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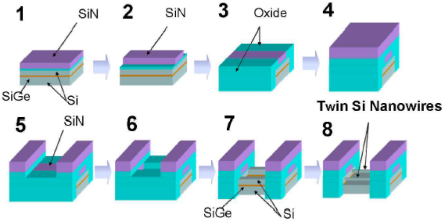
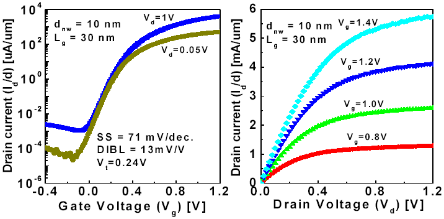
Quantum transport in cylindrical nanowire heterostructures

joint work with Roxana Racec (BTU Cottbus) and Hagen Neidhardt (WIAS)

Workshop "**Mathematical aspects of transport in mesoscopic systems**"
Dublin Institute for Advanced Studies, DIAS
Dublin, 4-7 December 2008

Twin Silicon Nanowire FET (TSNWFET)

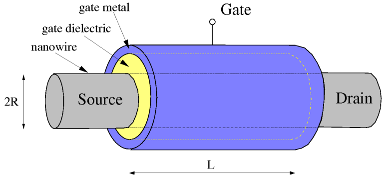




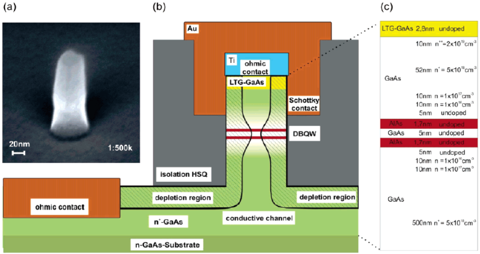
Sun Dae Suk, et al., IEDM Tech. Dig. p. 735, (2005)

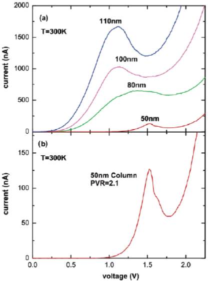
K. H. Cho, et al., Appl. Phys. Lett. **92**, 052102 (2008)

Our model:



Resonant tunneling in nanocolumns





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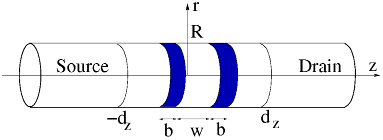
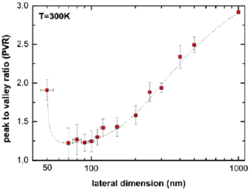
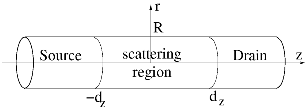




J. Wensorra, M. Lepsa et al., Nano Letters **5**, 2470, (2005)

Cylindrical coordinates (r θ z)



- one band envelope function in the effective mass aproximation

$$\left[-\frac{\hbar^2}{2\mu}\left(\frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial}{\partial r}\right)+\frac{1}{r^2}\frac{\partial^2}{\partial\theta^2}+\frac{\partial^2}{\partial z^2}\right)+V(r,z)\right]\Psi(r,\theta,z)=E\Psi(r,\theta,z)$$

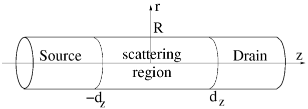
$$\Psi(r,\theta,z)=\frac{e^{im\theta}}{\sqrt{2\pi}}\psi(r,z),\qquad m=0,\pm1,\pm2,\ldots$$

$\Rightarrow$ 2D problem solved within scattering theory

$$\left[-\frac{\hbar^2}{2\mu}\left(\frac{\partial^2}{\partial r^2}+\frac{1}{r}\frac{\partial}{\partial r}-\frac{m^2}{r^2}+\frac{\partial^2}{\partial z^2}\right)+V(r,z)\right]\psi(r,z)=E\psi(r,z),$$

$$r\in[0,R],z\in(-\infty,\infty).$$

2D scattering theory in cylindrical coordinates for two leads



- ▷ definition of scattering region: constant potential outside it

$$V(r,z) = \begin{cases} V_1, & r \in [0,R], z < -d_z \\ V(r,z) & r \in [0,R], -d_z \le z \le d_z \\ V_2, & r \in [0,R], z > d_z \end{cases},$$

