

*Magnetotransport through systems
embedded in a quantum wire*

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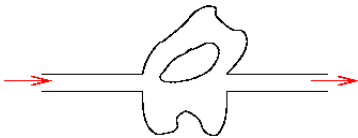
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Berlin, Februar, 2008

Aim

- Model of magnetotransport in a 2D quantum wire
- Embedded subsystems

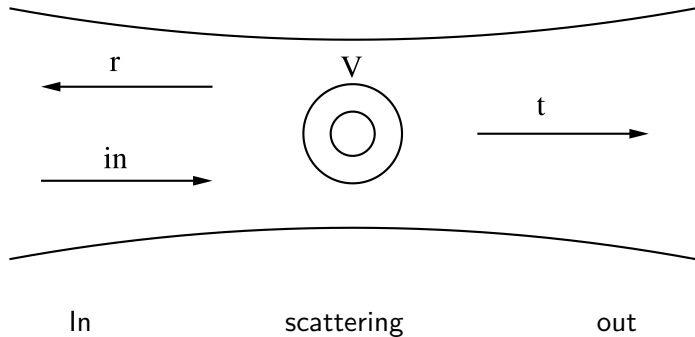


- Static and dynamic transport
- Effects \leftarrow geometry + magnetic field

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



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

Asymptotic regions, free parabolic wire, perpendicular magnetic field

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

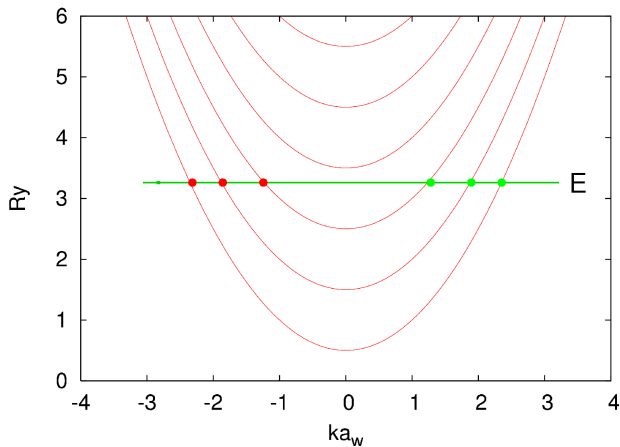
$$\psi^+(x, y, k_n) = e^{ik_n x} \phi_n(y - y_0)$$

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

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

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

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)

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

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

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)

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

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

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

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 $(E - E_n) = \frac{[k_n(E)]^2}{2} \frac{(\hbar\Omega_0)^2}{\hbar\Omega_w}$

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

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

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

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

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

Supplies

Wavefunctions

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

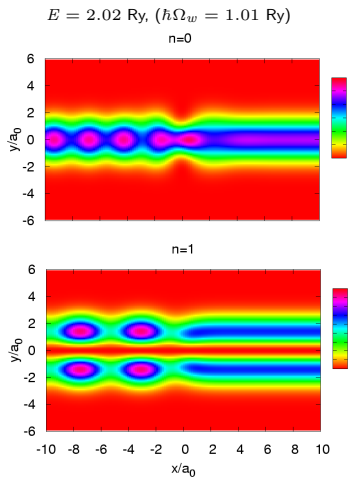
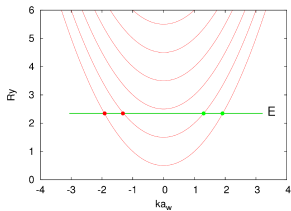
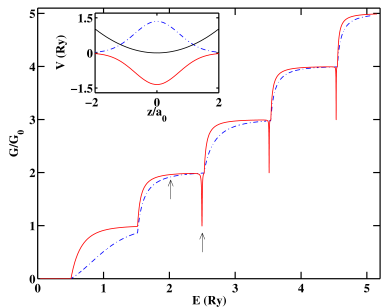
Transmission amplitudes

