

# *Geometrical effects in magnetotransport through systems embedded in a quantum wire*

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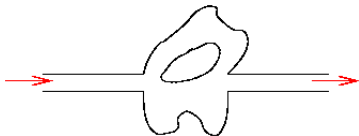
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[http://hartree.raunvis.hi.is/~vidar/Rann/Fyrirlestrar/MiaoLi\\_S.pdf](http://hartree.raunvis.hi.is/~vidar/Rann/Fyrirlestrar/MiaoLi_S.pdf)

MiaoLi, October, 2008

## Aim

- Model of magnetotransport in a 2D quantum wire
- Embedded subsystems, or two wires connected to another electronic system, simple or complex

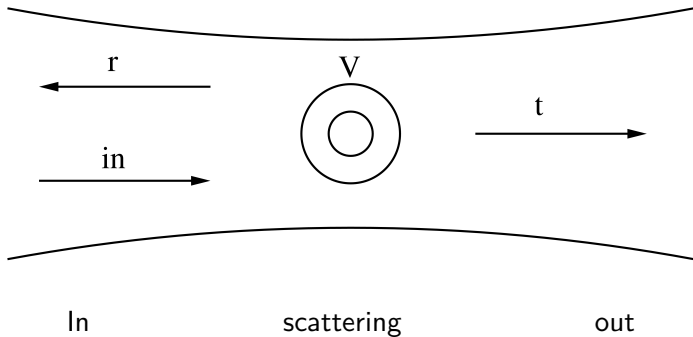


- Static transport
- Effects  $\leftarrow$  geometry + magnetic field

## Methods

- Scattering formalism, built on Lippmann-Schwinger approach
- Basis expansion – multimode transport – enhanced parallelization
- Cooperation and comparison with groups working on alternative approaches
  - Chi-Shung Tang: Wave function matching
  - Valeriu Moldoveanu: NEGF on a lattice.
- Analytical  $\rightarrow$  heavy numerical work

# Asymptotic regions



# No external magnetic field, $\mathbf{B} = 0$

## Quasi-one-dimensional scattering

Scattering state with in-energy  $E$

(Open system  $\rightarrow$  not eigenvalue problem)

$$\left( -\frac{\hbar^2}{2m^*} \left[ \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} \right] + V_c(y) + V_{sc}(\mathbf{r}) \right) \psi_E(\mathbf{r}) = E\psi_E(\mathbf{r})$$

Separation of variables, modes

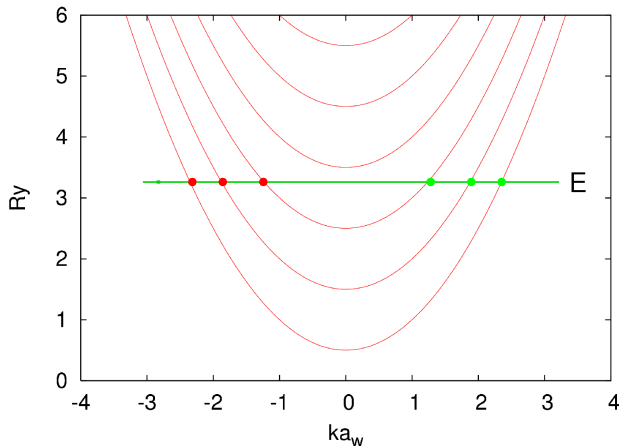
$$\left( -\frac{\hbar^2}{2m^*} \frac{d^2}{dy^2} + V_c(y) \right) \phi_n(y) = \varepsilon_n \phi_n(y)$$

In-state with energy  $E$  in **subband  $n$**

$$\psi_{nE}^{0,\pm}(\mathbf{r}) = e^{\pm ik_n(E)x} \phi_n(y)$$



## Ideal wire



In-, out- states with energy  $E$ , energy is conserved

Open system  $\rightarrow$  scattering boundary conditions

$$\psi_{nE}^+(\mathbf{r}) = \begin{cases} \psi_{nE}^{0,+}(\mathbf{r}) + \sum_{m,\text{prop}} r_{mn} \psi_{mE}^{0,-}(\mathbf{r}), & x \rightarrow -\infty \\ \sum_{m,\text{prop}} t_{mn} \psi_{mE}^{0,+}(\mathbf{r}), & x \rightarrow \infty \end{cases}$$

