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 conains 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. Please see references for details.

1 Quasi-classical problem

1.1 Poisson equation

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

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

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

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

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

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

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

The effective 3D density of states is given by

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

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:

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

Finally:

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

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:

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

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

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

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

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

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

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:

$$\int \frac{\mathrm{d}\psi_i}{\mathrm{d}z}\frac{\mathrm{d}\delta\phi}{\mathrm{d}z} + 4\pi \int \frac{\mathrm{d}n_0}{\mathrm{d}\phi_0}\psi_i \delta\phi = -\int \epsilon \frac{\mathrm{d}\psi_i}{\mathrm{d}z}\frac{\mathrm{d}\phi_0}{\mathrm{d}z} + 4\pi \int (N_D - n_0)\psi_i. \tag{10}$$

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

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

with

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

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

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

and

$$\int \frac{\mathrm{d}n_0}{\mathrm{d}\phi_0} \psi_i \psi_j = \sum_k w_k \frac{\mathrm{d}n}{\mathrm{d}\phi} \Big[\sum_l \phi_{0l} \psi_l(z_k) \Big] \psi_i(z_k) \psi_j(z_k). \qquad (14)$$

2 Quantum problem

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

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

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

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

where the effective 2D density of states is given by

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

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

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

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

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

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

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

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

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

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

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

with

$$T_{ij} = \frac{1}{2m} \int \frac{\mathrm{d}\psi_i}{\mathrm{d}z} \frac{\mathrm{d}\psi_j}{\mathrm{d}z}, \quad V_{ij} = \int V \psi_i \psi_j, \quad B_{ij} = \int \psi_i \psi_j, \tag{22}$$

where B is positive-definite.

3 ARPES signal calculation

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

$$I_0(E, k_x, k_z) \sim f_{\mathrm{FD}} \left[\frac{E - F}{T} \right] \times \\ \times \sum_n f_{\mathrm{D}} \left[E - E_n - \frac{k_x^2}{2m} \right] \left| \int \mathrm{d}z\, e^{-\mathrm{i}k_z z - z/\lambda} \psi_n(z) \right|^2, \tag{23}$$

where the Lorentz distribution

$$f_{\mathrm{D}}(E) \sim \frac{1}{1 + (E/\delta_D E)^2} \tag{24}$$

accounts for disorder.

If $\phi(z) = 0$, in the limit $L \to \infty$:

$$I_0(E, k_x, k_z) \sim f_{\mathrm{FD}} \left[\frac{E - F}{T} \right] \int \mathrm{d}k'_z\, f_{\mathrm{D}} \left[E - \frac{k_x^2 + k_z'^2}{2m} \right] \frac{1}{1 + [\lambda(k_z - k'_z)]^2}. \tag{25}$$

In the limit $\lambda \to \infty$ we recover a broadened parabolic spectrum:

$$I_0(E, k_x, k_z) \sim f_{\mathrm{FD}} \left[\frac{E - F}{T} \right] f_{\mathrm{D}} \left[E - \frac{k_x^2 + k_z^2}{2m} \right]. \tag{26}$$

At $k_z = 0$ we have:

$$I_0(E, k_x) \sim f_{\mathrm{FD}} \left[\frac{E - F}{T} \right] \sum_n f_{\mathrm{D}} \left[E - E_n - \frac{k_x^2}{2m} \right] \left[\int \mathrm{d}z\, e^{-z/\lambda} \psi_n(z) \right]^2. \tag{27}$$

To account for apparatus broadenings, we futher convolve $I_0(E, k_x)$ with two normal distributions

$$f_A(E) \sim \exp\left[-\frac{E^2}{2(\delta_A E)^2} \right], \quad f_A(k) \sim \exp\left[-\frac{k^2}{2(\delta_A k)^2} \right] \tag{28}$$

to obtain the final result:

$$I(E, k_x) \sim I_0(E, k_x) \star (f_A(E) \otimes f_A(k)) = \\ = \int \mathrm{d}k'_x \mathrm{d}E'\, f_A(E') f_A(k'_x) I_0(E - E', k_x - k'_x). \tag{29}$$