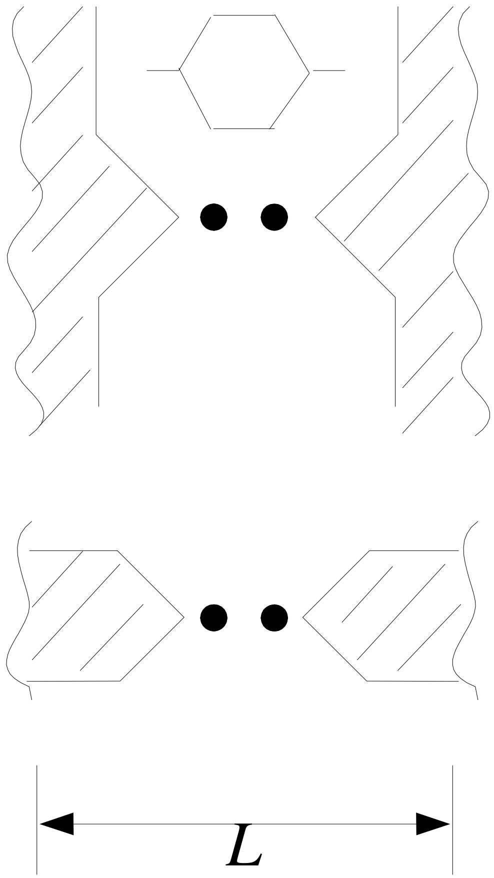
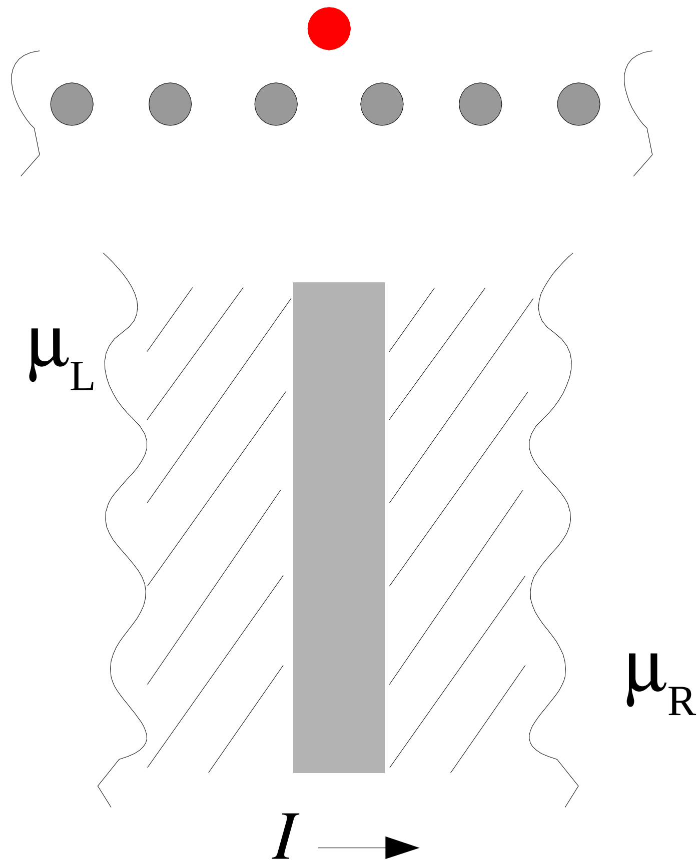
Coherent electron transport, Landauer-Buttiker approach





