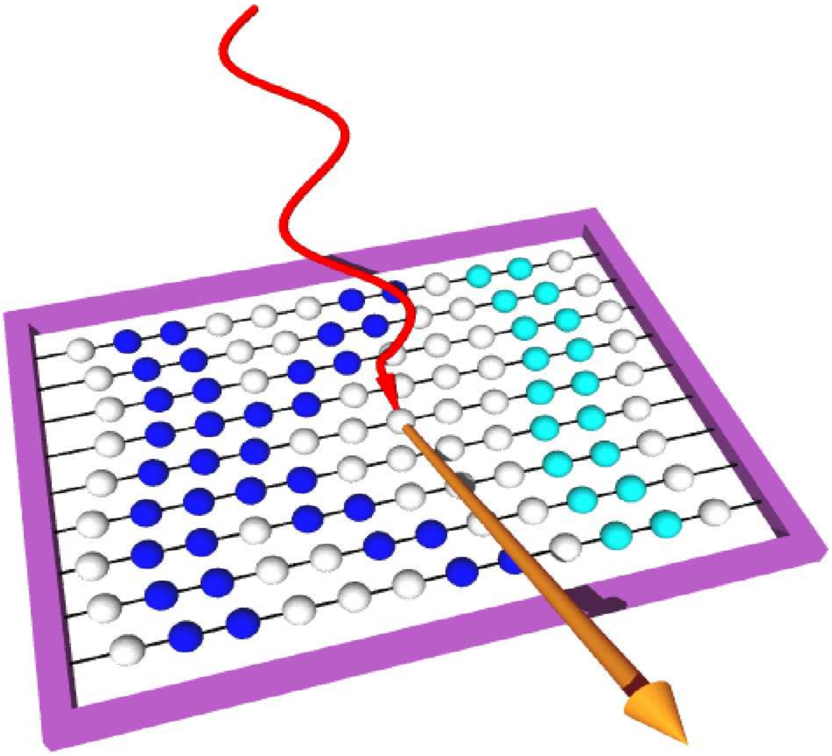
Electron-Scattering States of Solids

Oliver Tiedje

Kiel
1998



O. Tiedje, F. Starrost, C. Solterbeck, and W. Schattke

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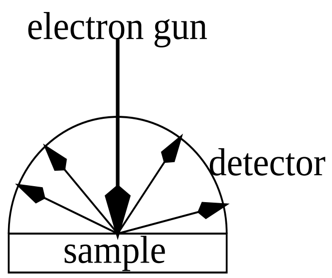
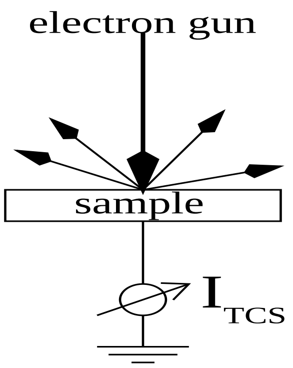
Experiments

1. VLEED



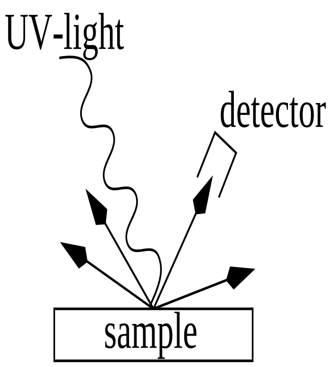
Schrödinger equation
with boundary condition
$\longrightarrow \Phi$

2. TCS



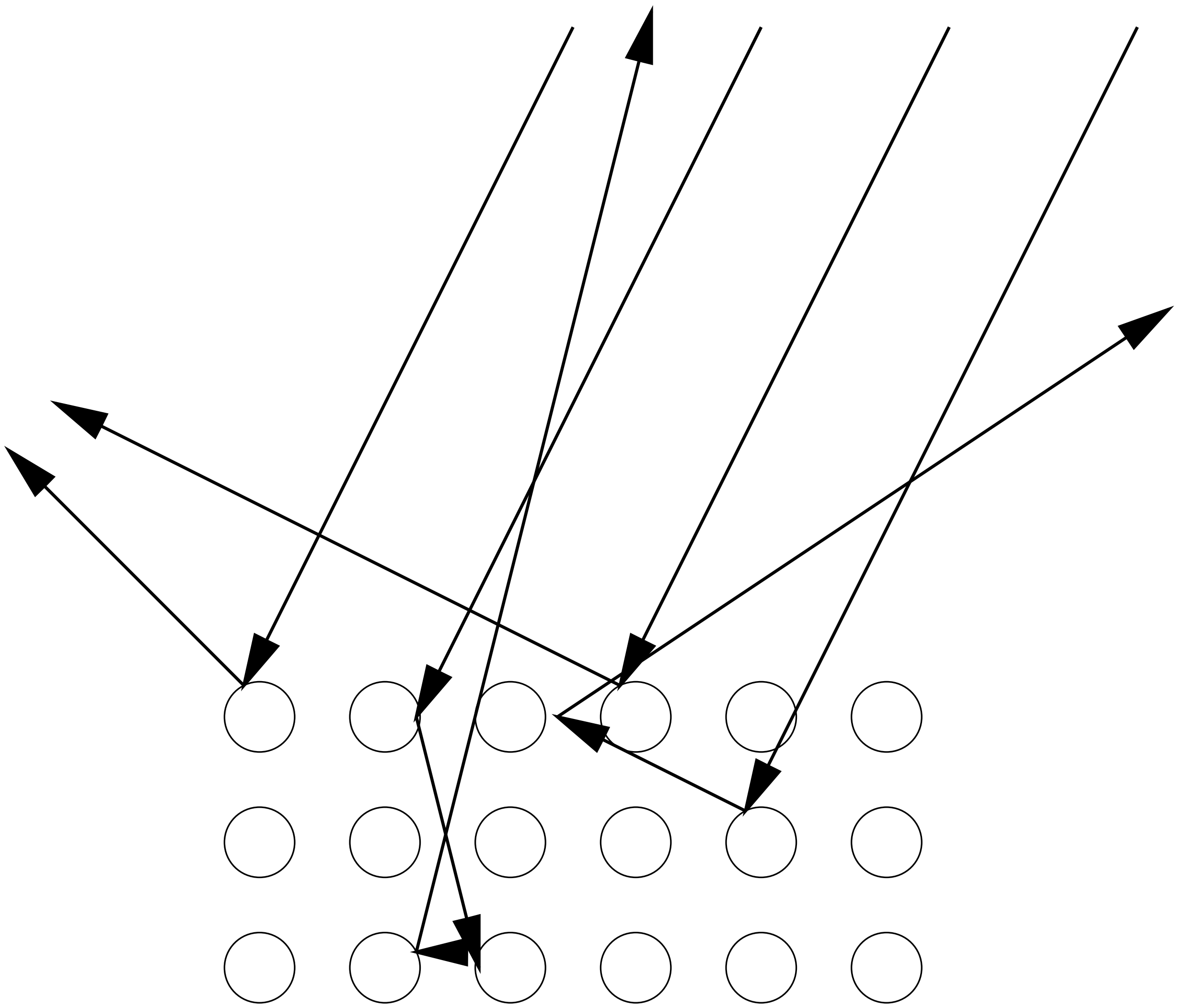
$$I \propto \Phi^* \nabla \Phi - \Phi \nabla \Phi^*$$