Landauer-Büttiker  $\rightarrow$  conductance

$$G = \frac{2e^2}{h} \text{Tr}[\mathbf{t}^\dagger \mathbf{t}]$$

## Coupled channel transport, (Cattapan and Maglione, Am. J. Phys. 71, 903 (2003))

Separation of variables, expansion in a basis

$$\psi_{nE}(\mathbf{r}) = \sum_m \varphi_{mE}^n(x) \phi_m(y)$$

Set of coupled 1D-equations

$$\left( \frac{d^2}{dx^2} + k_m^2(E) \right) \varphi_{mE}^n(x) = \frac{2m^*}{\hbar^2} \sum_{m'} V_{mm'}(x) \varphi_{m'E}^n(x)$$

Matrix elements

$$V_{mm'}(x) = \int dy \phi_m^*(y) V(\mathbf{r}) \phi_{m'}(y)$$

## External magnetic field, $\mathbf{B} \neq 0$

Asymptotic regions, free parabolic wire, perpendicular magnetic field

$$H_0 = \frac{\hbar^2}{2m^*} \left[ -i\nabla - \frac{eB}{\hbar c} y \hat{\mathbf{x}} \right]^2 + V_c(y)$$

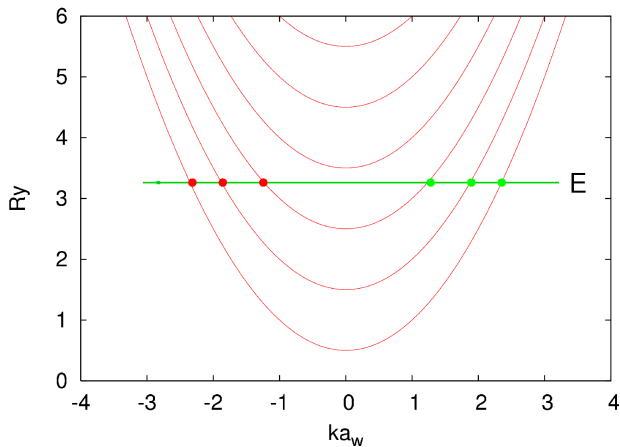
$$\psi^+(x, y, k_n) = e^{ik_n x} \phi_n(y - y_0)$$

$$E = \left( n + \frac{1}{2} \right) \hbar \Omega_w + \mathcal{K}_n(k_n)$$

$$\Omega_w = \sqrt{\omega_c^2 + \Omega_0^2}, \quad y_0 = k_n a_w^2 \frac{\omega_c}{\Omega_w}, \quad \omega_c = \frac{eB}{m^* c}$$

$$\mathcal{K}_n(k_n) = \frac{(k_n a_w)^2}{2} \left( \frac{\hbar^2 \Omega_0^2}{\hbar \Omega_w} \right), \quad a_w^2 \Omega_w = \frac{\hbar}{m^*}$$

## Asymptotic energy spectrum



In-, out- states, energy is conserved

## Consequences of $B \neq 0$

- Lorentz force couples the motion in  $x$ - and  $y$ -direction
- $\phi_n(y - y_0)$  with different  $y_0$ 's and  $n$ 's are not orthogonal
- No simple separation in modes, ( $k_n$  and  $y_0$  are related)

Mixed momentum-coordinate representation, S. A. Gurvitz, PRB 51, 7123 (1995)

$$\int dx \psi_E(x, y) e^{-ipx} = \Psi_E(p, y) \rightarrow \sum_n \varphi_n(p) \phi_n(p, y)$$

Separation in  $(p, y)$ -space,  $p$  is Fourier variable!