$I = ?$

$$L<l\,,\,L<L_\varphi\,,\,L\sim\lambda_F$$

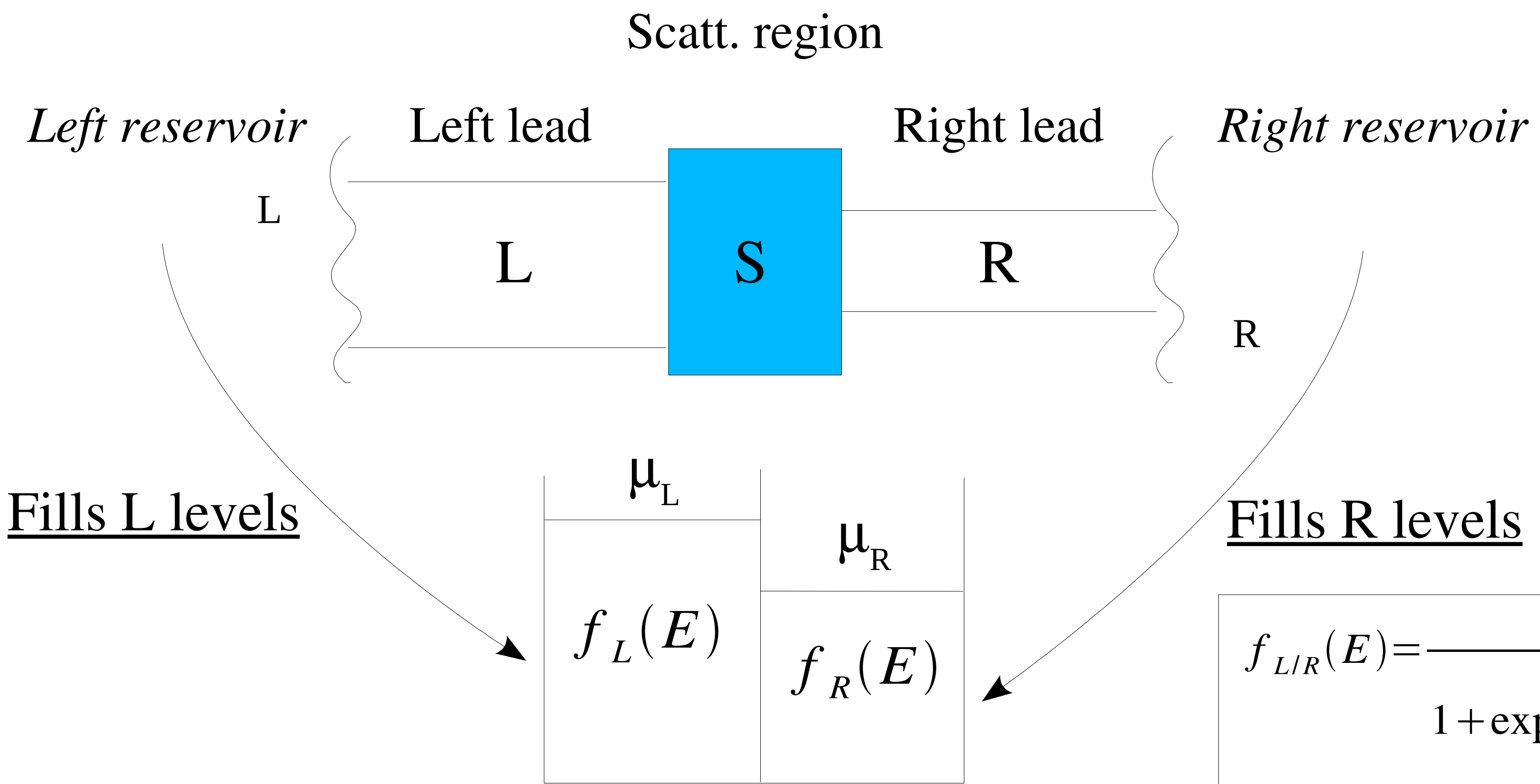
l - mean free path

L_φ - phase decoherence length

λ_F - wave length

Coherent ballistic transport, quantum mechanics is applicable, conductance is given by Landauer-Buttiker formula

Landauer-Buttiker formula



$$f_{L/R}(E)=\frac{1}{1+\exp\left[\frac{E-\mu_{L/R}}{kT}\right]}$$

Landauer-Buttiker formula:

