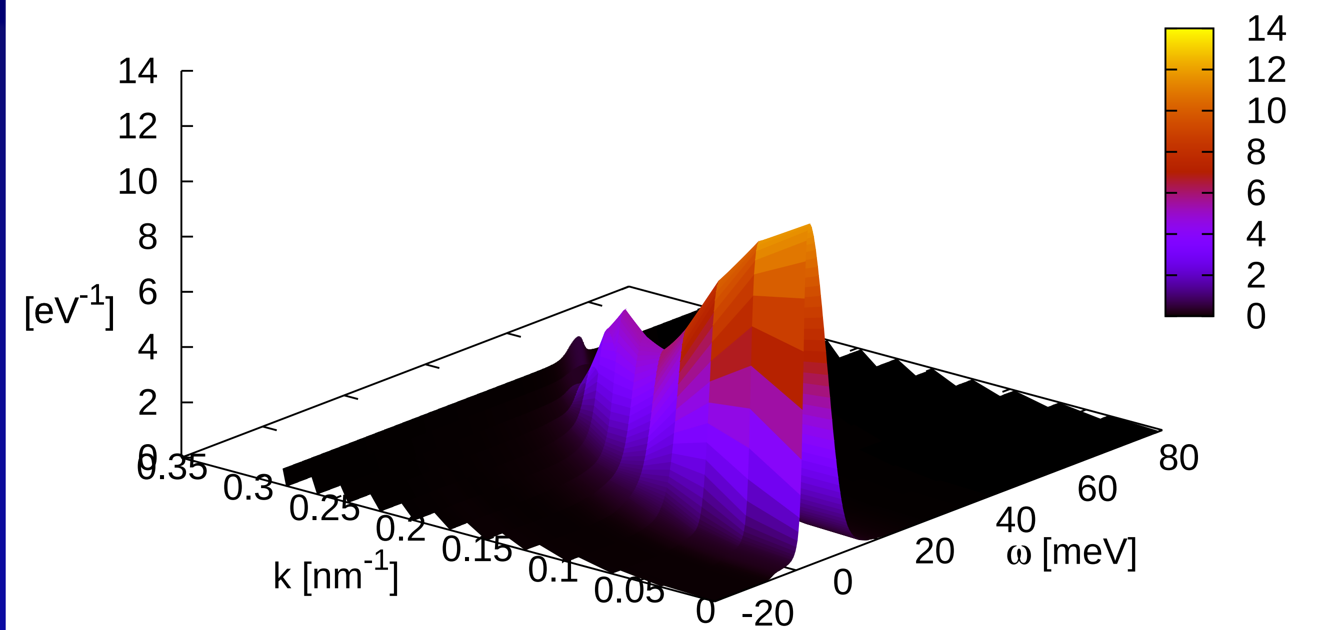
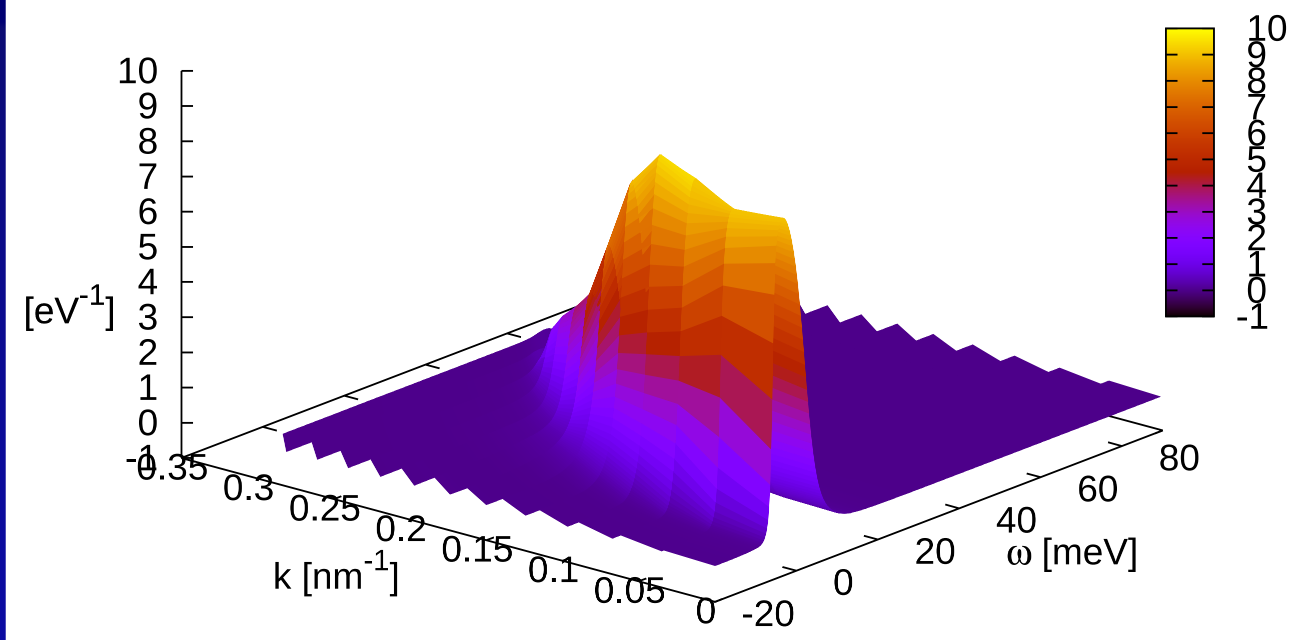
$G<(\omega,k,2,2)$