3. ARUPS

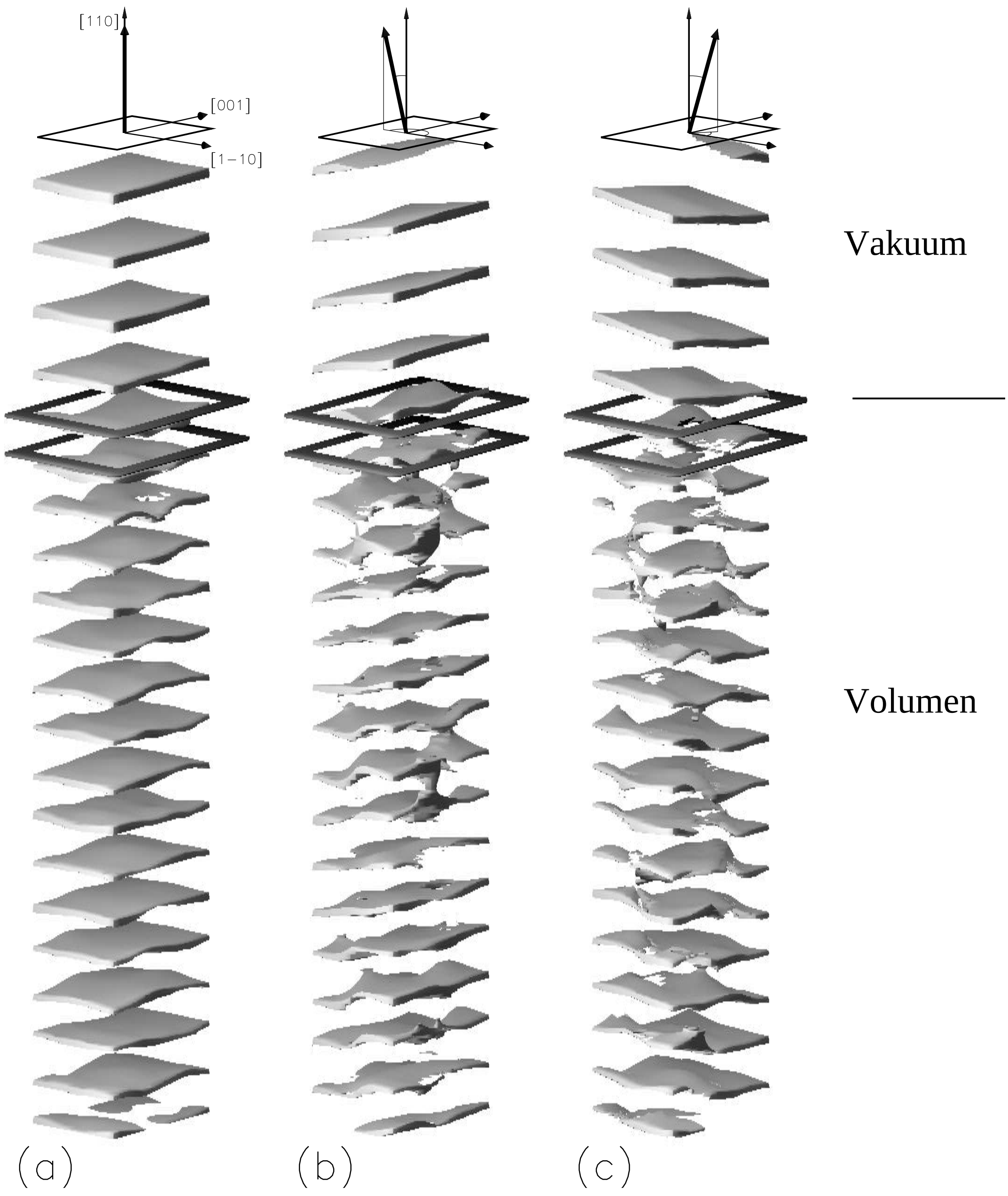


Fermi's Golden Rule
$I \propto \sum_n \delta(E - E_n)$
$| < \Phi^*(E + \hbar\omega)|\hat{O}|n > |^2$

Classical Scattering



Phase Isosurfaces GaAs(110)

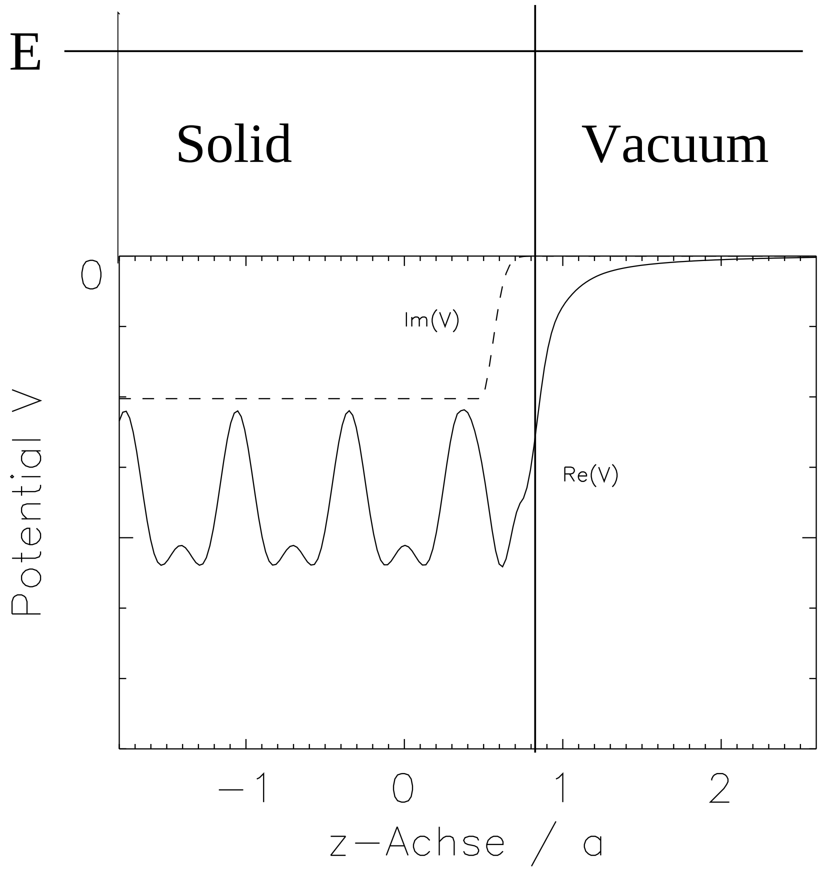


Calculation of Photoemission Final States

- Time Reverse of Electron Diffraction at Very Low Energies
- Half-Crystal
- Scattering States $\longrightarrow$ Boundary Condition
- Realistic Surface Potential (Non-Muffin-Tin)
- Time-Independent Schrödinger Equation
- Numerical Methods for Solving the Boundary Problem
- Important: Time and Memory
  (full hemisphere : $\approx$ 1500 final states)

Schrödinger Equation

$$(-\frac{1}{2}\Delta + V)\psi = E\psi$$



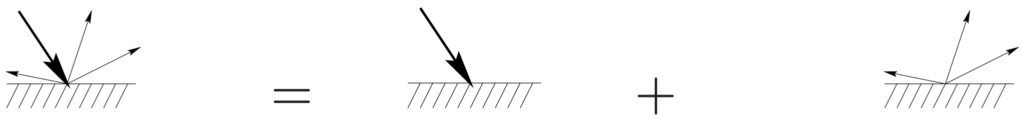
- Real part of V : atomic pseudo potential (with relaxation) + image charge potential
- Imaginary part of V : optical potential (inelastic many-particle effects)

Quantum Transmitting Boundary Method

- Parallel to the surface: Bloch condition
- Deep in the bulk: Zero ($\leftarrow$ optical potential)
- Vacuum: QTBM

$$\kappa_{\vec{g}} = -\sqrt{\frac{2m}{\hbar^2}(E - \Phi_{th}) - (\vec{k_{\|}} + \vec{g})^2}$$

$$\psi(\vec{\rho}, z) = \sum_{\vec{g} \in G} \phi^{+}_{\vec{g}} e^{\imath(\vec{k_{\|}}+\vec{g})\vec{\rho}+\imath\kappa_{\vec{g}}z} + \phi^{-}_{\vec{g}} e^{\imath(\vec{k_{\|}}+\vec{g})\vec{\rho}-\imath\kappa_{\vec{g}}z}$$



$$\begin{aligned} \hat{\psi}(\vec{g}, z) &= \frac{1}{|\Omega|} \int_{\Omega} \psi(\vec{\rho}, z) e^{-\imath(\vec{k_{\|}}+\vec{g})\vec{\rho}} d\vec{\rho} \\ \phi^{-}_{\vec{g}} &= -\phi^{+}_{\vec{g}} e^{2\imath\kappa_{\vec{g}}z} + \hat{\psi}(\vec{g}, z) e^{\imath\kappa_{\vec{g}}z} \end{aligned}$$

$$\int K(\rho - \rho', z)\psi(\rho', z_{max})d\rho' + f(z) = \psi(\rho, z),$$

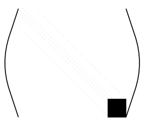
with known functions K and f.