Expansion in terms of eigenfunctions of the shifted harmonic oscillator  $\rightarrow$  transport mode “ $n$ ”

... transforms the Schrödinger equation (in  $q$ -space)

$$\mathcal{K}_n(q)\varphi_n(q) + \sum_{n'} \int \frac{dp}{2\pi} V_{nn'}(q, p)\varphi_{n'}(p) = (E - E_n)\varphi_n(q)$$

$$V_{nn'}(q, p) = \int dy \phi_n^*(q, y) V(q - p, y) \phi_{n'}(p, y)$$

$$V(q - p, y) = \int dx e^{-i(q-p)x} V_{sc}(x, y)$$

into a set of coupled **integral equations**,

$V_{sc}(x, y)$  is the scattering potential (**nonlocal**),  
(analytic matrix elements)

...rewrite

Nonlocal potential

$$\left[ -(qa_w)^2 + (k_n(E)a_w)^2 \right] \varphi_n(q) = \frac{2\hbar\Omega_w}{(\hbar\Omega_0)^2} \sum_{n'} \int \frac{dp}{2\pi} V_{nn'}(q, p) \varphi_{n'}(p)$$

Effective band momentum  $k_n(E)a_w = \sqrt{\frac{2(E - E_n)\hbar\Omega_w}{(\hbar\Omega_0)^2}}$

Free equation  $\left[ -(qa_w)^2 + (k_n(E)a_w)^2 \right] \varphi_n^0(q) = 0$

Suggests an interpretation...



... a Green function

$$\left[ -(qa_w)^2 + (k_n(E)a_w)^2 \right] G_E^n(q) = 1$$

Lippmann-Schwinger eq.'s in  $q$ -space

$$\varphi_n(q) = \varphi_n^0(q) + G_E^n(q) \sum_{n'} \int \frac{dp a_w}{2\pi} \tilde{V}_{nn'}(q, p) \varphi_{n'}(p)$$

$$\varphi = \varphi^0 + G \tilde{V} \varphi^0 + G \tilde{V} G \tilde{V} \varphi^0 + \dots \rightarrow (1 + G \tilde{T}) \varphi^0$$

$$\tilde{T}_{nn'}(q, p) = \tilde{V}_{nn'}(q, p) + \sum_{m'} \int \frac{dk a_w}{2\pi} \tilde{V}_{nm'}(q, k) G_E^{m'}(k) \tilde{T}_{nm'}(k, p).$$

Transformed into eq's for the T-matrix  
(convenient for numerical calculations)

# Supplies

## Wavefunctions

$$\psi_E(x, y) = e^{ik_n x} \phi_n(k_n, y) + \sum_m \int \frac{dq a_w}{2\pi} e^{iqx} G_E^m(q) \tilde{T}_{mn}(q, k_n) \phi_m(q, y)$$

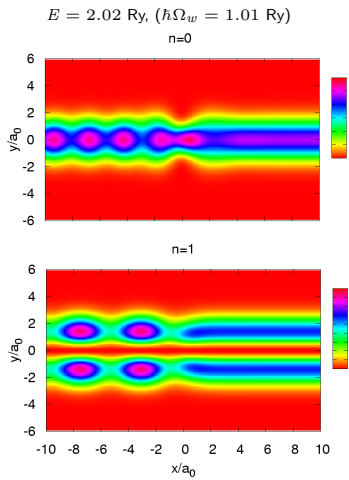
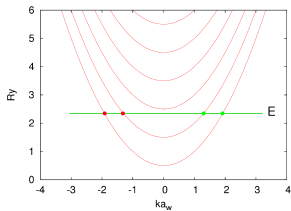
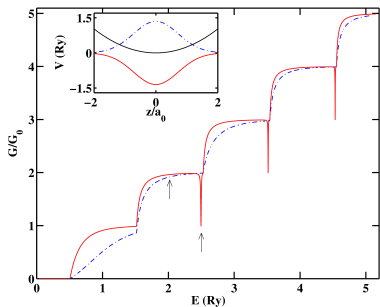
## Transmission amplitudes

$$t_{nm}(E) = \delta_{nm} - \frac{i\sqrt{(k_m/k_n)}}{4(k_m a_w)} \tilde{T}_{nm}(k_n, k_m)$$