- ▷ boundary conditions for no gate leakage current

$$\psi(R,z) = 0,\ z \in (-\infty, \infty)$$

- ▷ scattering boundary conditions on transport direction z

Asymptotic regions: definition of channels

- outside the scattering region: separation of variables

$$\psi(r,z) = \phi(r)\varphi(z), \qquad E = E_\perp + \varepsilon$$

♦ radial equation: transversal modes

$$-\frac{\hbar^2}{2\mu}\left(\frac{d^2}{dr^2} + \frac{1}{r}\frac{d}{dr} - \frac{m^2}{r^2}\right)\phi(r) = E_\perp \phi(r), \qquad r \in [0,R].$$

$$\phi(R) = 0 \Rightarrow \phi_n^{(m)}(r) = \frac{\sqrt{2}}{RJ_{|m|+1}(x_{mn})} J_m(x_{mn} r/R),$$

$$E_{\perp n}^{(m)} = \frac{\hbar^2}{2\mu}\left(\frac{x_{mn}}{R}\right)^2, n = 1,2,\dots$$

where x_{mn} is the nth root of Bessel function $J_m(x)$

$\Rightarrow \{\phi_n^{(m)}(r)\}$ orthonormal system of functions

Asymptotic regions: definition of channels

- transport direction: plane waves

$$\left[-\frac{\hbar^2}{2\mu}\frac{d^2}{dz^2}+V_s\right]\varphi(z)=\varepsilon\varphi(z), \qquad |z|>d_z,\ s=1,2$$

$$\varphi(\varepsilon,z)=\begin{cases}Ae^{ik_1z}+Be^{-ik_1z}, & z<-d_z\\ Ce^{ik_2z}+De^{-ik_2z}, & z>d_z,\end{cases},$$

ε has continuous spectrum, $k_s(\varepsilon)=\sqrt{(2\mu/\hbar^2)(\varepsilon-V_s)}$

A,B,C,D at most two of them are linearly independent

$\Rightarrow$ general solution: combination of channels $\phi_n^{(m)}(r)\varphi(\varepsilon,z)$.

Scattering states

- incident from source $s = 1$ (left)

$$\psi^{(1)}_{nm}(E,r,z) = \frac{1}{\sqrt{2\pi}} \begin{cases} e^{ik_{1nm}(z+d_z)}\phi^{(m)}_{n}(r) + \sum_{n'=1}^{\infty}\left(\hat{S}^{(m)}\right)^{T}_{1n,1n'}(E)e^{-ik_{1n'm}(z+d_z)}\phi^{(m)}_{n'}(r), & z \le -d_z \\ \sum_{n'=1}^{\infty}\left(\hat{S}^{(m)}\right)^{T}_{1n,2n'}(E)e^{ik_{2n'm}(z-d_z)}\phi^{(m)}_{n'}(r), & z \ge d_z \end{cases}$$

▷ $k_{snm}(E) = \sqrt{(2\mu/\hbar^2)(E - E^{(m)}_{\perp n} - V_s)}$, $s = 1,2$, $n \in \mathbb{N}_+$, $m \in \mathbb{Z}$

$E - E^{(m)}_{\perp n} - V_s > 0 \Rightarrow (snm) =$ open channel $\Rightarrow N_{sm}(E)$ nr. open channels

$E - E^{(m)}_{\perp n} - V_s < 0 \Rightarrow (snm) =$ closed channel

Scattering states

- incident from drain $s=2$ (right)

