
University of Glasgow
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VIA VERITAS VITA
The Non-equilibrium Green Function Approach to Quantum Transport in Nano Structures
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Short Course
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Outline

1. Introduction
1.1 Background
1.2 What is a Green Function?
1.3 Simple formalism: retarded Green function

2. The Schwinger- Keldysh-Kadanoff-Baym NEGF formalism
2.1 Birds eye view
2.2 Keldysh contours
2.3 Projection to real time domain

3. Computational Procedures
3.1 Equations of motion
3.2 Stationary case
3.3 Projection from open system to finite domain
3.4 Methodology
3.5 Pitfalls

4. Some Applications to Semiconductor Nano-Devices
Appendices
References

Present Collaborators
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Manuel Aldegunde, Raul Valin
University of Swansea, UK

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Appendices

This tutorial approach is under-pinned by background theory in Appendices.

1.**Representations and Pictures**

Schrödinger, Heisenberg, Dirac(Interaction), Density Matrix

2. **Time-dependent Perturbation Theory**

Evolution operator, Time-ordering operator

3. **Perturbation Theory at zero temperature**

The S-matrix, Dyson Equation

4. **Perturbation theory at Finite Temperature**

Complex time domain, ordering in imaginary time, The S-matrix, Dyson Equation

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Appendices contd…

5. **Non-Equilibrium Perturbation Theory**

Choice of NEGF approach, The Problem of non equilibrium,
The Keldysh Time-ordered Green Function
The Keldysh Contour, The Keldysh Kadanoff Baym time contour
The Green Function Zoo, Identities
Time-independent case, G^R and $G^<$,
Dyson equation of Motion on Keldysh Contour
Projection of equations of motion to real time
Langreth Rules
Equations of motion for no ISC stationary limit

6. **Visualisation of flows**
Velocity field, Vortices, vortices in atomistic devices, Trajectories and Experiment

7. **Selected Applications of NEGF to nanodevices**
The variability problem, interface roughness, Random dopant aggregation in source/drain extensions, Combined NEGF DFT studies of silicon SiO2 interfaces

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Appendices contd…

8. **Resonances in transmission**

What to Expect
Previous Studies
NEGF versions

9. **Selected personal references**

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1. Introduction

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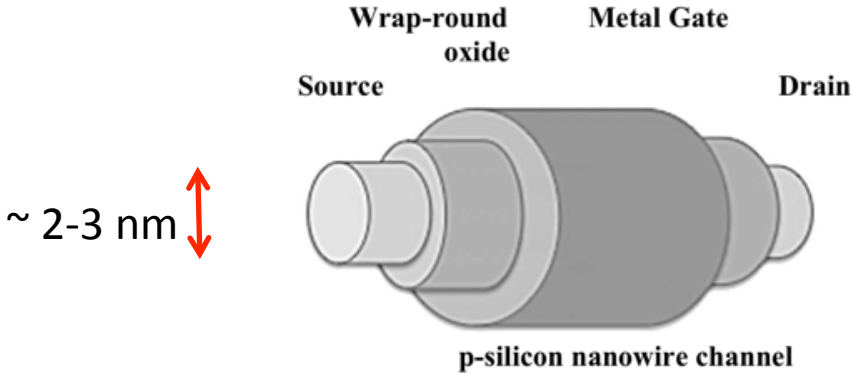
Source and Drain-Heavily doped n+ regions,atomistic effects
Plasmons, Image charge effects, electron correlations…..



P-type Silicon Channel
Laterally confined =>
sub-bands (size quantization)
Residual atomistic impurities
Non-bulk description

Wrap-round oxide
Surface interface roughness
Strong polar optical phonon scattering from surface
modes penetrate channel

Metal Gate

Plasmons
Image charge effects
Further interface issues

Strong, inhomogeneous self-consistent electrostatic potentials
Electrons in channel see bulk and interface phonons…..
Huge computational Problem: lots of many=body physics!

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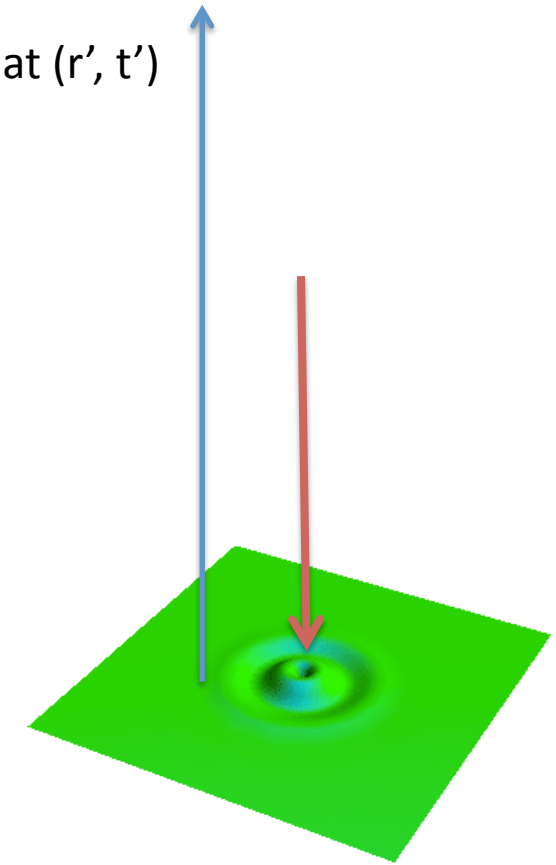
1.2 What is a Green Function?

Response at (r,t) after impulse at (r', t')



Retarded (causal Green Function)

G(r t; r' t')

Response at time t and place r to an impulse
at initial time t' and place r'

Example a drop of water falls into a bath of water

G(r t; r' t') =0 for t<t'

Antecedence Principle

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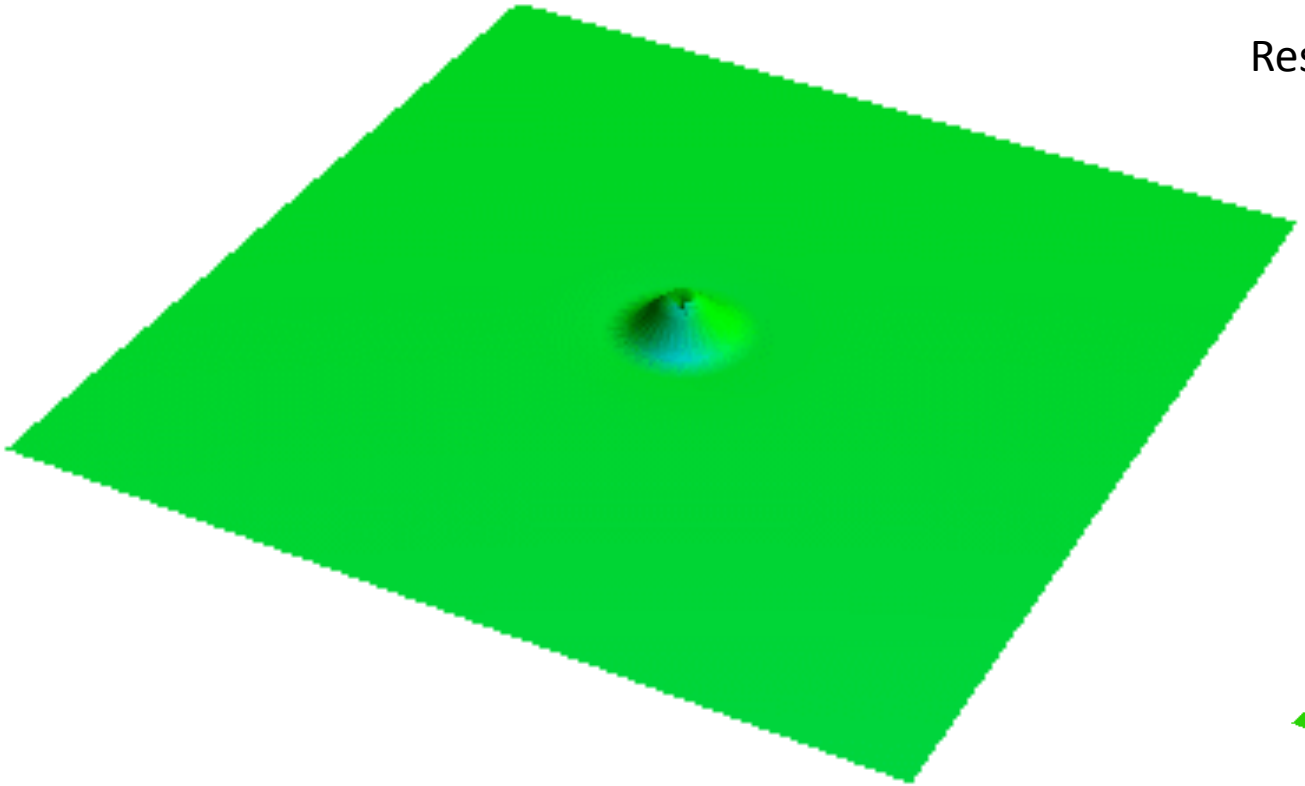
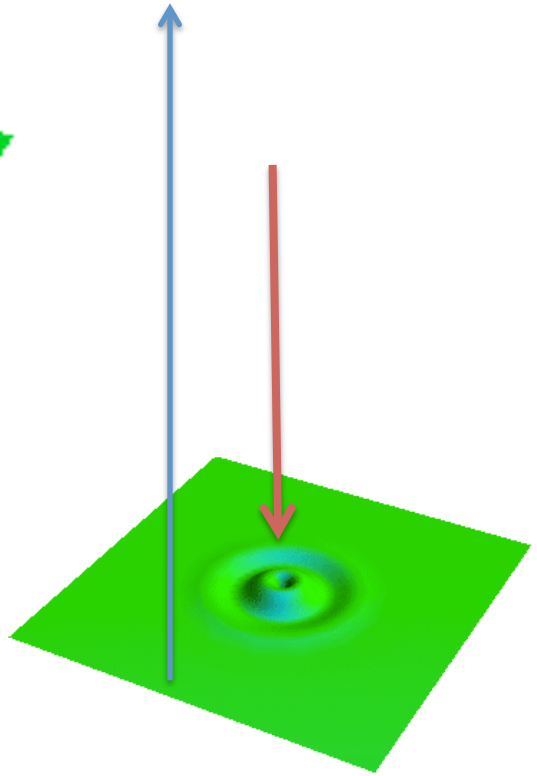
What is a Green Function?

Retarded
Green Function



Response after impulse



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Green function for classical diffusion

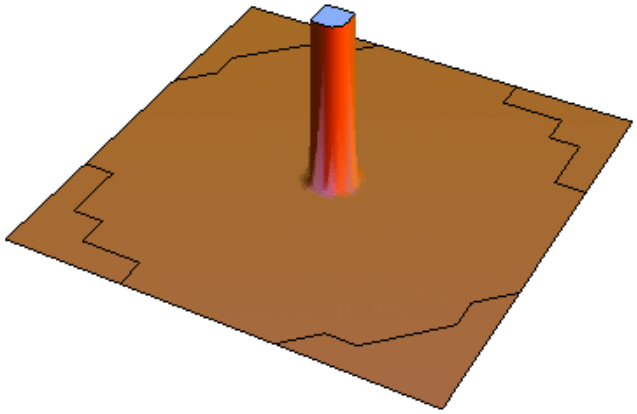
$$\frac{\partial \phi}{\partial t} - D\nabla^2 \phi = 0$$

$$\frac{\partial}{\partial t} g(\mathbf{x},t;\mathbf{x}_0,t_0) - D\nabla^2 g(\mathbf{x},t;\mathbf{x}_0,t_0) = \delta(\mathbf{x}-\mathbf{x}_0)\delta(t-t_0)$$

$$g(\mathbf{x},t,\mathbf{x}_0,t_0) = \frac{1}{(4\pi D(t-t_0))^{3/2}} \exp[-\frac{(\mathbf{x}-\mathbf{x}_0)^2}{4D(t-t_0)}]$$

Inject a tagged particle at $\mathbf{x}_0$, t_0

Probability density that it will be found at **x**, t is given by Green function $g(xt;x_0t_0)$



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Green function for Schrödinger Equation: free particle

Evolution of complex density field in space and time $\psi(\mathbf{x},t) =< \mathbf{x} \mid \psi;t >$

$$i\hbar \frac{\partial \mid \psi;t >}{\partial t} = H_0 \mid \psi;t >$$

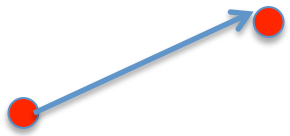
$$H_0 = -\frac{\hbar^2}{2m}\nabla^2$$

$$\frac{\partial \psi(\mathbf{x},t >}{\partial t} - \left(\frac{i\hbar}{2m}\right)\nabla^2\psi(\mathbf{x},t) = 0$$

Effective Diffusion Coefficient (units: Length^2/Time) $D_Q = i\frac{\hbar}{2m}$

Inject a particle at $\mathbf{x}_0,\ t_0$

Probability amplitude that it will be found at $\mathbf{x}_1,\ t_1$ is given by Green function $G_0(\mathbf{x}_1,t_1,\mathbf{x}_0,t_0)$ where



$$\frac{\partial}{\partial t}\ G_0(\mathbf{x},t,\mathbf{x}_0,t_0) - \left(\frac{i\hbar}{2m}\right)\nabla^2 G_0(\mathbf{x},t,\mathbf{x}_0,t_0) = \delta(\mathbf{x}-\mathbf{x}_0)\delta(t-t_0)$$

Impulse response Impulse

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Quantum "Diffusion": Green Function (retarded/causal)

$$G_0(\mathbf{x},t,\mathbf{x}_0,t_0) = \frac{1}{(4\pi\tilde{D}(t-t_0))^{3/2}}\exp[-\frac{(\mathbf{x}-\mathbf{x}_0)^2}{4\tilde{D}(t-t_0)}] \quad \vartheta(t-t_0)$$

$$D_Q = \frac{i\hbar}{2m}$$

Real diffusion in complex time

Serious differences with ordinary diffusion

Quantum equation of motion and time evolution is time-reversible

Form of the diffusion operator depends on kinetic energy operator

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1.3 Simple formalism:Retarded Green Function G^R

Things simplify if we treat stationary systems by Fourier transforming over time
Into energy space.

$$H = H_0 + V$$

$$i\hbar \frac{\partial |\psi;t>}{\partial t} = H|\psi;t>;$$

$$i\hbar \frac{\partial G^R(t,t')}{\partial t} - HG^R(t,t') = \delta(t-t')$$

$$G^R(t,t') = (1/i\hbar)\exp[-iH(t-t')/\hbar]\vartheta(t-t')$$

$$G^R(\mathbf{x},t;\mathbf{x}'t') \equiv <\mathbf{x}|G^R(t,t')|\mathbf{x}'>$$

$$G^R(\mathbf{x},t;\mathbf{x}'t') = 0 \quad for \quad (t-t') < 0$$

$$G^R(E) = \int_{-\infty}^{\infty} dt G^R(t,t')\exp[iE(t-t')/\hbar]\exp[-\eta(t-t')]$$

$$G^R(E) = \int_0^{\infty} dt(\frac{1}{i\hbar})\exp[-iHt]\exp[iE(t/\hbar]\exp[-\eta t]$$

$$G^R(E) = \frac{1}{E+i\eta-H} = (E+i\eta-H)^{-1}$$

$$limit \quad \eta \to 0^+$$

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Existence of a Self-Energy

Consider exact retarded Green Function

$$G^R = \{E + i\eta - H_0 - V\}^{-1}$$

$$G_0^R = \{E + i\eta - H_0\}^{-1}$$

$$G^R = G_0^R + G_0^R V G^R$$

V describes phase-breaking scattering

"Average" over scatterer degrees of freedom <……..>

$$< G^R >= G_0^R + G_0^R < VG^R >$$

A self-energy exists IF the second term factorizes as:

$$< VG^R >= \Sigma^R < G^R >$$

$$< G^R >= \{E + i\eta - H_0 - \Sigma^R\}^{-1}$$

Phase-breaking processes give rise to non-hermitian self-energy

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Advanced and Retarded Green Functions

$$G^R = \{E + i\eta - H_0 - \Sigma^R\}^{-1}; \qquad G^A = \{E - i\eta - H_0 - \Sigma^A\}^{-1}$$

$$G^R = \{G^A\}^+ \qquad (hermitian\ conjugate) \qquad \Sigma^R = \{\Sigma^A\}^+$$

$$\Delta^R = \frac{\Sigma^R + \Sigma^A}{2}; \qquad \Gamma^R = -\frac{\Sigma^R - \Sigma^A}{2i}$$

From causality-see later- the eigenvalues of Γ^R must be positive.

