Magnetotransport through systems embedded in a quantum wire

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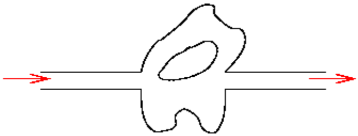
Tainan, September, 2007

Aim

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

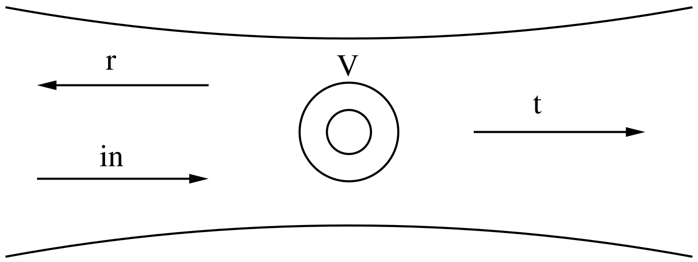


- Static transport
- Effects ← geometry + magnetic field

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 → heavy numerical work

Asymptotic regions



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

Quasi-one-dimensional scattering

Scattering state with in-energy E

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

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

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

Scattering boundary conditions

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

Landauer-Büttiker $\longrightarrow$ conductance

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

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

Separation of variables, expansion in a basis

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

Set of coupled 1D-equations

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

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

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

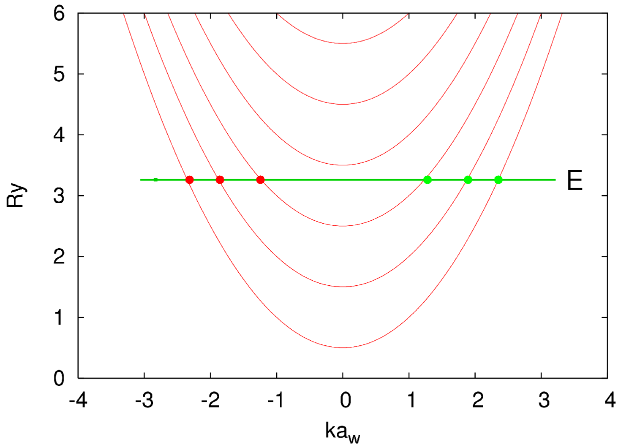
$$\psi^+(x,y,k_n) = e^{ik_n x}\phi_n(y-y_0)$$

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

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

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

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)

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

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

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 (in q-space)

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

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

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

into a set of coupled integral equations,

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

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

Wavefunctions

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

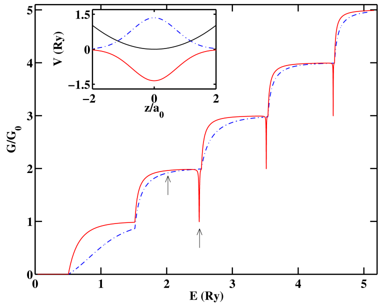
Transmission amplitudes

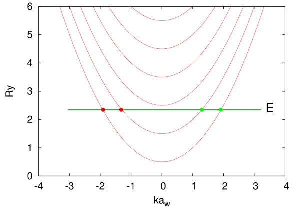
$$t_{nm}(E) = \delta_{nm} - \frac{i\sqrt{(k_m/k_n)}}{4(k_m a_w)}\tilde{T}_{nm}(k_n,k_m)$$

