The PWcond code: Complex bands, transmission, and ballistic conductance

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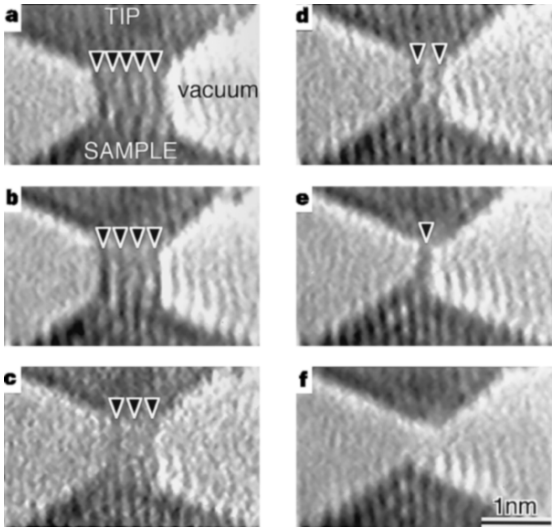
Outline

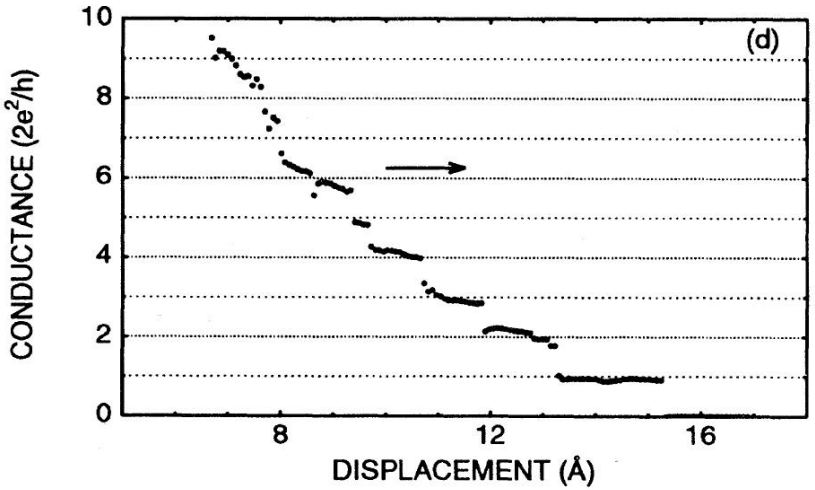
Ohm's law versus ballistic transport

According to the Ohm's law, the conductance G of a solid is

$$G = \frac{S}{L}\eta,$$

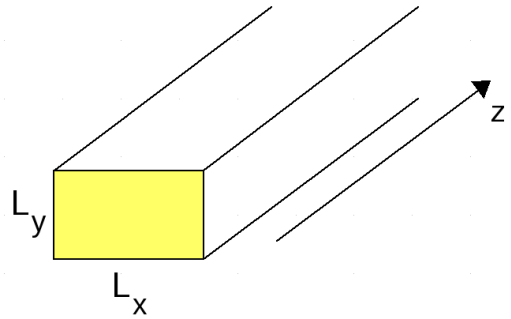
where S is its cross section, L its length and η the material dependent conductivity. Instead in very small contacts of nanometer size the measured conductance is:





Ohm law versus ballistic transport

The conductance is constant and independent of the length until the wire rearranges. At that point there is an abrupt jump. This behavior can be explained by the theory of ballistic transport valid when the system size is much smaller than the electron mean free path and comparable to the electron Fermi wavelength. Let us consider an ideal wire such as the following:



Electron energy levels of an ideal wire

The energy levels of this wire with rectangular cross section $S = L_x L_y$ are:

$$\varepsilon_{n_x,n_y,k_z} = \frac{\hbar^2\pi^2}{2m}\left[\left(\frac{n_x}{L_x}\right)^2 + \left(\frac{n_y}{L_y}\right)^2\right] + \frac{\hbar^2 k_z^2}{2m}$$

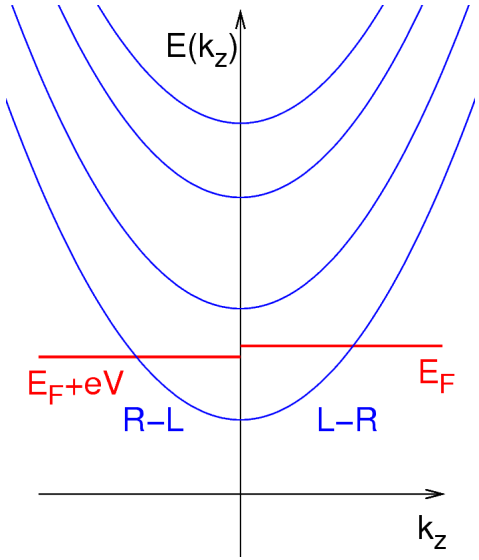
and are propagating states in the z direction, from left to right when $k_z > 0$, and from right to left when $k_z < 0$:

$$\psi_{n_x,n_y,k_z}(\mathbf{r}) = \frac{1}{\sqrt{L_x L_y L_z}} sin(k_x x) sin(k_y y) e^{ik_z z}.$$