The operator Δ^R re-normalises the electron spectrum via level shifts

The operator Γ^R describes the finite lifetime of the electronic states via level broadening.

$$G^R = \frac{1}{E + (i\eta + i\Gamma^R) - (H_0 - \Delta^R)}$$

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The Spectral Density Function

The spectral density operator is defined by:

$$A = -\frac{1}{2\pi i}\{G^R - G^A\}$$

In the "free" case:

$$A \to A_0 = -\frac{1}{2\pi i}\{\{E + i\eta - H_0\}^{-1} - \{E - i\eta - H_0\}^{-1}\}$$

$$= \frac{1}{\pi}\frac{\eta}{(E - H_0)^2 + \eta^2} \to \delta(E - H_0)$$

In the "interacting" case

$$A = -\frac{1}{2\pi i} < \{\{E + i\eta - H_0 - V\}^{-1} - \{E - i\eta - H_0 - V\}^{-1}\} >$$

$$= < \delta(E - H) >= -\frac{1}{2\pi i}\{\{E + i\eta - H_0 - \Sigma^R\}^{-1} - \{E - i\eta - H_0 - \Sigma^A\}^{-1}\}$$

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Density of States

The density of states

$$\rho(E) = \Omega^{-1}\ Trace[A] = \Omega^{-1}\ Trace < \delta(E - H) >$$

Example: free electrons in 1D – use momentum representation

$$< p \mid p' >= \delta(p - p') \ \ (orthornormality) \qquad \int_{-\infty}^{\infty} \mid p >< p \mid = 1 \ (completeness)$$

$$H \rightarrow \frac{\hat{p}^2}{2m} \rightarrow diagonal \qquad A(p, p'; E) = \delta(E - \frac{p^2}{2m})\ \delta(p - p')$$

$$\rho(E) = \Omega^{-1} \int_{-\infty}^{\infty} dp'' < p'' \mid \delta(E - \frac{p''^2}{2m})\ \delta(p'' - p') \sim 1/\sqrt{E}$$

Example:

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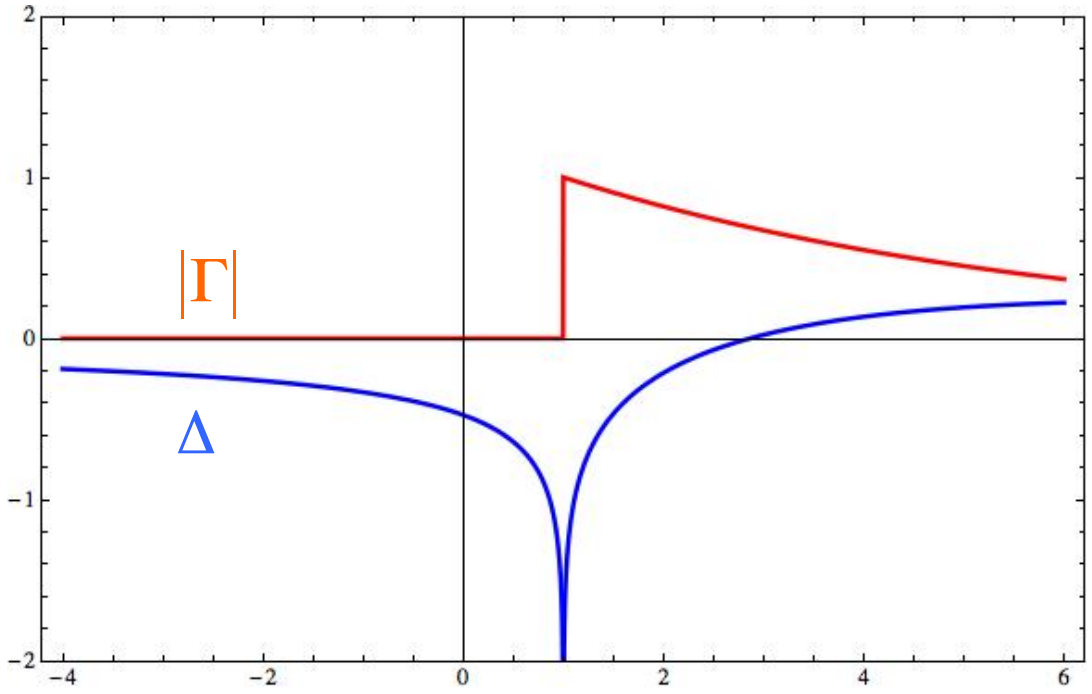
Electron – Phonon scattering: simple 1D model

Im self-energy

$$\Gamma = \alpha \, \mathrm{Exp}\left[-\frac{(\varepsilon - \varepsilon_0)}{\gamma}\right]\Theta[\varepsilon - \varepsilon_0]$$

Construct
Re self-energy
from Dispersion Relation



Spectral Function (strong coupling) in momentum representation as E[k] varied
From below optical phonon threshold to well above it.

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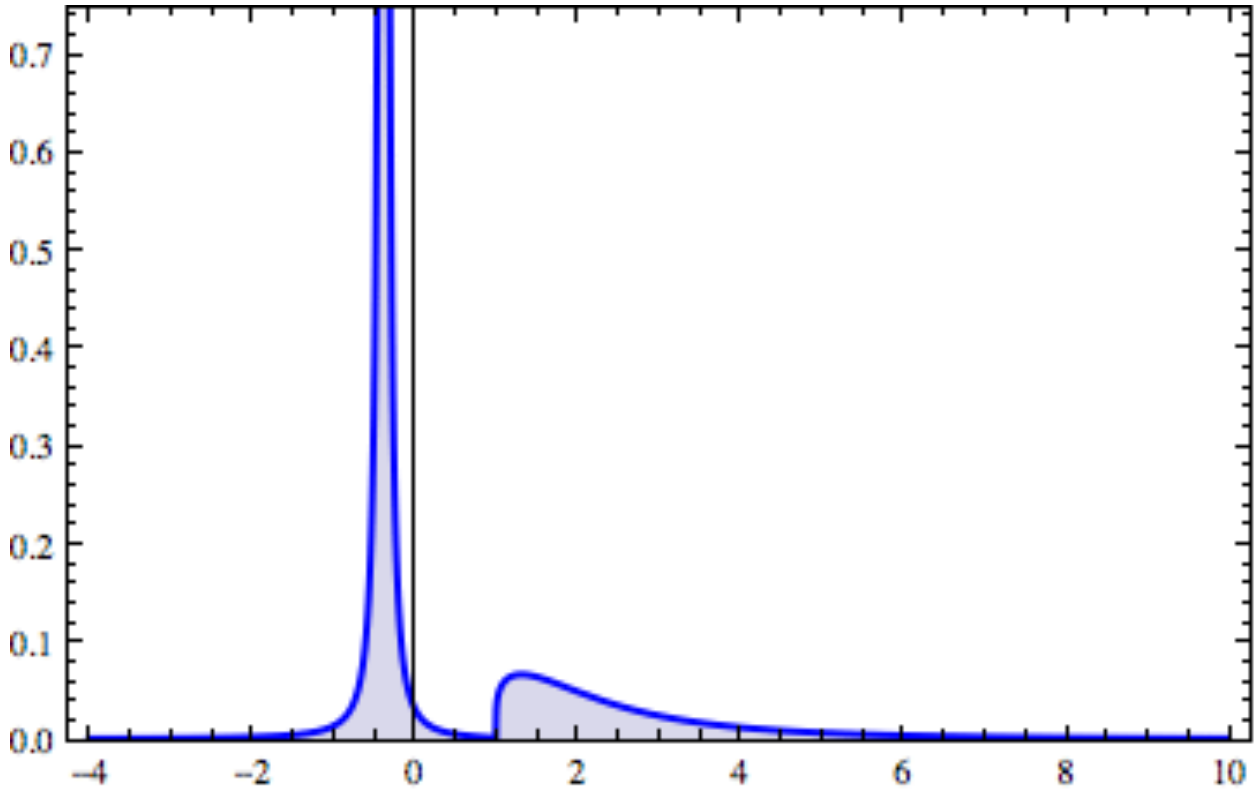
$$A(E;\ E[k]) = \frac{1}{\pi}\frac{\eta + \Gamma(E)}{(E - E[k] - \Delta(E))^2 + (\eta + \Gamma(E))^2} \qquad \eta \sim 0.1\ to\ show\ up\ \delta - fn$$



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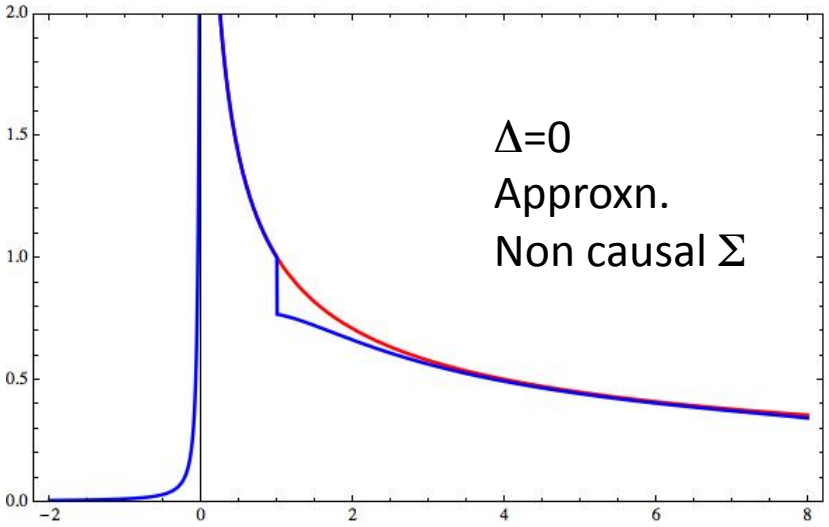
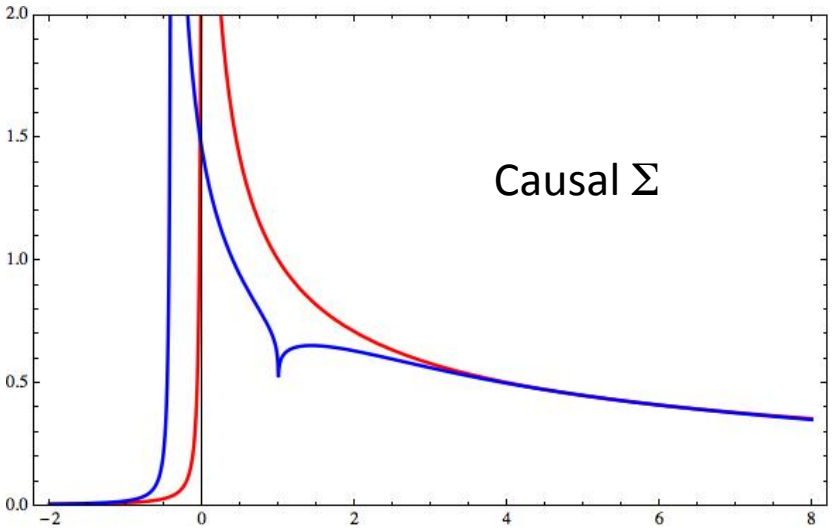
Comparison of 1D-DOS for Δ exact and Δ=0





Energy/$h\omega_0$

DOS unperturbed

DOS perturbed

Big differences

Up to 2 X Optical Phonon Energy

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2. The Schwinger-Keldysh-Kadanoff-Baym Formalism

J. Schwinger (1961)
L.V. Keldysh, (1964)
L.P. Kadanoff and G. Baym (1962).

Good Reviews

J. Rammer and H. Smith, Quantum field-theoretical methods in the transport theory of metals, Reviews of Modern Physics, 58, 323 (1986).

H. Haug and A. P. Jauho, Quantum kinetics in transport and optics of semiconductors (Springer, Heidelberg, 1996).

K. Balzer and M. Bonitz, Nonequilibrium Green's Functions Approach to Inhomogeneous Systems, Lecture Notes in Physics 867 (Springer, 2013).

S. Datta, Electronic transport in mesoscopic systems (Cambridge University Press, Cambridge, 1995): introductory

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Hamiltonian

Many-body Hamiltonian operator

$$H = H_0 + V + U$$

Non-interacting	Interactions	External perturbations
carriers	carrier-carrier	applied fields
phonons	carrier-impurity	thermal gradients
lattice structure	carrier-phonon	
…….		
device architecture	……..	

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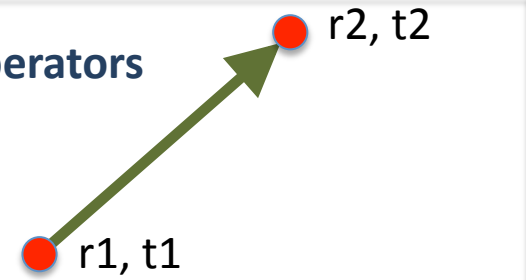
The One-Particle Green Function

Probability amplitude that a particle at r_1,t_1 is propagated to r_2, t_2 in space-time.

$$G(\boldsymbol{r}_1, t_1; \boldsymbol{r}_2, t_2)$$



Introduce electron annihilation and creation field operators

$\Psi^*(\mathbf{x}_1)$ *creates an electron at* $\mathbf{x}_1$

$\Psi(\mathbf{x}_2)$ *annihilates an electron at* $\mathbf{x}_2$

Anti – commutation relations

$$\Psi^*(\mathbf{x}_1)\Psi(\mathbf{x}_2)+\Psi(\mathbf{x}_2)\Psi^*(\mathbf{x}_1)=\{\Psi^*(\mathbf{x}_1),\Psi(\mathbf{x}_2)\}=\delta(\mathbf{x}_1-\mathbf{x}_2)$$

Example Hamiltonian:

$$G(\mathbf{x}_1,t_1;\mathbf{x}_2,t_2)\sim <\mathbf{T}\ \Psi^*_H(\mathbf{x}_1,t_1)\Psi_H(\mathbf{x}_2,t_2)>$$

$$H=\int d\mathbf{x}\{\Psi^*(\mathbf{x}\ )\{-\frac{\hbar^2}{2m}\nabla^2+V(\mathbf{x})+U(\mathbf{x})\}\Psi(\mathbf{x}\ )\}+$$

$$+\frac{1}{2}\int d\mathbf{x}_1\int d\mathbf{x}_2\{\Psi^*(\mathbf{x}_1)\Psi^*(\mathbf{x}_2)\ V_{Coulomb}(\mathbf{x}_1-\mathbf{x}_2)\Psi(\mathbf{x}_2)\Psi(\mathbf{x}_1)$$

What is the average?