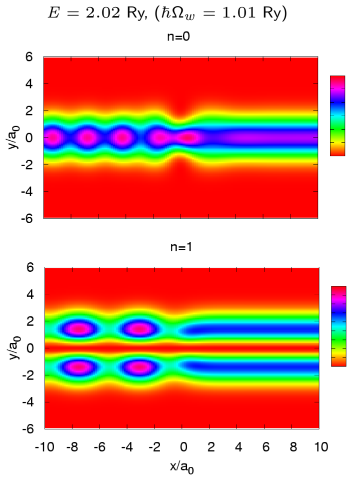
Conductance

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

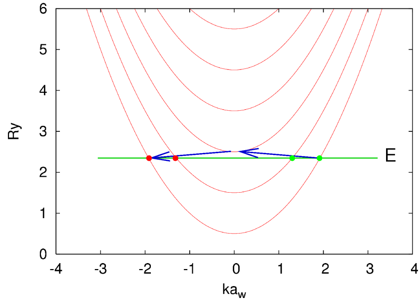
B=0, simple Gaussian hill or well



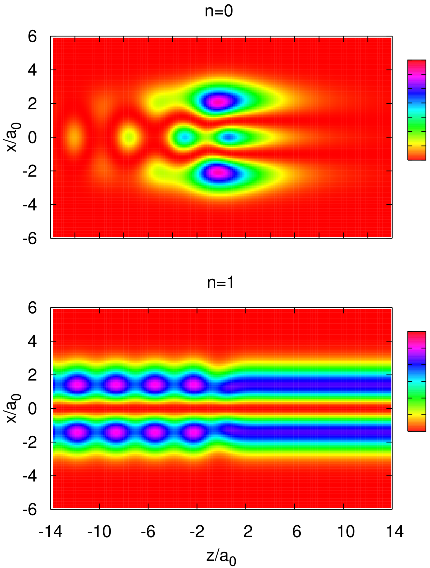




What causes a dip?

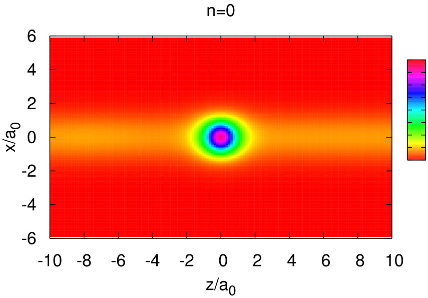


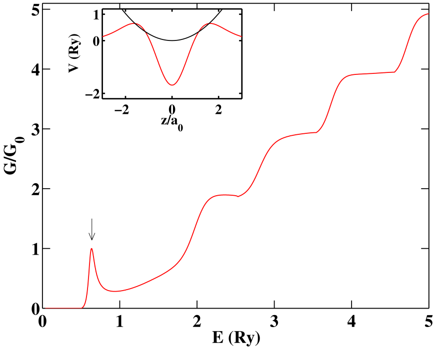
- Total reflection by an evanescent state
- Symmetry → selection rules
- All orders of scattering



Embedded dot, $B = 0$

- Total resonant transmission
- Finite lifetime



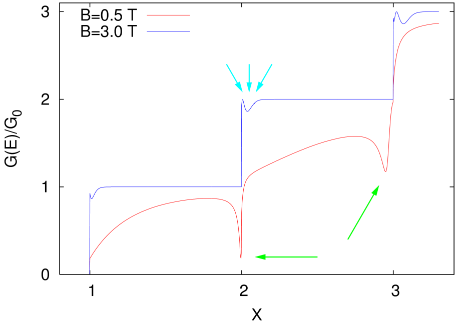


Phys. Rev. B **70** 245308, (2004)

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))

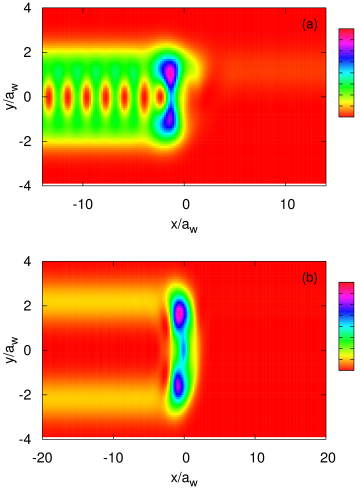


- $\hbar\Omega_0 = 1.0$ meV, broad wire
- $V_0 = -0.8$ meV, shallow dot
- $G_0 = \frac{2e^2}{h}$
- $\Omega_w = \sqrt{\omega_c^2 + \Omega_0^2}$
- $X = \frac{E}{\hbar\Omega_w} + \frac{1}{2}$

