Fano resonances in transport through two-dimensional quantum systems

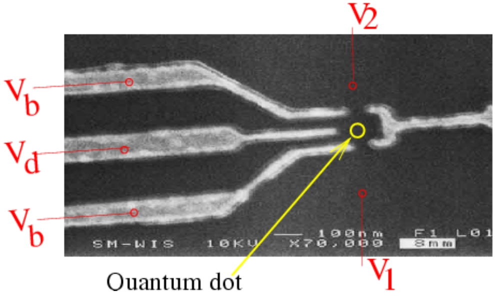
Roxana Racec
Brandenburg University of Technology, Cottbus
University of Bucharest

In cooperation with Paul Racec and Ulrich Wulf

Mesotrans 2008, WIAS Berlin

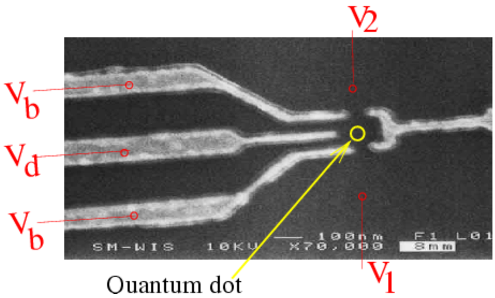
1. Experimental data

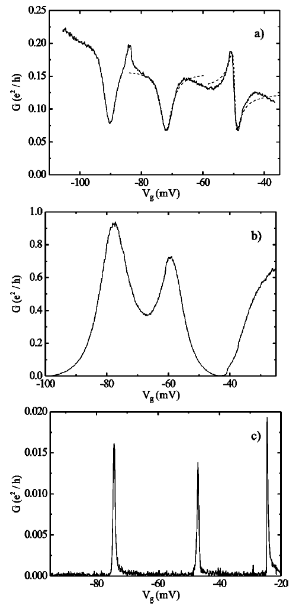
J. Goeres et al, PRB 62, 2188 (2000)



1. Experimental data

J. Goeres et al, PRB 62, 2188 (2000)





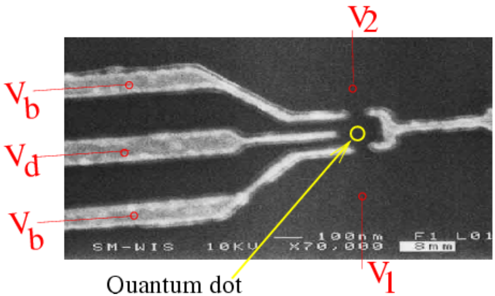
a) Fano-regime
strong coupling
between dot and contacts

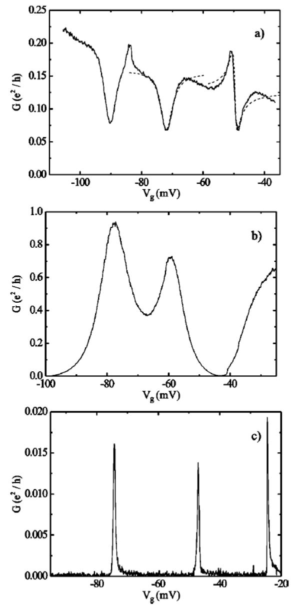
b) Kondo-regime
intermediate coupling

c) ideal Coulomb blockade
weak coupling

1. Experimental data

J. Goeres et al, PRB 62, 2188 (2000)





a) Fano-regime
strong coupling
between dot and contacts

b) Kondo-regime
intermediate coupling

c) ideal Coulomb blockade
weak coupling

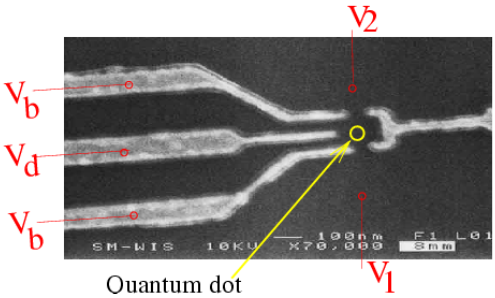
Fano regime:

$$G(e) \sim \frac{|\, e + q \,|^2}{e^2 + 1} \qquad e = \frac{E - E_0}{\Gamma/2}$$

q = complex asymmetry parameter

1. Experimental data

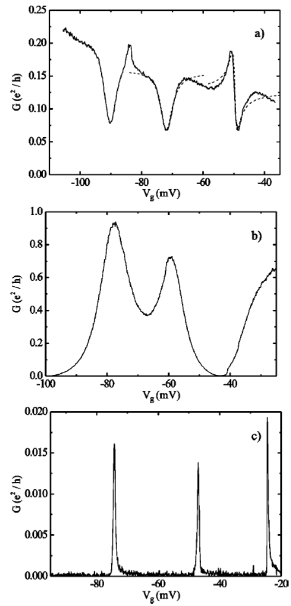
J. Goeres et al, PRB 62, 2188 (2000)