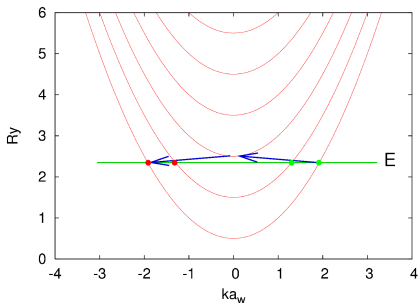
## Conductance

$$G(E) = \frac{2e^2}{h} \text{Tr}[\mathbf{t}^\dagger(E)\mathbf{t}(E)]$$

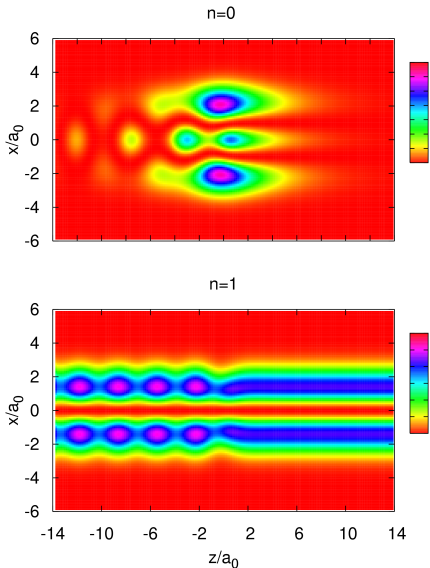
# B=0, simple Gaussian hill or well



## What causes a dip?

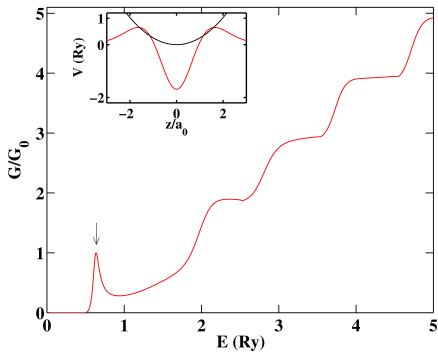
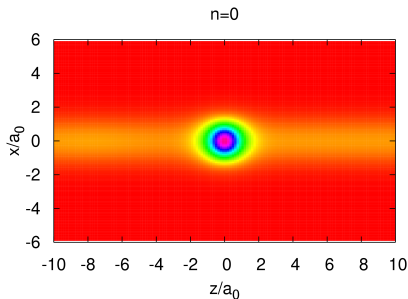


- Total reflection by an **evanescent** state
- Symmetry  $\rightarrow$  **selection** rules
- All **orders** of scattering



## Embedded dot, $B = 0$

- Total resonant transmission
- Finite lifetime

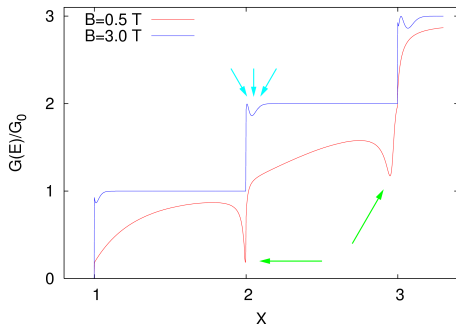


Phys. Rev. B **70** 245308, (2004)

# Magnetic field, $B \neq 0$

Small open quantum dot, (Phys. Rev. B **71**, 235302 (2005))

(Further systems in: PRB **70** 245308, (2004), Euro. Phys. J. B **45**, 339 (2005), and PRB **72**, 195331 (2005))

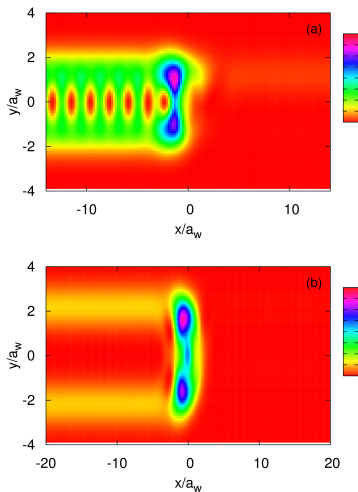


- $\hbar\Omega_0 = 1.0$  meV, broad wire
- $V_0 = -0.8$  meV, shallow dot
- $G_0 = \frac{2e^2}{h}$
- $\Omega_w = \sqrt{\omega_c^2 + \Omega_0^2}$
- $X = \frac{E}{\hbar\Omega_w} + \frac{1}{2}$

- Quantization, with or without  $B$ , symmetry breaking
- Lorentz force  $\rightarrow$  electrons bypass dot at high  $B$