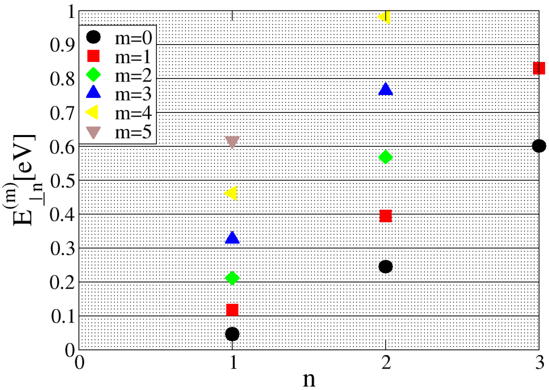
$$\psi_{nm}^{(2)}(E,r,z)=\frac{1}{\sqrt{2\pi}}\begin{cases}\sum_{n'=1}^{\infty}\left(\hat{S}^{(m)}\right)^T_{2n,1n'}(E)e^{-ik_{1n'm}(z+d_z)}\phi_{n'}^{(m)}(r), & z\leq -d_z\\ e^{-ik_{2nm}(z-d_z)}\phi_n^{(m)}(r)+\sum_{n'=1}^{\infty}\left(\hat{S}^{(m)}\right)^T_{2n,2n'}(E)e^{ik_{2n'm}(z-d_z)}\phi_{n'}^{(m)}(r), & \\ & z\geq d_z\end{cases}$$

▷ wave scattering matrix or generalized scattering matrix

$\hat{S}^{(m)}(E)$ has $N_{1m}(E)+N_{2m}(E)$ infinite columns

▷ consider $\hat{S}(E)$ infinite dimensional matrix,
but $(\hat{\Theta})_{sn,s'n'}=\theta(E-E_{\perp n}^{(m)}-V_s)\delta_{ss'}\delta_{nn'}$ "cuts" the meaningless terms

Open and closed channels



$$\mu = 0.19m_0,\ R = 5nm$$

Reflection and transmission probabilities

- density current

$$\vec{j}(\vec{r}) = \frac{\hbar}{2i\mu}\Big(\Psi(\vec{r})\nabla\Psi(\vec{r})^* - \Psi(\vec{r})^*\nabla\Psi(\vec{r})\Big)$$

- reflection probability from $(1n)$ into $(1n')$

$$R^{(1)}_{nn'} = \frac{k_{1n'}}{k_{1n}}|\hat{S}^T_{1n,1n'}|^2$$

- transmission probability from $(1n)$ into $(2n')$

$$T^{(1)}_{nn'} = \frac{k_{2n'}}{k_{1n}}|\hat{S}^T_{1n,2n'}|^2$$

Current scattering matrix

$$\hat{\tilde{S}}(E) \equiv \hat{K}^{1/2}(E)\hat{\Theta}(E)\hat{S}(E)\hat{K}^{-1/2}(E)$$

with $(\hat{K}(E))_{sn,s'n'} = k_{sn}(E)\delta_{ss'}\delta_{nn'}$, $\quad s,s' = 1,2,\ n,n' \in \mathbb{N}_+$

$$|\tilde{S}_{1n',1n}(E)|^2 = R^{(1)}_{nn'}(E) \qquad |\tilde{S}_{1n',2n}(E)|^2 = T^{(2)}_{nn'}(E)$$

$$|\tilde{S}_{2n',1n}(E)|^2 = T^{(1)}_{nn'}(E) \qquad |\tilde{S}_{2n',2n}(E)|^2 = R^{(2)}_{nn'}(E)$$

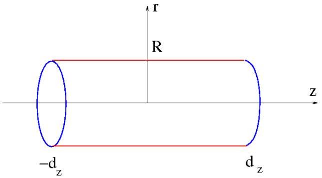
- $\hat{\tilde{S}}$ has $(N_1+N_2)\times(N_1+N_2)$ non-zero elements
- $\hat{\tilde{S}}\hat{\tilde{S}}^\dagger = \hat{\tilde{S}}^\dagger\hat{\tilde{S}} = \hat{1}$
- total tunneling coefficient

$$T^{(1)}(E) = \sum_{n,n'} T^{(1)}_{nn'}(E)$$

Wigner-Eisenbud problem

$$\left[-\frac{\hbar^2}{2\mu}\left(\frac{\partial^2}{\partial r^2}+\frac{1}{r}\frac{\partial}{\partial r}-\frac{m^2}{r^2}+\frac{\partial^2}{\partial z^2}\right)+V(r,z)\right]\chi_l(r,z)=E_l\chi_l(r,z), \quad l=1,2,\ldots$$