<....>

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2.1 Bird's Eye View 1

1. The Schwinger-Keldysh-Kadanoff-Baym Non-Equilibrium Green Function formalism

Open many-body systems driven far out of equilibrium by applied forces.
It is technically difficult but only the essence is necessary to use it.

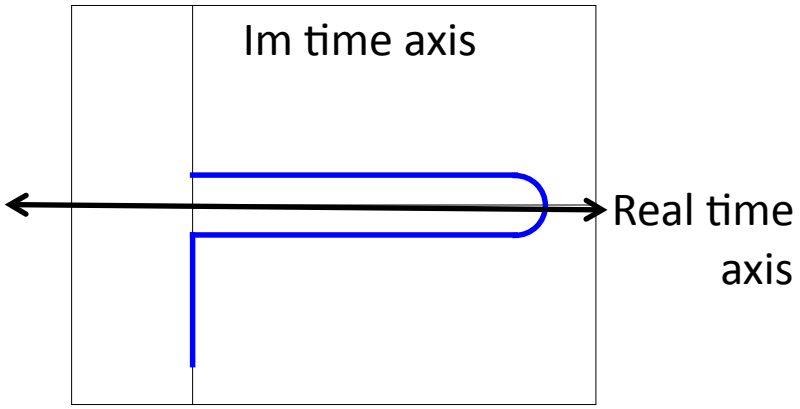
Miracle! S-K-K-B show that a non-equilibrium equivalent of zero temperature and finite temperature quantum statistical mechanics can be established with exactly the same structure in terms of double-time Green functions and self-energies (same Feynman diagrams). In the case of one-particle Green functions we can establish a Dyson equation in terms of a self-energy that contains all the interaction effects.

$$G(\mathbf{x},\tau;\mathbf{x}',\tau') = G_0(\mathbf{x},\tau;\mathbf{x}',\tau') + \iint dx''dx'''dt''dt''' G_0(\mathbf{x},\tau;\mathbf{x}'',\tau'')\Sigma(\mathbf{x}'',\tau'';\mathbf{x}''',\tau''')G(\mathbf{x}''',\tau''';\mathbf{x}',\tau')$$

$$or: \qquad G = G_0 + G_0\Sigma G$$

2. **The price is high**!

The variables τ, τ' etc are defined on a contour in **the complex time plane.**



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Bird's Eye View 2

3. Continuation to the **real time domain** is difficult and leads to a zoo of Green functions.

4. For **stationary systems** we only need two Green functions from the zoo:

They are: $G^R(E)$ the retarded Green function,and $G^<(E)$ the "less than" Green function.

Quantum states

Density of States

Local Density of States

Particle density and Current density

Generalised Wigner distribution

$$n(\mathbf{x},E) = iG^<(\mathbf{x},\mathbf{x};E)$$

$$\mathbf{J}(\mathbf{x},E) = -i\frac{e\hbar}{2m}\left(\nabla - \nabla'\right)G^<(\mathbf{x},\mathbf{x}';E)\,|_{\mathbf{x}=\mathbf{x}'}$$

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Bird's Eye View 3

5. We only need two equations of motion (non-linear integro-differential equations)

Plus coupling self-consistently to Maxwell's equations.

$$\left\{E - H_0 - U - \Sigma^R\right\} G^R = \mathbf{1}$$

$$G^<(E) = G^R \Sigma^< G^A$$

Generally GR is coupled to $G^<$ via the self-energy

6. **Snag: huge open many-body system**!

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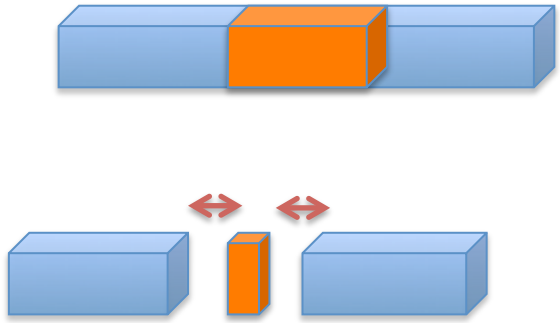
Bird's Eye View 4

7. Project the full system onto a finite "device" domain. Another Miracle!

Allow for coupling to environment at the device boundaries
by non-hermitian terms in the Hamiltonian: contact self-energies.
Just add to total self-energy:

$$\Sigma \rightarrow \Sigma_{scattering} + \Sigma_{contacts}$$



8. **For Ballistic transport**: ignore $\Sigma_{scattering}$

U(**x**,t) is just self-consistent electrostatic potential resulting from device architecture and the non-equilibrium flow.

Bird's Eye View 5

9. **Include atomistic charges non-perturbatively to represent impurity scattering**
since for less than ~1000 impurities in the device there is no self-averaging, the Kohn-Luttinger ansatz fails (Barker(2007)and the self-energy is not valid!

incorporate into H_0

10. Include **surface roughness scattering non-perturbatively** by varying interface profile.

incorporate into H_0

11. **For dissipative transport**: evaluate self-energy $\Sigma_{scattering}$
for scattering (elastic and inelastic)

This is the case for small nano-devices where if confinement ~ few nm
the density of states becomes quasi-1D (in sub-bands) and electron-phonon interactions are enhanced. SNAGS: possible non-diagonality, complicated dependence on all the GFs.

$$\Sigma_{scattering} = \Sigma_{scattering}[G^{<}, G^{R}]$$

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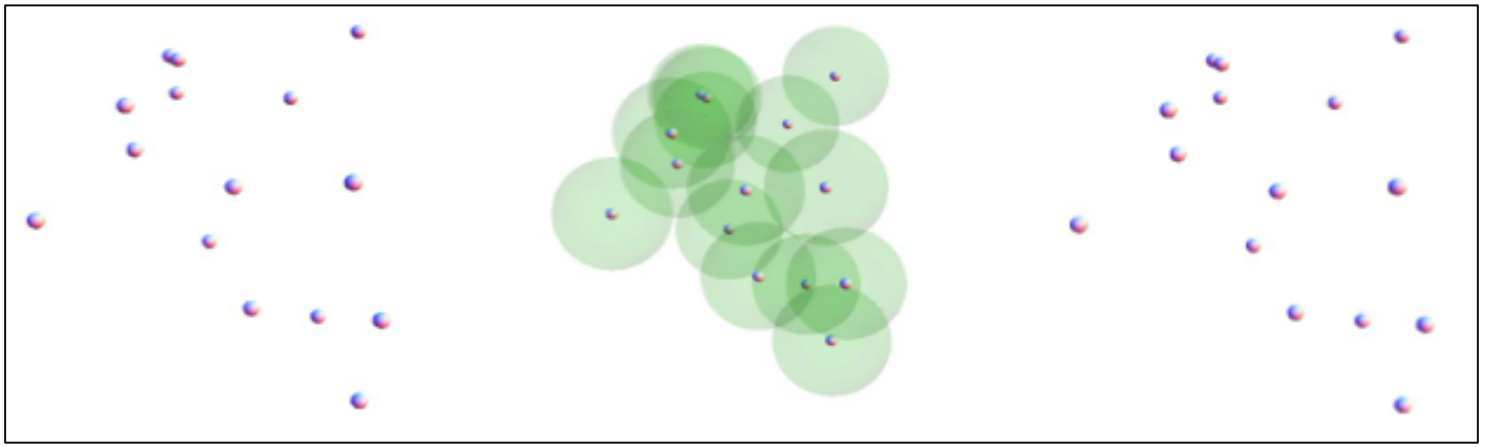
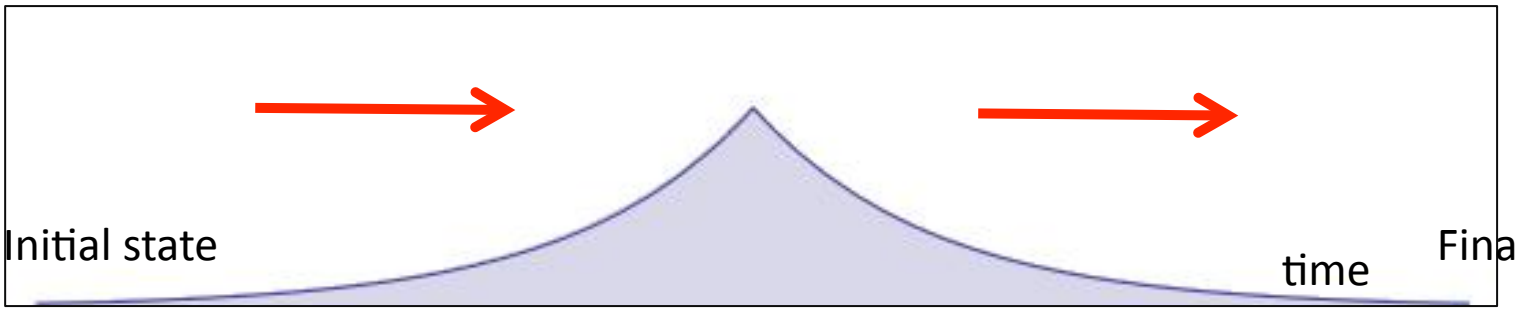
Adiabatic Switch-on and off of Interactions



$$H_{int}(t) = \exp[-\lambda|t|]\, H_{int}(0) \; ; \qquad \lambda \to 0^{+}$$



Usual Perturbation Theory requires initial and final states to differ only in phase.
How do we eliminate reference to the state at infinity?

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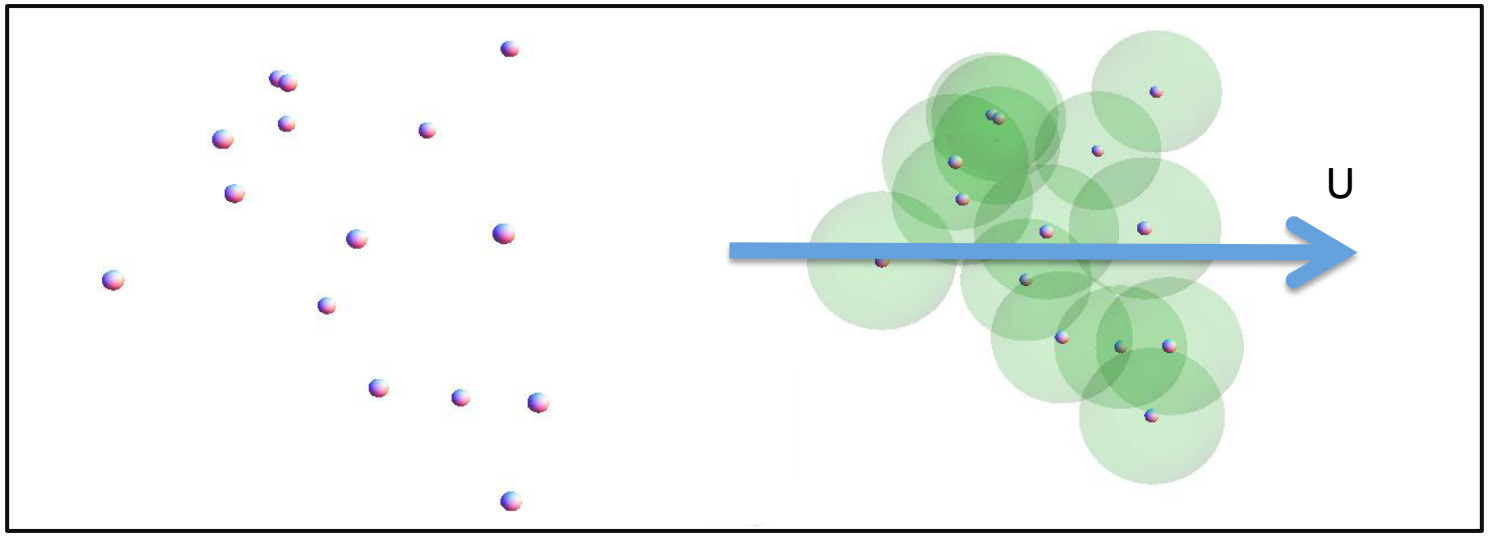
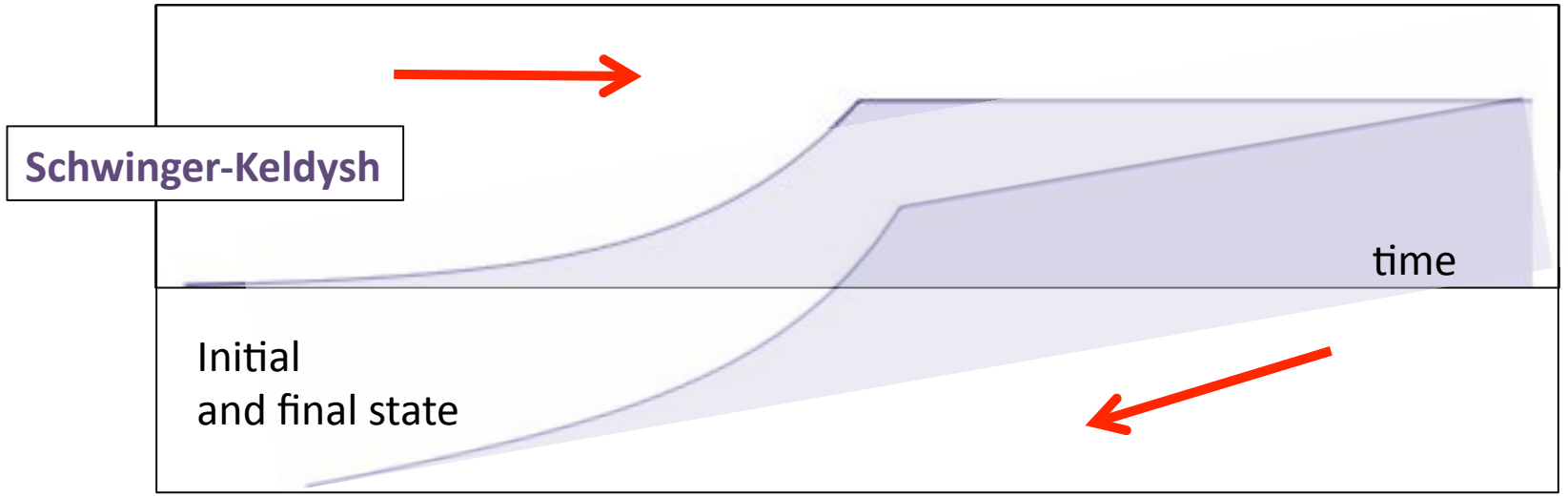
Adiabatic Switch-on of Interactions



$H_{int}(t) = \exp[-\lambda|t|]\, H_{int}(0)$ $t<t0$; $\lambda \to 0^{+}$; $Hint(0)+U(t)$ $t>t0$



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The Keldysh time-ordered Green Function

$$G(\mathbf{x},\tau;\mathbf{x}',\tau') = -i < \mathbf{T}_K \Psi(x,\tau)\Psi^*(x',\tau') >= Tr[\rho(H_0+V)\mathbf{T}_K \Psi_H(\mathbf{x},\tau)\Psi^*{}_H(\mathbf{x}',\tau')]A($$

$$H = H_0 + V$$

Heisenberg representation : operators evolve under full Hamiltonian $(H+U)$

$$A_H(t) = U^+(t,t_0)AU(t,t_0)$$

$\mathbf{T}_K$: Keldysh contour time ordering, put later Keldysh times τ,τ' to the left.