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

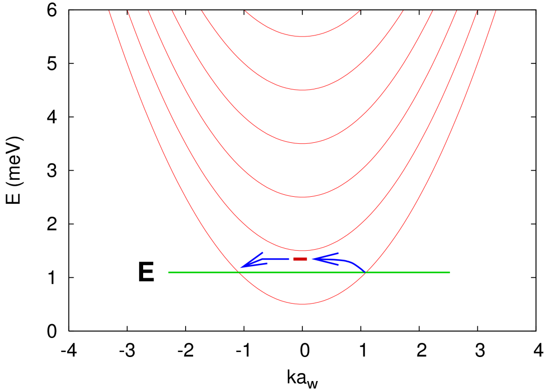
Lorentz force

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



Resonant backscattering caused by an evanescent state

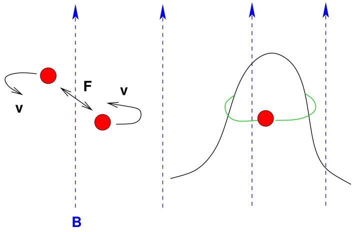
Selection rule broken by $\mathbf{B}$



- Scattering to all orders

Negative binding energy

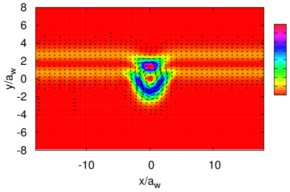
Small Gauss hill

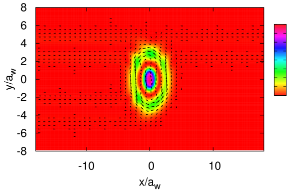


Probability density →

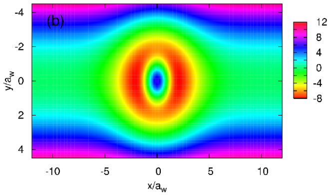
(Phys. Rev. B **72**, 153306 (2005))

Quasi-bound states

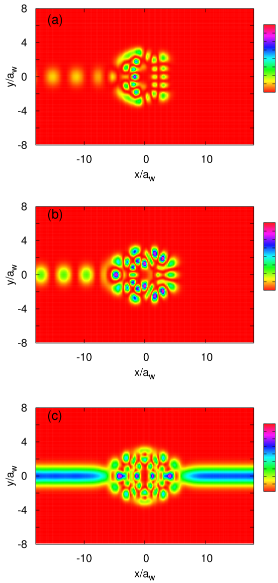




Quantum ring, $B = 0$



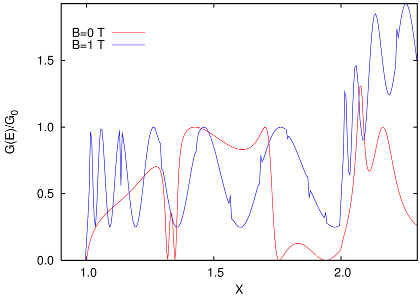
- Scarring of a wave function
  Persistence of eigenstates



$B \neq 0$

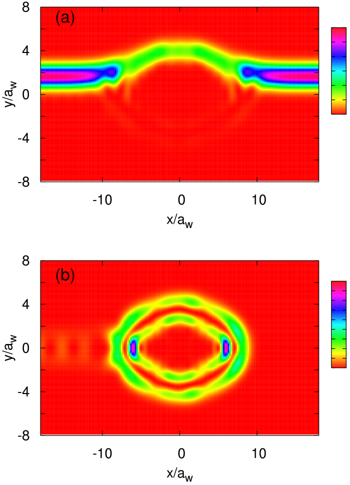
- Ahranov-Bohm oscillations
- Superimposed resonances

Conductance



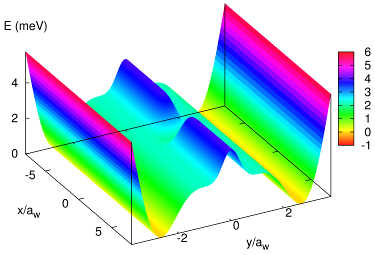
(Phys. Rev. B **71**, 235302 (2005))

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

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

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

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

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

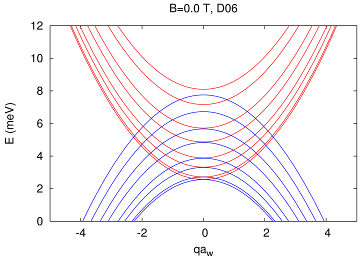
Nonpropagating modes, evanescent modes difficult, but necessary for Green function, (J.C.B. and P.N.B., Superlat. Microstr. **22**, 325 (1997), S.V.K. and M.A.L., PRB **60**, 13770 (1999))

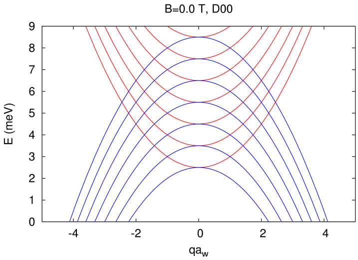
$$G_E^n(q) = \frac{1}{(k_n(E)a_w)^2 - (qa_w)^2 + i0^+}$$