Discretization

One way of solving a boundary problem is to discretize space to get a matrix problem:
Solve $Lu = f$!

Difficulties:

- PDE + Integral b.c. $\longrightarrow$ Irregular Pattern in the Matrix

  L= 

- Schrödinger $\longrightarrow$ Complex

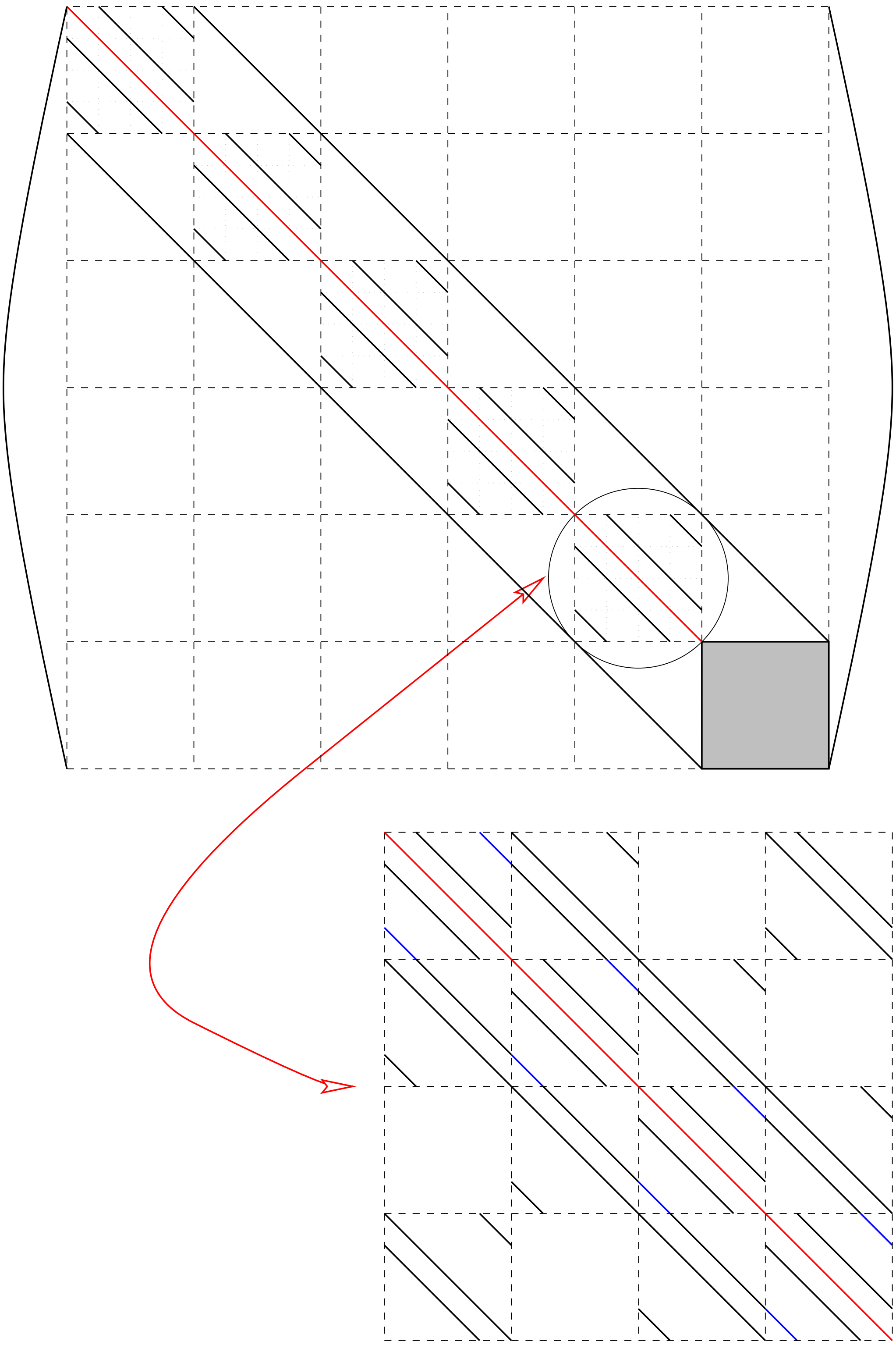
- Optical Potential $\longrightarrow$ Non-Hermitian

- $L = H - E \longrightarrow$ Indefinite

- Wave-Like Solutions $\longrightarrow$ Lower Bound for Grid Size $\longrightarrow$ Large Dimension ≈ 260000

Conventional direct solvers are impracticable, so iterative solver is needed.

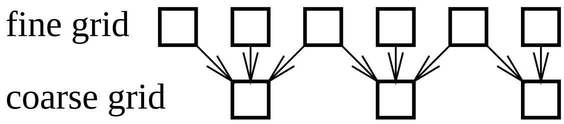
Matrix Pattern



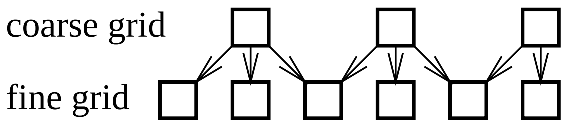
Multigrid

Most iterative solvers:
The low Fourier coefficients converge very slowly,
but the function is smoothed: $u_0 \xrightarrow{S} u_S$
The multigrid idea:
Solve the remaining problem $L\tilde{u} = Lu_S - f$ on a coarser grid!