defined on a closed domain



with mixed boundary conditions

$$\left.\frac{\partial\chi(r,z)}{\partial z}\right|_{z=\pm d_z} = 0 \qquad \text{(v. Neumann at interfaces to leads)}$$

$$\chi(R,z) = 0 \qquad \text{(Dirichlet otherwise)}$$

$\Rightarrow \{\chi_l(r,z)\}_{l\geq 1}$ orthonormal system of functions

Scattering wave function inside the scattering region

- expansion of scattering states in Wigner-Eisenbud functions

$$\psi_n^{(s)}(E,r,z) = \sum_{l=1}^{\infty} a_{ln}^{(s)}(E)\chi_l(r,z), \quad z \in [-d_z, d_z],\ r \in [0,R]$$

- define the R-function

$$R(E,r,z,r',z') \equiv \frac{\hbar^2}{2\mu}\sum_{l=1}^{\infty}\frac{\chi_l(r,z)\chi_l(r',z')}{E-E_l}\frac{\pi}{2d_z}$$

$\Rightarrow$

$$\psi_n^{(s)}(E,r,z) = \frac{2d_z}{\pi}\int_0^R dr'\, r' \left[R(E,r',-d_z,r,z)\left.\frac{\partial\psi_n^{(s)}(E,r',z')}{\partial z'}\right|_{z'=-d_z} - R(E,r',d_z,r,z)\left.\frac{\partial\psi_n^{(s)}(E,r',z')}{\partial z'}\right|_{z'=d_z}\right],$$

Relation between R and S-matrix

- continuity of the wave function

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

where define the R-matrix: real and symmetric

$$\hat{R}_{sn,s'n'}(E) = \int_0^R dr\, r \int_0^R dr'\, r' R(E; r, (-1)^s d_z, r', (-1)^{s'} d_z)\, \phi_n(r)\phi_{n'}(r')$$

▷ $\hat{R}$ infinite dimensional matrix

R-matrix representation of $\tilde{S}$ matrix

- current scattering matrix

$$\hat{\tilde{S}}(E) = \hat{\Theta}(E)\left[\hat{1} - 2\left(\hat{1} + i\hat{\Omega}(E)\right)^{-1}\right]\hat{\Theta}(E),$$

with the symmetric and complex matrix

$$\hat{\Omega}(E) = \hat{K}^{1/2}(E)\hat{R}(E)\hat{K}^{1/2}(E) = \sum_{l=1}^{\infty} \frac{\vec{\alpha}_l(E)\,\vec{\alpha}_l^T(E)}{E - E_l}$$

where

$$(\vec{\alpha}_l)_{sn}(E) = \frac{\hbar}{\sqrt{2\mu}} k_{sn}^{1/2}(E) \int_0^R dr\, r\, \chi_l(r, (-1)^s d_z)\phi_n(r), \quad s = 1, 2,\ n \geq 1.$$

▷ $\hat{\Omega}$ infinite dimensional matrix

Resonances

Split $\hat{\Omega}$ matrix around a Wigner-Eisenbud energy E_λ

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

$$\Rightarrow \hat{\tilde{S}} = \hat{\tilde{S}}_\lambda + 2i \frac{\hat{\Theta} \vec{\beta}_\lambda \vec{\beta}_\lambda^T \hat{\Theta}}{E - E_\lambda - \bar{\mathscr{E}}_\lambda(E)}$$