$k_x = n_x\pi/L_x$ and $k_y = n_y\pi/L_y$ are instead quantized and n_x and n_y are positive integers.

Conductance of an ideal wire

When the wire is connected on the left to a reservoir with levels occupied up to E_F and on the right to a reservoir with levels occupied up to $E_F + eV$ (V is an electrostatic potential) a current I flows.



When E_F crosses only one level of the wire the conductance $G = I/V$ can be calculated as follows.

Conductance of an ideal wire

An electron in a state k contributes a current $I = envk$ where $n = 1/L$ is the linear density and $v_k = \frac{1}{\hbar}\frac{\partial \varepsilon_k}{\partial k}$ is the electron speed (the subscript z is omitted). Accounting for spin degeneracy, the total current from left to right is:

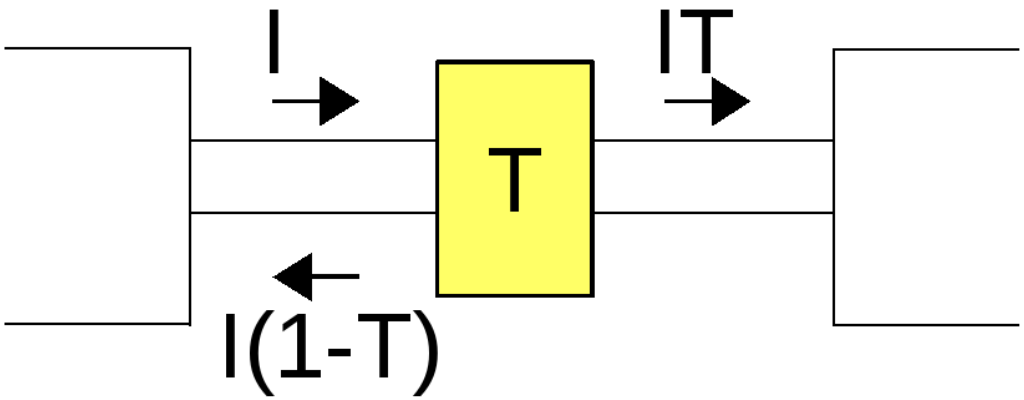
$$I_{L\to R} = \frac{2e}{L}\sum_k v_k = \frac{e}{\pi}\int_0^{k_F} \frac{1}{\hbar}\frac{\partial \varepsilon_k}{\partial k} dk = \frac{2e}{h}\int_0^{\varepsilon_F} d\varepsilon$$

Similarly, the current from right to left is: $I_{R\to L} = \frac{2e}{h}\int_0^{\varepsilon_F + eV} d\varepsilon$.
The total current is $I = \frac{2e^2}{h}V$ and the conductance:

$$G = 2e^2/h$$

is constant.

Conductance from transmission: Büttiker Landauer formula

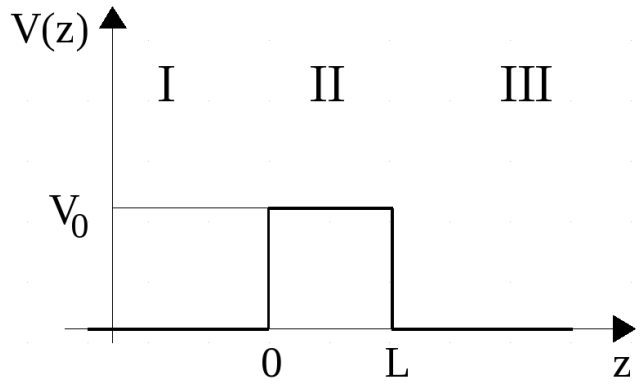


If the wire contains a scattering region with a finite transmission T, the current is IT and the conductance is proportional to the transmission $T(E_F)$ calculated at the Fermi level:

$$G = \frac{2e^2}{h} T(E_F)$$

Transmission in the square potential barrier

For instance the transmission with a barrier potential



is calculated by solving the scattering equation

$$-\frac{\hbar^2}{2m}\frac{d^2}{dz^2}\psi(z) + V(z)\psi(z) = E\psi(z)$$

at energy E in the regions I, II, and III and the solution is matched at the interfaces $z = 0$ and $z = L$.

