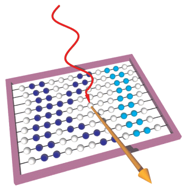

Wave Functions of Electron-Scattering States at Low Energy

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Wave Functions of Scattering States

Calculating direct solutions of the Schrödinger equation with scattering asymptotics has several advantages over the traditional description of multi-scattering processes and the notoriously unstable matching procedures.

The calculations are simple, stable and can be done fast for realsitic potentials, eg. near a surface.

The explicit derivation of the wave function offers a convenient approach for the interpretation of electron spectroscopy at very low energies.

There is more than one way to calculate the wave functions. Several decisions have to be made:

- which equation to solve;
- which representation and discretization to use;
- which numerical techniques to apply.

The following combinations have been shown to work:

- Schrödinger equation in full direct space;
- Lippman-Schwinger equation in the Laue representation;
- Schrödinger equation in the Laue representation.

From these techniques optimal methods can be developed to satisfy the increasing demands for efficiency, flexibility, and accuracy.

Topics

The charge density describes the surface sensitivity and its dependence on angle and kinetic energy.

A Fourier analysis of the phases provides perpendicular wave vectors and gives the relation to band structure.

New aspects arise with spatial modulations of the wave function.

Calculation

Schrödinger equation, full direct space

- sparse system matrix
- one dense block because of boundary conditions
- low memory requirement
- solver: QMR, multi-grid *with problems*

Lippman-Schwinger equation, Laue representation

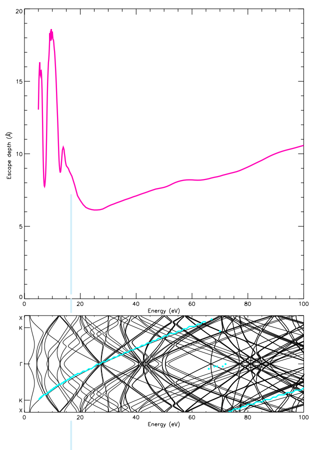
- dense system matrix, but factorizing into two simple matrices allows for more efficiency
- easy boundary conditions
- modest memory requirement
- Nyström discretization in full direct space would lead to a sparse potential matrix and thus ease the application of multi-grid methods
- solver: QMR

Schrödinger equation, Laue representation

- band system matrix
- easy boundary conditions
- high memory requirement
- solver: LU, multi-grid
- very fast

Escape Depth and Energy

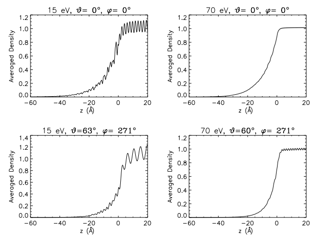
GaAs(110) ▪ Normal incidence



Plasma frequency

- Below the plasma frequency the escape depth is strongly dependend on the band structure.

Averaged charge density



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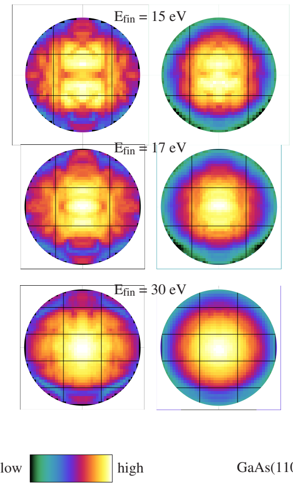
URL: **http://www.tp.cau.de/schattke/**

Escape Depth and Angle

Full hemisphere

Escape depth **Charge in crystal**



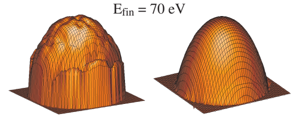
GaAs(110)

- Band structure effects are visible but less important for the increased surface sensitivity at large angles.
- Escape depth (exponent) underestimates the surface sensitivity at large angles.

Full hemisphere

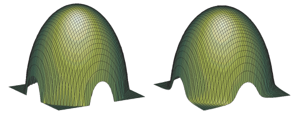
Escape depth **Charge in crystal**

E_{fin} = 70 eV

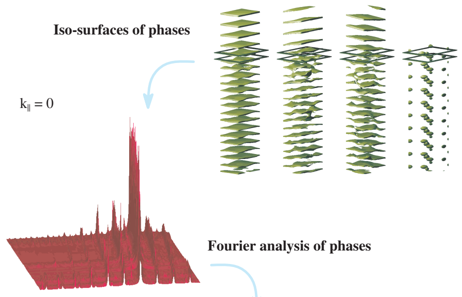


GaAs(110)

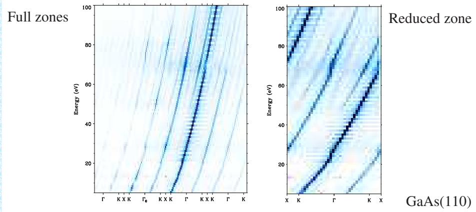
Cosine model **Free electron with optical potential**



Phase and Perpendicular Wave Vector



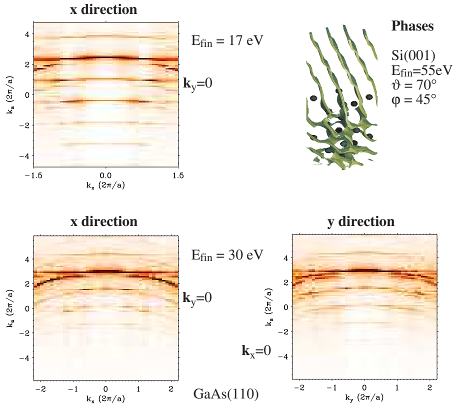
"Band structure" of scattering states



GaAs(110)

- The tail of the wave function inside the solid exhibits several distinct $k_\perp$.
- The high coherence in normal emission is lost with increasing angles.

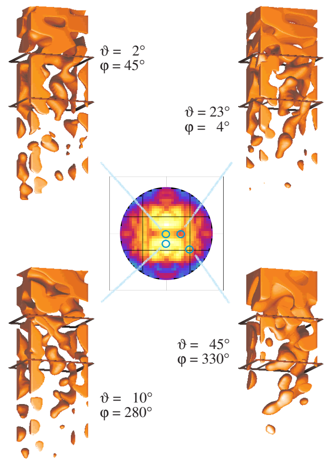
Angular distribution of $k_\perp$



GaAs(110)

Localization of Charge Density

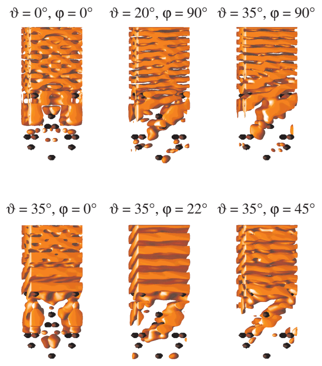
Iso-surfaces of charge density



E_{fin} = 15 eV GaAs(110)

- Scattering states bear a rich spatial structure.
- Charge localizations at bonds, in crystal planes etc. might provide help for the analysis of spectra.

Iso-surfaces of charge density



E_{fin} = 55 eV Si(001)