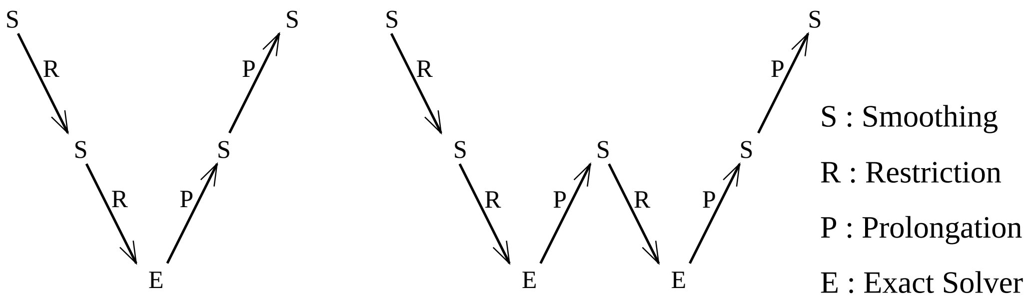
Restriction



Prolongation

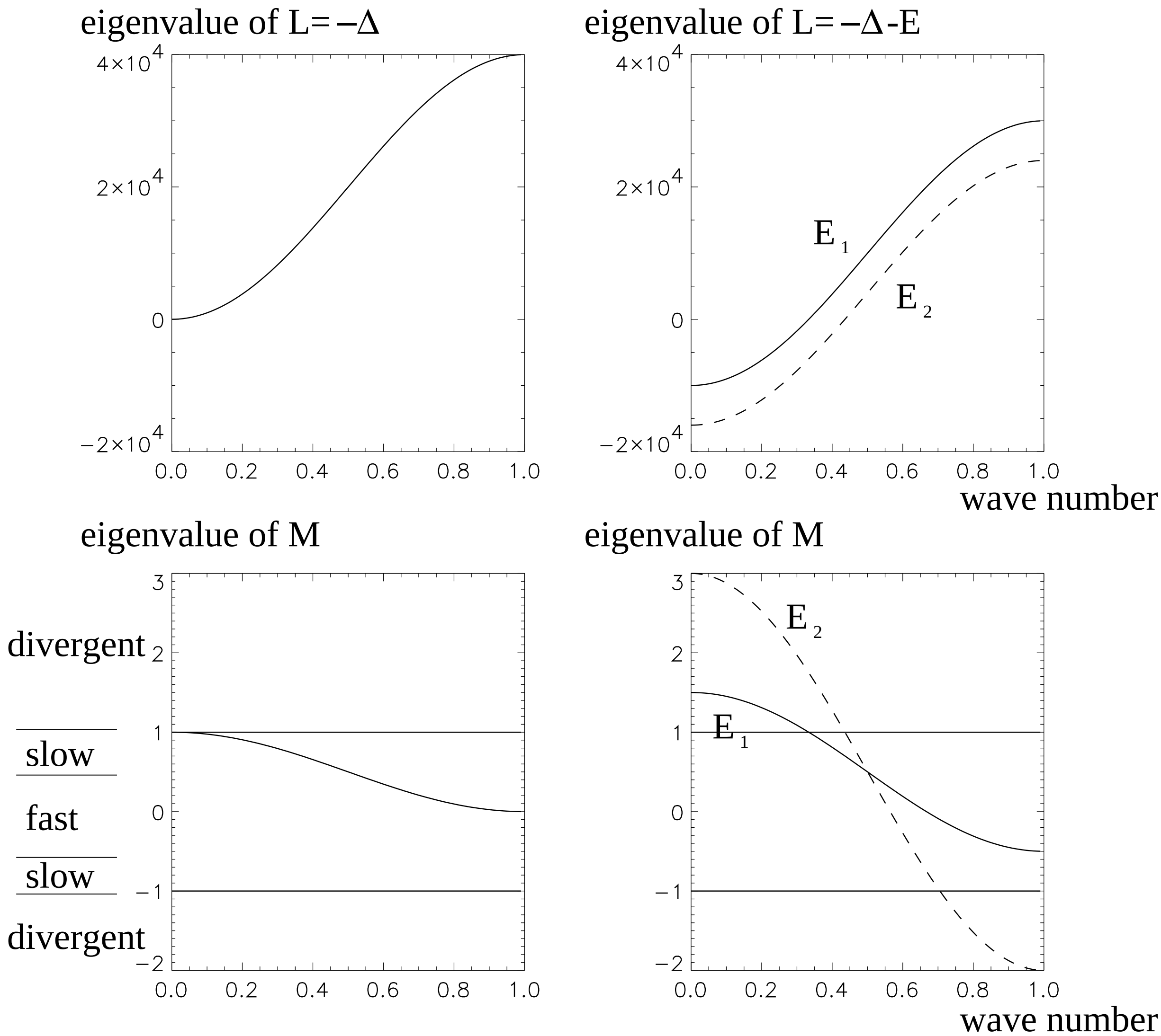


You can arrange these parts like this:



V-cycle W-cycle

Smoothing Property



$M = \mathbf{1} - \omega D^{-1} L \quad , \quad \omega \approx \frac{1}{2}$

Jacobi iteration : $u^{j+1} = M u^j + \omega D^{-1} f$

Defect $d = Lu - f$: $d^{j+1} = LML^{-1} d^j$

$h_{max} \propto \frac{1}{\sqrt{E}}$

Comparison with Other Methods

Schrödinger equation in direct space

- finite differences
- sparse matrix
- solver QMR, (multi-grid)

Schrödinger equation in Laue representation

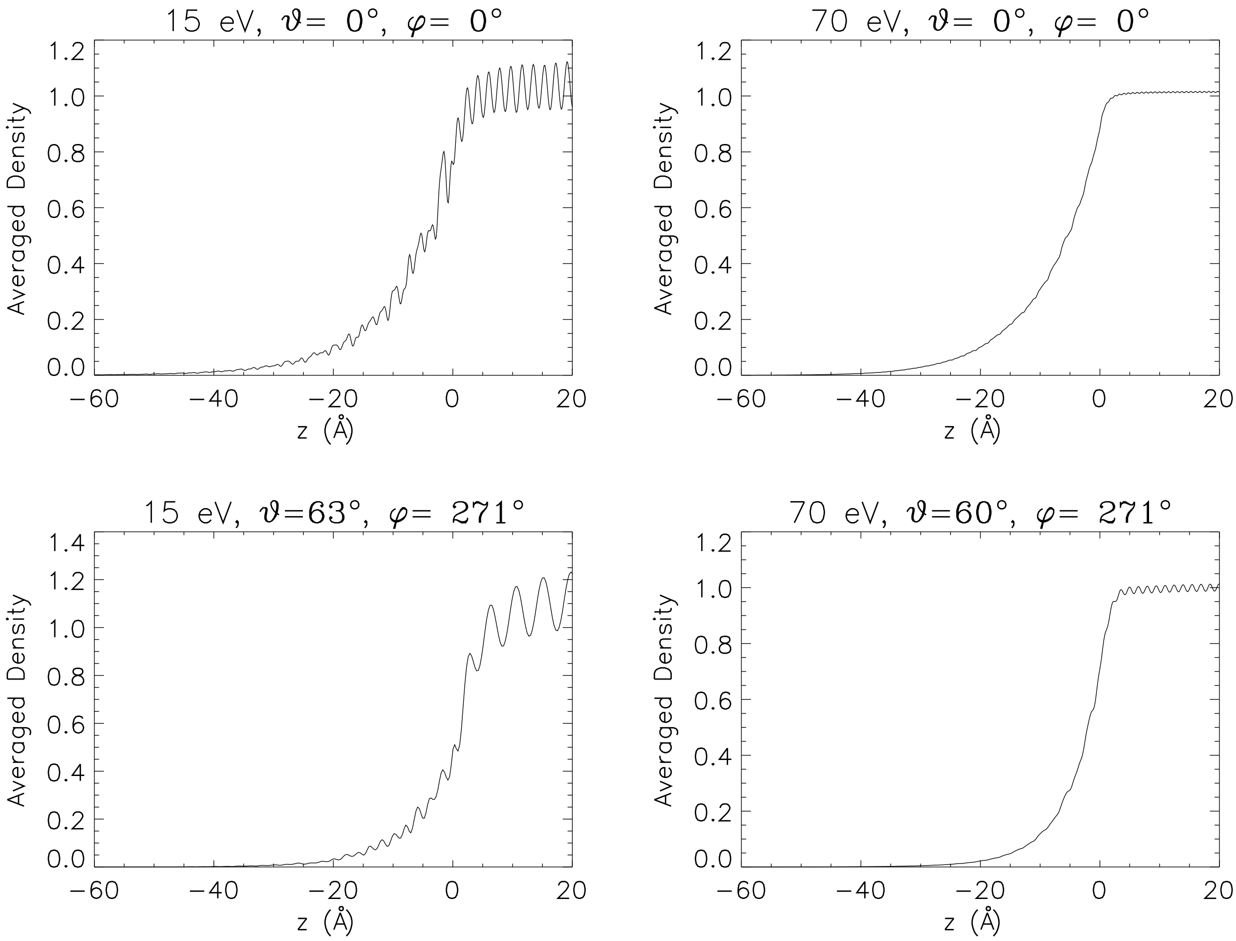
- fourier transformation in xy-direction
- band matrix
- solver LU, multi-grid