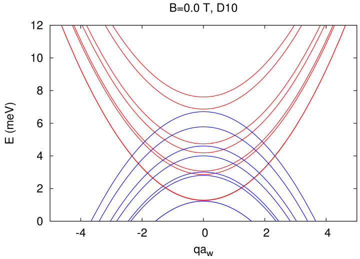
Evanescent modes have complex $k_n(E)$

Energy bands, $B = 0$

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

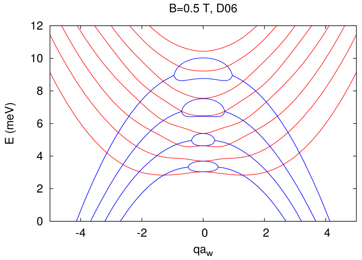


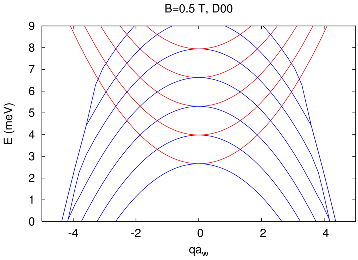


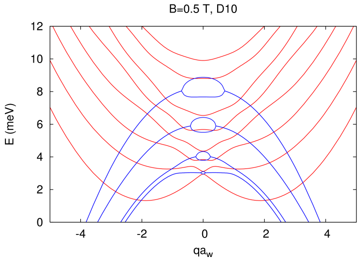


Energy bands, $B = 0.5\,T$

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





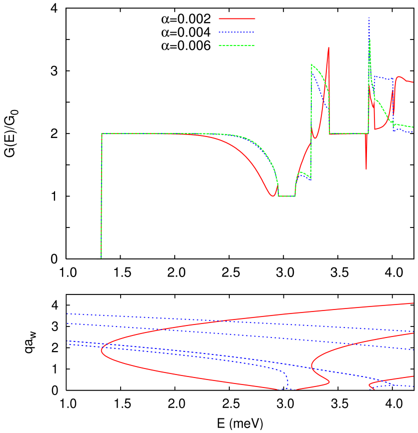


Conductance

(Phys. Rev. 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

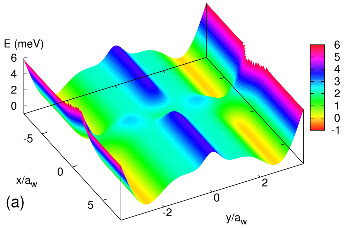


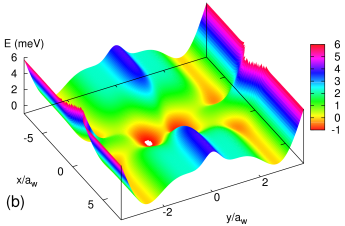
Edge blocker ± resonator

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

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

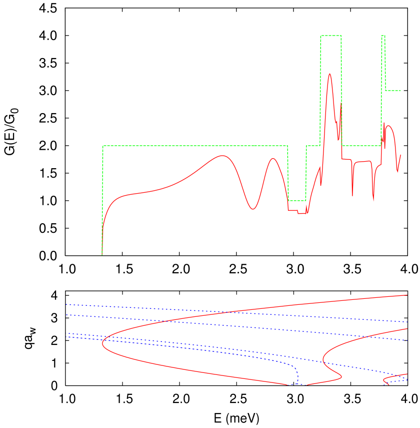
System



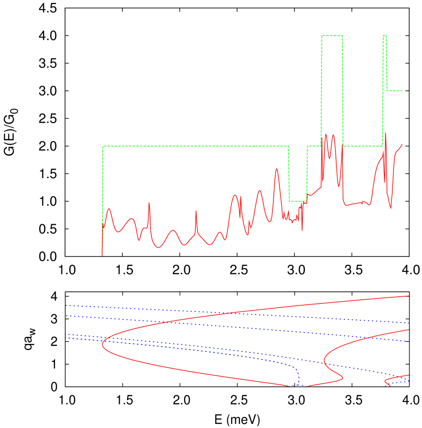


Conductance, $B = 0.5$ T