Fano regime:

$$G(e) \sim \frac{|\, e + q \,|^2}{e^2 + 1} \qquad e = \frac{E - E_0}{\Gamma/2}$$

q = complex asymmetry parameter



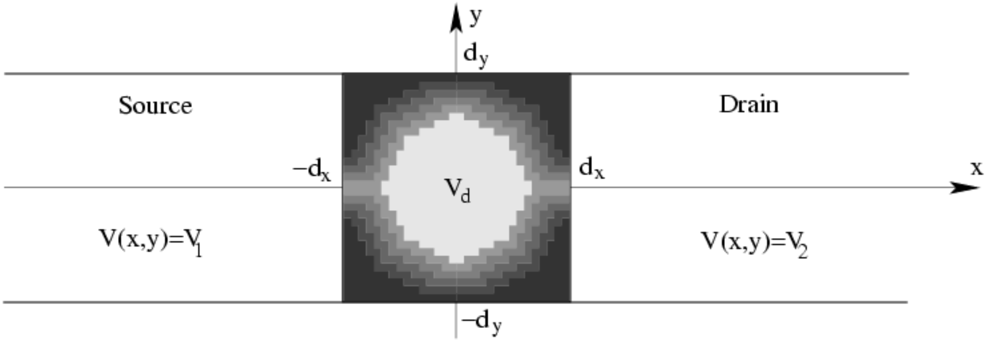
a) Fano-regime
strong coupling
between dot and contacts

b) Kondo-regime
intermediate coupling

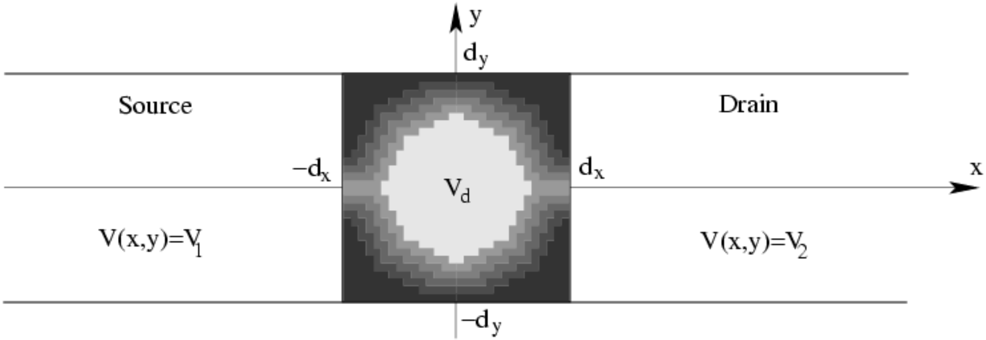
c) ideal Coulomb blockade
weak coupling

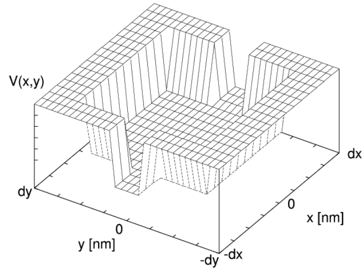
Quasi 1D Model: E.R. Racec and U. Wulf, PRB 64, 115318 (2001)

2. Scattering potential

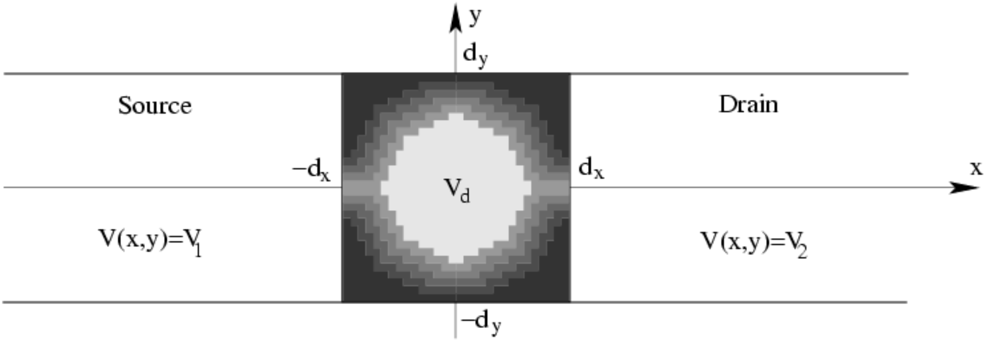


2. Scattering potential





2. Scattering potential



3. 2D-Schrödinger equation

$$\left[-\frac{\hbar^2}{2m^*}\left(\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}\right)+V(x,y)\right]\Psi(x,y)=E\Psi(x,y)$$