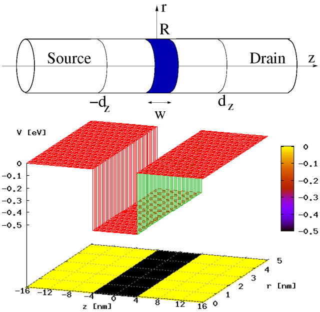
Poles of the $\tilde{S}$ matrix

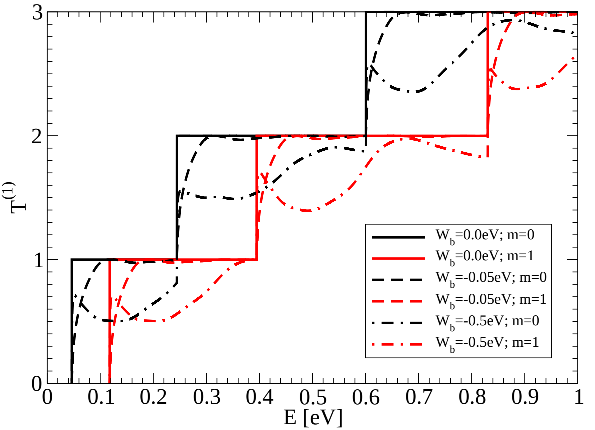
$$\boxed{E - E_\lambda - \bar{\mathscr{E}}_\lambda(E) = 0} \quad \Rightarrow \quad \bar{E}_{0\lambda} = E_{0\lambda} - i\,\Gamma_\lambda/2$$

where

$$\vec{\beta}_\lambda = (1 + i\hat{\Omega}_\lambda)^{-1} \vec{\alpha}_\lambda, \quad \bar{\mathscr{E}}_\lambda(E) = -i\vec{\beta}_\lambda^T \cdot \vec{\alpha}_\lambda, \quad \hat{\tilde{S}}_\lambda = \hat{\Theta}\left[\hat{1} - 2(1 + i\hat{\Omega}_\lambda)^{-1}\right]\hat{\Theta}.$$

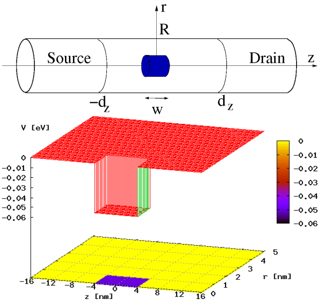
Quantum dot with same radius

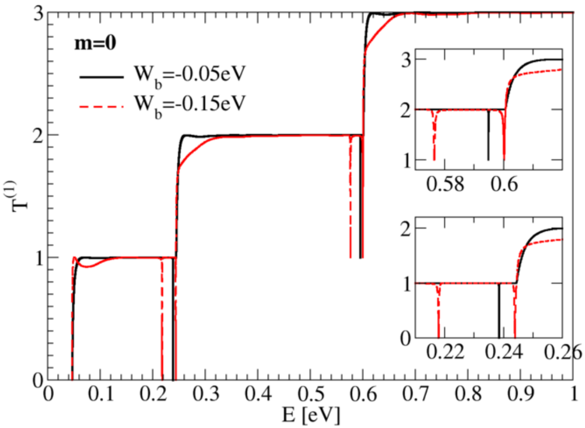




- ▷ separable potential: $V(r,z) = V(z)$ $\Rightarrow$ no channel mixing
- ▷ increasing well depth $\Rightarrow$ deviations from steps at $E_{\perp,n}^{(m)}$

Quantum dot surrounded by host material





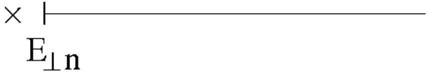
- ▷ nonseparable potential: $V(r,z) \neq V(z) \Rightarrow$ channel mixing
- ▷ dips due to quasi-bound states of evanescent channels

Channel mixing

- ▷ interchannel potential

$$V_{nn'}(z) := \int_0^R \phi_n(r) V(r,z) \phi_{n'}(r)\, r dr.$$

- ▷ attractive potential $\Rightarrow V_{nn}(z) < 0 \Rightarrow$ at least one bound state



- ▷ through channel mixing it becomes a quasi-bound state (resonance) whose real part gets embedded into continuum spectrum of the lower channel

- ▷ P.F. Bagwell (1990) for δ potential
  S.A. Gurvitz and Y.B. Levinson (1993) for extended potential
  J.U. Nöckel and A.D.Stone (1994) Fano profile
  V. Gudmundsson (2004) and (2005) for quantum wire tailored in 2DEG

Channel mixing

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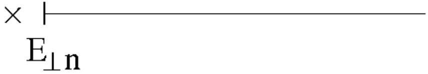