Lippman-Schwinger equation in Laue representation

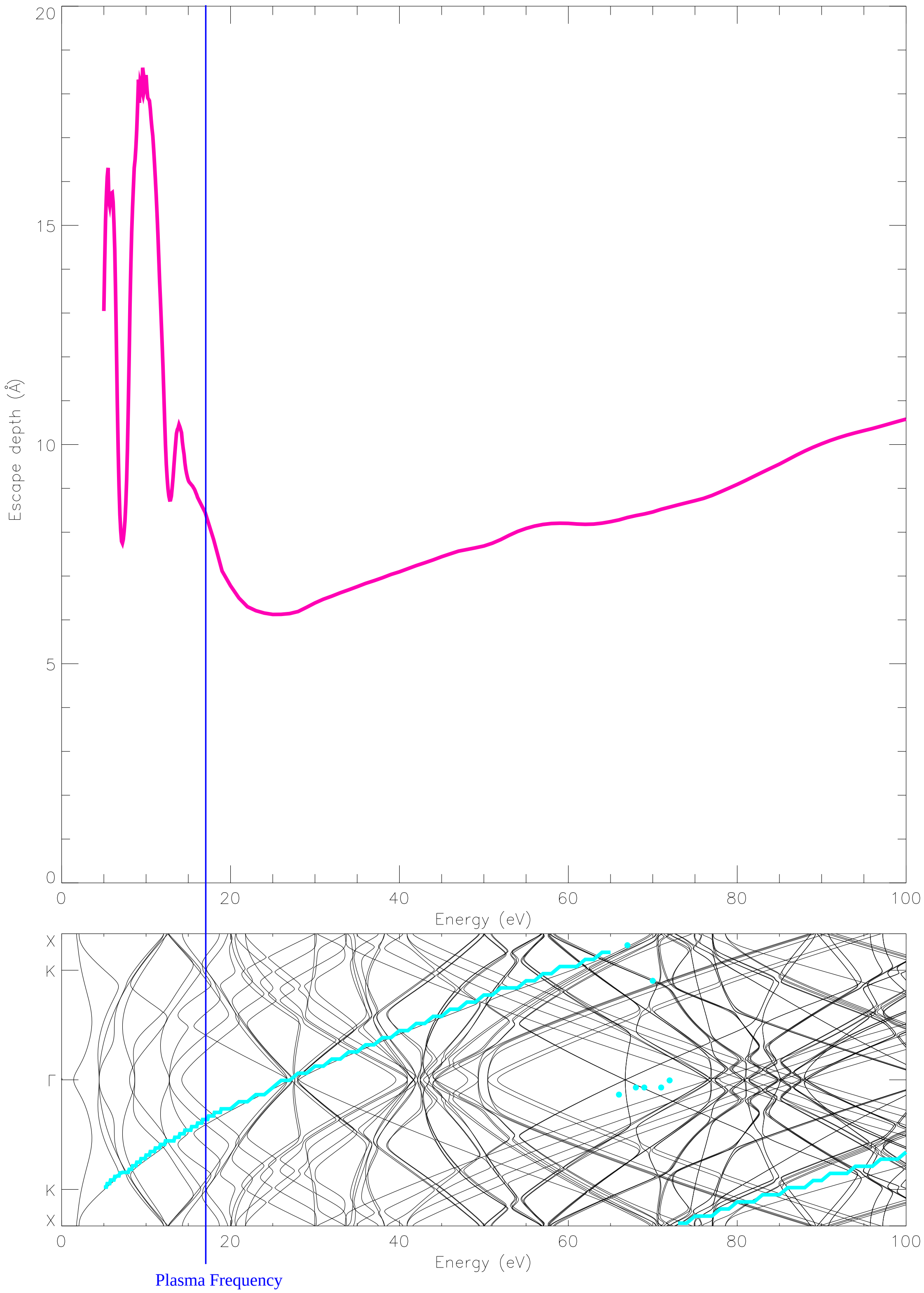
- integral equation (Green's function)
- dense matrix
- solver QMR

Averaged Charge Density

GaAs(110)



'Universal Curve' of Escape Depth

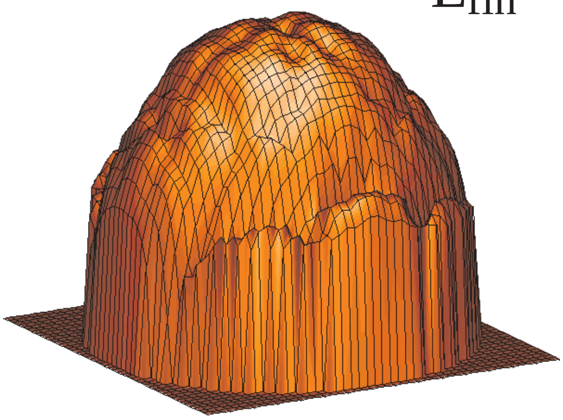


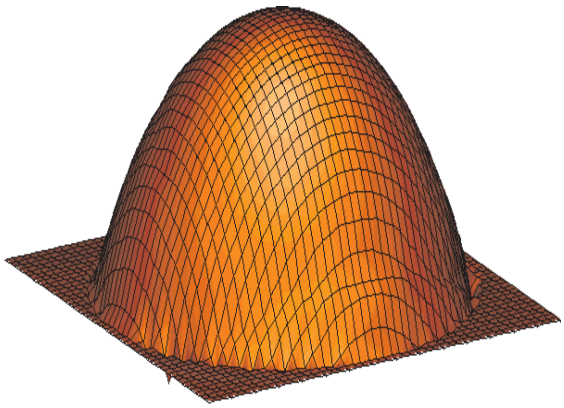
Angular Dependence of Escape Depth

Full hemisphere

Escape depth | **Charge in crystal**

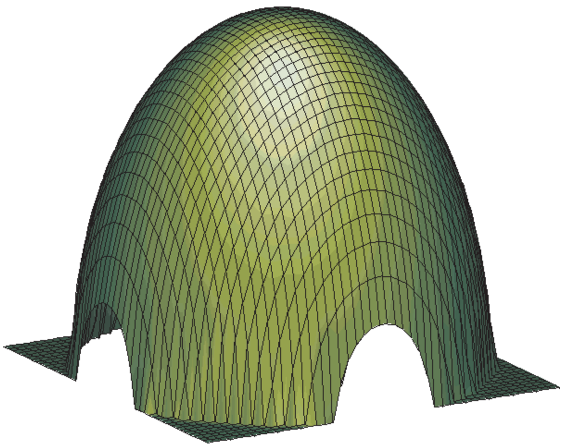
$E_{fin} = 70$ eV



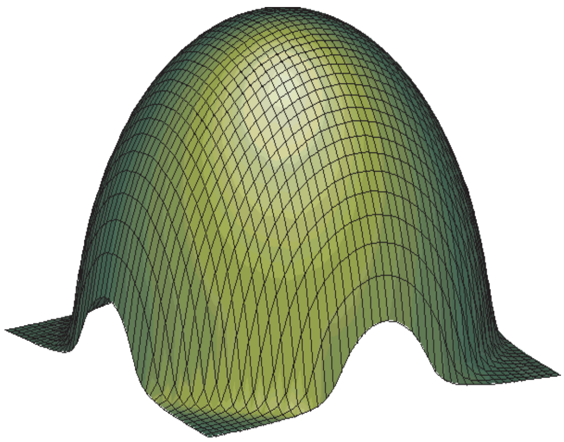


GaAs(110)