(use, fermion rules $\times(-1)$ per interchange),

$$\rho(H) = exp[-\beta(H-\mu N)]/Z$$

This Green function has the same perturbation theoretic structure as zero temperature or finite temperature Theory. Use **Interaction picture**.
In particular, G satisfies a Dyson equation.

Evolution operator-integral equation :

Why Time-ordered?

$$U(t,t_0) = \mathbf{1} - (i/\hbar)\int_{t_0}^{t} dt' H_H(t',t_0)U(t',t_0)$$

Iterating gives

$$U(t,t_0) = \mathbf{1} + \sum_{p=1}^{\infty} (-i/\hbar)^p \int_{t_0}^{t} dt_1 \int_{t_0}^{t_1} dt_2 \ldots \int_{t_0}^{t_{p-1}} dt_p H_H(t_1,t_0)\times$$

$$\times H_H(t_2,t_0)\times \ldots H_H(t_p,t_0)$$

using time ordering operator $\mathbf{T}$ this becomes

$$U(t,t_0) = \mathbf{1} +$$

$$+\mathbf{T}\sum_{p=1}^{\infty} \frac{(-i/\hbar)^p}{p!} \int_{t_0}^{t} dt_1 \int_{t_0}^{t} dt_2 \ldots \int_{t_0}^{t} dt_p H_H(t_1,t_0)H_H(t_2,t_0)\times \ldots H_H(t_p,t_0)$$

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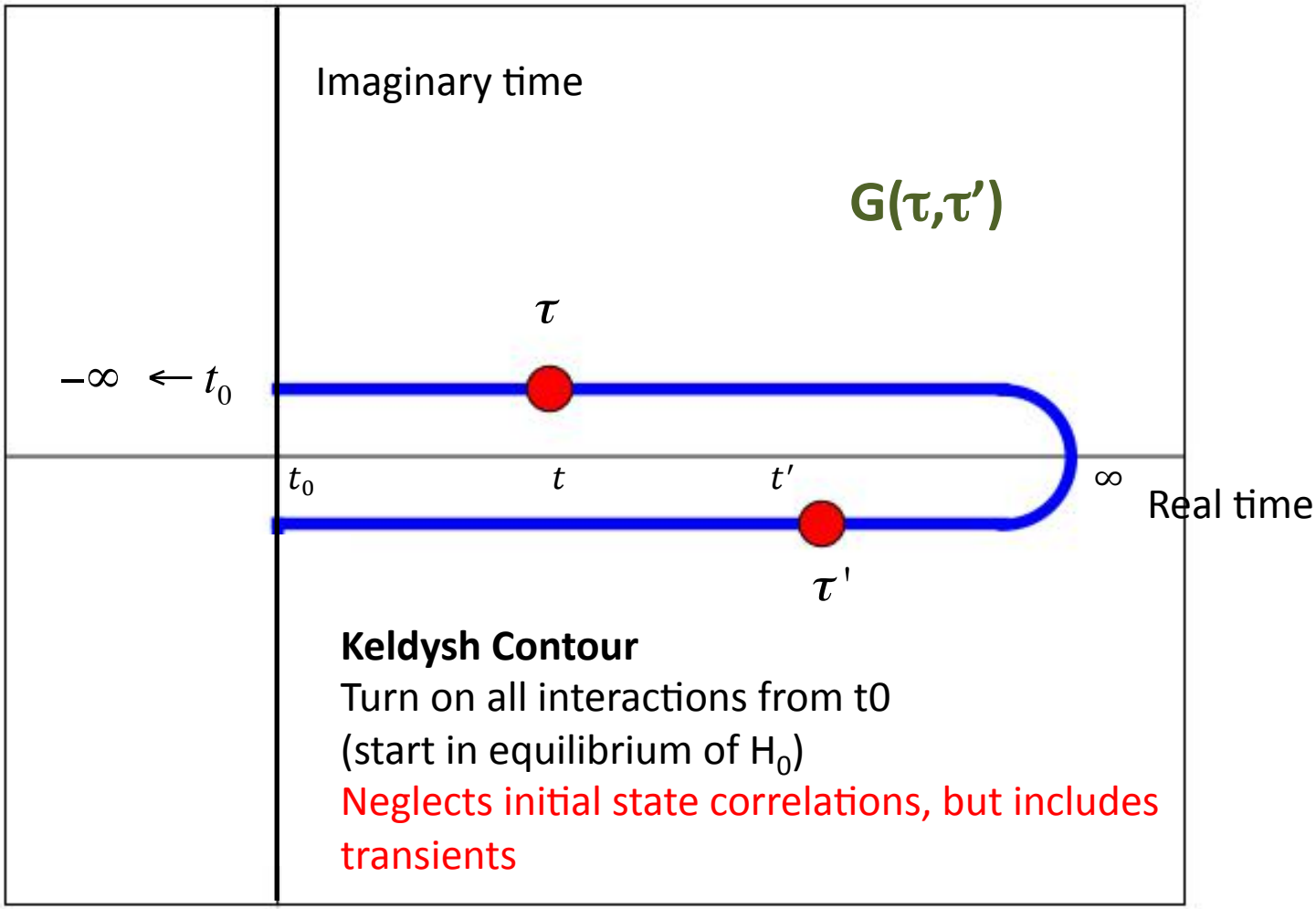
The Green Function defined on the Keldysh contour



Keldysh Contour

Turn on all interactions from t0

(start in equilibrium of H_0)

Neglects initial state correlations, but includes transients

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The Green Function Zoo: distinguished by ordering on the Keldysh contour

$$G(\mathbf{x},\tau;\mathbf{x}',\tau') \equiv <\mathbf{x}\,|\,G(\tau,\tau')\,|\,\mathbf{x}'>$$

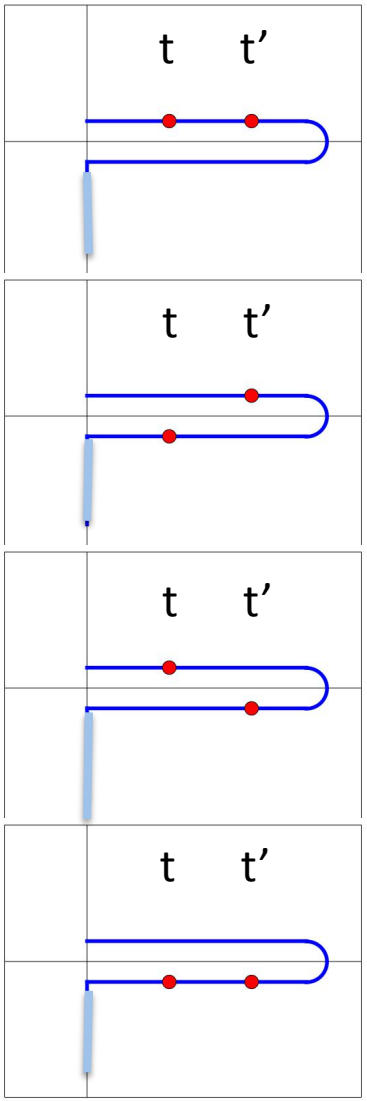
$$= -i\hbar <T_K \psi_h(\mathbf{x},\tau)\psi_h^+(\mathbf{x}',\tau')$$

$$= G_T(\mathbf{x},\tau;\mathbf{x}',\tau') \quad t,t' \text{ on upper contour}$$

$$= G^>(\mathbf{x},\tau;\mathbf{x}',\tau') \quad t \text{ on lower contour},\ t' \text{ on upper contour}$$

$$= G^<(\mathbf{x},\tau;\mathbf{x}',\tau') \quad t \text{ on upper contour},\ t' \text{ on lower contour}$$

$$= G_{T^*}(\mathbf{x},\tau;\mathbf{x}',\tau') \quad t,t' \text{ on lower contour}$$



G_T

$G^>$

$G^<$

G_{T^*}

< Less Than; > Greater Than; T time-ordered, T* anti-time ordered

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Not all Non-Equilibrium Green Functions are independent

We choose initially

$G_T(\mathbf{x},\tau;\mathbf{x}',\tau')$ t, t' *on upper contour*

$G^{>}(\mathbf{x},\tau;\mathbf{x}',\tau')$ t *on lower contour*, t' *on upper contour*

$G^{<}(\mathbf{x},\tau;\mathbf{x}',\tau')$ t *on upper contour*, t' *on lower contour*

then by observing the inter-relationships

Retarded	$G^R = G_T - G^<$
Advanced	$G^A = G_T - G^>$
Lesser Than	$G^<$

Only 3 independent Green functions typical choice:

$G^<$ statistics initial state

G^R, G^A dynamics

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Identities

$$G^R = G_T - G^< = G^> - G_{T*}$$

Retarded Green Function

$$G^R(\mathbf{x},t;\mathbf{x}',t') = -i\hbar\vartheta(t-t') < \{\psi(\mathbf{x},t),\psi^*(\mathbf{x}',t')\} >$$

$$G^A = G_T - G^> = G^< - G_{T*}$$

Advanced Green Function

$$G^A(\mathbf{x},t;\mathbf{x}',t') = i\hbar\vartheta(t'-t) < \{\psi(\mathbf{x},t),\psi^*(\mathbf{x}',t')\} >$$

Spectral Function

$$A = G^R - G^A = G^> - G^<$$

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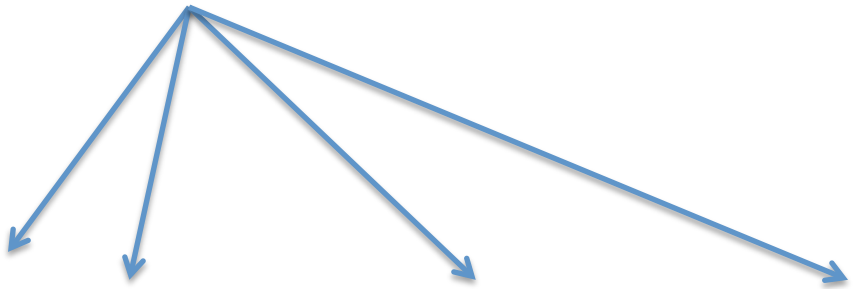
3: Computational Procedure

Start from the Dyson equation on Keldysh contour

$$G = G_0 + G_0 \Sigma G$$

$$G(\mathbf{x}\tau;\mathbf{x}'\tau' = G_0(\mathbf{x}\tau;\mathbf{x}'\tau') +$$



$$\int dx''dx''' \int_K d\tau'' \int_K d\tau''' G_0(\mathbf{x}\tau,\mathbf{x}''\tau'')\Sigma(\mathbf{x}''\tau'',\mathbf{x}'''\tau''')G(\mathbf{x}'''\tau''';\mathbf{x}'\tau')$$

Transform to Real Times: complicated projection (see Appendices)

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3.1:Equations of Motion

Project the Dyson equation from Keldysh contour to real time :
Keep U explicitly as a perturbation here. **Integrals over time and space implicit here.**

$$G = G_0 + G_0(U + \Sigma)G$$

Dyson equation on Keldysh contour

$$G^R = G_0^R + G_0^R U G^R + G_0^R \Sigma^R G^R = \{G_0^{R\ -1} - U - \Sigma^R\}^{-1}$$

First Keldysh equation

$$G^< = G_0^< + G_0^R U G^< + G_0^< U G^A + G_0^R \Sigma^R G^< + G_0^R \Sigma^< G^A + G_0^< \Sigma^A G^A$$

$$G^< = \{1 + G^R(U + \Sigma^R)\} G_0^< \{1 + (U + \Sigma^A)G^A\} + G^R \Sigma^< G^A$$

Vanishes in steady state, no ISCs

Second Keldysh equation

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3.2: Stationary case

The stationary case is determined by transforming to the time variables T_1= (t-t'); setting T_2=(t+t')/2 and setting time derivatives in d/dT_2 to zero. Finally introduce energy-dependent NEGF by Fourier transforming over T_1.

$$G^<(\mathbf{x},\mathbf{x}';E) = \lim_{T_2 \to 0} \int_{-\infty}^{\infty} dT_1 \exp(iET_1/\hbar)\, G^<(\mathbf{x},\mathbf{x}';T_1,T_2)$$

$$G^R = \{G_0^{R\ -1} - U - \Sigma^R\}^{-1}$$

$$G_0^{R\ -1} = \{E + i\eta - H_0\}$$

$$G^< = G^R \Sigma^< G^A$$

Huge simplification
IF self-energies
Are diagonal

$$\{E + \hbar^2 \frac{\nabla^2}{2m} - U(\mathbf{x})\} G^R(\mathbf{x},\mathbf{x}';E) = \delta(\mathbf{x}-\mathbf{x}') + \int d\mathbf{x}''\ \Sigma^R(\mathbf{x},\mathbf{x}'';E) G^R(\mathbf{x}'',\mathbf{x}';E)$$

$$\{E + \hbar^2 \frac{\nabla^2}{2m} - U(\mathbf{x})\} G^<(\mathbf{x},\mathbf{x}';E) = \int d\mathbf{x}''\ \Sigma^<(\mathbf{x},\mathbf{x}'';E) G^A(\mathbf{x}'',\mathbf{x}';E) + \int d\mathbf{x}''\ \Sigma^R(\mathbf{x},\mathbf{x}'';E) G^<(\mathbf{x}'',\mathbf{x}';E)$$

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G^R and $G^<$

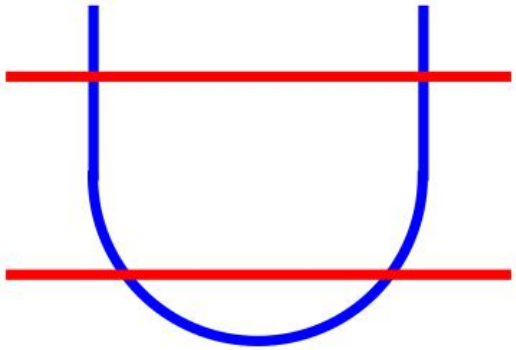
The Retarded Green Function G^R
Describes the Electronic States
(DYNAMICS)