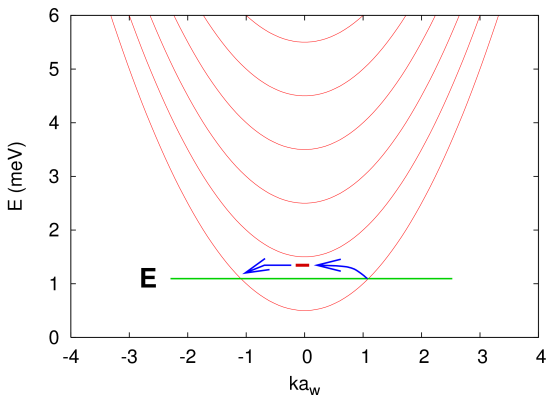
## Lorentz force

- $B = 0.6$  T, or  $B = 1.2$  T
- Separation of in- and out-states
- Interference
- Telltale symmetry



# Resonant backscattering caused by an evanescent state

Selection rule broken by **B**

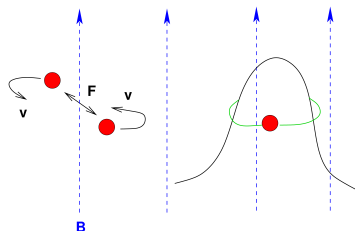


- Scattering to all orders



# Negative binding energy

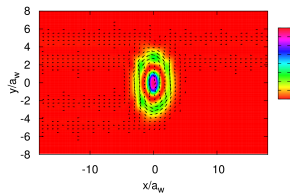
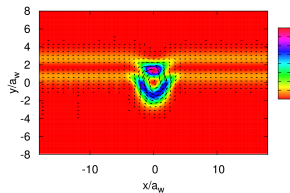
## Small Gauss hill



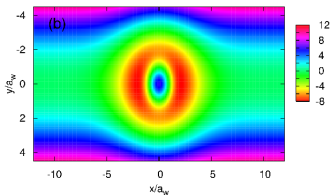
Probability density  $\rightarrow$

(Phys. Rev. B **72**, 153306 (2005))

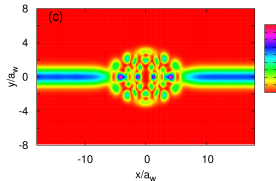
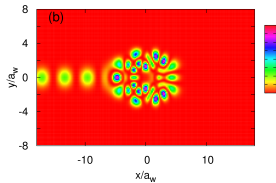
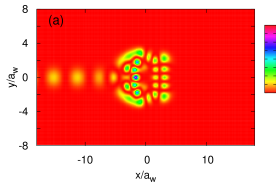
## Quasi-bound states



# Quantum ring, $B = 0$



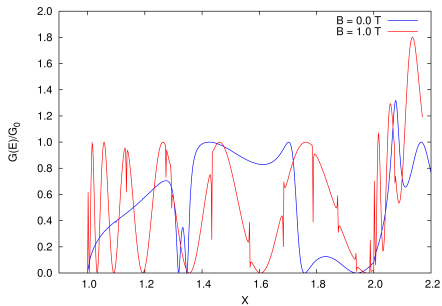
- Scarring of a wave function
- Persistence of eigenstates



$B \neq 0$

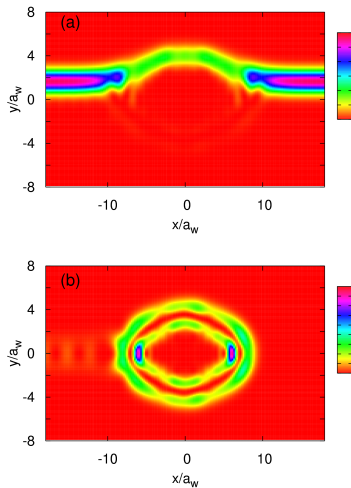
- Aharonov-Bohm oscillations
- Superimposed resonances

Conductance



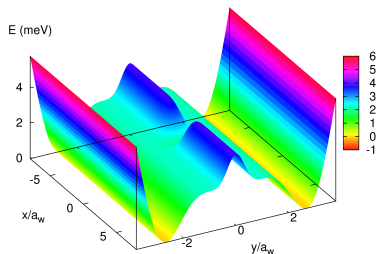
(Phys. Rev. B **71**, 235302 (2005))