Transmission in the square potential barrier - II

In region I, the solution is searched as an incident and a reflected wave:

$$\psi(z) = e^{ikz} + re^{-ikz}$$

In region III, the solution is a transmitted wave:

$$\psi(z) = te^{ikz}$$

where $\frac{\hbar^2 k^2}{2m} = E$. In region II:

$$\psi(z) = Ae^{ik_1 z} + Be^{-ik_1 z}$$

The continuity of the solution and of its first derivative at $z = 0$ and $z = L$ gives the scattering state at energy E, that is the four parameters r, t, A, B. The current in region III is $I_{III} = |t|^2 \hbar k/m$ while the current of the incident wave is $I = \hbar k/m$ so the transmission is $T = I_{III}/I = |t|^2$.

Transmission with real atoms

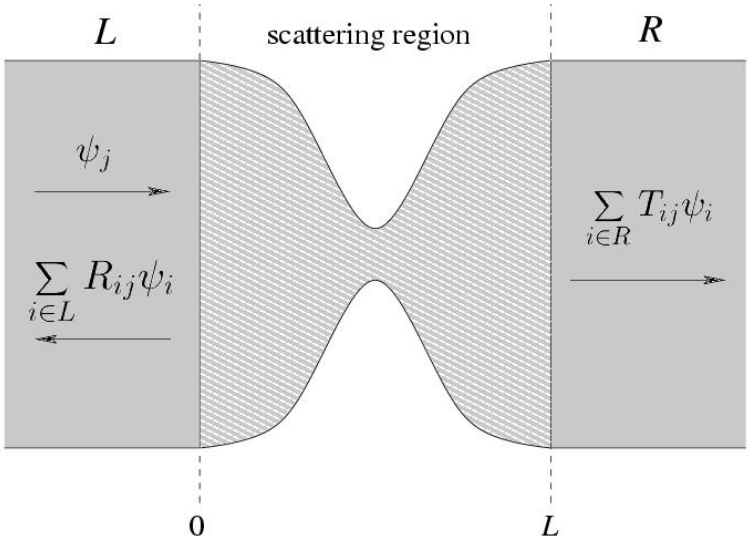
In real materials the problem is three dimensional and at a given energy E there might be several propagating states. However, the major difficulty is that the interaction of electrons and ions is described not only by a local potential but also by nonlocal pseudopotentials that are non vanishing in spheres about each atom:

$$V^{PS} = \sum_{I} \sum_{\substack{\tau,\ell,m \\ \tau',\ell',m'}} D^{\gamma(I)}_{\tau,\ell,m;\tau',\ell',m'} |\beta^{I}_{\tau,\ell} Y^{I}_{\ell,m}\rangle\langle Y^{I}_{\ell',m'} \beta^{I}_{\tau',\ell'}|,$$

so the scattering equation is an integro-differential equation. The problem has been solved efficiently by Choi and Ihm, Phys. Rev. B **59**, 2267 (1999) for norm conserving pseudopotentials.

The PWcond code: transmission for real materials

The PWcond code calculates the transmission, by considering the solutions of the scattering equation with the following asymptotic form:



where $i \in L$ ($i \in R$) are all the propagating and decaying states on the left (right) leads. Using T_{ij} the total transmission is $T = \sum_{ij} \frac{I_i}{I_j} |T_{ij}|^2$ and the sum is over all the states propagating from left to right, j on the left lead and i on the right lead. I_i and I_j are the currents carried by the state i and j respectively.

The PWcond code: the scattering equation

The scattering equation is the following (in a.u.):

$$-\frac{1}{2}\nabla^2|\psi\rangle + V_{\rm eff}|\psi\rangle + \sum_{l,m,n} \bar{D}^l_{m,n}|\beta^l_m\rangle\langle\beta^l_n|\psi\rangle = E|\psi\rangle$$

where $V_{\rm eff}$ is the effective potential (sum of the local, Hartree and exchange and correlation potentials), $\bar{D}^l_{m,n} = D^l_{m,n} - Eq_{m,n}$ are the coefficients of the nonlocal pseudopotential corrected for the presence of the overlap matrix, and $|\beta^l_m\rangle$ are the projectors of the nonlocal pseudopotential. m and n are a shorthand for $\{\tau, \ell, m\}$ and $\{\tau', \ell', m'\}$. $V_{\rm eff}$ and the coefficients $\bar{D}^l_{m,n}$ are calculated in a self-consistent calculation by the `pw.x` code.