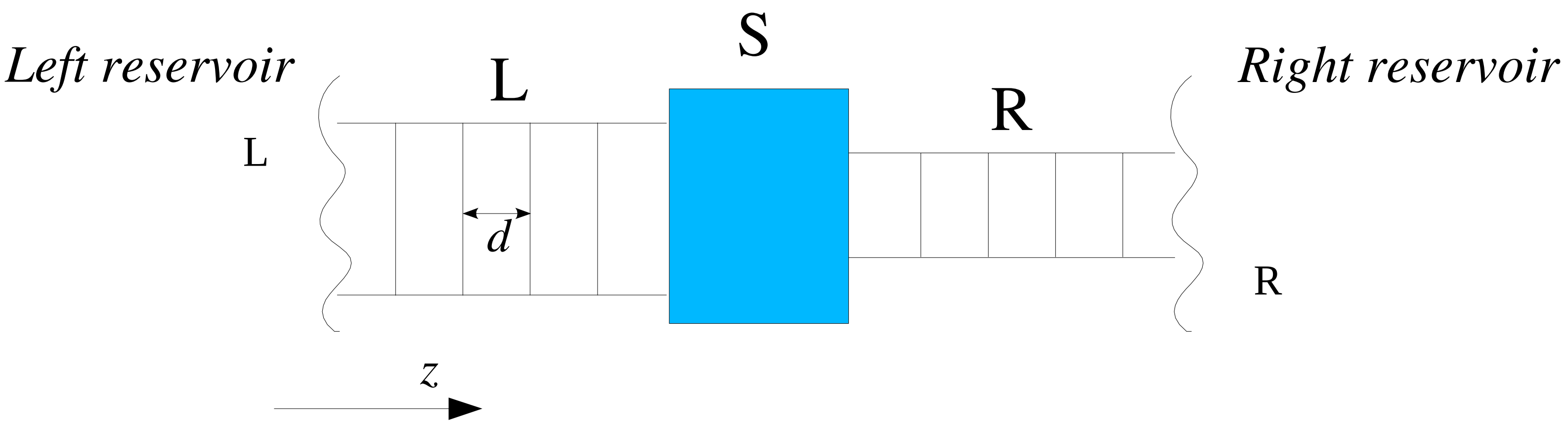
$$I=\frac{e}{h}\int T(E)[f_L(E)-f_R(E)]dE$$

Zero temperature, $I=\frac{e}{h}\int_{\mu_R}^{\mu_L} T(E)dE$

In the linear response regime, at infinitely small voltage, $\mu_L-\mu_R=e\delta V$,

$$G=\frac{I}{\delta V}=\frac{e^2}{h}T(E_F).$$

Asymptotic wave functions in the leads, complex band structure

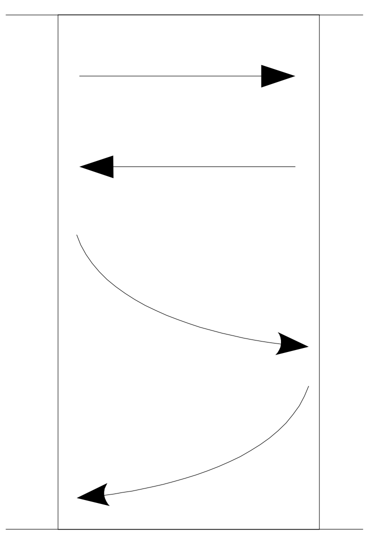


The leads are preriodic in the direction of transport, the *z* axis:

$$\varphi(x,y,z) = \exp(ikz)\,u(x,y,z) \quad \text{- Bloch form}$$

At fixed energy E:

L or R



$\varphi^{+}_{L/R,j}$ - propagating to the right, real k, $M_{L/R}(E)$

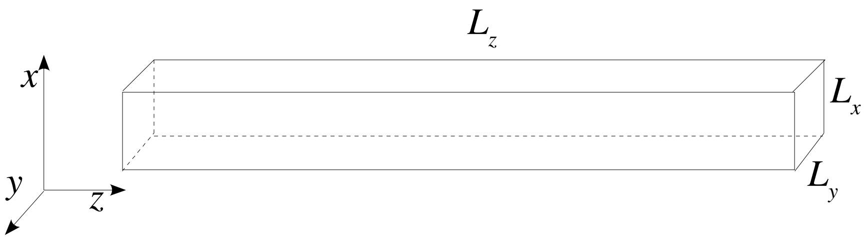
$\varphi^{-}_{L/R,j}$ - propagating to the left, real k, $M_{L/R}(E)$

(number of modes or channels)

$\tilde{\varphi}^{+}_{L/R,j}$ - decaying to the left, complex k, $\mathrm{Im}k > 0$, Infinite number

$\tilde{\varphi}^{-}_{L/R,j}$ - decaying to the right, complex k, $\mathrm{Im}k < 0$, Infinite number

Complex band structure, example: hard wall potential



$$V(x,y,z)=\begin{cases}0, & 0<x<L_x, \quad 0<y<L_y \\ \infty, & \text{otherwise}\end{cases}$$

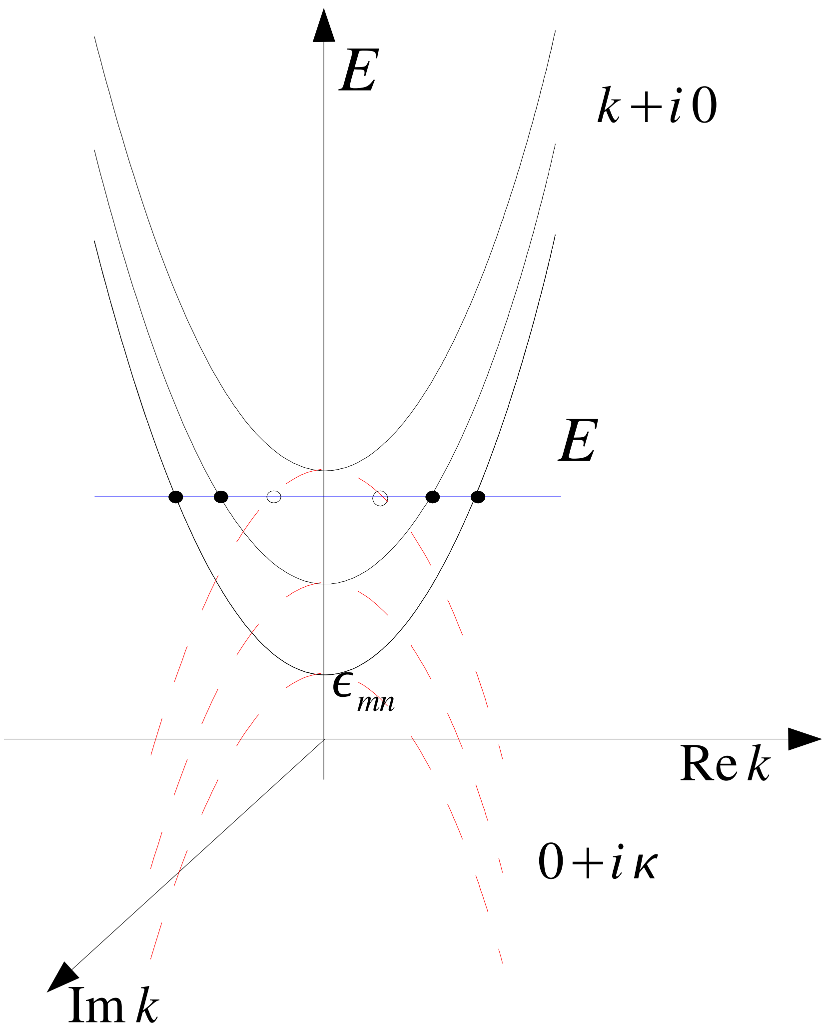
$$\varphi_{mnk}=\frac{1}{\sqrt{L_z}}\chi_{mn}(x,y)\exp(ikz) \qquad \chi_{mn}(x,y)=\frac{1}{\sqrt{L_x L_y}}\sin\left\{m\frac{\pi}{L_x}x\right\}\sin\left\{n\frac{\pi}{L_y}y\right\}$$

$$E=\epsilon_{mnk}=\epsilon_{mnk}+\frac{\hbar^2 k^2}{2\mu}, \quad \epsilon_{mn}=\frac{\hbar^2\pi^2}{2\mu L_x^2}m^2+\frac{\hbar^2\pi^2}{2\mu L_y^2}n^2$$