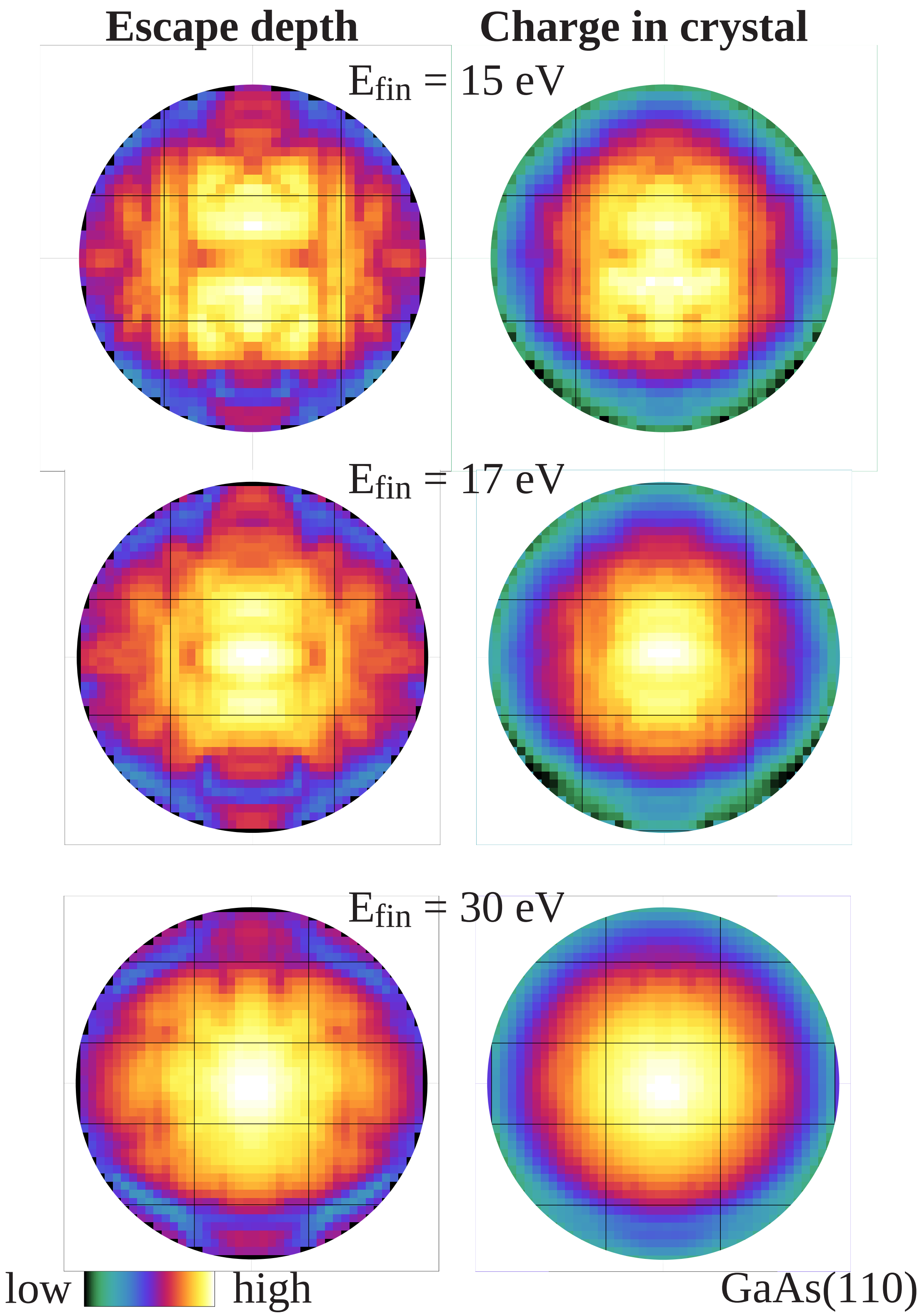
Cosine model



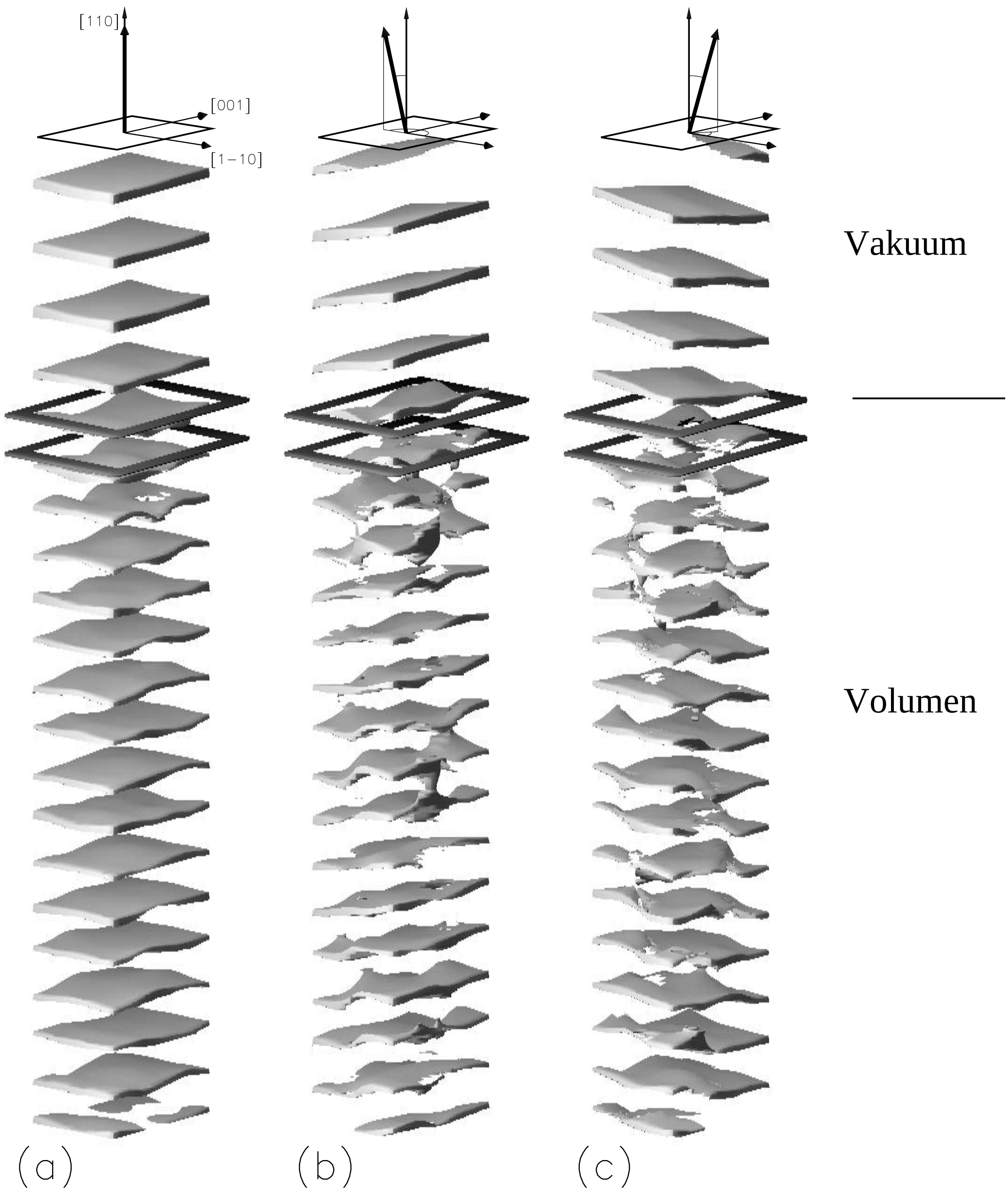
Free electron with optical potential