Periodic boundary conditions

Perpendicularly to the transport direction we use the Bloch theorem. Defining the atomic positions with a Bravais lattice $\mathbf{R}_\perp$ and positions $\mathbf{d}_s$ we search the scattering state as:

$$\psi_{\mathbf{k}_\perp}(\mathbf{r}_\perp + \mathbf{R}_\perp, z) = e^{i\mathbf{k}_\perp \cdot \mathbf{R}_\perp} \psi_{\mathbf{k}_\perp}(\mathbf{r}_\perp, z)$$

so that the matrix element

$$\langle \beta^l_m | \psi_{\mathbf{k}_\perp} \rangle = e^{i\mathbf{k}_\perp \cdot \mathbf{R}_\perp} \langle \beta^s_m | \psi_{\mathbf{k}_\perp} \rangle.$$

The scattering equations for different $\mathbf{k}_\perp$ are decoupled and are:

Periodic boundary conditions

$$\left[-\frac{1}{2}\nabla^2 + V_{\text{eff}}\right]|\psi_{\mathbf{k}_\perp}\rangle + \sum_{s,m} C_m^s \sum_{\mathbf{R}_\perp} e^{i\mathbf{k}_\perp\cdot\mathbf{R}_\perp}|\beta_m^l\rangle = E|\psi_{\mathbf{k}_\perp}\rangle$$

where

$$C_m^s = \sum_n \bar{D}_{m,n}^s \langle\beta_n^s|\psi_{\mathbf{k}_\perp}\rangle$$

This is an integro-differential equation that can be solved by standard techniques.

Solution of an integro-differential equation - I

An integro-differential equation can be solved by solving separately an homogeneous system:

$$\left[-\frac{1}{2}\nabla^2 + V_{\text{eff}}\right]|\phi_p\rangle = E|\phi_p\rangle$$

and many inhomogeneous systems:

$$\left[-\frac{1}{2}\nabla^2 + V_{\text{eff}}\right]|\phi_{s,m}\rangle + \sum_{\mathbf{R}_\perp} e^{i\mathbf{k}_\perp\cdot\mathbf{R}_\perp}|\beta_m^l\rangle = E|\phi_{s,m}\rangle$$

obtained by setting to 0 all the coefficients $C_{m'}^{s'}$ but the coefficient C_m^s which is set to 1.

Solution of an integro-differential equation - II

Both the homogeneous and the inhomogeneous equations are solved by expanding the solution in plane waves in the *xy* plane. For instance:

$$\phi_p(\mathbf{r}) = \sum_{\mathbf{G}_\perp} c_p(\mathbf{G}_\perp, z) e^{i(\mathbf{k}_\perp + \mathbf{G}_\perp)\cdot \mathbf{r}_\perp}$$

so the homogeneous equation becomes a system of coupled second order ordinary differential equations for the N_{2D} functions $c_p(\mathbf{G}_\perp, z)$. Here N_{2D} is the number of $\mathbf{G}_\perp$ vectors in the perpendicular direction. There are therefore $2N_{2D}$ independent solutions. Similarly we find N_{orb} solutions of the inhomogeneous systems, where N_{orb} is the total number of nonlocal projectors that are nonzero in the region where the equation is solved.

Solution of an integro-differential equation - III

The solution of the original integro-differential equation can be written as:

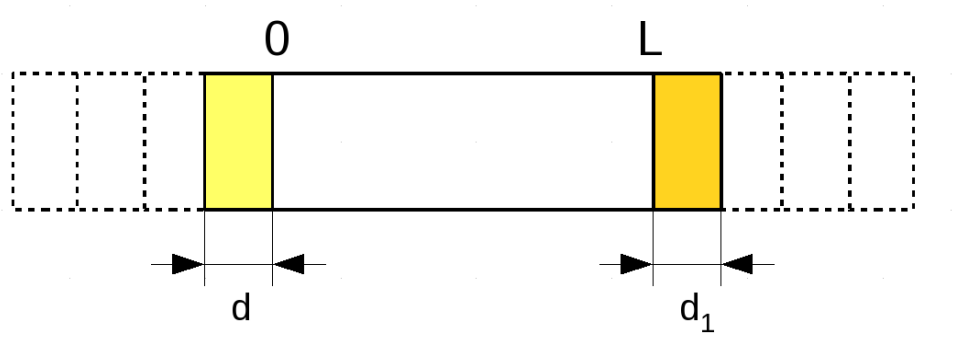
$$|\psi\rangle = \sum_p a_p |\phi_p\rangle + \sum_{s,m} C_m^s |\phi_{s,m}\rangle$$

where the coefficients a_p are determined by the boundary conditions while C_m^s have been defined before. Inserting this solution, they satisfy the equation:

$$C_m^s = \sum_{n,p} a_p \bar{D}_{m,n} \langle \beta_n^s | \phi_p \rangle + \sum_{n,s',m'} C_{m'}^{s'} \bar{D}_{m,n} \langle \beta_n^s | \phi_{s',m'} \rangle$$

Therefore the solution is known after determining the $2N_{2D} + N_{\text{orb}}$ coefficients a_p and C_m^s.