14
12
10
8
6
4
2
0
[eV-1]
0.35
0.3
0.25
0.2
0.15
0.1
0.05
0
k [nm-1]
-20
0
20
40
60
80
ω [meV]

G<(ω,k,1,1)



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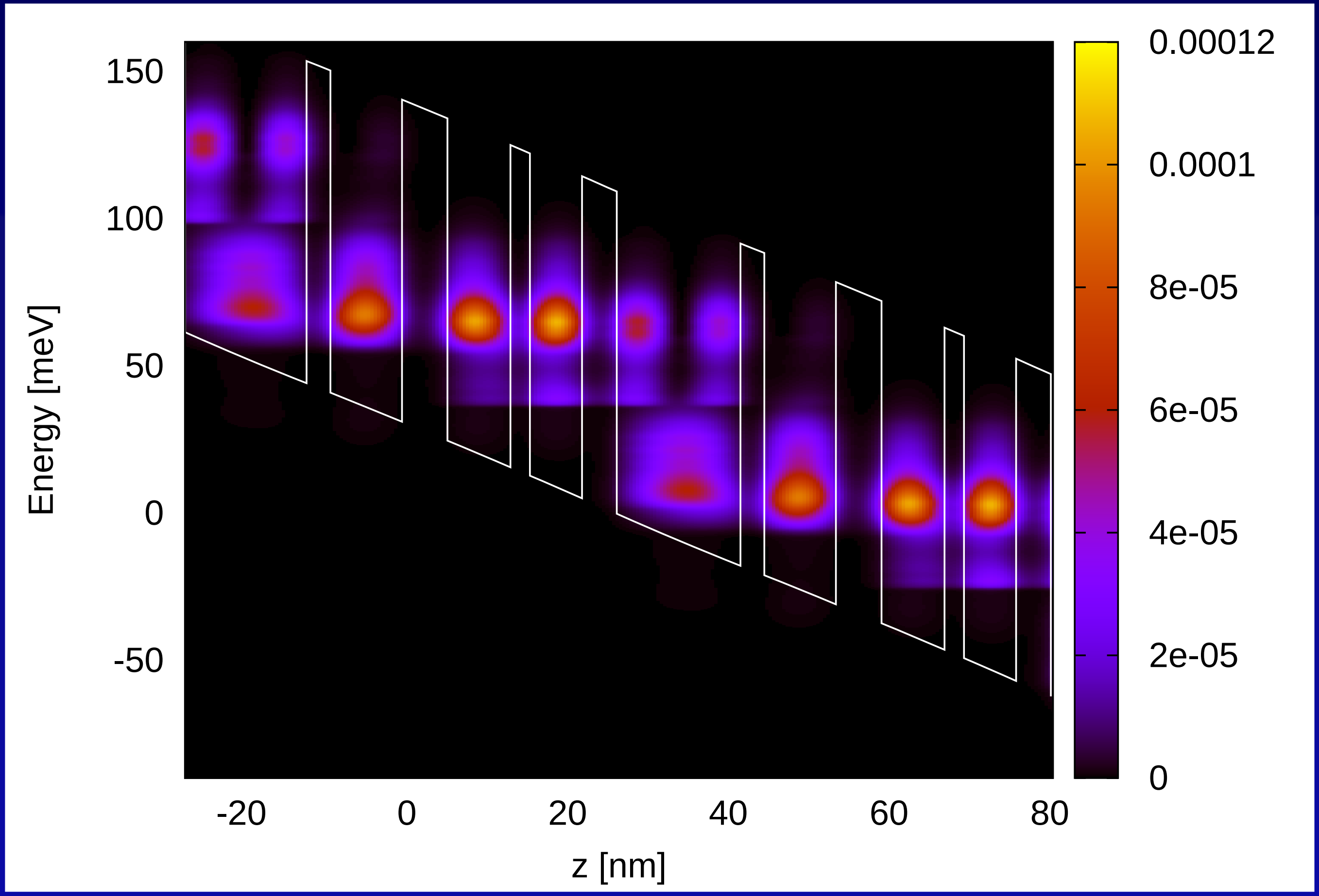
Energetically and Spatially Resolved Density