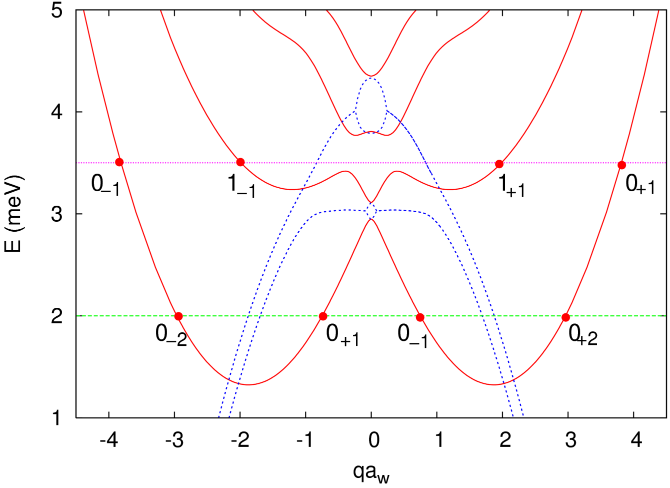
Edge blocker



Edge blocker + Resonator

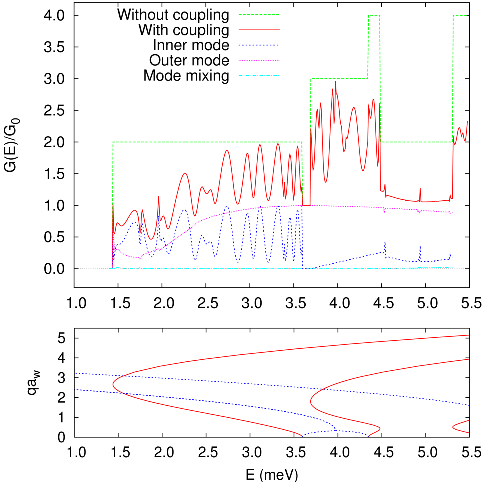


Character of in-states

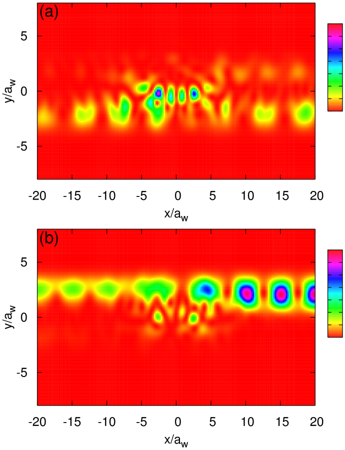


Conductance, $B = 0.8$ T

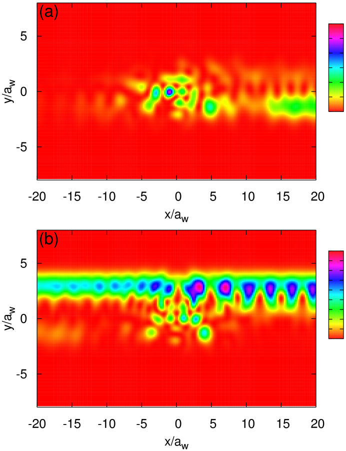
Edge blocker + resonator



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



$E = 1.69$ meV, $(0_{+1},\ 0_{+2})$



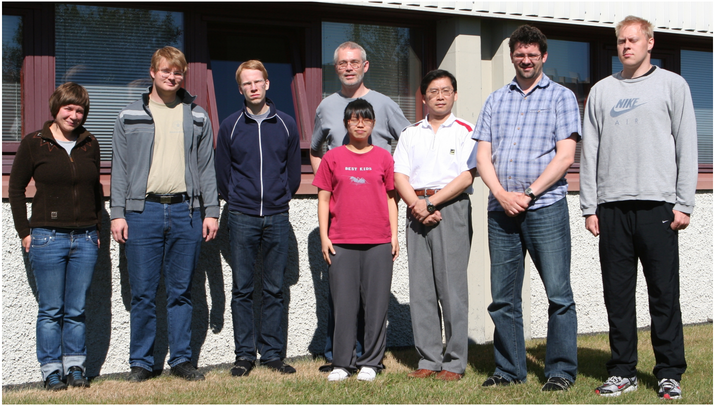
$E = 2.07$ meV, $(0_{+1},\ 0_{+2})$

Summary

- General scattering potentials – embedded systems
- Magnetic field
- General confinement
- Heavy numerical – analytical calculations
- Single-electron formalism

- Interplay of geometry and magnetic field $\rightarrow$ interference
- Scattering to all orders
- Resonances
- Extensions: t-dependence, Coulomb-interaction

Cooperation



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