The leads: complex bands



In the leads we can search the solution of the problem in one periodic unit cell with the boundary conditions:

$$\psi_k(\mathbf{G}_\perp, z+d) = e^{ikd}\psi_k(\mathbf{G}_\perp, z)$$

This relationship together with the corresponding conditions for the derivatives with respect to z:

$$\psi'_k(\mathbf{G}_\perp, z+d) = e^{ikd}\psi'_k(\mathbf{G}_\perp, z)$$

gives $2N_{2D}$ conditions.

The leads: complex bands II

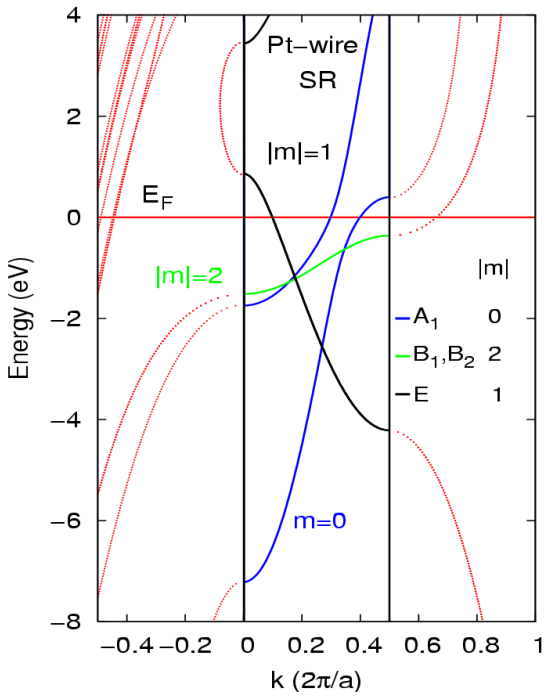
Together with the N_{orb} conditions on the C_m^s this leads to a generalized eigenvalue problem:

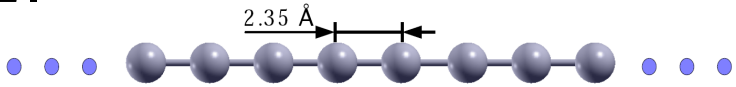
$$AX = e^{ikd}BX$$

where X is a vector that contains the coefficients a_p and the C_m^s.

An example: the infinite Pt monatomic wire

Usually, for each energy E, there are only a few real values of k. The others are complex and correspond to Bloch functions that decay or diverge exponentially. We can plot the values of k for many values of the energy E.





In the central panel the bands with real k.
In the left panel the bands with imaginary k.
In the right panel the bands with $\Re k = \pi/d$ as a function of $\Im k + \pi/d$.

Current of a propagating Bloch state

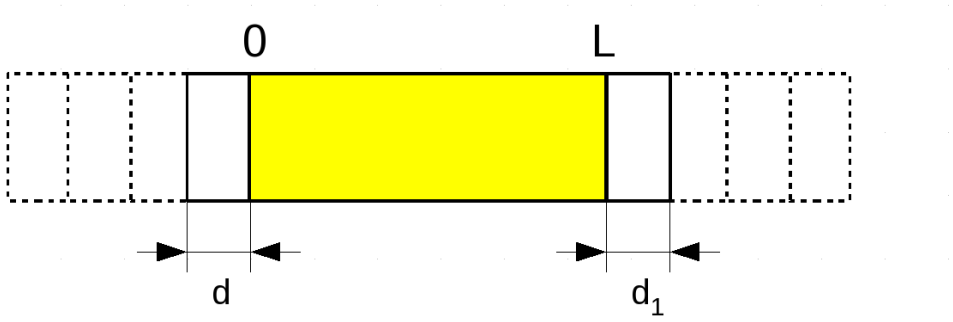
In order to calculate the transmission at energy E, we need the current of each propagating state. In the points z_0 where the plane perpendicular to the transport direction does not cross any nonlocal sphere, we have:

$$I_k^0 = 2\Im \int_S \psi_k^*(\mathbf{r}_\perp, z_0) \left. \frac{\partial \psi_k(\mathbf{r}_\perp, z)}{\partial z} \right|_{z_0} d^2 r_\perp$$

