# *Magnetotransport in a double quantum wire*

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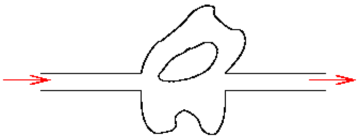
http://hartree.raunvis.hi.is/~vidar/Rann/Fyrirlestrar/RCAS_L1.pdf

RCAS, November 28, 2006

## Aim

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



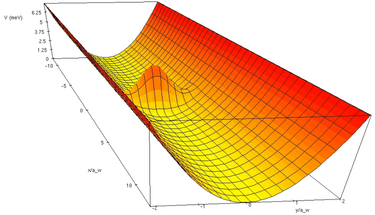
- Static transport
- Time-dependent transport

## Methods

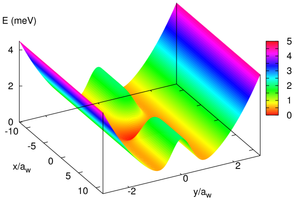
- Scattering formalism, built on Lippmann-Schwinger approach
- Basis expansion – multimode transport – enhanced parallelization
- Cooperation and comparison with groups working on alternative approaches
    - Chi-Shung Tang: Wave function matching
    - Valeriu Moldoveanu: NEGF on a lattice.
- DFT, biased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

# Outlines

## Parabolic wire + smooth scatterer

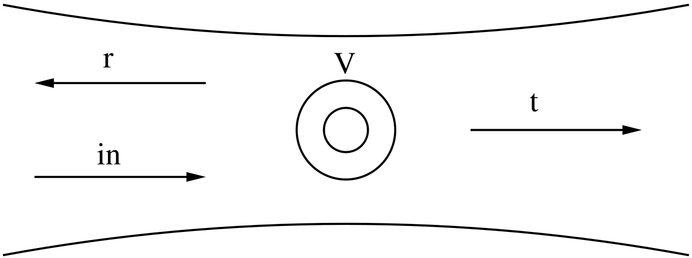



## Double wire + scattering window




Start with a single wire to explain the formalism

# Asymptotic regions




In scattering out

# Asymptotic regions

## Free parabolic wire, perpendicular magnetic field

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

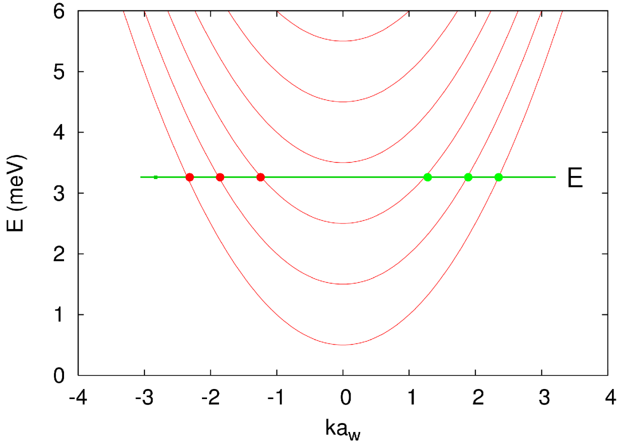
$$\psi^+(x,y,k_n) = e^{ik_nx}\chi_n(y-y_0)$$

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

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

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

# Asymptotic energy spectrum




In-, out- states, energy is conserved

# Consequences of $B \neq 0$

- Lorentz force couples the motion in $x$- and $y$-direction
- $\chi_n(y - y_0)$ 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)

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

$$\Psi_E(p,y) = \sum_n \varphi_n(p) \phi_n(p,y)$$

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

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

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

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

into a set of coupled integral equations,

$V_{sc}(x,y)$ is the scattering potential,
(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 $\quad (E - E_n) = \frac{[k_n(E)]^2}{2}\frac{(\hbar\Omega_0)^2}{\hbar\Omega_w}$

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

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

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

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

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

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

# Supplies

## Conductance, transmission amplitudes, wavefunctions

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

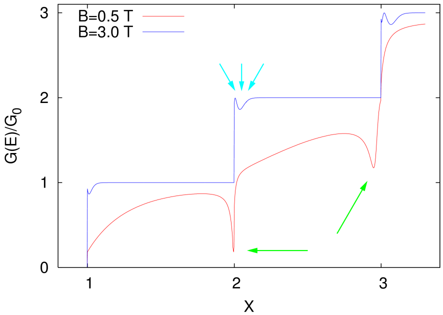
$$t_{nm}(E) = \delta_{nm} - \frac{i\sqrt{(k_m/k_n)}}{2(k_m a_w)}\left(\frac{\hbar\Omega_0}{\hbar\Omega_w}\right)^2 \tilde{T}_{nm}(k_n, k_m)$$