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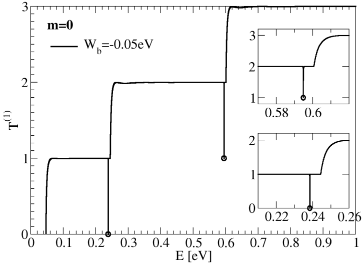
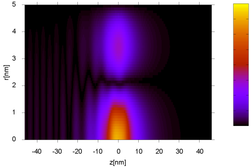
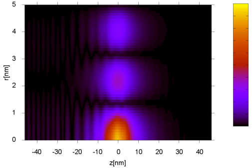
Quantum dot surrounded by host material: localization probability density





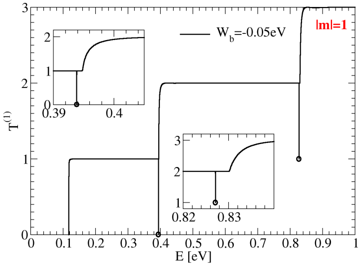
$E = 0.238eV,\ n = 1$

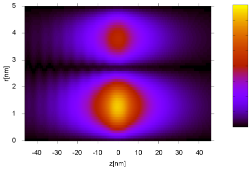


$E = 0.594eV,\ n = 2$

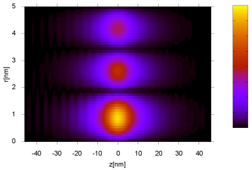
- maximum around quantum well, decreases exponentialy to left and right
- number of nodes give information about the evanescent channel
- resonant back-reflection

Quantum dot surrounded by host material: localization probability density





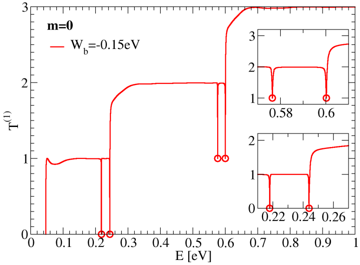
$E = 0.393eV, n = 1$

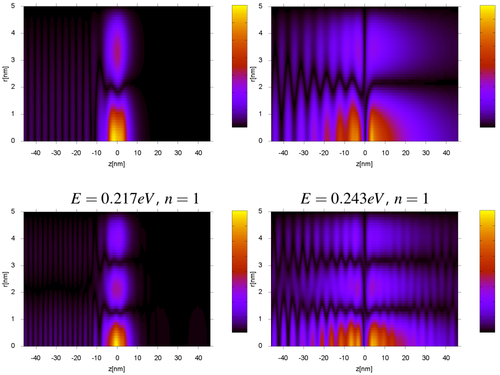


$E = 0.827eV, n = 2$

- similar pictures for $m \neq 0$, but $\psi(r = 0, z) = 0$

Quantum dot surrounded by host material: deeper well



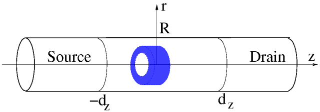


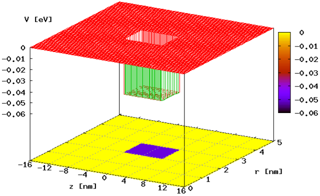
$E = 0.217eV, n = 1$ $E = 0.243eV, n = 1$

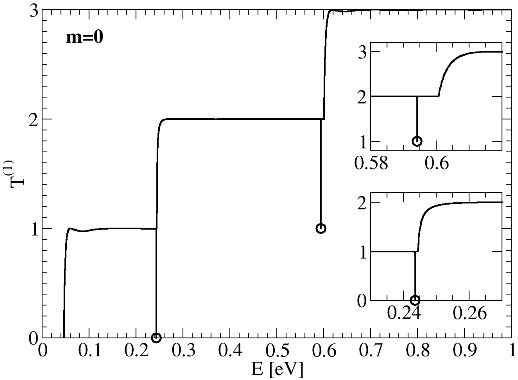
$E = 0.576eV, n = 2$ $E = 0.600eV, n = 2$