If the plane cross nonlocal spheres we have a correction term:

$$I_k = I_k^0 - 2\Im \left[\sum_{l,m,n} \bar{D}^l_{m,n} \langle \beta_n | \psi_k \rangle \int_{-\infty}^{z_0} d\, z \int_S \beta^l_m(\mathbf{r} - \mathbf{R}_l) \psi_k^*(\mathbf{r}) d^2 \mathbf{r}_\perp \right]$$

The solution of the scattering equation



Once we have all the propagating and decaying states in the two leads, we can solve the scattering equation in the scattering region. Here the solution is

$$|\psi\rangle = \sum_p a_p |\phi_p\rangle + \sum_{s,m} C^s_m |\phi_{s,m}\rangle$$

The solution of the scattering equation - II

In the left lead the solution is

$$|\psi\rangle = |\psi_j\rangle + \sum_{i \in L} R_{i,j} |\psi_i\rangle$$

where j is a state propagating from left to right and the sum over i is over all states propagating from right to left or decaying in the left lead. In the right lead the solution is:

$$|\psi\rangle = \sum_{i \in R} T_{i,j} |\psi_i\rangle$$

where the sum over i is over all the states propagating from left to right or decaying in the right lead.

The solution of the scattering equation - III

The continuity of the solution and of its derivative at $z = 0$ and $z = L$, the conditions on the C^s_m coefficients, and the additional relationship between C^s_m and the coefficients $C^s_{m,i}$ calculated with the Bloch functions $|\psi_i\rangle$:

$$C^s_{m,j} + \sum_{i \in L} R_{i,j} C^s_{m,i} = C^s_m$$

for all atom s whose sphere crosses the $z = 0$ boundary and

$$\sum_{i \in R} T_{i,j} C^s_{m,i} = C^s_m$$

for all atom s whose sphere crosses the $z = L$ boundary,

The solution of the scattering equation - IV

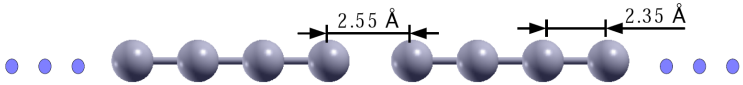
give a linear system:

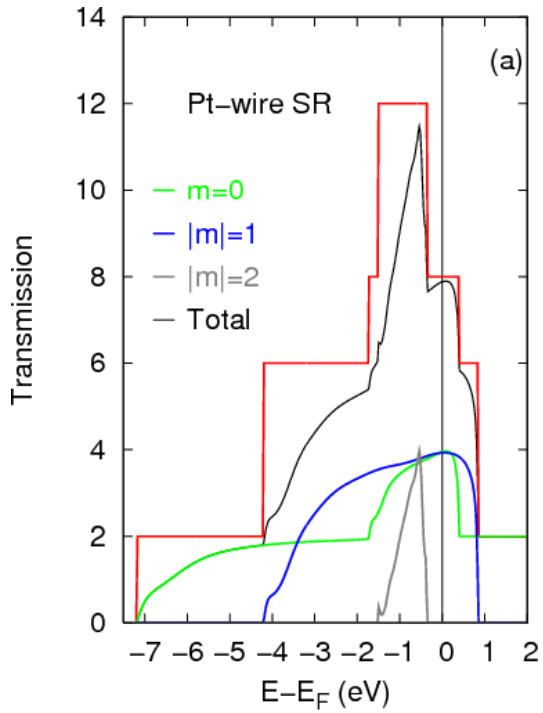
$$AY = B$$

whose solution Y are the coefficients a_p, C^s_m, $R_{i,j}$, $T_{i,j}$. Solving this system for all states j propagating in the left region we get the coefficients $T_{i,j}$ and hence the total transmission.
$T = \sum_{ij} \frac{l_i}{l_j} |T_{i,j}|^2$

An example: transmission of a Pt wire with a defect

The transmission as a function of energy





Spin-orbit coupling with PPs

A scalar relativistic pseudo-potential:

$$V^{PS} = \sum_{I} \sum_{\substack{\tau,\ell,m \\ \tau',\ell',m'}} D^{\gamma(I)}_{\tau,\ell,m;\tau',\ell',m'} |\beta^{I}_{\tau,\ell} Y^{I}_{\ell,m}\rangle\langle Y^{I}_{\ell',m'} \beta^{I}_{\tau',\ell'}|,$$