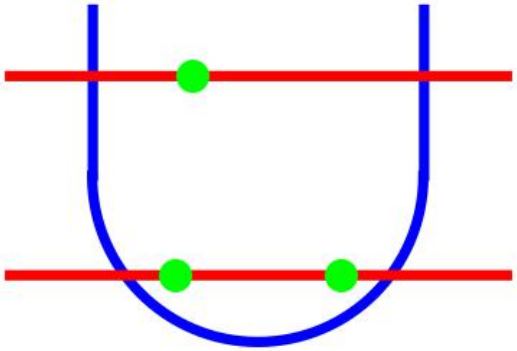
Confinement-sub bands et
Applied field shifts
Resonances
Bound states
Lifetime of states

$$\{E - H_0 - e\varphi - \Sigma^R\}G^R = 1$$

The Lesser than Green Function $G^<$
Describes the Occupancy of States
(STATISTICS)

$$\mathbf{G}^< = G^R \Sigma^< G^A$$





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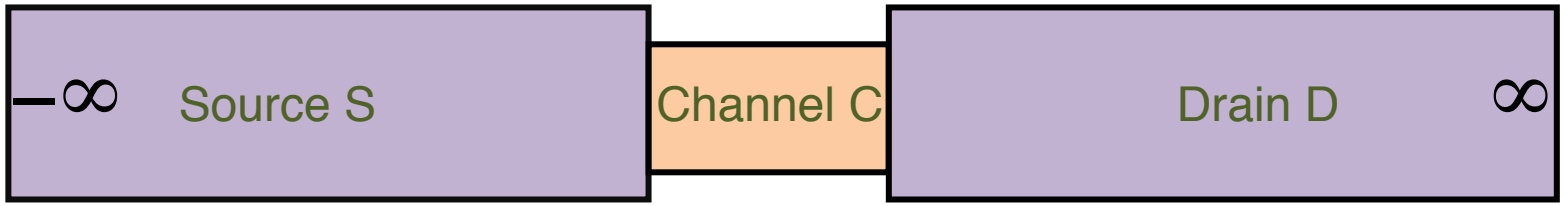
3.3:Projection from Open System to Finite Domain



$$G_R^{-1} \bullet G_R = \mathbf{1}$$

$$\begin{bmatrix} (E+i\eta)1-H_S & \Lambda_{SC} & 0 \\ \Lambda_{CS} & (E+i\eta)1-H_C & \Lambda_{CD} \\ 0 & \Lambda_{DC} & (E+i\eta)1-H_D \end{bmatrix} \begin{bmatrix} G_{SS} & G_{SC} & G_{SD} \\ G_{CS} & G_{CC} & G_{CD} \\ G_{DS} & G_{DC} & G_{DD} \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}$$

Block Matrix Form

$$\{(E+i\eta)1-H_S\}G_{SC}+\Lambda_{SC}G_{CC}=0 \qquad (1st\ row->2nd\ column)$$

$$solve\ formally\ for\ \ G_{SC}=-\{(E+i\eta)1-H_S\}^{-1}\Lambda_{SC}G_{CC}$$

$$similarly,\ \ solve\ formally\ for\ G_{DC}=-\{(E+i\eta)1-H_D\}^{-1}\Lambda_{DC}G_{CC}$$

$$substitute\ \ in$$

$$\Lambda_{CS}G_{SC}+\{(E+i\eta)1-H_C\}G_{CC}+\Lambda_{CD}G_{DC}=1\ (2nd\ row->2nd\ column)$$

$$gives\ closed\ equation\ for\ G_{CC}$$

C. Caroli, R. Combescot, D. Lederer, P. Nozieres and D. Saint-James, (1971).

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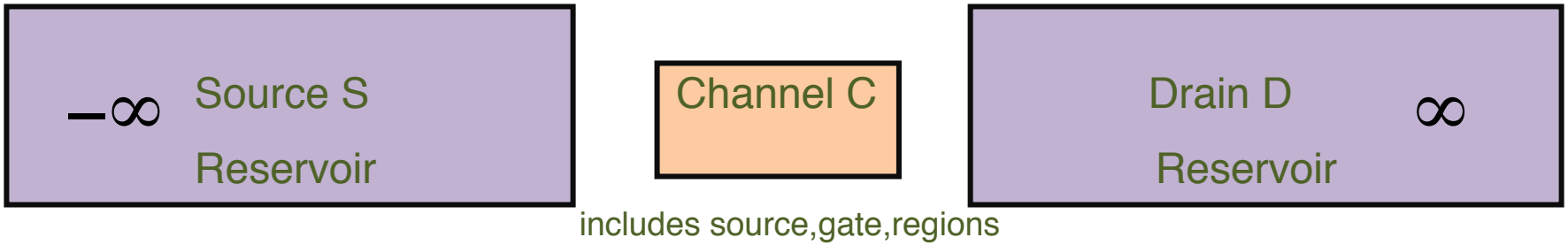
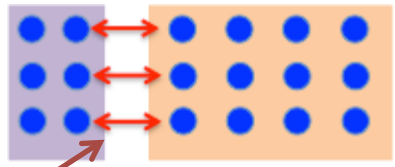
Projection from Open System to Finite System



$$G_{CC} = [(E + i\eta) - H_C - \Sigma_C]^{-1}$$ NEGF for Finite System

$$\Sigma_C = \Lambda_{CS} G^0{}_{SS} \Lambda_{SC} + \Lambda_{CD} G_{DD}{}^0 \Lambda_{DC} = \Sigma_{CS} + \Sigma_{CD}$$

$$G^0{}_{SS} = [(E + i\eta) - H_S]^{-1};\ G^0{}_{DD} = [(E + i\eta) - H_D]^{-1}$$



Coupling to reservoirs

Executed by

Contact self-energy

Non-zero at interface

Contact Green Functions

Details depend on model

Numerics: use discrete matrices for G_{CC}, H_C, Σ_C

NOTE:
Channel refers to the Simulation Domain: it usually includes the true source and drain regions

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Form of Green Function G^R

$$G_R^{-1} \sim \{E + i\eta + \frac{\hbar^2}{2m}\frac{d^2}{dx^2} - U(x) - \Sigma_R(x,x)\};\ t = \frac{\hbar^2}{2m\delta x^2}$$

$$\sim \begin{bmatrix} E+U+\Sigma+2t & -t & 0 & 0 \\ -t & E+U+\Sigma+2t & -t & 0 \\ 0 & -t & E+U+\Sigma+2t & -t \\ 0 & 0 & -t & E+U+\Sigma+2t \end{bmatrix}$$

Simple tri-diagonal matrix **provided self-energy is diagonal**

Straightforward to handle.

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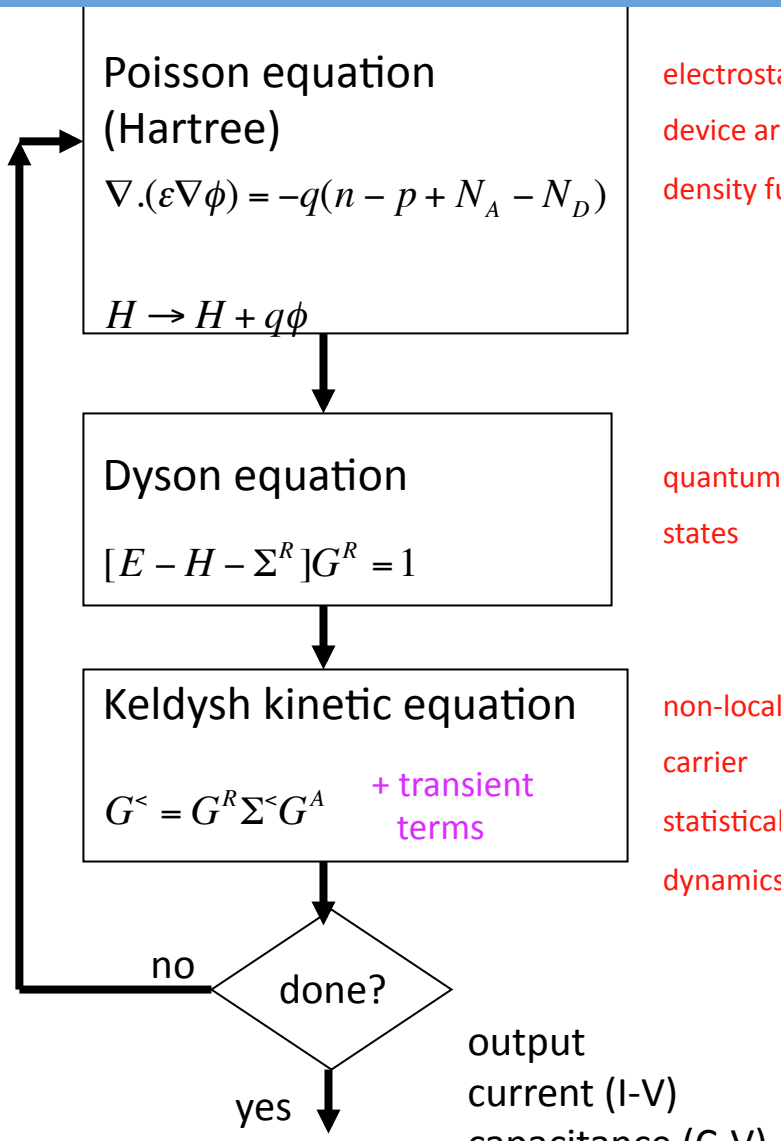
3.4:Methodology-Device modelling with NEGF Green functions



electrostatics

device architecture

density functional

quantum

states

non-local

carrier

statistical

dynamics

Schwinger Keldysh Kadanoff Baym kinetic equations

$$(\frac{\partial}{\partial t} + \frac{\partial}{\partial t'} + \frac{i}{\hbar}[H(\mathbf{x}) - H(\mathbf{x}')])G^<(\mathbf{x},t;\mathbf{x}',t')$$
$$= \frac{i}{\hbar}\int d^3x''dt''\{$$
$$\Sigma^R(\mathbf{x},t;\mathbf{x}'',t'')G^<(\mathbf{x}'',t'';\mathbf{x}',t') - G^<(\mathbf{x},t;\mathbf{x}'',t'')\Sigma^A(\mathbf{x}'',t'';\mathbf{x}',t')\}$$
$$+\frac{i}{\hbar}\int d^3x''dt''\{$$
$$\Sigma^<(\mathbf{x},t;\mathbf{x}'',t'')G^A(\mathbf{x}'',t'';\mathbf{x}',t') - G^R(\mathbf{x},t;\mathbf{x}'',t'')\Sigma^<(\mathbf{x}'',t'';\mathbf{x}',t')\}$$

Boltzmann transport equation

$$(\frac{\partial}{\partial t} + \mathbf{v}.\nabla + q\mathbf{E}.\nabla_p)f(\mathbf{x},\mathbf{p},t)$$
$$= \sum_{\mathbf{p}'}\{f(\mathbf{x},\mathbf{p}',t)R(\mathbf{p}',\mathbf{p}) - f(\mathbf{x},\mathbf{p},\mathbf{t})R(\mathbf{p},\mathbf{p}')\}$$

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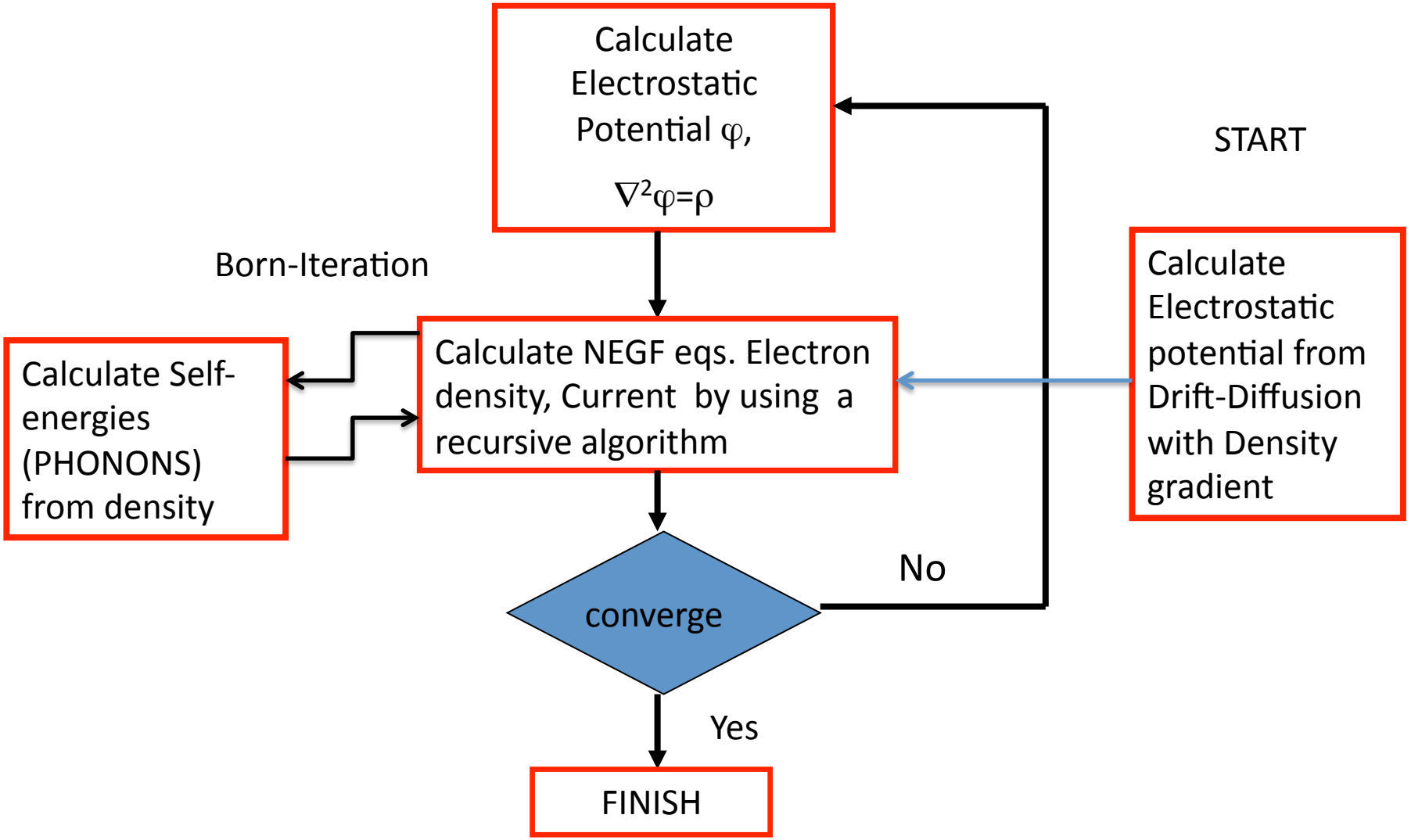
Device modelling with NEGF Green functions 2