$m, \; n$ – integers, numbering transverse subbands

$k=\sqrt{\frac{2\mu}{\hbar^2}(E-\epsilon_{mn})}$ and is real or *imaginary*, depending on *E*,

Complex band structure, example: hard wall potential



if $E > \epsilon_{mn}$

$$\varphi_j^{\pm} = \frac{1}{\sqrt{L_z}} \chi_{mn}(x, y) \exp(\pm ikz) \qquad k = \sqrt{\frac{2\mu}{\hbar^2}(E - \epsilon_{mn})}$$

propagating to the right and to the left modes

Number of modes or channels, $M(E)$ = number of real bands crossing E = number of $\epsilon_{mn} < E$, 2 in our case

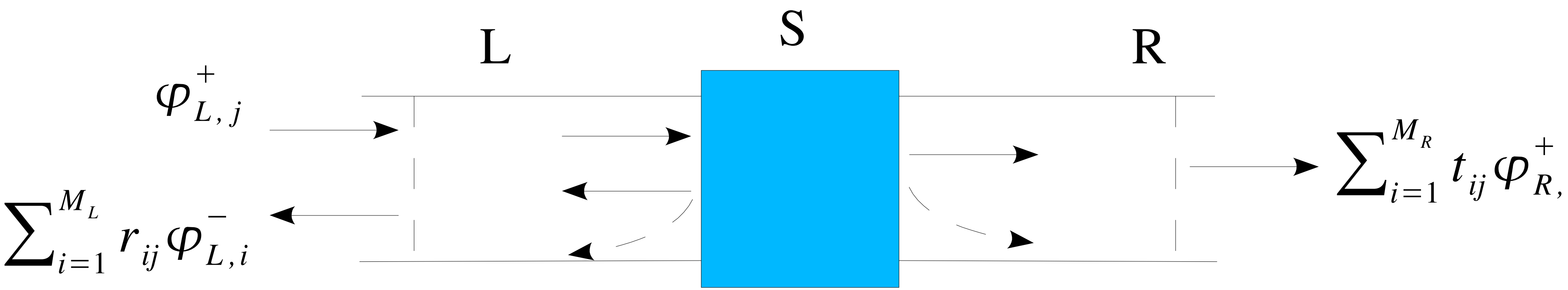
if $E < \epsilon_{mn}$

$$k = \pm i\kappa$$

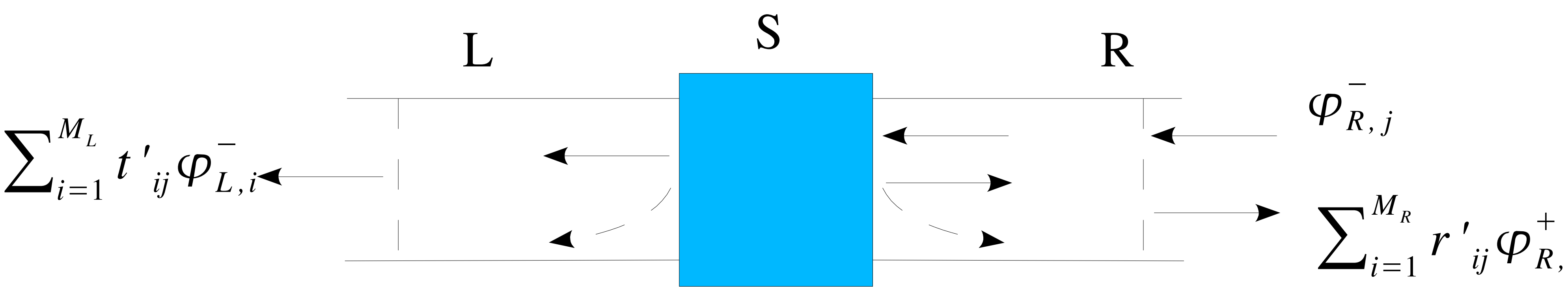
$$\tilde{\varphi}_j^{\pm} = \frac{1}{\sqrt{L_z}} \chi_{mn}(x, y) \exp(\mp\kappa z) \qquad \kappa = \sqrt{\frac{2\mu}{\hbar^2}(\epsilon_{mn} - E)}$$