3. 2D-Schrödinger equation

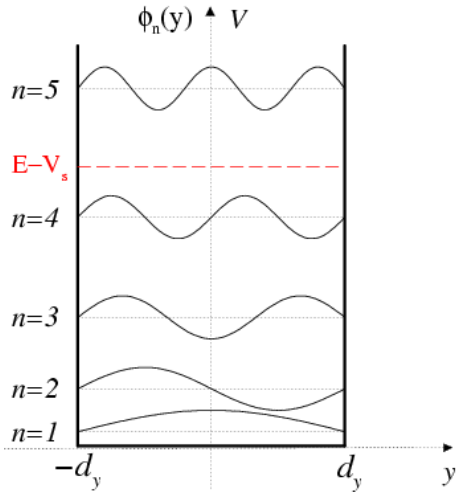
3.1. Contact regions (V_1, V_2 = constant)

$$\Psi(E; x, y) \sim e^{\pm i k_{sn} x} \phi_n(y)$$

3. 2D-Schrödinger equation

3.1. Contact regions (V_1, V_2 = constant)

$$\Psi(E;x,y) \sim e^{\pm i k_{sn} x} \phi_n(y)$$



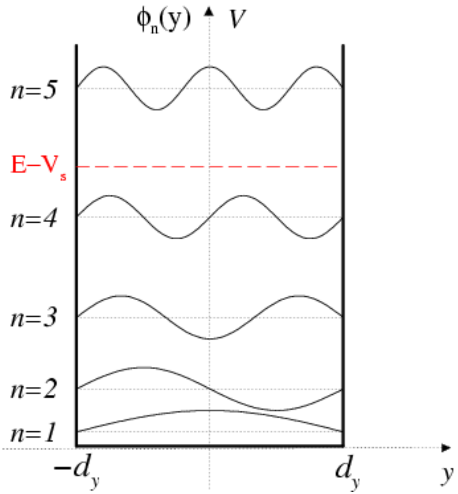
$$\phi_n(y) = \frac{1}{\sqrt{d_y}} \sin\left[\frac{n\pi}{2d_y}(y+d_y)\right]$$

$$E_{yn} = \frac{\hbar^2}{2m^*}\left(\frac{\pi}{2d_y}\right)^2 n^2, \quad n \geq 1$$

3. 2D-Schrödinger equation

3.1. Contact regions (V_1, V_2 = constant)

$$\Psi(E;x,y) \sim e^{\pm i k_{sn} x}\phi_n(y)$$



$$\phi_n(y) = \frac{1}{\sqrt{d_y}} \sin\left[\frac{n\pi}{2d_y}(y+d_y)\right]$$

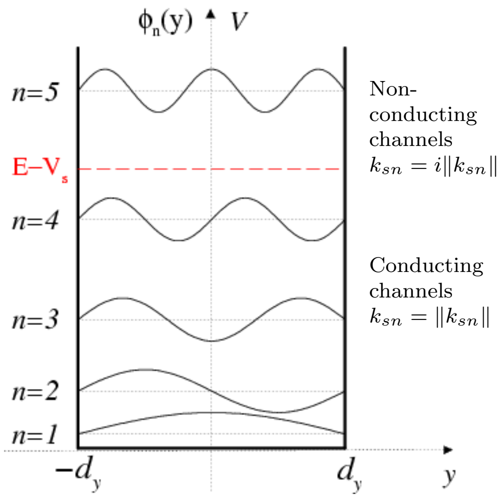
$$E_{yn} = \frac{\hbar^2}{2m^*}\left(\frac{\pi}{2d_y}\right)^2 n^2, \quad n \geq 1$$

Every (s,n) defines an energy channel associated with E.