Probability density



# Nonparabolic confinement, double quantum wire

## System



Scattering potential = window  
between wires

## Mode expansion

$(q, y)$ -representation

Use eigenfunctions for parabolic  
confinement  $\phi_m(q, y)$  as basis

$$\Psi_E(q, y) = \sum_n \varphi_n(q) \Phi_n(q, y)$$

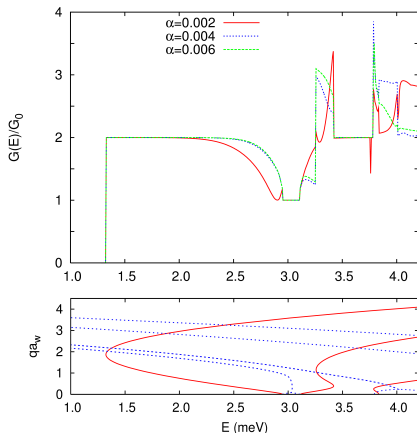
$$\Phi_n(q, y) = \sum_m c_{nm}(q) \phi_m(q, y)$$

# Conductance

(Phys. Rev. B **74**, 125302 (2006))

- Not monotonically increasing steps
- Electron- and hole-like states, different Lorentz force
- Small window  $\rightarrow$  weak interwire processes

## Different lengths of window

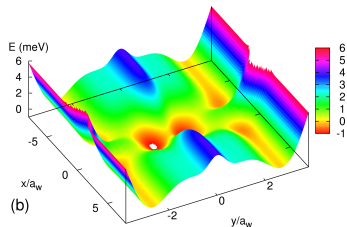
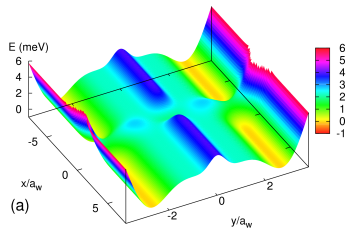


# Edge blocker $\pm$ resonator

(Phys. Rev. B **74**, 195323 (2006))

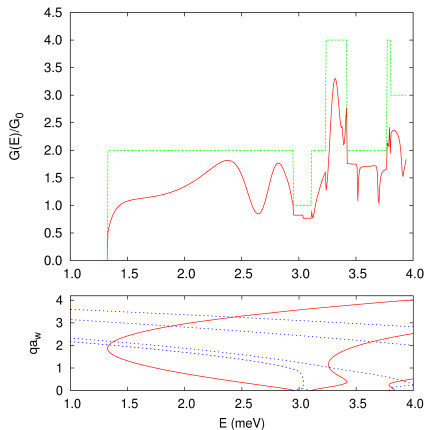
- Enhanced interwire processes
- Intermediate  $B \rightarrow a_w$  comparable with system sizes
- Intermediate Lorentz force