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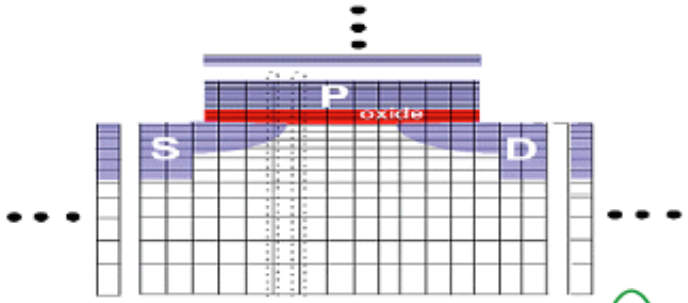
2D MOSFET simulation scheme



Svizhenko, M. P. Anantram, T. R. Govindan, B. Biegel, and R. Venugopal (2002)

$$(E-H)\Psi = 0 \rightarrow (EI - H - \Sigma^r)G^r = \delta$$

$$(EI - H - \Sigma^r)G^< = \Sigma^< G^a$$

$$(EI - H - \Sigma^r)G^> = \Sigma^> G^a$$

← Kinetics

Statistics

Hamiltonian of Device
Atomistic: DFT, Tight-binding, …

in-scattering & out-scattering
Statistical mechanics

Self-energies → Scattering rate
electron-phonon
contacts

Breakthrough approach

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Visualisation

Local Density of States LDOS

$$\rho(E;\mathbf{r}) = -\frac{1}{\pi}\mathrm{Im}\,G^{R}(\mathbf{r},\mathbf{r}\,;E) = A(\mathbf{r},E)$$

Carrier charge density

$$n(E;\mathbf{r}) = -\frac{2e}{\pi}\mathrm{Im}\,G^{<}(\mathbf{r},\mathbf{r}\,;E)$$

Current density

$$\mathbf{J}(E;\mathbf{r}) = -e\frac{\hbar}{4\pi}\mathbf{m}^{*-1}\,.\,(\nabla-\nabla')G^{<}(\mathbf{r},\mathbf{r}'\,;E)\Big|_{r\to r'}$$

Velocity field

$$\mathbf{v}(E;\mathbf{r}) = \frac{\mathbf{J}(E;\mathbf{r})}{n(E;\mathbf{r})}$$

See Appendices

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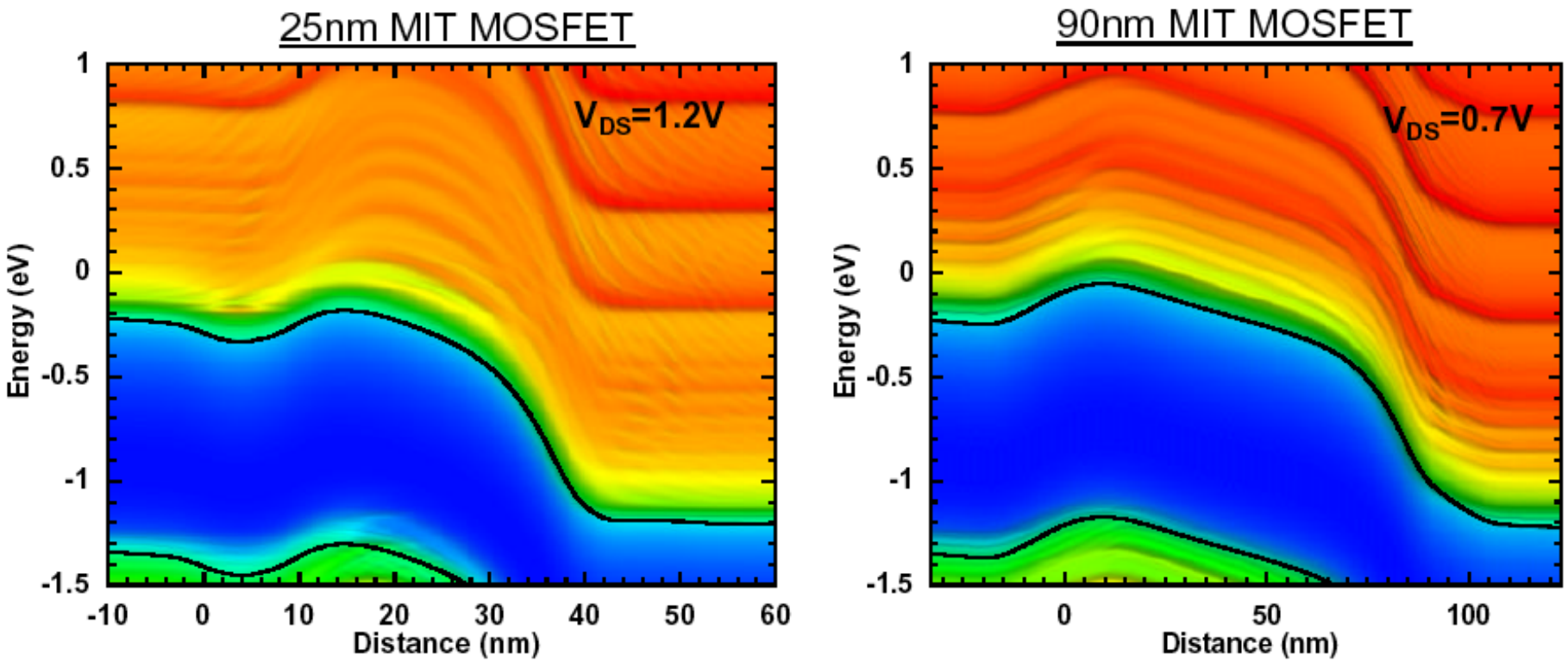
Quantum mechanical DOS (spectral function) data taken at Si-SiO2 interface

MOSFET sub-bands by Green Functions



Striations in DOS plots are sub-bands. Spectral shift evident near source barrier. Multiple sub-bands are required for accurate scattering calculations

First calculated by Jovanovich 2001

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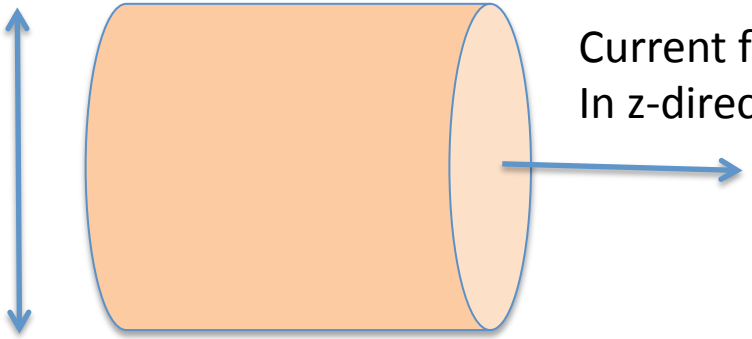
Mode Space Decomposition



J. R. Barker, M. Finch, J. Pepin and M. Laughton, *Theory of non-linear transport in quantum waveguides*, Solid State Electronics **32**, 1155 (1989).

R. Venugopal1, Z. Ren, S. Datta, M. S. Lundstrom, and D. Jovanovic, *Simulating quantum transport in nanoscale transistors: Real versus mode-space approaches*, Journal of Applied Physics, **92**, 3730 (2002).

Transverse motion is confined
Discrete modes: each 1D residual motion (z)
Use NEGF for each valley and mode
Get coupling between valleys/modes

$$-\frac{\hbar^2}{2}\left\{\frac{\partial}{\partial x}\left(\frac{1}{m_x^v}\frac{\partial}{\partial x}\right)+\frac{\partial}{\partial x}\left(\frac{1}{m_x^v}\frac{\partial}{\partial x}\right)+V_c(x,y,z)+e\phi(x,y,z_j)\right\}\Psi_j^{v,n}(x,y)=E_j^{v,n}\Psi_j^{v,n}(x,y)$$

$G^{R,\,v,n}(z,z';E)$ Bare confinement potential, electrostatic potential

$$G_0^{R,\,v,n}(z,z';E)\sim -i\frac{m_z^v}{\hbar^2 K}\exp[iK\,|z-z'|];\qquad K=\left(\frac{2m_z^v}{\hbar^2}\right)^{1/2}\left(E-E^{v,n}+i\eta\right)^{1/2}$$

v = valley index
n = mode index

Can be much faster but various caveats

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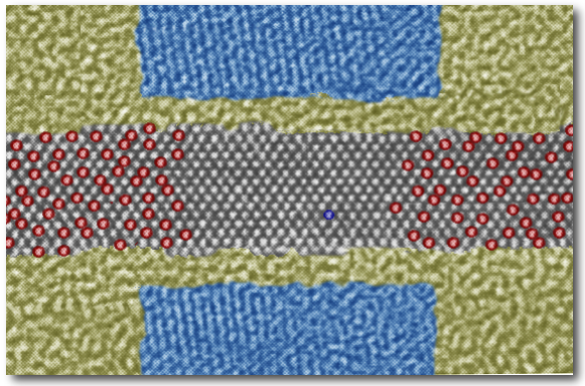
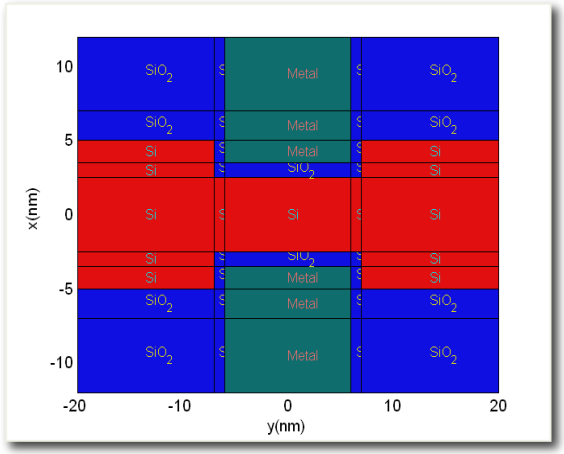
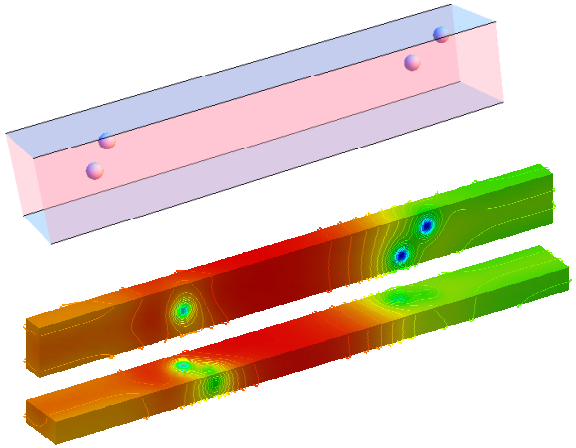
2D & 3D atomistic ballistic simulations

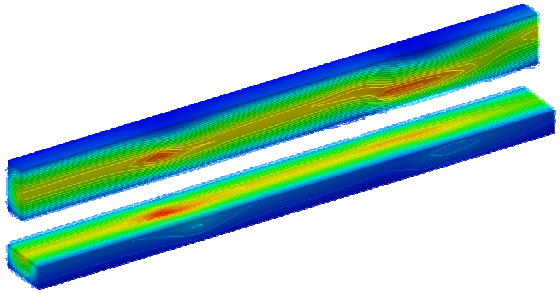




4 nm channel:
Meandering current flow
3D contours of jz



4 nm channel:
Potential Distribution



A. Martinez, J.R. Barker, A. Svizhenko, M.P. Anantram, M. Bescond, A. Asenov, *Ballistic Quantum Simulators for Studying Variability in Nanotransistors*, Journal of Computational and Theoretical Nanoscience, **5**, 2289 (2008)

2D and 3D device simulation
Self-Consistent Poisson-NEGF

Volume discretization

3D variable space mesh

Parallelized Recursive techniques

Includes precision description of rough interfaces and atomistic dopants non-perturbatively

Tight binding band structure confined Silicon nanowire devices

Unique dielectric assignment

Reviews detailed algorithms

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Dissipation: Electron-Phonon Interactions

For narrow silicon nanowires the transport is not ballistic.

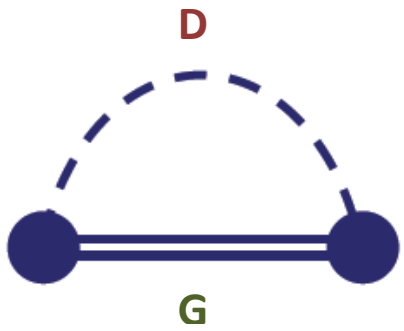
* Quasi-1D density of states due to confinement enhances electron-phonon interactions
* Long range polar optical phonon – electron interactions from oxide interface

The Generic Lowest order Self-Energy for Electron-Phonon scattering

Self-consistent Born Approximation for the lesser self-energy

$$\Sigma^{<}(\mathbf{r}_1,\mathbf{r}_2;\varepsilon) = (2\pi)^{-3}\int d^3q\,|U(\mathbf{q})|^2\,\exp[i\mathbf{q}.(\mathbf{r}_1-\mathbf{r}_2)]\;\times$$

$$\{n_q G^{<}(\mathbf{r}_1,\mathbf{r}_2;\varepsilon-\hbar\omega_q)+(n_q+1)G^{<}(\mathbf{r}_1,\mathbf{r}_2;\varepsilon+\hbar\omega_q)\}$$



$$\{E - H_0 - \Sigma^R\}G^R = 1$$

$$\Sigma^R = G^R D^R + G^R D^< + G^< D^R$$

$$G^< = G^R \Sigma^< G^A$$

$$\Sigma^< = G^< D^<$$

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Do not de-couple !!

Example: de-coupling approximation for electron-phonon interaction

$$\{E - H_0 - \Sigma^R\}G^R = 1$$

$$\Sigma^R = G^R D^R + G^R D^< + G^< D^R$$

$$G^< = G^R \Sigma^< G^A$$

$$\Sigma^< = G^< D^<$$

This approximation neglects the statistical component of the retarded self energy:

Leads to serious violations of the Pauli Exclusion Principle.