3. 2D-Schrödinger equation

3.1. Contact regions (V_1, V_2 = constant)

$$\Psi(E; x, y) \sim e^{\pm i k_{sn} x} \phi_n(y)$$



$$\phi_n(y) = \frac{1}{\sqrt{d_y}} \sin\left[\frac{n\pi}{2d_y}(y + d_y)\right]$$

$$E_{yn} = \frac{\hbar^2}{2m^*}\left(\frac{\pi}{2d_y}\right)^2 n^2, \quad n \geq 1$$

$$k_{sn} = \sqrt{\frac{2m^*}{\hbar^2}(E - E_{yn} - V_s)}$$

$s = 1, 2,\ n \geq 1$

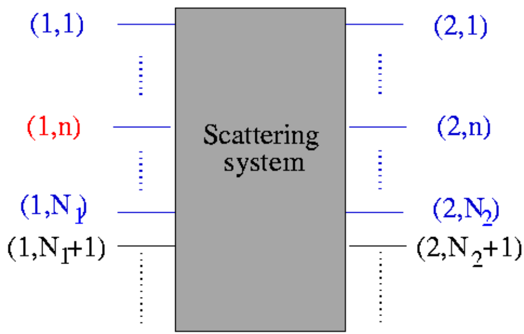
Every (s, n) defines an energy channel associated with E.

Scattering function in contacts for the conducting channel (1,n)

$$\Psi_n^{(1)}(E;x,y) = \begin{cases} \psi^{in}_{1n,1n}(E) e^{ik_{1n}(x+d_x)} \phi_n(y) \\ + \sum_{n'=1}^{\infty} \psi^{out}_{1n,1n'}(E) e^{-ik_{1n'}(x+d_x)} \phi_{n'}(y), & x \leq -d_x \\ \\ \sum_{n'=1}^{\infty} \psi^{out}_{1n,2n'}(E) e^{i\,k_{2n'}\,(x-d_x)} \phi_{n'}(y), & x \geq d_x \end{cases}$$

Conducting channels $n \leq N_1$

Nonconducting channels $n > N_1$



Conducting channels $n \leq N_2$

Nonconducting channels $n > N_2$

Scattering function in contacts for the conducting channel (1,n)

$$\Psi_n^{(1)}(E;x,y) = \begin{cases} \psi^{in}_{1n,1n}(E) e^{ik_{1n}(x+d_x)}\phi_n(y) \\ + \sum_{n'=1}^{\infty} \psi^{out}_{1n,1n'}(E) e^{-ik_{1n'}(x+d_x)}\phi_{n'}(y), & x \le -d_x \\ \\ \sum_{n'=1}^{\infty} \psi^{out}_{1n,2n'}(E) e^{i\,k_{2n'}\,(x-d_x)}\phi_{n'}(y), & x \ge d_x \end{cases}$$

$$\psi^{in}_{sn,s'n'}(E) = \frac{\theta(E - E_{yn} - V_s)}{\sqrt{2\pi}}\delta_{ss'}\delta_{nn'}$$

Scattering function in contacts for the conducting channel (1,n)

$$\Psi_n^{(1)}(E;x,y) = \begin{cases} \psi^{in}_{1n,1n}(E) e^{ik_{1n}(x+d_x)}\phi_n(y) \\ +\sum_{n'=1}^{\infty} \psi^{out}_{1n,1n'}(E) e^{-ik_{1n'}(x+d_x)}\phi_{n'}(y), & x \le -d_x \\ \\ \sum_{n'=1}^{\infty} \psi^{out}_{1n,2n'}(E) e^{i\,k_{2n'}\,(x-d_x)}\phi_{n'}(y), & x \ge d_x \end{cases}$$

$$\psi^{in}_{sn,s'n'}(E) = \frac{\theta(E - E_{yn} - V_s)}{\sqrt{2\pi}} \delta_{ss'}\delta_{nn'}$$

Definition of the S-matrix:

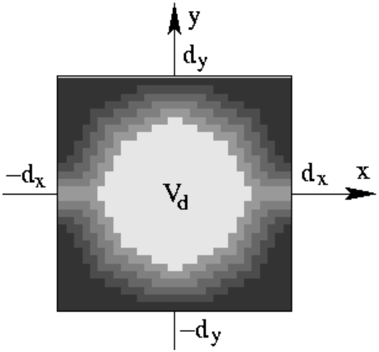
$$\hat{\Psi}^{out} = \hat{S}(E)\hat{\Psi}^{in},$$