decaying to the right and to the left modes

S-matrix and transmission coefficient



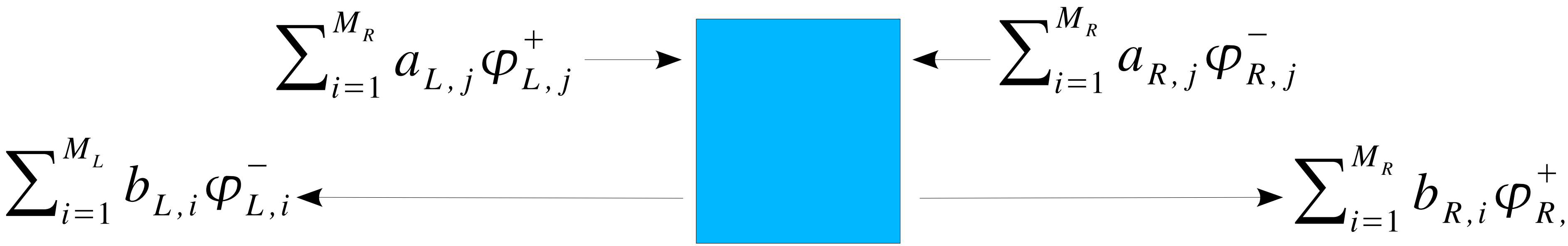
The scattering state $\Phi^{+}_{L,j}$ originated from $\varphi^{+}_{L,j}$, $M_L(E)$



The scattering state $\Phi^{-}_{R,j}$ originated from $\varphi^{-}_{R,j}$, $M_R(E)$

General solution of the SE at the energy E is a linear combination $\left\{\Phi^{+}_{L,j}, \Phi^{-}_{R,j}\right\}$

S-matrix and transmission coefficient (continuation)



Related by means of S-matrix:

$$[a]=\begin{bmatrix} a_L \\ a_R \end{bmatrix}$$ - given

$$[b]=[S][a]$$

$$[b]=\begin{bmatrix} b_L \\ b_R \end{bmatrix}$$ - to find

$$[S]=\begin{bmatrix} [r] & [t'] \\ [t] & [r'] \end{bmatrix} \quad M_L + M_R$$

$$M_L + M_R$$

Ballistic transport with PWCOND code

Running sequence:

1. Supercell pw.x calculations

↓

- Self-consistent potential for left/right leads and the scattering region

2. pwcond.x calculation

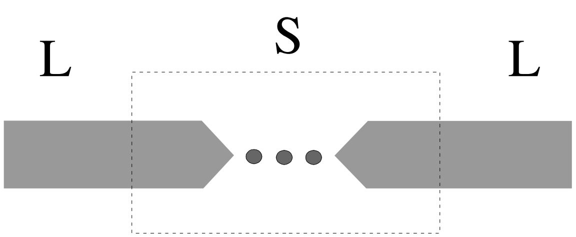
↓

- Complex band structure (CBS) of the leads
- Transmission coefficients for each propagating channel of the left lead