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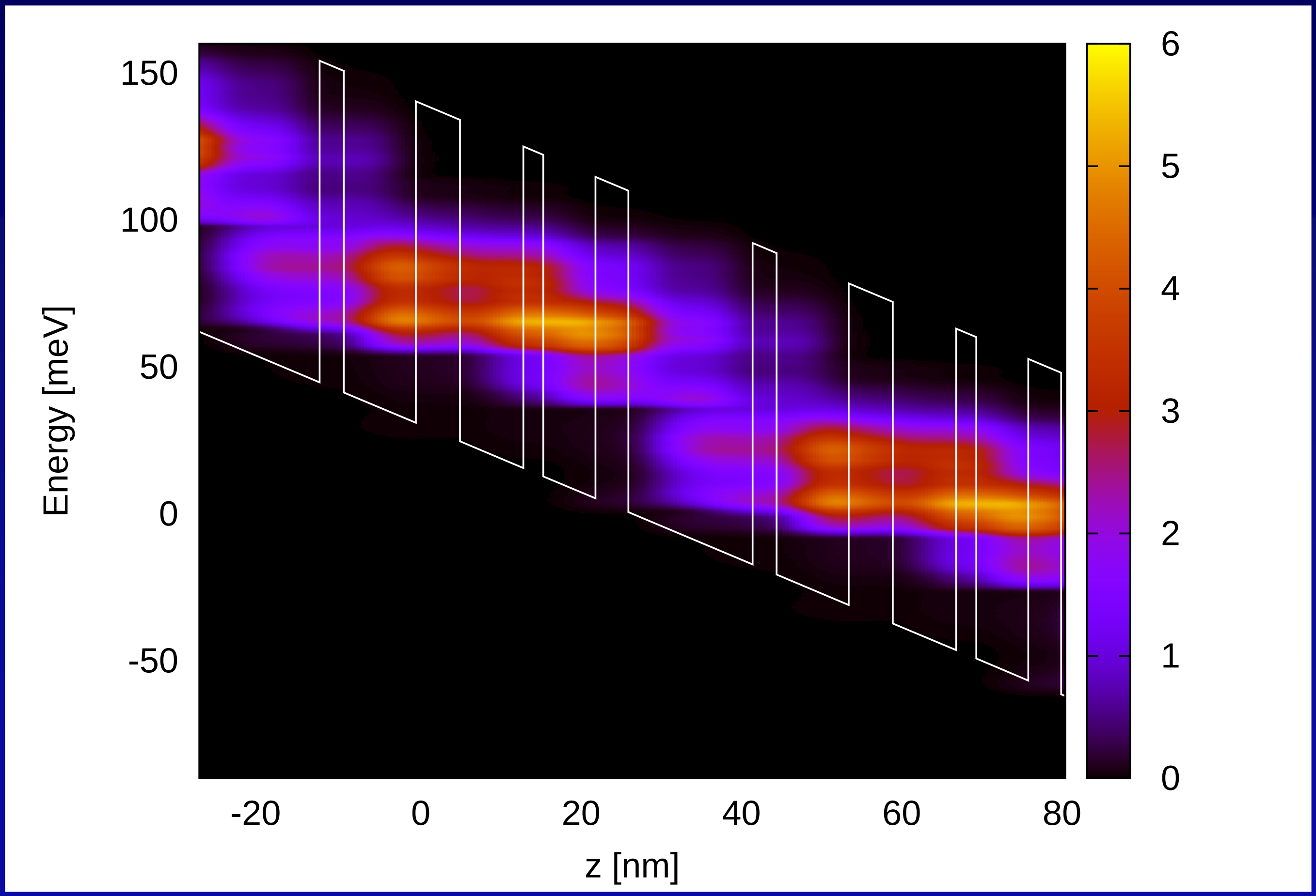
Energetically and Spatially Resolved Current



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