3. 2D-Schrödinger equation

3.2. Scattering Region (Nonseparable potential)

$$\Psi_n^{(s)}(E;x,y) = \sum_{l=1}^{\infty} a_{ln}^{(s)}(E)\chi_l(x,y)$$

Eigenvalue problem of the isolated dot $\Rightarrow \chi_l(x,y)$, $l \geq 1$



$$\left[-\frac{\hbar^2}{2m^*}\left(\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}\right)+V(x,y)\right]\chi_l = E_l\chi_l$$

$$\frac{\partial \chi_l}{\partial x}(x=\pm d_x, y) = 0$$

$$\chi_l(x, y=\pm d_y) = 0$$

Scattering functions inside the scattering region

$$\vec{\Psi}(E;x,y) = \frac{i}{\sqrt{2\pi}}\hat{\Theta}\,[\hat{1} - \hat{\mathcal{S}}^T]\,\hat{K}\,\vec{R}(x,y)$$

$$\hat{\Theta}_{sn,s'n'} = \theta(N_s - n)\delta_{ss'}\delta_{nn'}$$

$$\mathbf{K}_{sn,s'n'} = \frac{k_{sn}}{\pi/2d_x}\delta_{ss'}\delta_{nn'}$$

$$\vec{R}(x,y) = \frac{\hbar^2}{2m^*}\frac{\pi}{2d_x}\sum_{l=1}^{\infty}\frac{\vec{\chi}^{(l)}\chi_l(x,y)}{E - E_l}$$

$$\vec{\chi}^{(l)}_{sn} = \int_{-d_y}^{d_y} dy\ \chi_l[(-1)^s d_x, y]\ \Phi_n(y)$$

Relation between S-matrix and R-matrix

$$\hat{\mathcal{S}} = \left[\hat{1} - 2(\hat{1} + i\,\hat{R}\hat{K})^{-1}\right]\hat{\Theta}$$

R matrix

$$\hat{R} = \frac{\hbar^2}{2m^*}\frac{\pi}{2d_x}\sum_{l=1}^{\infty}\frac{\vec{\chi}^{(l)}(\vec{\chi}^{(l)})^T}{E - E_l}$$

4. Conductance

The conductance at $T = 0$:

$$G(V_d) = \frac{2e^2}{h} \sum_{n,n'=1}^{N} \mid \hat{\mathbf{S}}_{1n,2n'}(E = E_F; V_d) \mid^2$$

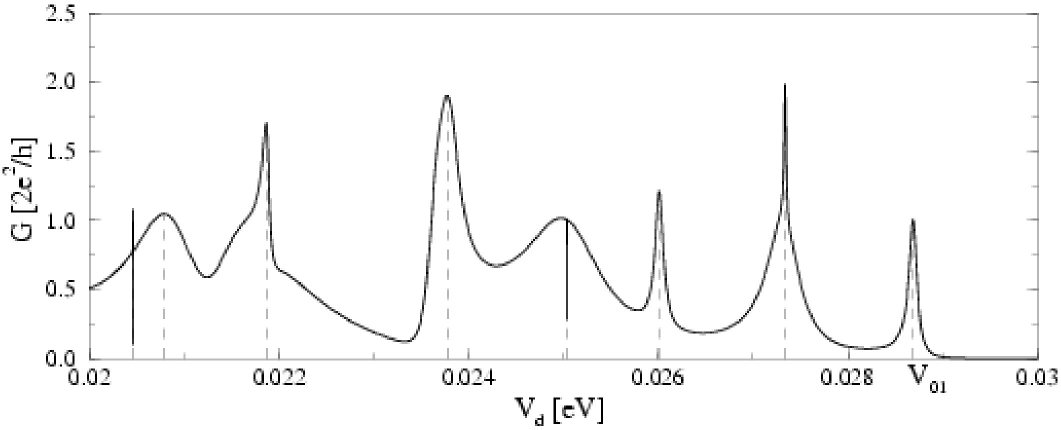
R-matrix representation of the current transmission matrix **S**

$$\hat{\mathbf{S}} = \hat{\Theta} \frac{1 - i\hat{\Omega}}{1 + i\hat{\Omega}} \hat{\Theta}$$

$$\hat{\mathbf{\Omega}} = \sum_{l=1}^{\infty} \frac{\vec{\alpha}_l \vec{\alpha}_l^T}{E - E_l}$$