- nodes in the z-direction for higher-order quasi-bound states

Core/shell quantum ring

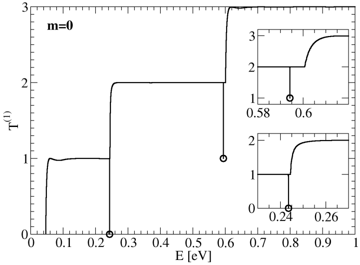


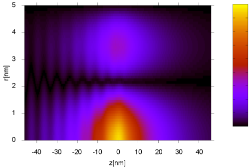




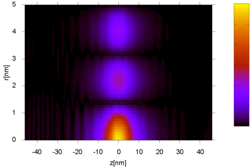
▷ same quantum well, but off-centered

Core/shell quantum ring: localization probability density





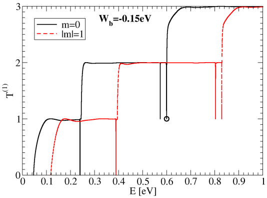
$E = 0.243eV, n = 1$

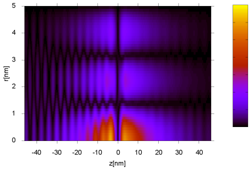


$E = 0.594eV, n = 2$

▷ extension of the quasi-bound states over whole cylinder radius

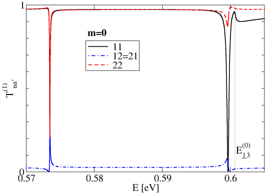
Core/shell quantum ring: deeper quantum well

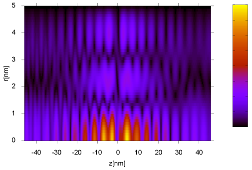




$E = 0.599eV$, $n = 1$

Interband and intraband tunneling

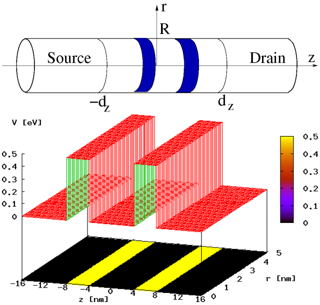


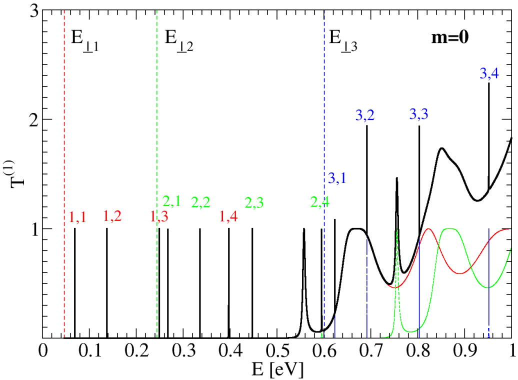


$E = 0.599eV$, $n = 2$

- ▷ nodes in the z-direction for higher-order quasi-bound states
- ▷ interference patterns decided by interband and intraband tunneling

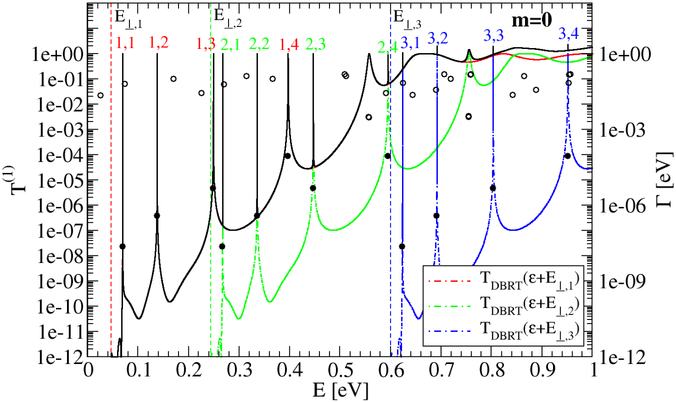
Double-barrier heterostructure along the nanowire