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

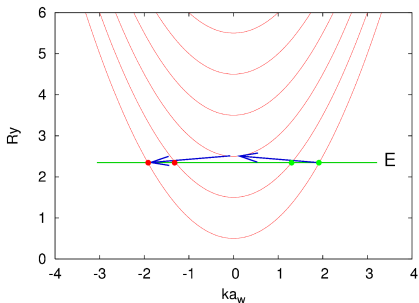
Conductance

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

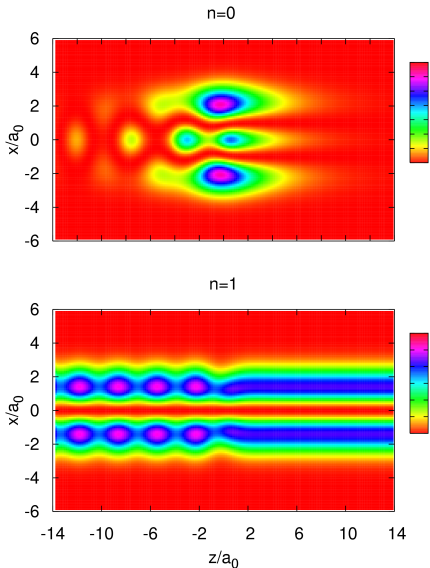
B=0, simple Gaussian hill or well



What causes a dip?

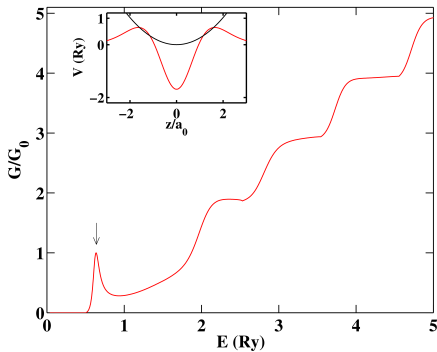
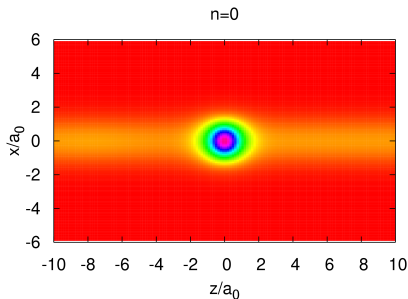


- Total reflection by an **evanescent** state
- Symmetry \rightarrow **selection** rules
- All **orders** of scattering



Embedded dot, $B = 0$

- Total resonant transmission
- Finite lifetime

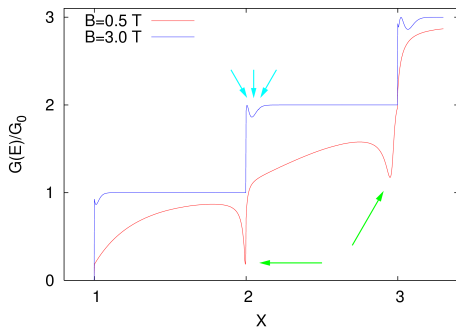


Phys. Rev. B **70** 245308, (2004)

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))

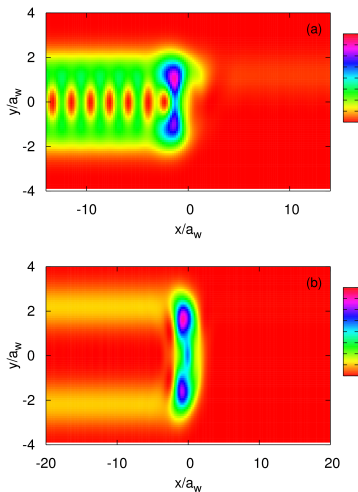


- $\hbar\Omega_0 = 1.0$ meV, broad wire
- $V_0 = -0.8$ meV, shallow dot
- $G_0 = \frac{2e^2}{h}$
- $\Omega_w = \sqrt{\omega_c^2 + \Omega_0^2}$
- $X = \frac{E}{\hbar\Omega_w} + \frac{1}{2}$

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

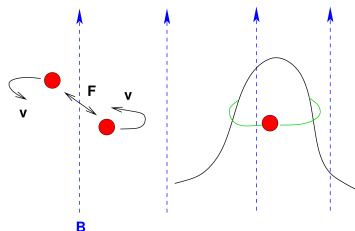
Lorentz force

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



Negative binding energy

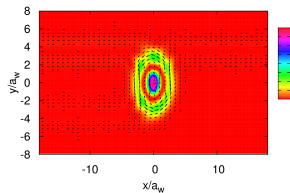
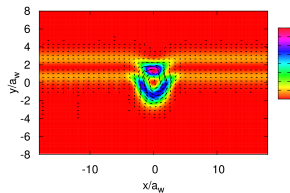
Small Gauss hill