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

# Elastic scattering

Attractive well - 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))

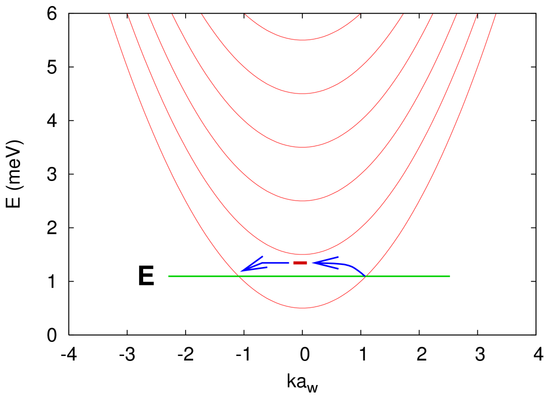



- $\hbar\Omega_0 = 1.0$ meV, broad wire
- $V_0 = -0.8$ meV, shallow dot
- $G_0 = \frac{2e^2}{h}$
- $\Omega_w = \sqrt{\omega_c^2 + \Omega_0^2}$
- $X = \frac{E}{\hbar\Omega_w} + \frac{1}{2}$

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

# perturbative view

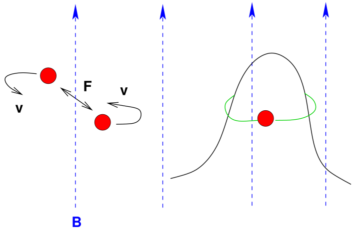
## Resonant backscattering caused by an evanescent state




- The Lippmann-Schwinger eq's include scattering to all orders

# Example 1, negative binding energy

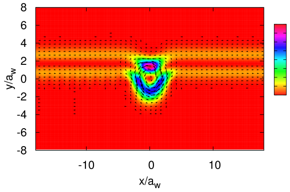
## Small Gauss hill

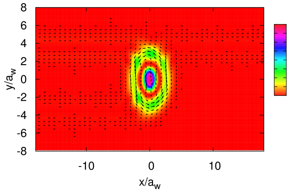



Probability density →

(Phys. Rev. B72, 153306 (2005))

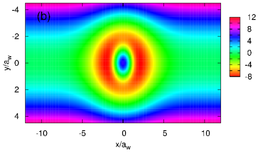
## Quasi-bound states



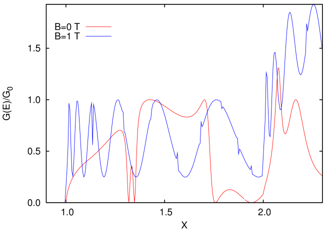



# Example 2, large quantum ring, Ahranov-Bohm oscillations

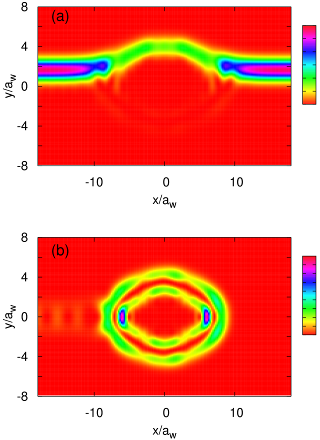
## System, (Phys. Rev. B71, 235302 (2005))




## Conductance

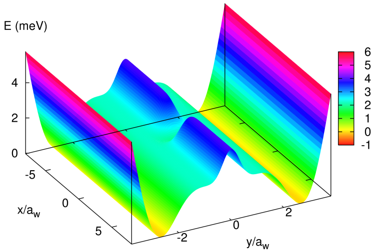



## Probability density



# 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

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

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

# Energy spectrum, asymptotic region

Energy subbands not generally equidistant

$$E_n(q) = E_n^0 + \epsilon(n,q) + \frac{(qa_w)^2}{2}\frac{(\hbar\Omega_0)^2}{\hbar\Omega_w}$$

$$E_n^0 = \hbar\Omega_w(n+1/2)$$

Band momentum

$$[k_n(E)a_w]^2 = 2\left[E - E_n^0 - \epsilon(n,q)\right]\frac{\hbar\Omega_w}{(\hbar\Omega_0)^2}$$