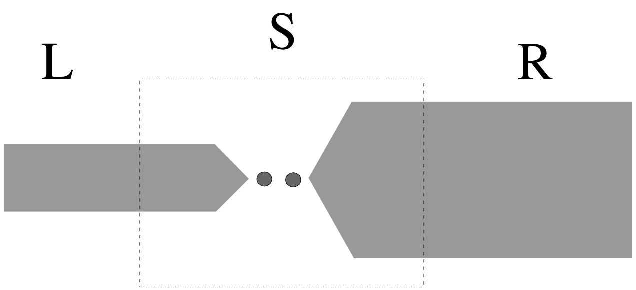
Three kinds of calculations controlled by IKIND flag

1. IKIND = 0 : CBS of the lead

2. IKIND = 1 : The scattering problem with ***identical*** leads



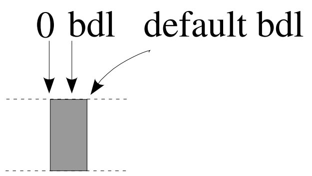
3. IKIND = 2 : The scattering problem with ***different*** leads



Separate files for LEADS and SCATTERING region

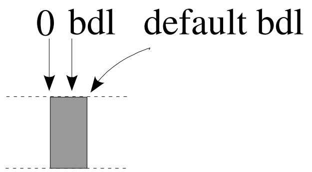
- IKIND = 0

lead plefixl = '...'

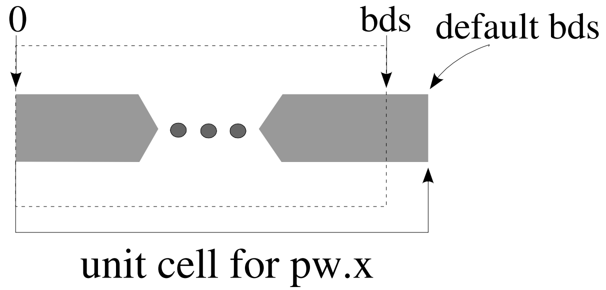


- IKIND = 1

left (right) lead plefixl = '...'

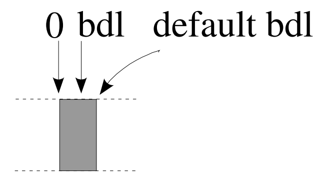


scattering region plefixs = '...'

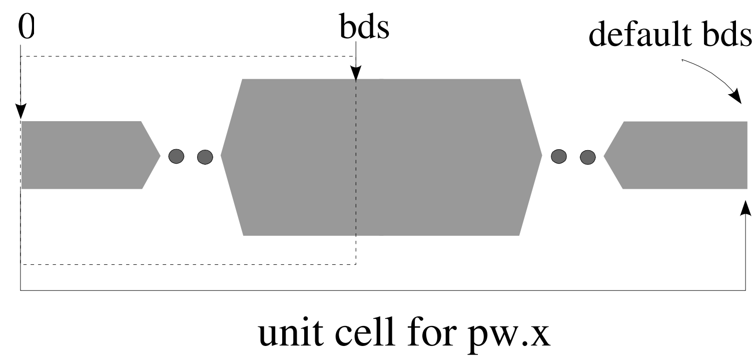


- IKIND = 2

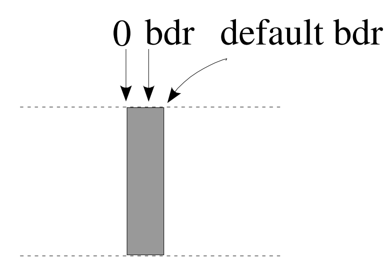
left lead plefixl = '...'



scattering region plefixs = '...'