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Constraints

If the transport is not ballistic it is necessary to use the many-body descriptions of self-energies. Several constraints emerge:

Continuity equation

Microscopic Conservation laws

Causality requirements-analyticity

Non-locality conditions

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Charge and Current Conservation

$$\frac{\partial n(\mathbf{x},t)}{\partial t} + \nabla \bullet j(\mathbf{x},t) = 0$$

In stationary case: the current density must be constant in space

$$\nabla \bullet \mathbf{j}(\mathbf{r};E) = \frac{e}{h}\left\{G^R\Sigma^< - \Sigma^< G^A \quad + G^<\Sigma^A - \Sigma^R G^<\right\} = 0$$

This is a constraint on $G^<$

This fails for the Born approximation:

$$\Sigma^<(\mathbf{r}_1,\mathbf{r}_2;\varepsilon) = (2\pi)^{-3}\int d^3q\,|U(\mathbf{q})|^2\,\exp[i\mathbf{q}.(\mathbf{r}_1-\mathbf{r}_2)]$$
$$\{n_q G_0^<(\mathbf{r}_1,\mathbf{r}_2;\varepsilon-\hbar\omega_q) + (n_q+1)G_0^<(\mathbf{r}_1,\mathbf{r}_2;\varepsilon+\hbar\omega_q)\}$$

But holds for the generalised Born approximation

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Other Conservation Laws

More generally, the microscopic continuity of momentum, energy (and angular momentum) is required

$$\frac{\partial n(\mathbf{x},t)}{\partial t} + \nabla \bullet j(\mathbf{x},t) = 0$$

$$\frac{\partial \mathbf{P}(t)}{\partial t} + \int d\mathbf{x}\ \{\nabla U(\mathbf{x},t)\} n(\mathbf{x},t) = 0$$

$$\frac{\partial W(t)}{\partial t} + \int d\mathbf{x}\ \{\nabla U(\mathbf{x},t)\} \bullet \mathbf{j}(\mathbf{x},t) = 0$$

These fail for the Born approximation:

But hold for the generalised Born approximation

Ward Identities

Conservation laws hold if Self-energy derived from particular "dressed" Feynman diagrams

$$\Sigma = \frac{\delta \Phi[G]}{\delta G}$$

Using the Luttinger-Ward functional Φ

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Causality and Dispersion Relations

The retarded Green function $G^R(t,t')$ is zero for $t<t'$
Fourier transforming over $(t-t')$ to energy space it follows that
$G^R(E)$ has poles only in the LH of the complex energy plane.
It is a causal function. Similarly it is often assumed that the self-energy has a similar analytic structure. Both the Green function and self energy then satisfy Dispersion relations of the form of a Hilbert transform:

$$\mathrm{Re}\,\Sigma^R(E) = -\frac{P}{\pi}\int_{-\infty}^{\infty}\frac{|\,\mathrm{Im}\,\Sigma^R(E')\,|}{E'-E}$$

Useful for computing
The Real part from a model of the Imaginary part

Problems:
(1) Cannot set Re Σ to zero
(2) Care needed if Re part and Imaginary part are disjoint: get distributions
(3) The dispersion relation may be invalid:
Σ need not be causal to make G causal.
(4) Accurate dispersion relation needed to ensure Spectral density sum rule
Otherwise density of states errors.
Barker and Martinez (2013)

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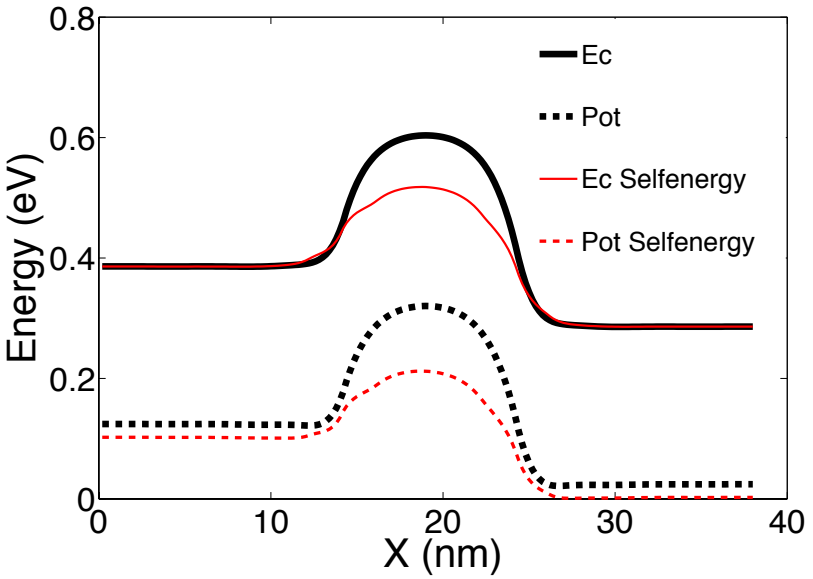
Electrostatic self-energy

- Gate all around nanowire device
- Many body dynamic correlation model due to dielectric surfaces follows from refs:



J.R. Barker (2013)

C. Li et al, Phys. Rev. B **80**, 195318 (2009).

C. Delerue, M. Lannoo, *Nanostructures*, Springer (2004).

This conference (C-5)

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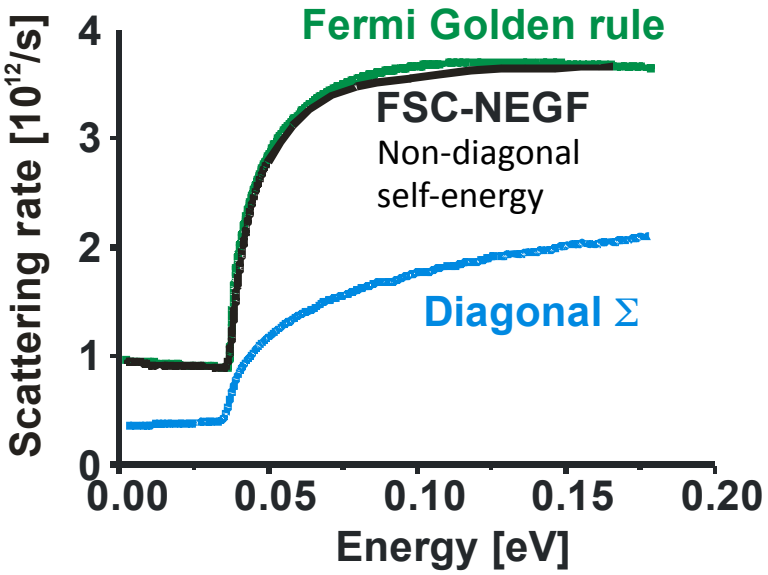
Non-Local (non-diagonal) Self-Energy

For a variety of electron-phonon interactions e.g polar optical coupling the corresponding self-energy is non-local i.e non-diagonal in position basis.

Huge increase in computational complexity



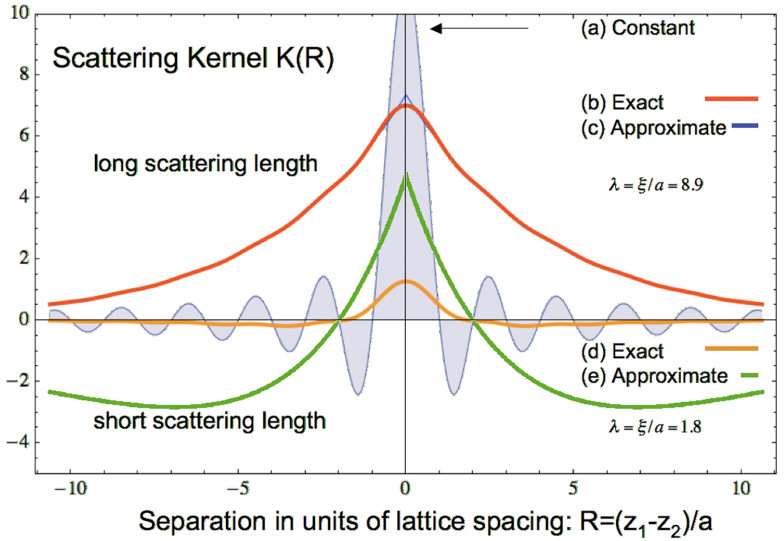
Test case: Kubis (2009)

Bulk GaAs @ 300 K

n = 10^{16} cm^{-3}, m = -0.08 eV

$$K = C\int_{-\pi/a}^{\pi/a} dq_z \, |U(\mathbf{q})|^2 \exp[iq_z(z_1 - z_2)]$$

$$C = e^2 \frac{\hbar\omega_0}{2\varepsilon_0}\left(\frac{1}{\varepsilon_\infty} - \frac{1}{\varepsilon_s}\right); \qquad |U(\mathbf{q})|^2 = C\frac{q_\perp^2 + q_z^2}{(q_\perp^2 + q_z^2 + \xi^{-2})^2}$$



Barker (2012)

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3.4 Approximations and Pitfalls

Self-energy approximations

Need to be self-consistent with **Ward identities** to maintain **current conservation**

Need **non-locality** in general or fails in known limits: **realistic scattering rates**

Full momentum and energy conservation needed: realistic momentum and energy relaxation – **conservation laws**

Inelastic scattering cannot be approximated by elastic scattering:
or energy relaxation and statistical distributions become invalid (non-equilibrium)

Causality conditions must be respected (failures in density of states etc)

Use coupled equations: many-body effects and Pauli exclusion

Computational Issues

Non-locality breaks the fast compact algorithms.
Iterative self-consistent schemes required: convergence issues

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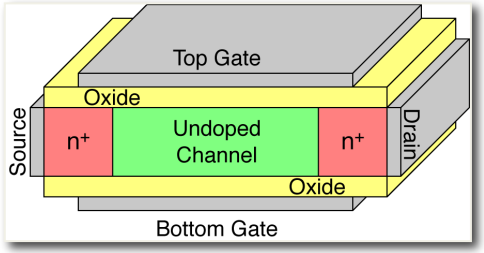
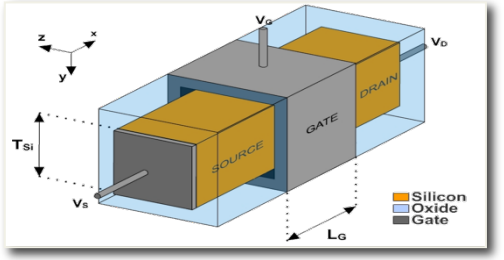
4. Applications to 3D Semiconductor Nano-Devices

Double gate MOSFET

Silicon nanowire wrap-round gate MOSFET





Atomistic variability

Resonances

Vortex flows

Source-drain extensions- impurity aggregations

Interface roughness

Strained systems

Architecture dependent dynamics

Dissipation

Electrostatic Self-Energy

Causality issues

http://johnreginaldbarker.co.uk/

silicon

silicon germanium

III-V

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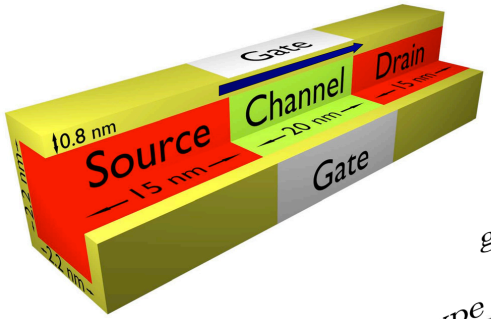
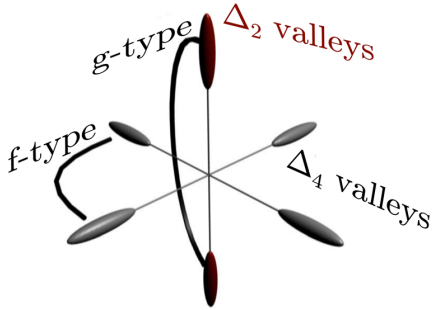
3D-Mode space nano-transistor with dissipation





Effective Mass from Tight binding

Inelastic, Local Self-Energy in
Self-Consistent Born Approximation
3 types of f and g
inter-valley optical phonons,
intra-valley acoustic phonons,

Violations of Mattheisen's Rule
of the order of 13%

M. Aldegunde, A. Martinez and J. R. Barker, *Study of individual phonon scattering mechanisms and the validity of Matthiessen's rule in a gate-all-around silicon nanowire transistor,* Journal of Applied Physics, **113**, 014501 (2013)

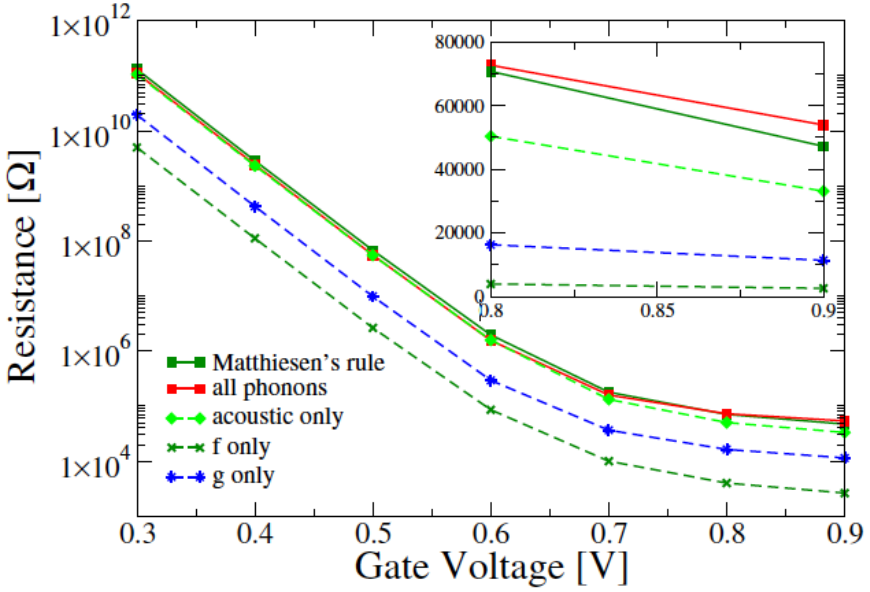


FIG. 8. Resistances of the 20 nm gate length silicon nanowire (S), (A), (G and (F) transistors. The inset represents the data for high drain bias cond tions in linear scale.

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Example of atomistic effects:

Resonances due to single positively charged dopant

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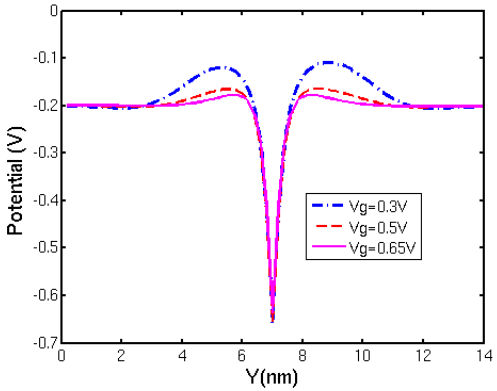
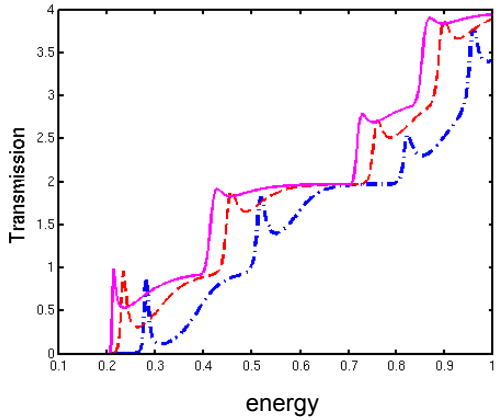
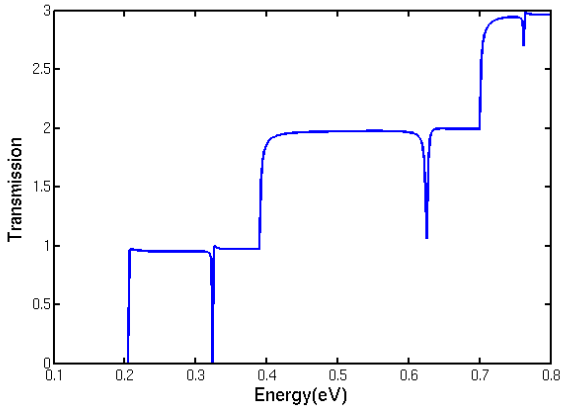
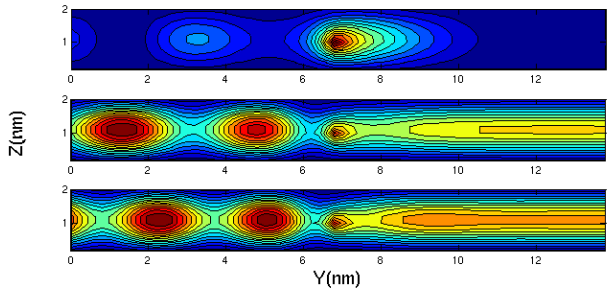
Gated Silicon quantum wire
Positive point charge at centre of channel
Self-consistent (Hartree) screening is obtained non-perturbatively.
Polarisation effects due to SiO_2 included

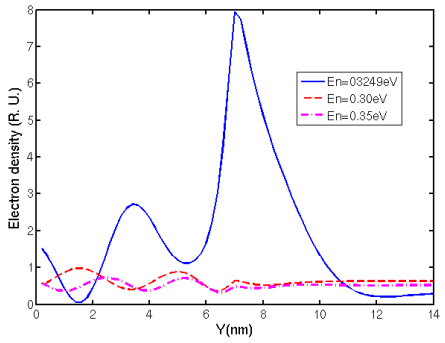
cross – section 2.2 nm × 2.2 nm
channel length 10 nm
gate length 6 nm
oxide thickness 0.8 nm
doped (uniformly) p - type at 10^{20} cm^{-3}











Shape of self-consistent screened potential is altered by gate potential.
Observe Breit-Wigner and asymmetric Fano resonances in energy continuum.

