

ARPES signal calculation in a slab with a depletion/accumulation surface layer (quasi-1D model)

https://github.com/eugnsp/surface_arpes

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This document contains a succinct description of equations that are numerically solved in the code. No attempt has been made to present mathematically and/or physically rigorous derivations.

1 Quasi-classical problem

1.1 Poisson equation

To find the potential profile $\phi(z)$, we solve the 1D Poisson equation:

$$-\frac{d}{dz} \left[\epsilon \frac{d\phi(z)}{dz} \right] = 4\pi [N_D - n(z)], \quad (1)$$

where N_D is the (spatially uniform) density of ionized donors, and $n(z)$ is the electron density. It is given by

$$n(z) = N_c^{3D} f_{FD}^{1/2} \left[-\frac{E_c(z) - F}{T} \right] = N_c^{3D} f_{FD}^{1/2} \left[-\frac{E_{c0} - \phi(z) - F}{T} \right] \quad (2)$$

where N_c is the effective 3D density of states, f_{FD}^α is the Fermi-Dirac integral of order α ,

$$f_{FD}^\alpha(x) = \frac{1}{\Gamma(\alpha+1)} \int_0^\infty dt \frac{t^\alpha}{1 + e^{t-x}}, \quad (3)$$

F is the Fermi level, E_{c0} is the conduction band minimum, and T is the lattice temperature.

The effective 3D density of states is given by

$$N_c^{3D} = 2 \left[\frac{mT}{2\pi} \right]^{3/2}, \quad (4)$$

where m is the electron effective mass.

The zero level of energy is chosen such that $E_{c0} = 0$. Then the arbitrary additive constant in the potential $\phi(x)$ is chosen such that $\phi(x) = 0$ corresponds to charge neutrality:

$$N_D = N_c^{3D} f_{FD}^{1/2} \left[\frac{F}{T} \right], \quad \text{or} \quad F = T \{f_{FD}^{1/2}\}^{-1} \left[\frac{N_D}{N_c^{3D}} \right]. \quad (5)$$

Finally:

$$n(\phi) = N_c^{3D} f_{FD}^{1/2} \left[\frac{\phi + F}{T} \right], \quad \frac{dn}{d\phi} = \frac{N_c^{3D}}{T} f_{FD}^{-1/2} \left[\frac{\phi + F}{T} \right]. \quad (6)$$

The Poisson equation (1) is a non-linear equation. To solve it, we employ the Newton's method. Linearizing for $\phi(z) = \phi_0(z) + \delta\phi(z)$, we get:

$$-\frac{d}{dz} \left[\epsilon \frac{d\delta\phi(z)}{dz} \right] + 4\pi \frac{dn_0}{d\phi_0} \delta\phi(z) = \frac{d}{dz} \left[\epsilon \frac{d\phi_0(z)}{dz} \right] + 4\pi [N_D - n_0(z)], \quad (7)$$

where $n_0(z) = n(\phi_0(z))$.

Boundary conditions. The boundary conditions for eq. (1) are:

$$\phi(0) = \phi_b, \quad \frac{d\phi(L)}{dz} = E(L) = 0, \quad (8)$$

where L is the system length, chosen such that $L \gg$ screening length. Corresponding boundary conditions for eq. (7) are:

$$\delta\phi(0) = 0, \quad \frac{d\delta\phi(L)}{dz} = 0. \quad (9)$$

The initial guess for $\phi_0(z)$ is obtained from local charge neutrality inside the system. Hence, we start Newton's iterations from $\phi_0(0) = \phi_b$, $\phi_0(z > 0) = 0$.

Finite elements discretization. Galerkin's method is used for numerical solution of eq. (7). We multiply it by the test function $\psi_i(z)$ and integrate by parts taking into account the boundary conditions:

$$\begin{aligned} \int dz \frac{d\psi_i}{dz} \frac{d\delta\phi}{dz} + 4\pi \int dz \frac{dn_0}{d\phi_0} \psi_i \delta\phi &= \\ &= - \int dz \epsilon \frac{d\psi_i}{dz} \frac{d\phi_0}{dz} + 4\pi \int dz (N_D - n_0) \psi_i. \end{aligned} \quad (10)$$

Expanding $\delta\phi(z)$ over $\psi_i(z)$, $\delta\phi(x) = \sum_j \delta\phi_j \psi_j(z)$, = we obtain the matrix equation:

$$\sum_j (S_{ij} - M_{ij}) \delta\phi_j = r_i \quad (11)$$

with

$$\begin{aligned} S_{ij} &= \int dz \epsilon \frac{d\psi_i}{dz} \frac{d\psi_j}{dz}, \quad M_{ij} = -4\pi \int dz \frac{dn_0}{d\phi_0} \psi_i \psi_j, \\ r_i &= - \sum_j S_{ij} \phi_{0j} + 4\pi \int dz (N_D - n_0) \psi_i. \end{aligned} \quad (12)$$

Integrals are calculated using Gauss quadratures $\{z_k, w_k\}$. In particular:

$$\int dz n_0 \psi_i = \sum_k w_k n[\phi_0(z_k)] \psi_i(z_k) = \sum_k w_k n \left[\sum_l \phi_{0l} \psi_l(z_k) \right] \psi_i(z_k), \quad (13)$$

and

$$\int dz \frac{dn_0}{d\phi_0} \psi_i \psi_j = \sum_k w_k \frac{dn}{d\phi} \left[\sum_l \phi_{0l} \psi_l(z_k) \right] \psi_i(z_k) \psi_j(z_k). \quad (14)$$