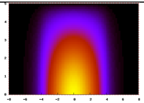
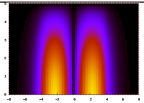
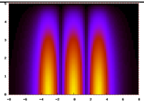
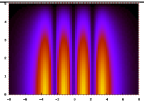
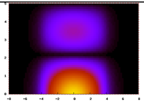
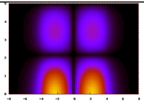
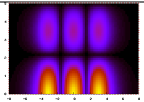
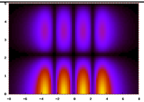
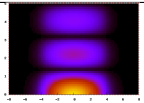
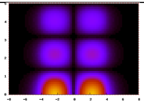
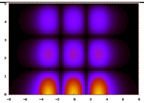
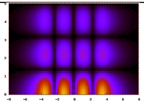
- ▷ sharp peaks in transmission coefficient

Double-barrier heterostructure along the nanowire



- $V(r,z) = V_{DBRT}(z) \Rightarrow T^{(1)}_{nn}(E) = T_{DBRT}(\varepsilon + E^{(m)}_{\perp,n})$
- poles of the $\hat{\hat{S}}$-matrix denoted by symbols
- resonant poles well separated by others

Double-barrier heterostructure along the nanowire: localization probability density

(n,i)	i=1	i=2	i=3	i=4
n=1				
n=2				
n=3				

- the peaks indexed by (n,i)
  - n denotes the incident channel
  - i denotes the resonance between the barriers
- similar pictures for $m \neq 0$, but $\psi(r=0,z)=0$

Conclusions

- solution of 3D Schrödinger equation for cylindrical symmetric open systems
- R-matrix formalism for cylindrical coordinates
- efficient numerical method
- for attractive nonseparable scattering potential $\Rightarrow$ dips in tunneling coefficient due to quasi-bound states of the evanescent channels
- for non-uniform potential along the nanowire $\Rightarrow$ peaks in tunneling coefficient due to quasi-bound-states between barriers
- quantitative description of peaks through the poles of the $\hat{\hat{S}}$-matrix

P.N. Racec, E. R. Racec, H. Neidhardt, WIAS Preprint 1376 (2008)

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- Gheorghe Nenciu (Bucharest)

Thank you for your attention!

General solution

$$\psi(E,r,z) = \begin{cases} \sum_{n=1}^{\infty} \left(a_n(E) e^{ik_{1n}(z+d_z)} + b_n(E) e^{-ik_{1n}(z+d_z)} \right) \phi_n(r), & z \leq -d_z \\ \sum_{n'=1}^{\infty} \left(c_n(E) e^{ik_{2n}(z-d_z)} + d_n(E) e^{-ik_{2n}(z-d_z)} \right) \phi_n(r), & z \geq d_z \end{cases}$$

$$k_{sn}(E) = \sqrt{(2\mu/\hbar^2)(E - E_{\perp n} - V_s)},\ s = 1,2,\ \text{n=1,2,...}$$

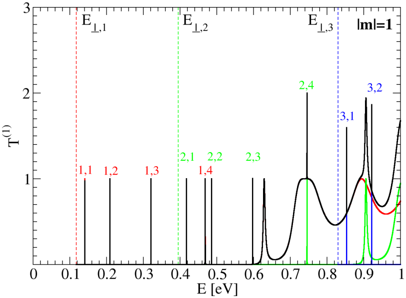
General solution

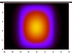
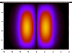
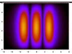
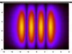
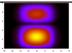
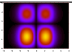
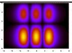
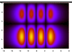
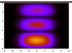
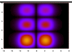
- the outcoming- and ingoing coefficients are related throught wave transmission matrix $\hat{S}$

$$\begin{pmatrix} b_1(E) \\ b_2(E) \\ \vdots \\ c_1(E) \\ c_2(E) \\ \vdots \end{pmatrix} = \hat{S}(E) \begin{pmatrix} a_1(E) \\ a_2(E) \\ \vdots \\ d_1(E) \\ d_2(E) \\ \vdots \end{pmatrix}$$

$(\hat{S}(E))_{sn,s'n'}, \quad s,s' = 1,2, \quad n,n' = 1,2,\ldots \Rightarrow$ infinite dimensional matrix

Double-barrier heterostructure along the nanowire



(n,i)	i=1	i=2	i=3	i=4
n=1				
n=2				
n=3				

▷ similar pictures for $m \neq 0$, but $\psi(r=0,z)=0$