## System

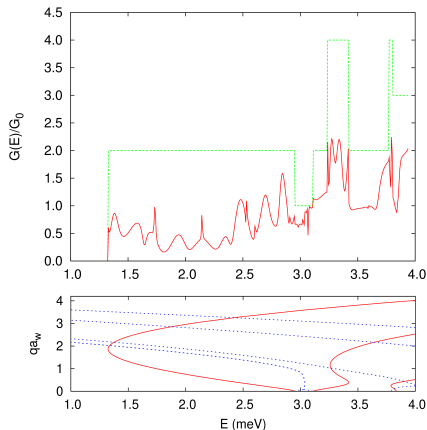


# Conductance, $B = 0.5$ T

## Edge blocker

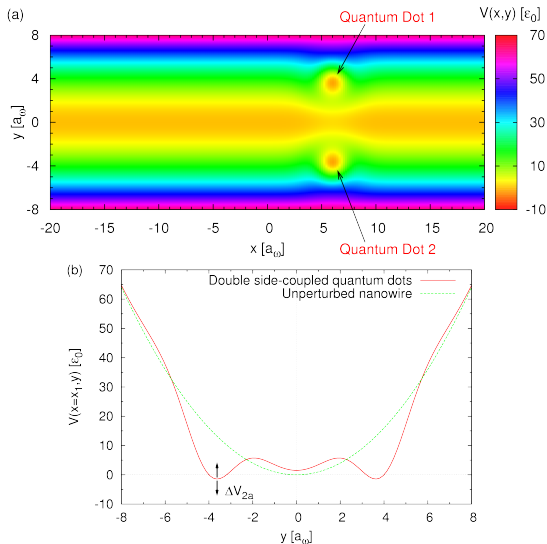


## Edge blocker + Resonator

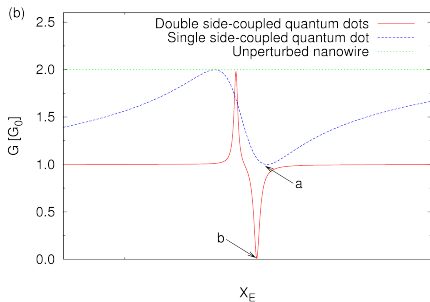
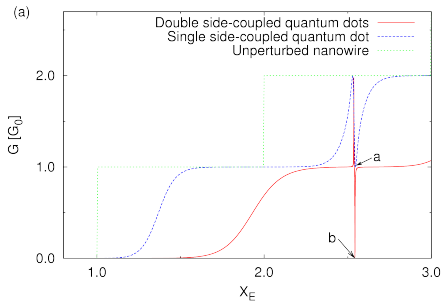


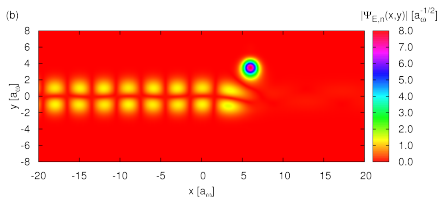
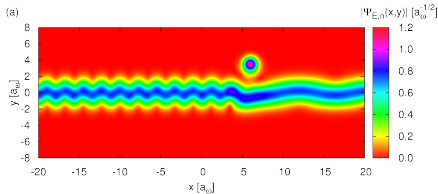
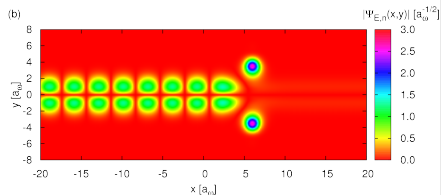
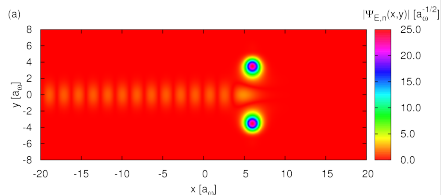
# Side-coupled quantum dots

Phys. Rev. B78, 165318 (2008)

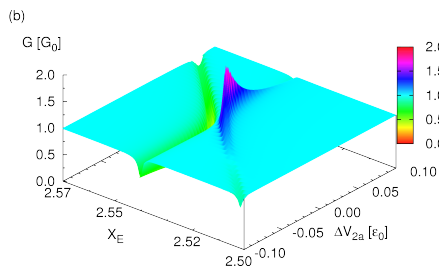
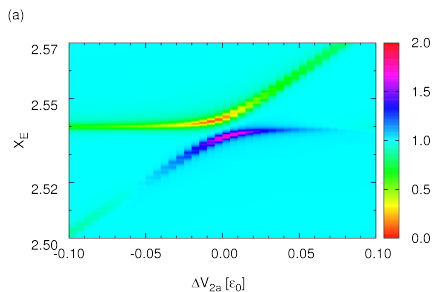


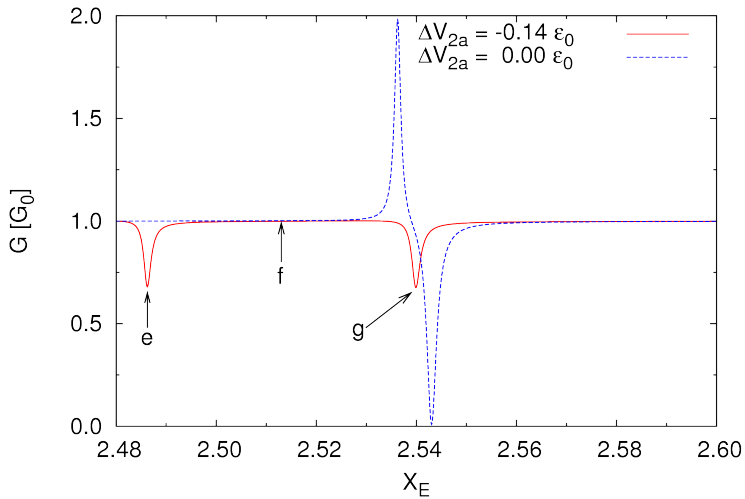




**a****b**

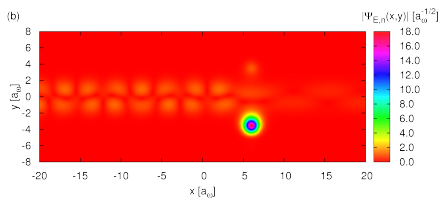
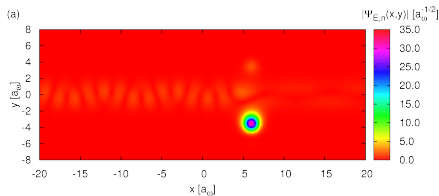
# Skewing of one dot