2 Quantum problem

To account for quantum effects, we solve the Schrödinger and the Poisson equations self-consistently. First, we solve the Schrödinger equation

$$\frac{1}{2m} \frac{d^2}{dz^2} \psi(z) + V(z) \psi(z) = E \psi(z) \quad (15)$$

with $V(z) = -\phi(z)$, and then use the first-order perturbation theory to turn a linear Poisson equation into a non-linear one with the electron density given by

$$n(\phi, z) = N_c^{2D} \sum_n |\psi_n^{(0)}(z)|^2 f_{FD}^0 \left[\frac{\phi(z) - \phi^{(0)}(z) + F - E_n^{(0)}}{T} \right], \quad (16)$$

where the effective 2D density of states is given by

$$N_c^{2D} = \frac{mT}{\pi}. \quad (17)$$

and summation is performed over all eigenstates $\{\psi_n^{(0)}(z), E_n^{(0)}\}$ that were obtained by solving (15) with the potential $V(z) = -\phi_0^{(0)}(z)$. The derivative of $n(\phi, z)$ is

$$\frac{dn}{d\phi} = \frac{N_c^{2D}}{T} \sum_n |\psi_n^{(0)}(z)|^2 f_{FD}^{-1} \left[\frac{\phi(z) - \phi^{(0)}(z) + F - E_n^{(0)}}{T} \right]. \quad (18)$$

The initial approximation for $\phi(z)$ is obtained from the solution of the quasi-classical problem (1)–(2).

The Fermi–Dirac integrals $f_{FD}^0(x)$ and $f_{FD}^{-1}(x)$ have closed forms:

$$f_{FD}^0(x) = \ln[1 + e^x], \quad f_{FD}^{-1}(x) = \frac{1}{1 + e^{-x}} = f_{FD}(-x), \quad (19)$$

where $f_{FD}(x)$ is the Fermi–Dirac distribution.

Boundary conditions. The potential barriers at the system boundaries are assumed to be infinitely high, so we put

$$\psi(z=0) = \psi(z=L) = 0. \quad (20)$$

Finite elements discretization. Here we also use the Galerkin's method. Eq. (15) reduces to a generalized eigenvalue problem:

$$\sum_j (T_{ij} + V_{ij}) \psi_j = E_n B_{ij} \psi_j \quad (21)$$

with

$$T_{ij} = \frac{1}{2m} \int dz \frac{d\psi_i}{dz} \frac{d\psi_j}{dz}, \quad V_{ij} = \int dz V \psi_i \psi_j, \quad B_{ij} = \int dz \psi_i \psi_j, \quad (22)$$

where B is positive-definite.

3 ARPES signal calculation

The intensity of the ARPES signal at $k_y = 0$ is given by:

$$I^0(k_x, k_z, E) \sim f_{\text{FD}} \left[\frac{E - F}{T} \right] \sum_n f_{\text{D}} \left[E - E_n - \frac{k_x^2}{2m} \right] |\varphi_n(k_z)|^2, \quad (23)$$

where

$$\varphi_n(k_z) = \int dz e^{-ik_z z - z/\lambda} \psi_n(z), \quad (24)$$

and the Lorentz distribution

$$f_{\text{D}}(E) \sim \frac{1}{1 + (E/\delta_D E)^2} \quad (25)$$

accounts for disorder.

If $\phi(z) = 0$, in the limit $L \rightarrow \infty$ and $\lambda \rightarrow \infty$ we recover a broadened parabolic spectrum:

$$I^0(E, k_x, k_z) \sim f_{\text{FD}} \left[\frac{E - F}{T} \right] f_{\text{D}} \left[E - \frac{k_x^2 + k_z^2}{2m} \right]. \quad (26)$$

To account for instrumental broadenings, we further convolve $I_0(k_x, k_z, E)$ with two normal distributions (broadening over k_z is assumed to be negligible)

$$f_A(k) \sim \exp \left[-\frac{k^2}{2(\delta_A k)^2} \right] \quad \text{and} \quad f_A(E) \sim \exp \left[-\frac{E^2}{2(\delta_A E)^2} \right] \quad (27)$$

to obtain the final result:

$$\begin{aligned} I(k_x, k_z, E) &\sim I^0(k_x, k_z, E) \star (f_A(k_x) \otimes \delta(k_z) \otimes f_A(E)) \sim \\ &\sim \int dk'_x dE' I^0(k_x - k'_x, k_z, E - E') f_A(k'_x) f_A(E'). \end{aligned} \quad (28)$$

Let's introduce a partial intensity function

$$I_n^0(k_x, E) \sim f_{\text{FD}} \left[\frac{E - F}{T} \right] f_{\text{D}} \left[E - E_n - \frac{k_x^2}{2m} \right] \quad (29)$$

and its convolution

$$I_n(k_x, E) \sim \int dk'_x dE' I_n^0(k_x - k'_x, E - E') f_A(k'_x) f_A(E'). \quad (30)$$

Then $I(k_x, k_z, E)$ can be written as

$$I(k_x, k_z, E) \sim \sum_n I_n(k_x, E) |\varphi_n(k_z)|^2. \quad (31)$$

We want to compute three types of spectra: $I(k_x, 0, E)$, $I(0, k_z, E)$, and $I(k_x, k_z, F)$.

1. At $k_z = 0$ we have:

$$I(k_x, E) \sim \sum_n I_n(k_x, E) |\varphi_n(0)|^2. \quad (32)$$

2. At $E = F$ we have:

$$I(k_x, k_z) \sim \sum_n I_n(k_x, F) |\varphi_n(k_z)|^2. \quad (33)$$

3. At $k_x = 0$ we have:

$$I(k_z, E) \sim \sum_n I_n(0, E) |\varphi_n(k_z)|^2. \quad (34)$$