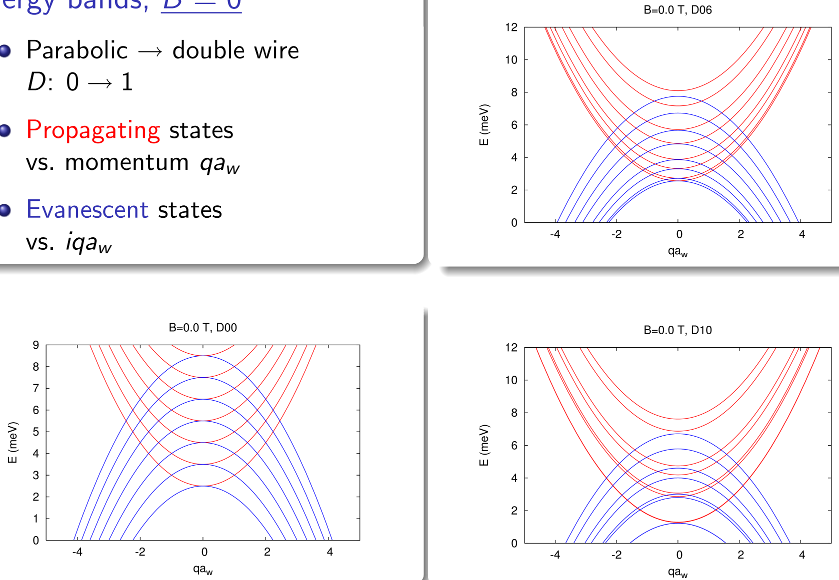
Nonpropagating modes, evanescent modes difficult, but necessary for Green function, (J.C.B. and P.N.B., Superlat. Microstr. 22, 325 (1997), S.V.K. and M.A.L., PRB 60, 13770 (1999))

$$G_E^n(q) = \frac{1}{(k_n(E)a_w)^2 - (qa_w)^2 + i0^+}$$

Evanescent modes have complex $k_n(E)$

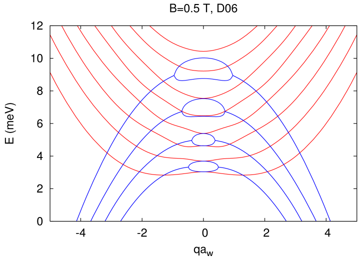
# Energy bands, $\underline{B = 0}$

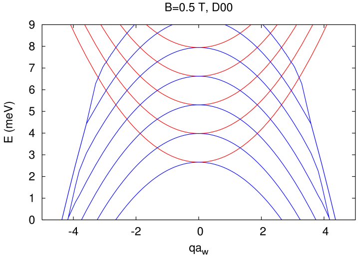
- Parabolic $\longrightarrow$ double wire
  $D$: $0 \to 1$
- Propagating states
  vs. momentum $qa_w$
- Evanescent states
  vs. $iqa_w$

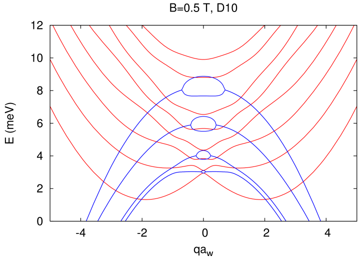


# Energy bands, $B = 0.5\,T$

- Parabolic $\rightarrow$ double wire
  $D$: $0 \rightarrow 1$
- Propagating states
  vs. momentum $qa_w$
- Evanescent states
  vs. $iqa_w$



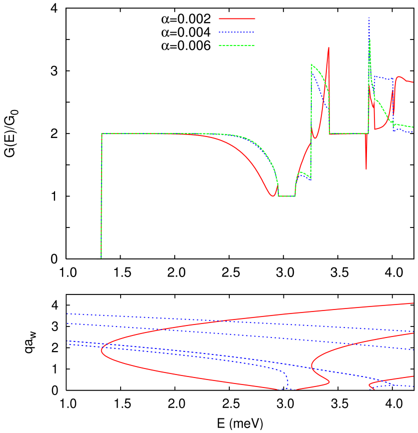



# Conductance

(Phys. Rev. B74, 125302 (2006))

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

## Different lengths of window

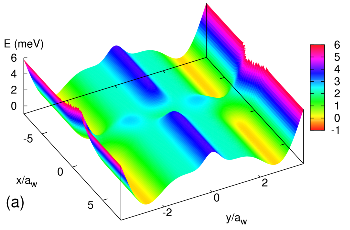


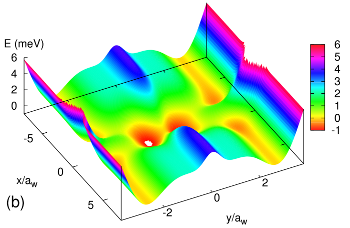
# Edge blocker $\pm$ resonator

(Phys. Rev. B74, 195323 (2006))