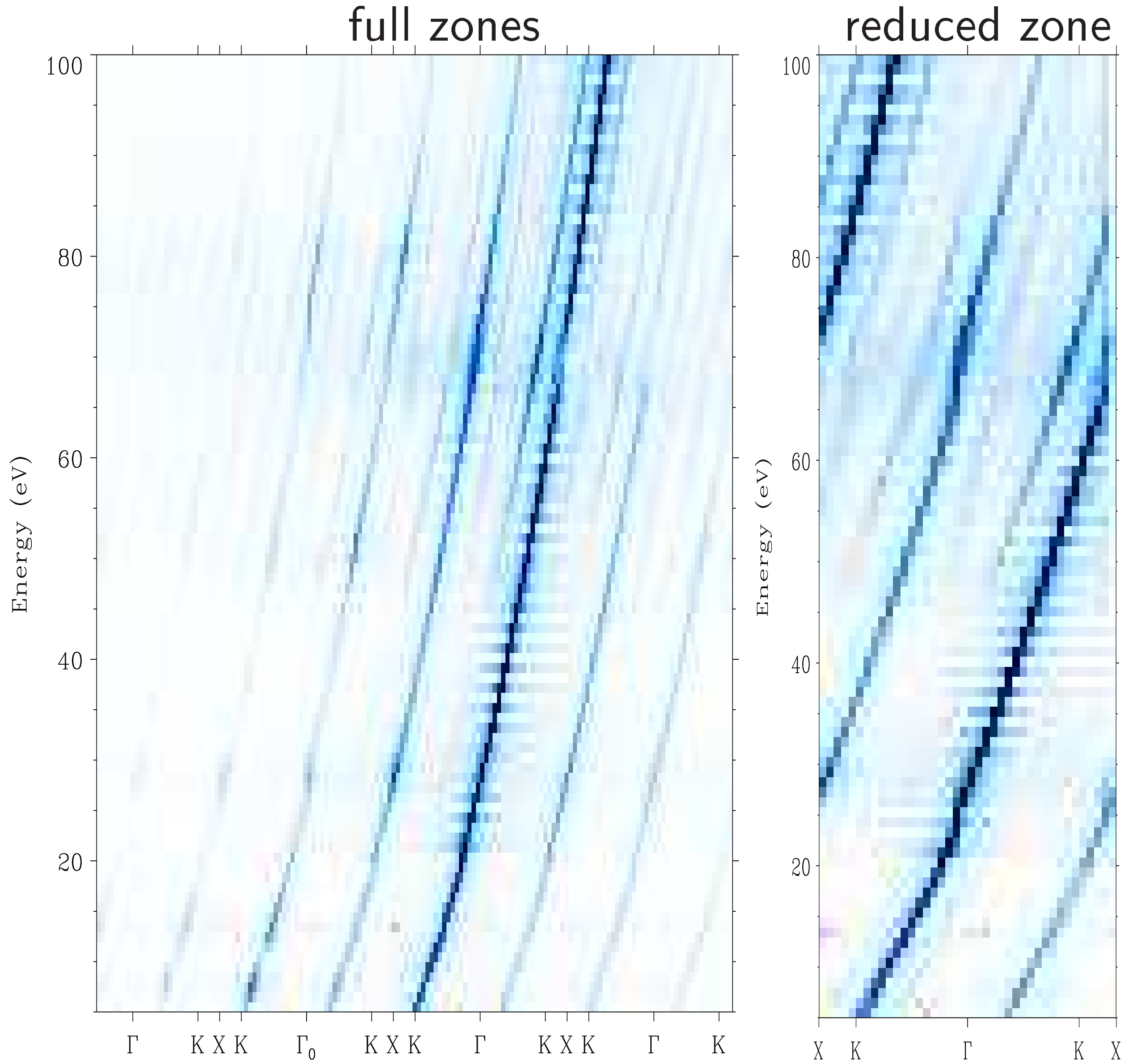
Angular Dependence of Escape Depth



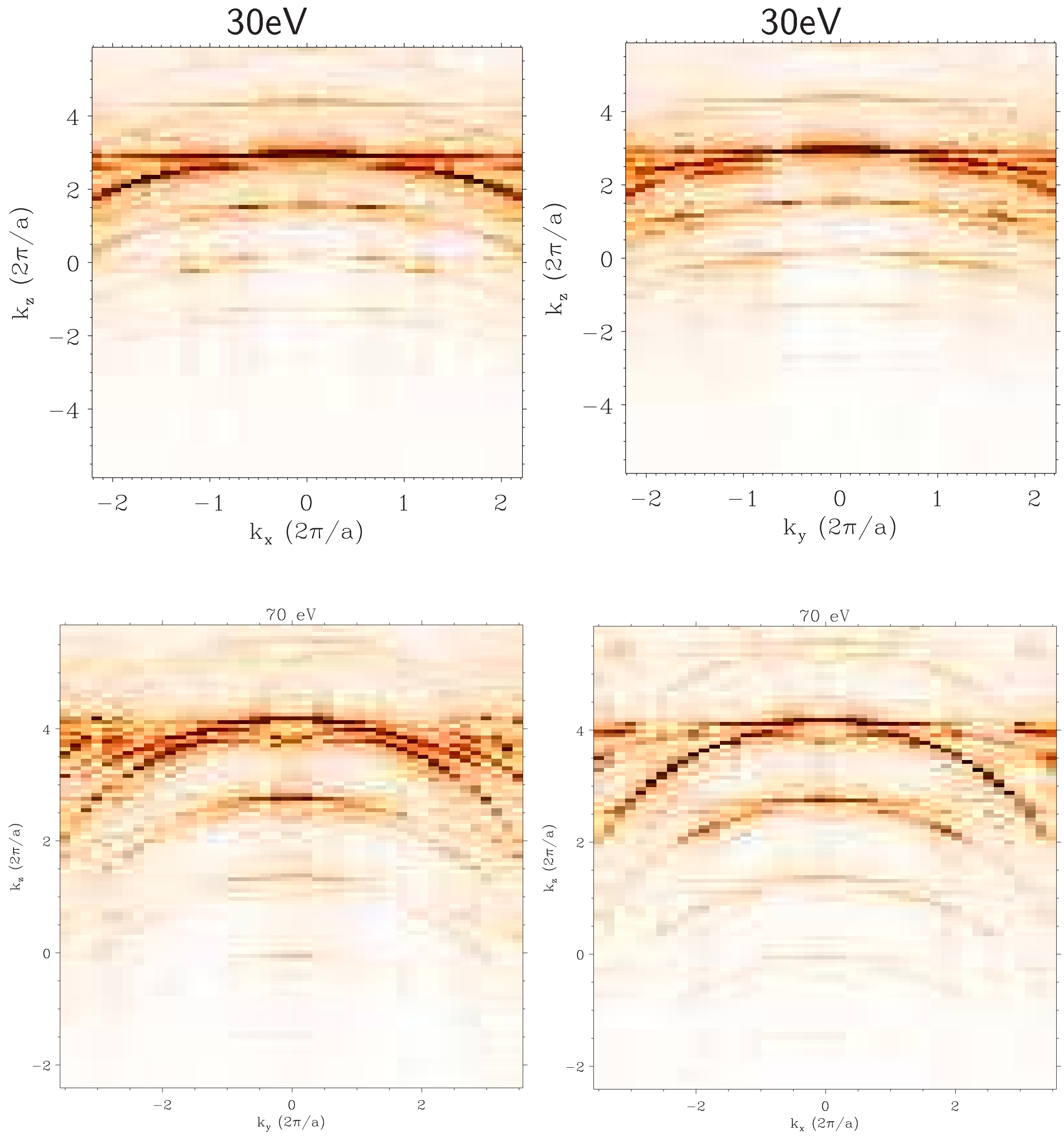
Phase Isosurfaces GaAs(110)