A pseudopotential with spin-orbit coupling:

$$V^{PS,\sigma,\sigma'}_{\text{with s.o.}} = \sum_{I} \sum_{\substack{\tau,\ell,j,m_j \\ \tau',\ell',j',m_{j'}}} D^{\gamma(I)}_{\tau,\ell,j,m_j;\tau',\ell',j',m_{j'}} |\beta^{I}_{\tau,\ell,j} \tilde{Y}^{\sigma,I}_{\ell,j,m_j}\rangle\langle \tilde{Y}^{\sigma',I}_{\ell',j',m_{j'}} \beta^{I}_{\tau',\ell',j'}|,$$

$$V^{PS,\sigma,\sigma'}_{\text{with s.o.}} = \sum_{I} \sum_{\substack{\tau,\ell,j,m \\ \tau',\ell',j',m'}} D^{\gamma(I),\sigma,\sigma'}_{\tau,\ell,j,m;\tau',\ell',j',m'} |\beta^{I}_{\tau,\ell,j} Y'^{I}_{\ell,m}\rangle\langle Y'^{I}_{\ell',m'} \beta^{I}_{\tau',\ell',j'}|,$$

Transmission with spin-orbit coupling

The scattering equation is the following:

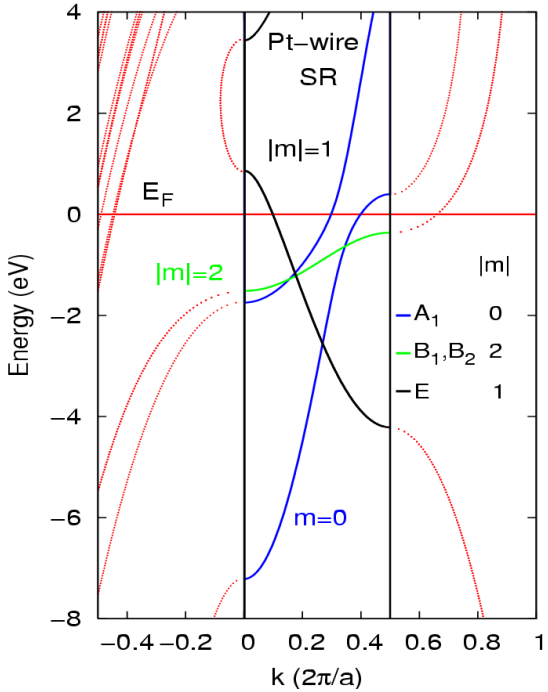
$$-\frac{1}{2}\nabla^2|\psi^\sigma\rangle+\sum_{\sigma'} V_{\rm LOC}^{\sigma,\sigma'}|\psi^{\sigma'}\rangle+\sum_{I,m,n}\sum_{\sigma'}\bar{D}_{m,n}^{I,\sigma,\sigma'}|\beta_m^I\rangle\langle\beta_n^I|\psi^{\sigma'}\rangle = E|\psi^\sigma\rangle$$

where $V_{\rm LOC}^{\sigma,\sigma'}$ is a local potential ($V_{\rm LOC}^{\sigma,\sigma'} = V_{\rm eff}\delta^{\sigma,\sigma'} - \mu_B \mathbf{B}_{xc}\cdot\boldsymbol{\sigma}^{\sigma,\sigma'}$) and $\bar{D}_{m,n}^{I,\sigma,\sigma'} = D_{m,n}^{I,\sigma,\sigma'} - Eq_{m,n}^{\sigma,\sigma'}$ are the coefficients of the nonlocal pseudopotential corrected for the presence of the overlap matrix. $V_{\rm LOC}^{\sigma,\sigma'}$ and the coefficients $\bar{D}_{m,n}^{I,\sigma,\sigma'}$ are calculated in a self-consistent calculation by the `pw.x` code.

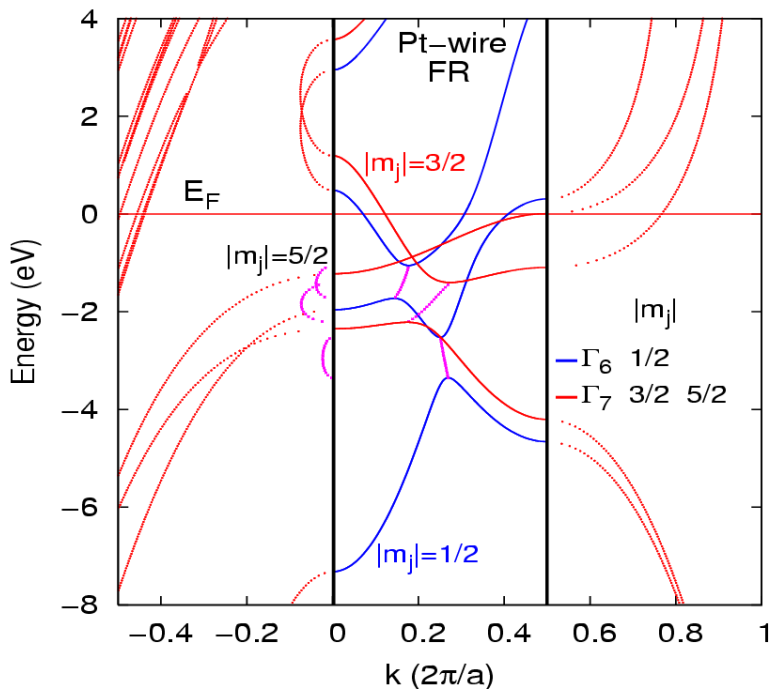
An example: the infinite Pt monatomic wire