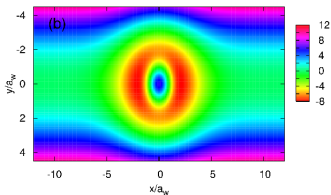
Probability density \rightarrow

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

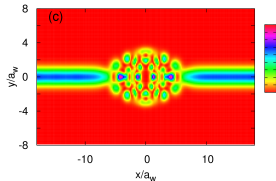
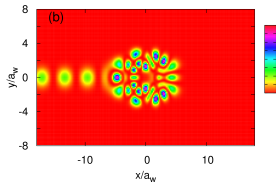
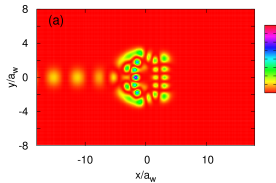
Quasi-bound states



Quantum ring, $B = 0$



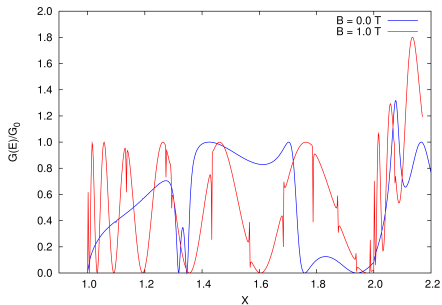
- Scarring of a wave function
- Persistence of eigenstates



$B \neq 0$

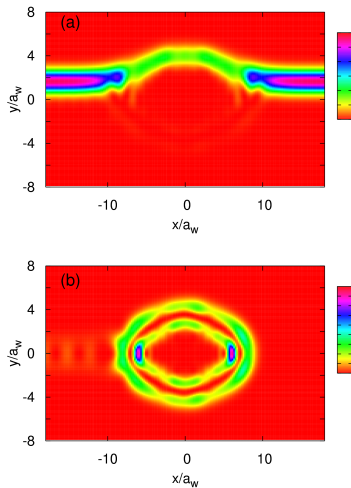
- Aharonov-Bohm oscillations
- Superimposed resonances

Conductance



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

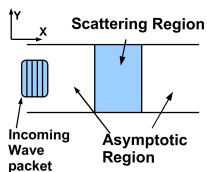
Probability density



Two cases of time-dependent magnetotransport

Wave packet transport

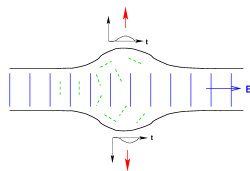
- Static potential
- Elastic scattering
- Life-time of quasi-bound states and resonances
- Delay times



(Phys. Rev. B 76, 195314 (2007))

Modulation of a current

- Plane in-wave \rightarrow sharp in-energy E
- Time-dependent potential
- Potential flashed smoothly on and off, not periodic
- Inelastic scattering

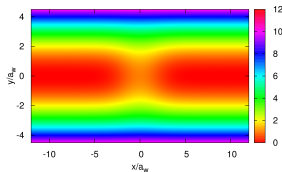
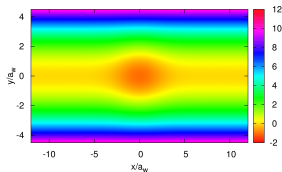
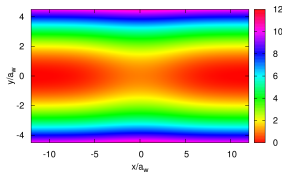
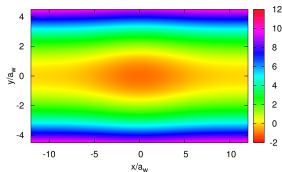


(Phys. Rev. B 77, 035329 (2008))

Current modulation

$$V_{\text{sc}}(\mathbf{r}, t) = V_0 e^{-\beta r^2} e^{-\gamma t} \cos(\Omega t),$$

view at $t = 0$:



$V_0 = \pm 1.0 \text{ meV}$, $\Omega = 0.2\Omega_w$, $\gamma = 1.0\Omega_w^2$, $\beta = 1$ or $4 \times 10^{-4} \text{ nm}^{-2}$, \rightarrow **one smooth flash**

Plane in-wave

$$\varphi_m^0(q, \omega) = (2\pi)^2 \delta(q - k_n) \delta(\omega - \omega_{nq}^0) \delta_{m,n}$$