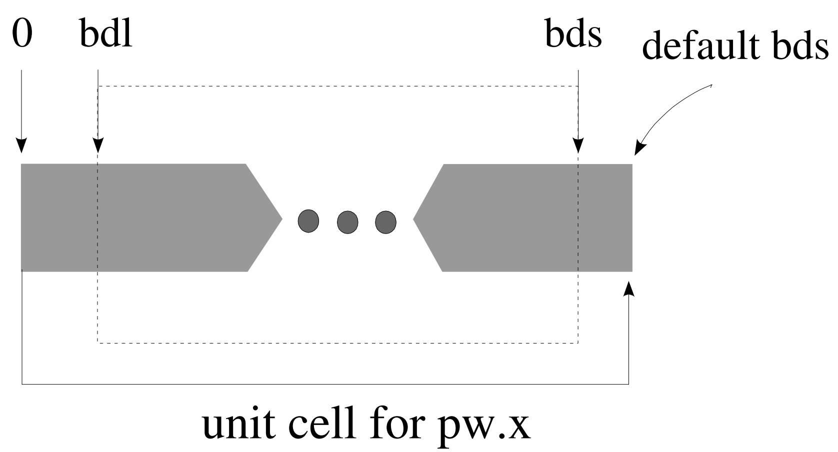
right lead plefixr = '...'



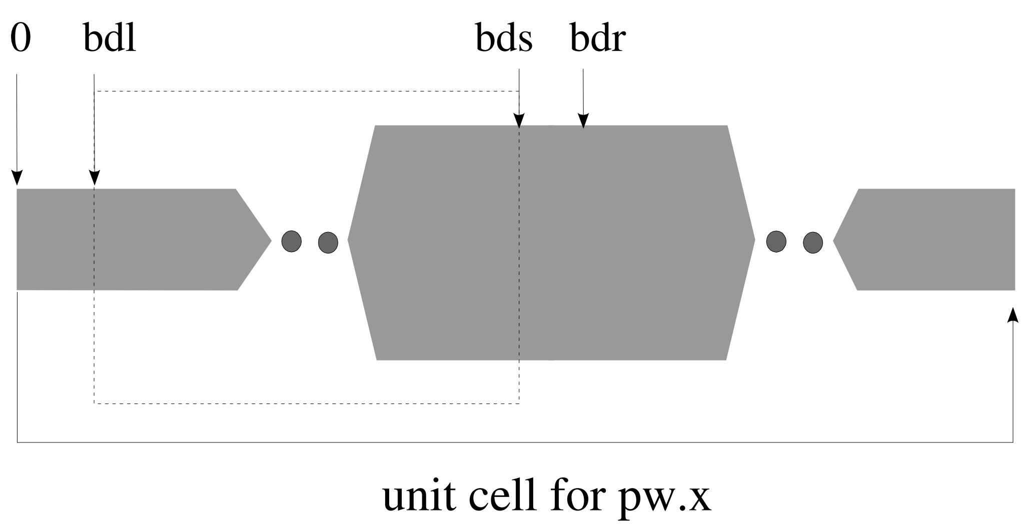
A single file containing all the regions

plefixt = '...'

- IKIND = 1



- IKIND = 2



Input variables of PWCOND (see Doc/INPUT_PWCOND.txt)

&inputcond

Already discussed

ikind,
prefixl, prefixs, prefixr, prefixt,
bdl, bds, bdr

Controlling the accuracy:

ewind,
epsproj,
nz1

Larger ewind and nz1, and smaller epsproj
↓
higher accuracy

Output of CBS and transmission

band_file,
tran_file

Mesh in energy

energy0 - initial energy (in eV from Ef)
denergy - step in energy (in eV)

/

nkpts		- number of (kx,ky) points
kx(1) ky(1) weight(1)		followed by kx, ky, and
kx(2) ky(2) weight(2)		the weight
. . .		
nenergy		- number of energies

If denergy = 0 the list of energies is provided after nenergy

References

- *Books on electron transport:*
  S. Datta "Electronic transport in mesoscopic systems";
  D.K. Ferry and S.M. Goodnick "Transport in nanostructures"

- *Details of the method implemented in PWCOND:*
  H.J. Choi and J. Ihm, Phys. Rev. B 59, 2267 (1999);
  A. Smogunov, A. Dal Corso, and E. Tosatti, Phys. Rev. B 70, 045417 (2004)