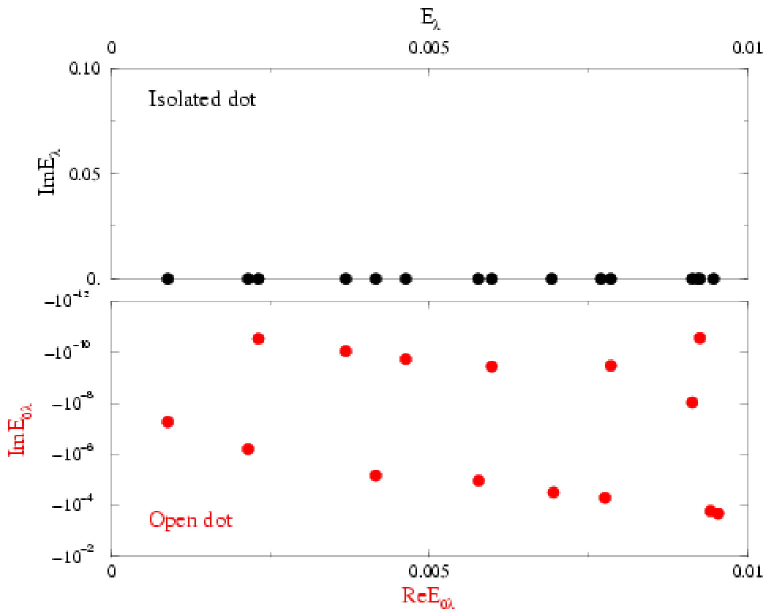
$$(\vec{\alpha}_l)_{sn} = \frac{\hbar}{\sqrt{2m}} k_{sn}^{1/2} \int_{-d_y}^{d_y} dy \ \chi_l[(-1)^s d_x, y] \ \Phi_n(y)$$

4. Conductance



5. Resonance energies

$$\hat{\mathbf{S}} = \hat{\Theta}\frac{1 - i\hat{\Omega}}{1 + i\hat{\Omega}}\hat{\Theta} \qquad \Rightarrow \qquad 1 + i\hat{\Omega}(\bar{E}_{0\lambda}) = 0$$



Calculation of the resonance energies

$$\hat{\mathbf{\Omega}} = \sum_{l=1}^{\infty} \frac{\vec{\alpha}_l \vec{\alpha}_l^T}{E - E_l} = \frac{\vec{\alpha}_\lambda \vec{\alpha}_\lambda^T}{E - E_\lambda} + \hat{\mathbf{\Omega}}_\lambda$$

Analytical expression for S-matrix

$$\hat{\mathbf{S}}(E) = \hat{\mathbf{S}}_\lambda(E) + 2i \frac{\vec{\beta}_\lambda \vec{\beta}_\lambda^T}{E - E_\lambda - \bar{\mathcal{E}}_\lambda(E)}$$

$$\hat{\mathbf{S}}_\lambda(E) = \hat{\Theta} \frac{1 - i\hat{\mathbf{\Omega}}_\lambda}{1 + i\hat{\mathbf{\Omega}}_\lambda} \hat{\Theta}, \qquad \vec{\beta}_\lambda = \hat{\Theta}(1 + i\hat{\mathbf{\Omega}}_\lambda)^{-1} \vec{\alpha}_\lambda, \qquad \bar{\mathcal{E}}_\lambda(E) = -i\vec{\alpha}_\lambda^T \vec{\beta}_\lambda$$

Analytical expression for S-matrix

$$\hat{\mathbf{S}}(E) = \hat{\mathbf{S}}_\lambda(E) + 2i \frac{\vec{\beta}_\lambda \vec{\beta}_\lambda^T}{E - E_\lambda - \bar{\mathcal{E}}_\lambda(E)}$$

- Resonance energy

$$E - E_\lambda - \bar{\mathcal{E}}_\lambda(E) = 0 \quad \Rightarrow \quad E = \bar{E}_{0\lambda}$$

- Isolated resonance: $\hat{\mathbf{S}}_\lambda(E)$ is slowly varying.

  A Laurent expansion yields a Fano line shape.

  Interacting resonances: $\hat{\mathbf{S}}_\lambda(E)$ has the same form as $\hat{\mathbf{S}}(E)$

  $\Rightarrow$ iterative procedure possible

$$\hat{\mathbf{S}}(E) = \hat{\Theta} \frac{1 - i\hat{\mathbf{\Omega}}}{1 + i\hat{\mathbf{\Omega}}} \hat{\Theta}, \qquad \hat{\mathbf{\Omega}} = \sum_{l=1}^{\infty} \frac{\vec{\alpha}_l \vec{\alpha}_l^T}{E - E_l}$$

$$\hat{\mathbf{S}}_\lambda(E) = \hat{\Theta} \frac{1 - i\hat{\mathbf{\Omega}}_\lambda}{1 + i\hat{\mathbf{\Omega}}_\lambda} \hat{\Theta}, \qquad \hat{\mathbf{\Omega}}_\lambda = \sum_{l \neq \lambda} \frac{\vec{\alpha}_l \vec{\alpha}_l^T}{E - E_l}$$

6. Conductance in the Fano approximation

$$G(V_0 + \delta V) \simeq \frac{2e^2}{h} \sum_{n,n'=1}^{N} \mid \hat{\mathbf{S}}_{1n,2n'}(E_F - \delta V; V_0) \mid^2$$