Green function

$$\{\hbar\omega - \hbar\omega_{nq}^0\} G_0^n(q, \omega) = 1$$

T -matrix

$$T_{nn'}(q\omega, p\nu) = V_{nn'}^{\text{sc}}(q\omega, p\nu) + \sum_{m'} \int \frac{dk}{2\pi} \frac{d\omega'}{2\pi} V_{nm'}^{\text{sc}}(q\omega, k\omega') G_0^{m'}(k\omega') T_{m'n'}(k\omega', p\nu)$$

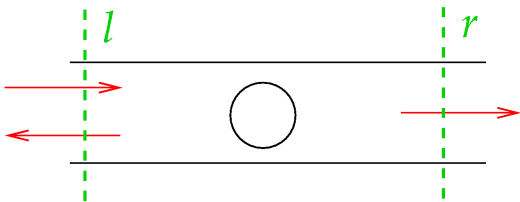
and full wave function

$$\Psi(\mathbf{r}, t) = e^{i(k_n x - \omega_{nk}^0 t)} \phi_n(k_n, y) + \sum_m \int \frac{dq}{2\pi} \frac{d\omega}{2\pi} e^{i(qx - \omega t)} G_0^m(q\omega) T_{mn}(q\omega, k_n \omega_{nk}^0) \phi_m(q, y)$$

Left and right current of state α

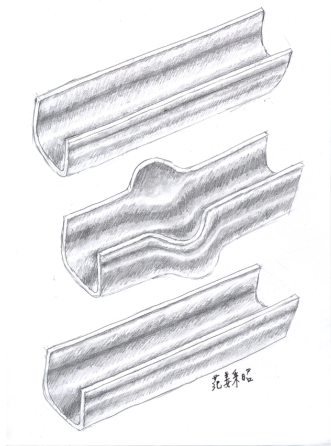
$$(I_{\alpha}^{r,l}(t))_x = \frac{\hbar}{m^*} \Re \left\{ \int_{-\infty}^{\infty} dy (\Psi_{\alpha}^{r,l})^* D_x \Psi_{\alpha}^{r,l} \right\}$$

with $\hbar D_x = (p_x + (e/c)A_x) = \hbar(-i\partial_x - y/l^2)$



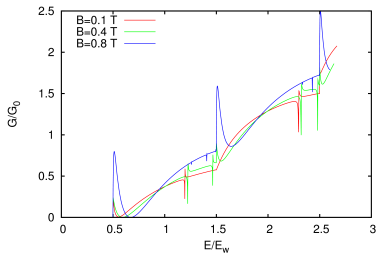
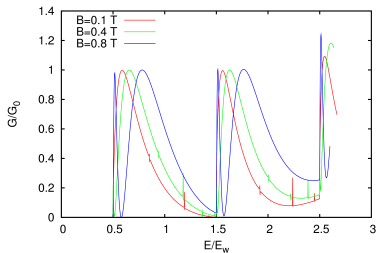
- Contributions from any point in sc-region for all earlier times
- Calculate for state α at Fermi energy
- Inelastic, any outstate possible, evanescent states explicitly in G

Smooth well-like pulse



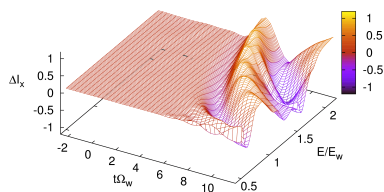
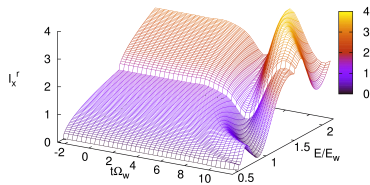
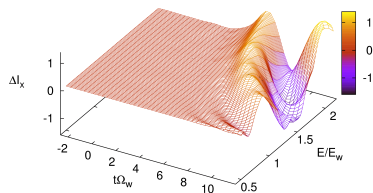
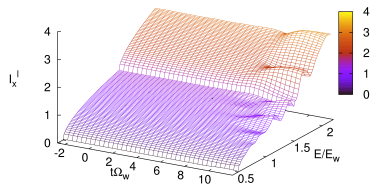
$$\beta = 1 \times 10^{-4} \text{ nm}^{-2}, \quad \beta = 4 \times 10^{-4} \text{ nm}^{-2}$$