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

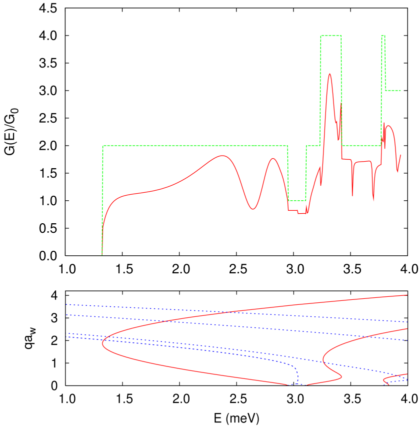
## System



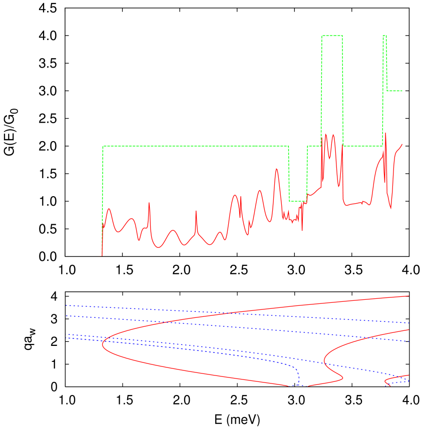



# Conductance, $B = 0.5$ T

## Edge blocker

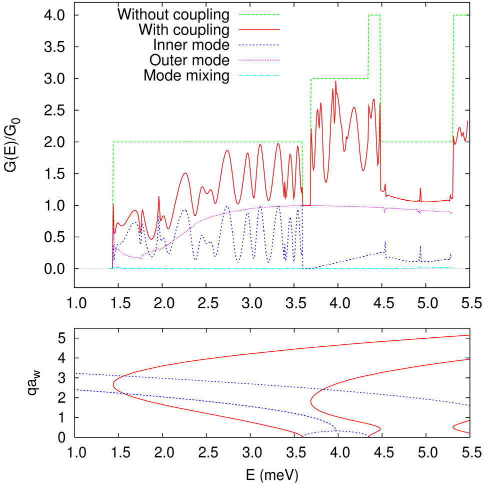



## Edge blocker + Resonator

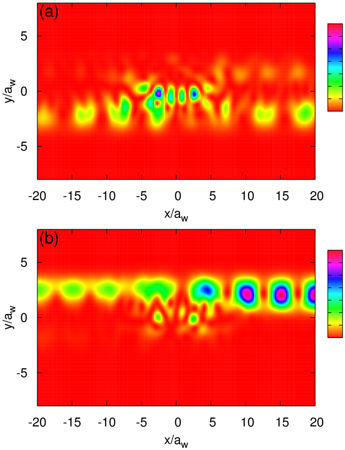


# Conductance, $B = 0.8$ T

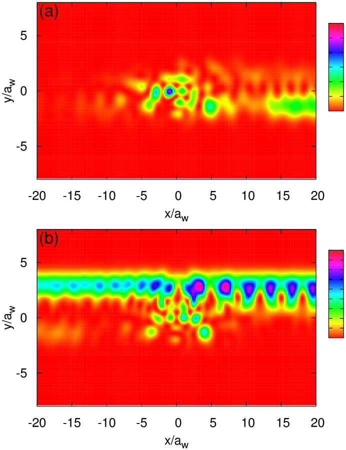
## Edge blocker + resonator



# Probability density - interwire processes, $B = 0.8$ T




E = 1.69 meV




E = 2.07 meV

# Summary

- Magnetotransport in quantum wires
- General scattering potential (embedded system) and confinement.
- Intra- and interwire processes in double quantum wires
- Time-dependent phenomena

## Cooperation + funding

Researchers:

- Chi-Shung Tang (RCAS)
- Valeriu Moldoveanu (Bukarest)
- Andrei Manolescu (SI, UI)
- Ingibjörg Magnúsdóttir

Students:

- Jens H. Bárðarson
- Wing Wa Yu
- Yu-Yu Lin
- Guðný Guðmundsdóttir
- Gunnar Þorgilsson
- Harpa Óskarsdóttir
- Ómar Valsson

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