$V_d = V_0$ maximum in conductance for which $E_{0\lambda} \simeq E_F$

- Isolated resonance

$$G = G_{nc} + G_c^{bg} \frac{\mid v + q_\lambda \mid^2}{v^2 + 1},$$

with

$$v = \frac{\delta V}{\Gamma_\lambda / 2}.$$

- Two interacting resonances

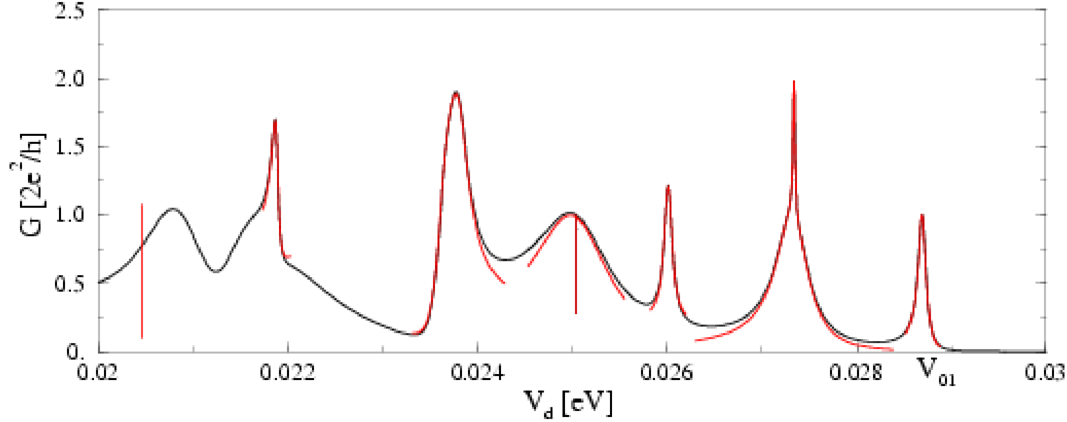
$$G = G_{nc} + G_c^{bg} \frac{\mid v + q_\lambda \mid^2}{v^2 + 1} + (G_c')^{bg} \frac{\mid v' + q_{\lambda'} \mid^2}{v'^2 + 1},$$

with

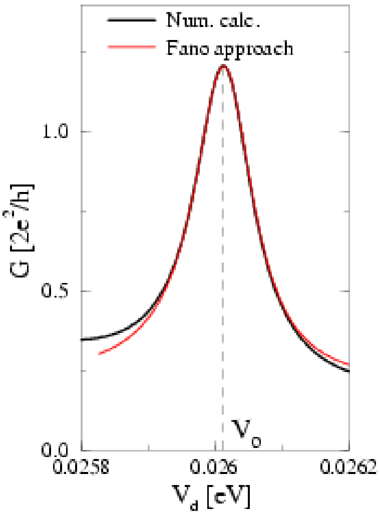
$$v' = \frac{\delta V + E_{0\lambda} - E_{0\lambda'}}{\Gamma_{\lambda'}/2}$$