Static conductance

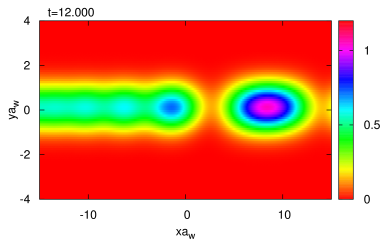
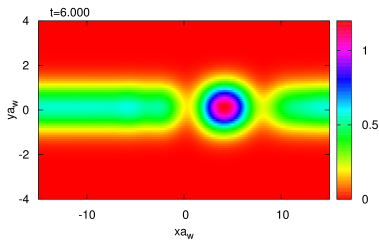
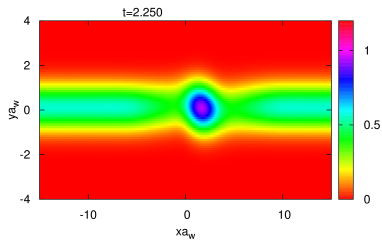
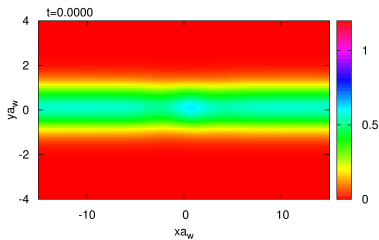


I_x^l and I_x^r , $B = 0.1$ T, $V_0 = -1$ meV

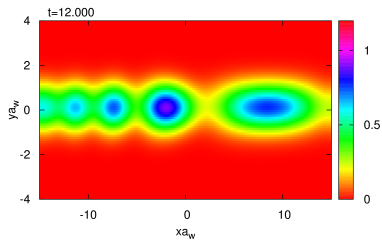
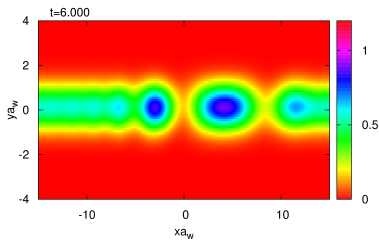
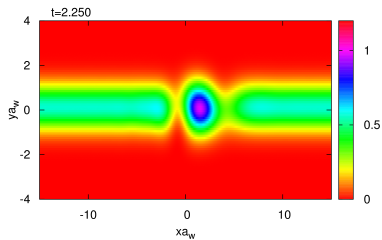
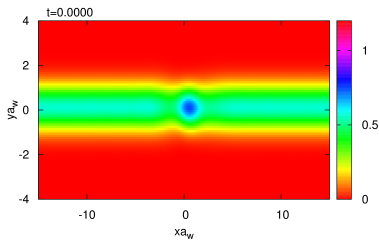
$I_x^l - I_x^r$, $\beta = 1 \times 10^{-4}$ nm $^{-2}$, $\beta = 4 \times 10^{-4}$ nm $^{-2}$



$$|\Psi|^2, B = 0.1 \text{ T}, V_0 = -1 \text{ meV}, \beta = 1 \times 10^{-4} \text{ nm}^{-2}, E = 0.75 E_w$$



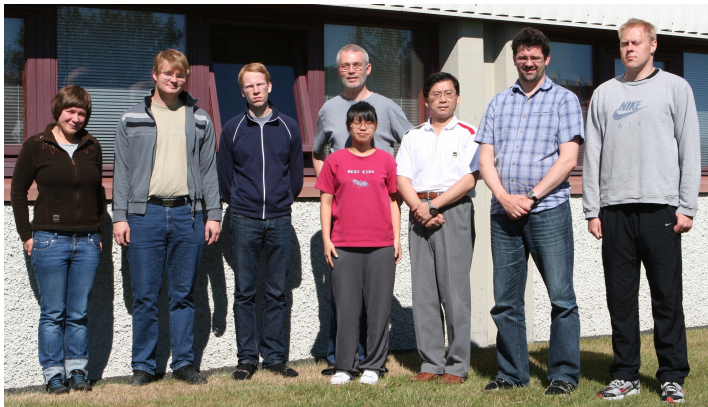
$$|\Psi|^2, B = 0.1 \text{ T}, V_0 = -1 \text{ meV}, \beta = 4 \times 10^{-4} \text{ nm}^{-2}, E = 0.75 E_w$$



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, open systems
 - Current modulation
 - Releasing of quasi-bound states
 - Time-dependence → inelastic processes

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