The complex bands are the following:

Scalar relativistic

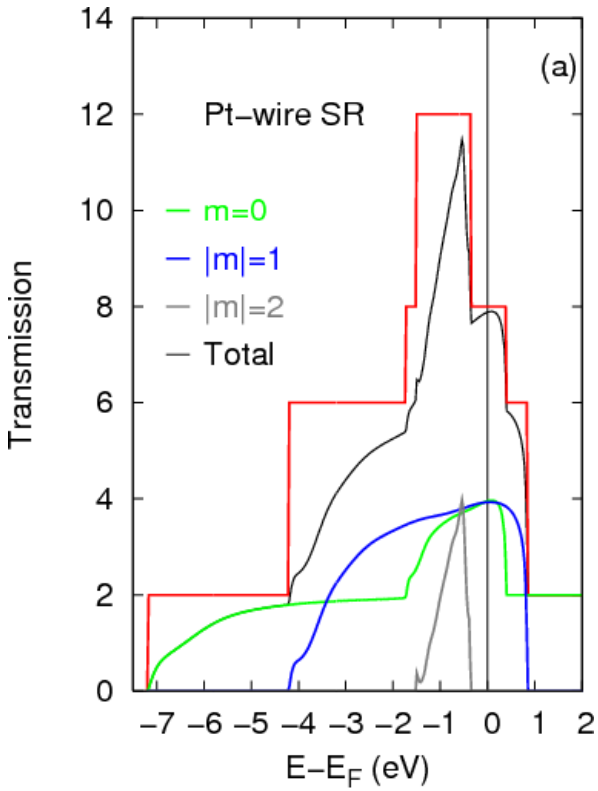


Fully relativistic

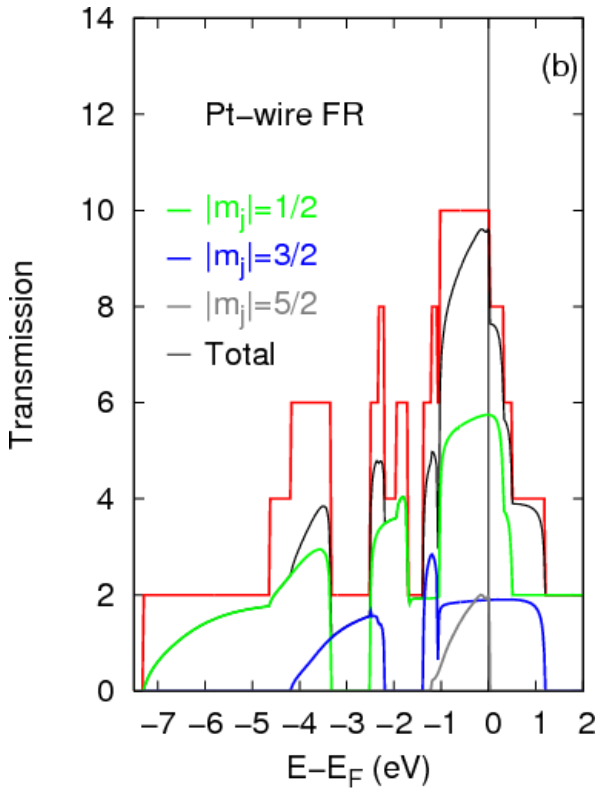


An example: the infinite Pt monatomic wire with a defect

Scalar relativistic



Fully relativistic



Bibliography

1 H.J. Choi and J. Ihm, Phys. Rev. B **59**, 2267 (1999).

2 A. Smogunov, A. Dal Corso, and E. Tosatti, Phys. Rev. B **70**, 045417 (2004).

3 A. Dal Corso and A. Mosca Conte, Phys. Rev. B **71**, 115106 (2005).

4 A. Dal Corso, A. Smogunov, and E. Tosatti, Phys. Rev. B **74**, 045429 (2006).