q_λ, $q_{\lambda'}$ = complex asymmetry parameters

Conductance in the Fano approximation

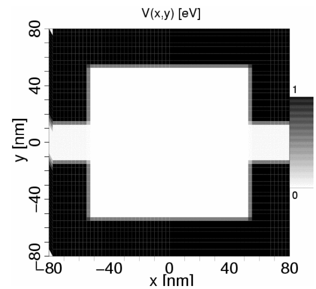


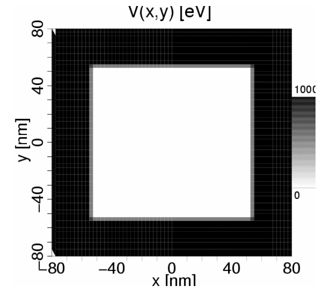
One isolated resonance



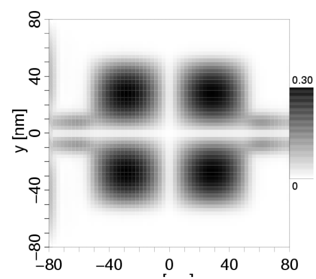
Open dot

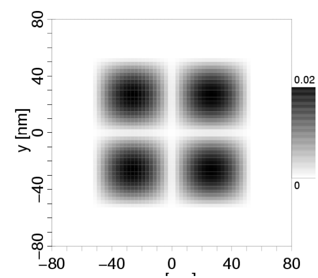
Isolated dot



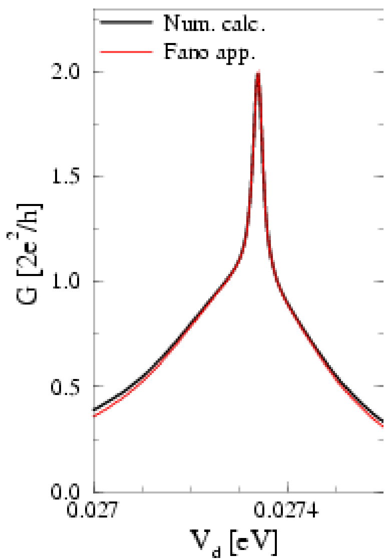


$\mid \psi_1^{(1)}(E_F; x, y) \mid^2$ for $V_d = V_0$



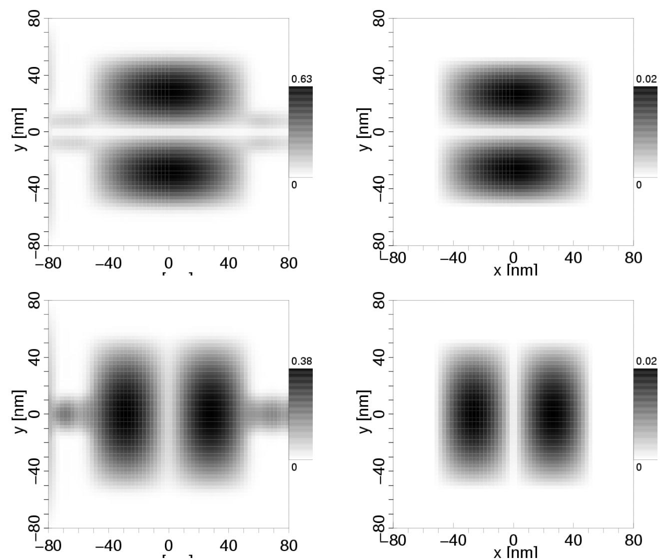


Two interacting resonances with different symmetry on y

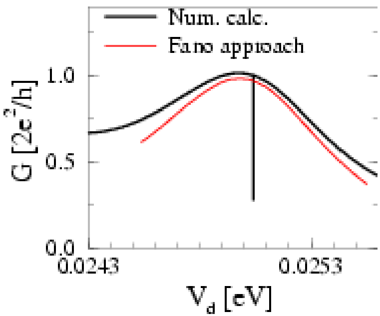


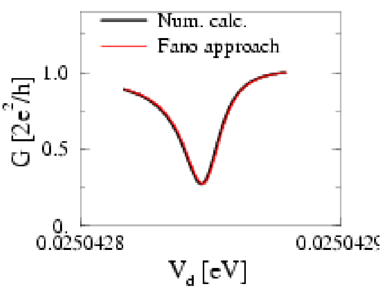
Open dot   Isolated dot

$|\psi_1^{(1)}(E_F; x, y)|^2$



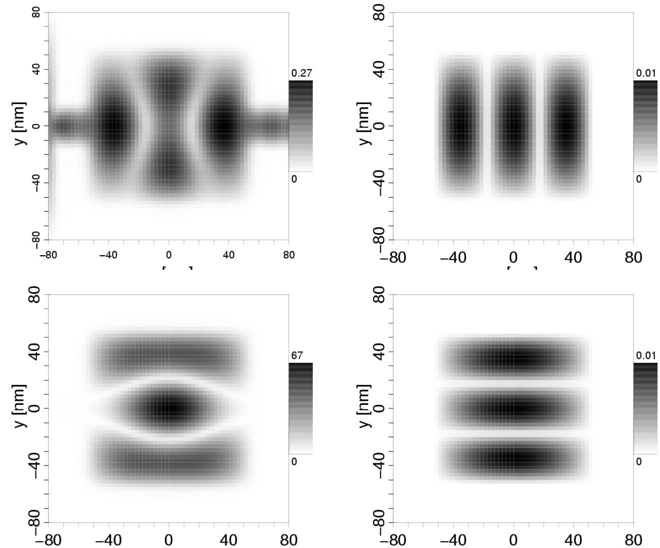
Two interacting resonances with the same symmetry on y





Open dot Isolated dot

$\mid \psi_1^{(1)}(E_F; x, y) \mid^2$



7. Conclusions

- We derived an analytical expression for the S-matrix suitable for the description of Fano resonances: decomposition in background part and resonant part.

- isolated resonance: resonant part interacting with a slowly varying background yields Fano resonance shape for the conductance.

- interacting resonances: iterative procedures yields more complex shapes for the conductance maxima and other structure types.