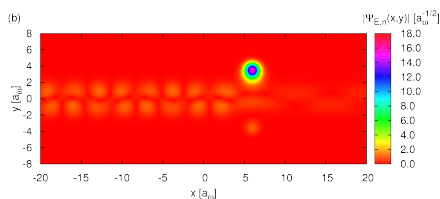
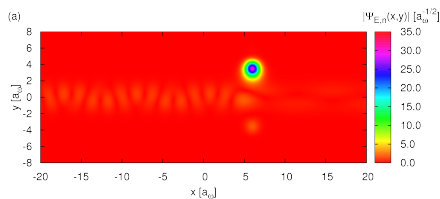


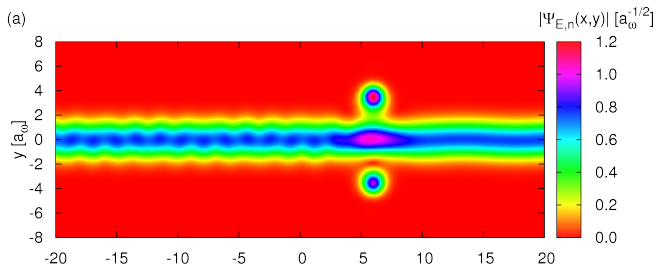
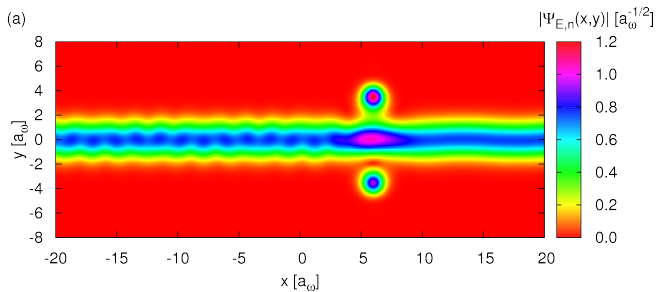
# Switching

e



og

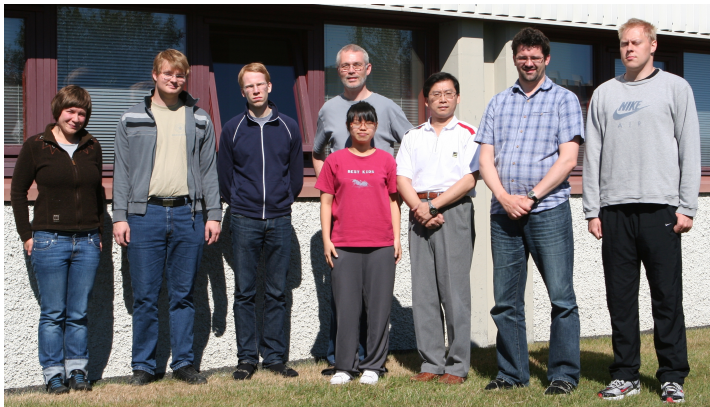




# Summary

- General scattering potentials – embedded systems
  - Magnetic field
  - General confinement
  - Heavy numerical – analytical calculations
  - Single-electron formalism
- Interplay of geometry and magnetic field → interference
  - Scattering to all orders
  - Resonances
  - Extensions: t-dependence, Coulomb-interaction

## Cooperation



Ingibjörg Magnúsdóttir  
Gunnar Þorgilsson  
Yu-Yu Lin  
Wing Wa Yu

Guðný Guðmundsdóttir  
Kristinn Torfason  
Chi-Shung Tang  
Andrei Manolescu

Jens H. Bárðarson  
Ómar Valsson  
Cai-Jhao Fan-Jiang  
Valeriu Moldoveanu