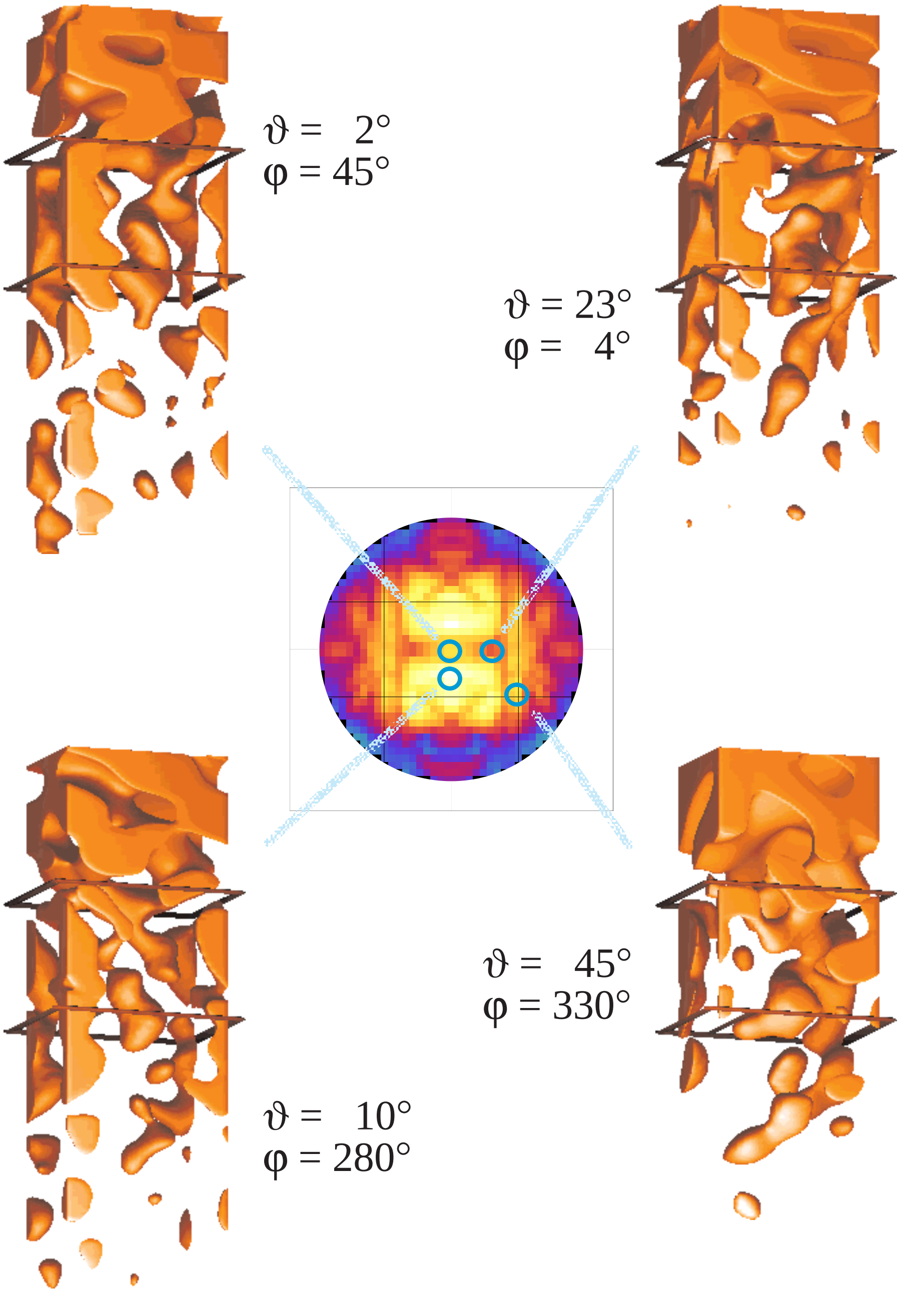
'Band Structure'



Angular Dependence of the Wave Vector



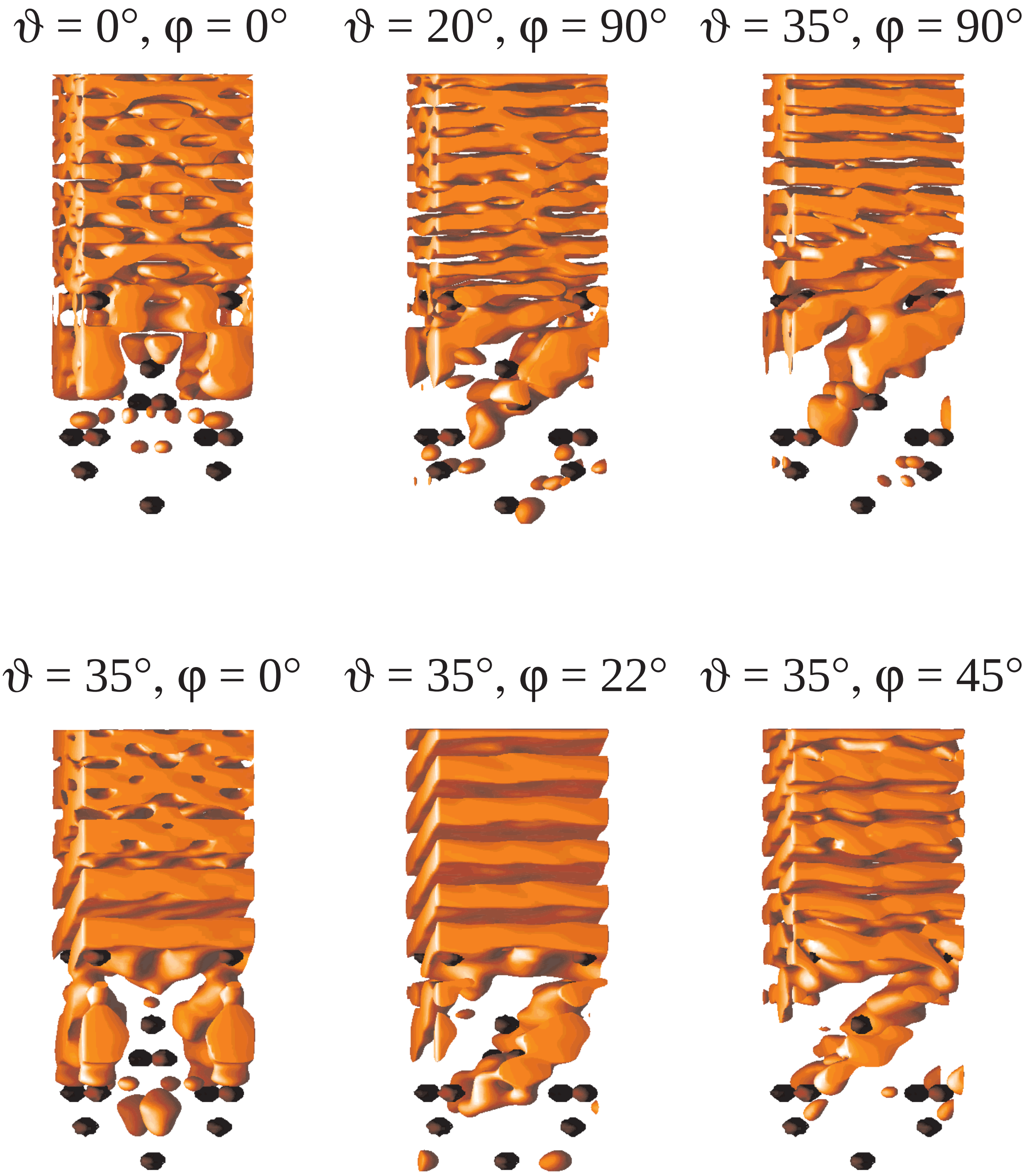
Charge Localization



E_{fin} = 15 eV

GaAs(110)

Charge Localization



$E_{fin} = 55$ eV

Si(001)

Methods and Results

Methods:

- Plane Waves in xy-direction (Phys. Rev. B **55)**
- Schrödinger Eq. in Direct Space (J. Electron Spectrosc., in press)
- Green's Function Technique (Lippman-Schwinger) (do.)

Results:

- Escape Depth
- Density Localization
- Phase Coherence

$\longrightarrow$ Photoemission