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Resonances due to single positively charged dopant

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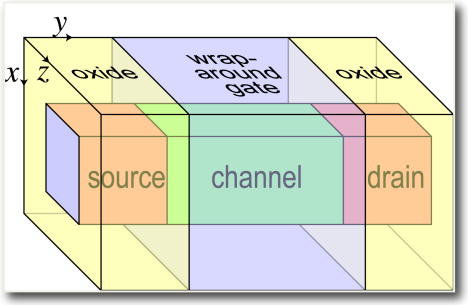
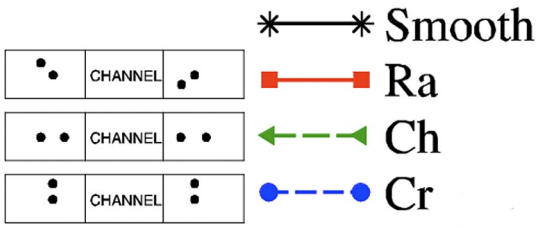
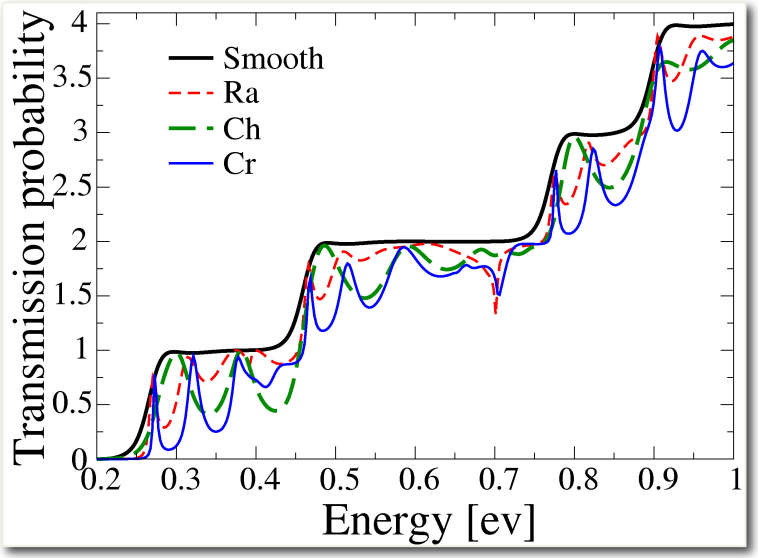
Ab initio coherent scattering from discrete dopants in the source and drain of a nanowire transistor using 3D NEGF simulations

N. Seoane, A. Martinez, A. R. Brown, J.R. Barker and A. Asenov (2008)







silicon nanowire MOSFET

active channel

4 nm X 2.2 nm

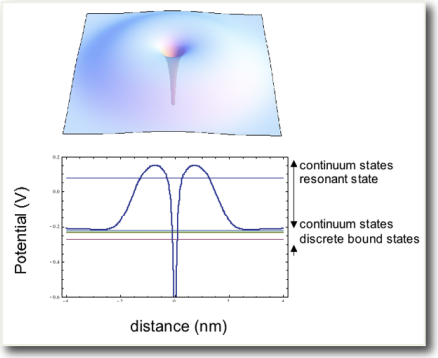
X 2.2 nm

A range of resonant tunnelling resonances from Sombrero potentials

Breit-Wigner and Fano Resonances

Mostly compatible with independent centres

Some evidence of cluster scattering



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CONCLUSION

Here endeth the tutorial and brief overview.

Lots remains to be done:

Initial state correlations

Time correlations

Time dependent NEGF

Better models for contact self-energies

Many-body processes

……

Finally, the References and Appendices provide background material and further details

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References and 7 Appendices

with more details

see pdf file

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Appendix 1: Representatiuons and Pictures

Use Dirac notation (understand operator or c-number from context)

Eigenvalues a (real) of a Hermitian operator A

$$A\,|a\rangle = a\,|a\rangle$$

orthonormality

$$\langle a\,|a'\rangle = \delta_{aa'}$$

$$\{|a\rangle\}\ complete\ set \qquad \sum_a |a\rangle\langle a| = \mathbf{1}$$

Canonically conjugate observables

$$[q,p] = qp - pq = i\hbar$$

$$Expansion\ of\ arbitrary\ ket\ |\psi\rangle = \sum_a |a\rangle\langle a|\psi\rangle = \sum \langle a|\psi\rangle\,|a\rangle$$

Schrödinger Picture: state vectors evolve in time under action of the Hamiltonian H

$$i\hbar\frac{\partial}{\partial t}|\psi;t\rangle = H\,|\psi;t\rangle$$

Expectation value of observable A

$$\langle A[t]\rangle = \langle\psi;t|\,A\,|\psi;t\rangle$$

Position representation

$$x\,|x\rangle = x\,|x\rangle \qquad \int dx\,|x\rangle\langle x| = 1$$

$$\langle x\,|x'\rangle = \delta(x-x')$$

Wavefunction

$$\psi(x;t) = \langle x\,|\psi\ ;t\rangle$$

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Evolution Operator and Heisenberg Picture

$$i\hbar\frac{\partial}{\partial t}|\psi;t>=H|\psi;t>$$

$$|\psi;t>=U(t,t_0)|\psi;t_0>$$

$$i\hbar\frac{\partial}{\partial t}U(t,t_0)=HU(t,t_0)$$

$$Boundary\ \ condition: U(t_0,t_0)=\mathbf{1}$$

$$Unitarity:\ \ UU^{+}=\mathbf{1}$$

Heisenberg Picture: state vectors constant in time; operators evolve

$$|\psi>_H=U^{+}(t,t_0)|\psi\ ;t>=U^{+}(t,t_0)U(t,t_0)|\psi\ ;t_0>$$

$$A_H(t)=U^{+}(t,t_0)AU(t,t_0)$$

$$i\hbar\frac{d}{dt}A_H(t)=i\hbar U^{+}(t,t_0)\frac{\partial}{\partial t}A(t)U(t,t_0)$$
$$+[A_H(t),H_H(t)]$$

Expectation values

$$_H<\psi|A_H(t)|\psi>_H=$$
$$<\psi\ ;t_0|U^{+}(t,t_0)AU(t,t_0)|\psi\ ;t_0>=$$
$$<\psi\ ;t|A|\psi\ ;t>$$

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Interaction aka Dirac Picture

Suppose Hamiltonian splits into an unperturbed and perturbed part

$$H = H_0 + V$$

$$H_0 \ \ time-independent; \ \ V(t) generally \ \ time \ \ dependent$$

$$|\psi;t>_I \equiv \exp[i(t-t_0)H_0/\hbar]\,|\psi;t>$$

$$A_I(t) \equiv \exp[i(t-t_0)H_0/\hbar]A\exp[-i(t-t_0)H_0/\hbar]$$

State vector evolves under interactions $V_I(t)$
Operators evolve under H_0

$$i\hbar\frac{d}{dt}|\psi;t>_I = V_I(t)\,|\psi;t>_I \qquad V_I(t) = \exp[i(t-t_0)H_0/\hbar]V\exp[-i(t-t_0)H_0/\hbar]$$

$$i\hbar\frac{d}{dt}A_I(t) = [\,A_I(t), H_0\,]$$

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Density Matrix

$$Pure\ \ state\ |\psi;t>$$

$$\rho(t) = |\psi;t><\psi;t|$$

$$i\hbar\frac{\partial}{\partial t}\rho(t) = [H,\rho(t)]$$

$$Mixed\ \ state;\ \ if\ \ probability\ \ of\ \ state\ |\psi_n;t>\ \ is\ \ P_n:$$

$$\rho(t) = \sum_n |\psi_n;t> P_n <\psi_n;t|$$

Equation of motion

$$i\hbar\frac{\partial}{\partial t}\rho(t) = [H,\rho(t)]$$

Expectation value

$$< A(t) >= Tr[\rho(t)A] = \sum_n \sum_a P_n |\psi_n;t><\psi_n;t|a><a|A|a><a|$$

$$= \sum_a <a|A|a>$$

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Appendix 2: Time-dependent Perturbation Theory 1

$$Let\ \ H = H_0 + V(t)$$

$$\rho(t_0) = \sum_n \ |\psi_n > f_n < \psi_n|$$

$$\rho(t) = \sum_n \ |\psi_n;t > f_n < \psi_n;t| = \sum_n U(t,t_0)|\psi_n > f_n < \psi_n|U^*(t,t_0)$$

Probability of being in a state $|\psi_n>$ is then

$$<\psi_n|\rho(t)|\psi_n> = \sum_{n'} f_{n'} |<\psi_n|U(t,t_0)|\psi_{n'}>|^2 = \sum_{n'} f_{n'} P[n,n']$$

$$P[n,n'] = |<\psi_n|U(t,t_0)|\psi_{n'}>|^2 \quad Transition\ \ probability$$

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Appendix 2: Time-dependent Perturbation Theory 2

From Appendix 1: for $t > t_0$ in Heisenberg picture

$$H_H(t,t_0) = \exp[i(t-t_0)H/\hbar]H(t_0)\exp[-i(t-t_0)H/\hbar]$$

$$i\hbar\frac{\partial}{\partial t}U(t,t_0) = H_H(t,t_0)U(t,t_0)$$

using $BC: \quad U(t_0,t_0) = \mathbf{1}$

solution satisfies integral equation:

$$U(t,t_0) = \mathbf{1} - (i/\hbar)\int_{t_0}^{t} dt' H_H(t',t_0)U(t',t_0)$$

Iterating gives

$$U(t,t_0) = \mathbf{1} + \sum_{p=1}^{\infty} (-i/\hbar)^p \int_{t_0}^{t} dt_1 \int_{t_0}^{t_1} dt_2 \ldots \int_{t_0}^{t_{p-1}} dt_p H_H(t_1,t_0)H_H(t_2,t_0)\times\ldots H_H(t_p,t_0)$$

using time ordering operator $\mathbf{T}$ this becomes

$$U(t,t_0) = \mathbf{1} + \mathbf{T}\sum_{p=1}^{\infty} \frac{(-i/\hbar)^p}{p!} \int_{t_0}^{t} dt_1 \int_{t_0}^{t} dt_2 \ldots \int_{t_0}^{t} dt_p H_H(t_1,t_0)H_H(t_2,t_0)\times\ldots H_H(t_p,t_0)$$

$$U(t,t_0) = \mathbf{T}\exp[-(i/\hbar)\int_{t_0}^{t} dt_1 \; H_H(t_1,t_0)]$$

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Appendix 2: Time-dependent Perturbation Theory 3

From Appendix 1: for $t > t_0$; in Dirac picture

$$V_I(t,t_0) = \exp[i(t-t_0)H_0/\hbar]V\exp[-i(t-t_0)H_0/\hbar]$$

$$i\hbar\frac{\partial}{\partial t}U_I(t,t_0) = V_I(t,t_0)U_I(t,t_0)$$

using *BC*: $U(t_0,t_0) = \mathbf{1}$

Interaction/Dirac picture is best for setting up Feynman diagrams etc

solution satisfies integral equation:

$$U_I(t,t_0) = \mathbf{1} - (i/\hbar)\int_{t_0}^{t} dt' V_I(t',t_0)U_I(t',t_0)$$

Iterating gives

$$U_I(t,t_0) = \mathbf{1} + \sum_{p=1}^{\infty} (-i/\hbar)^p \int_{t_0}^{t} dt_1 \int_{t_0}^{t_1} dt_2 \ldots \int_{t_0}^{t_{p-1}} dt_p V_I(t_1,t_0)V_I(t_2,t_0)\times\ldots V_I(t_p,t_0)$$

using time ordering operator $\mathbf{T}$ this becomes

$$U_I(t,t_0) = \mathbf{1} + \mathbf{T}\sum_{p=1}^{\infty} \frac{(-i/\hbar)^p}{p!} \int_{t_0}^{t} dt_1 \int_{t_0}^{t} dt_2 \ldots \int_{t_0}^{t} dt_p V_I(t_1,t_0)V_I(t_2,t_0)\times\ldots V_I(t_p,t_0)$$

$$U_I(t,t_0) = \mathbf{T}\exp[-(i/\hbar)\int_{t_0}^{t} dt_1\ V_I(t_1,t_0)]$$

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Appendix 3: Perturbation Theory at zero temperature

This problem is long-established in perturbation theory
Assume many-body system is in the ground state

$$\rho(t_0) = |\Psi_0><\Psi_0|$$

ground state of exact time independent Hamiltonian $H = H_0 + V.$

$$G(\mathbf{x},t;\mathbf{x},t') = < G > = < \Psi_0 | \mathbf{T}\{\Psi(\mathbf{x},t)\Psi^*(\mathbf{x}',t')\} | \Psi_0 >$$

In terms of $|\Psi_{00}>$ the ground state of H_0 it can be shown that

$$G(\mathbf{x},t;\mathbf{x},t') = \frac{< \Psi_{00} | \mathbf{T}\{S(\infty,-\infty)\Psi_I(\mathbf{x},t)\Psi_I{}^*(\mathbf{x}',t')\} | \Psi_{00} >}{< \Psi_{00} | S(\infty,-\infty) | \Psi_{00}>}$$

here the S-matrix is defined as

$$S(\infty,-\infty) = \mathbf{T}\exp[-(1/\hbar)\int_{-\infty}^{\infty} dt'' V_I(t'')]$$

The time-ordering operator is slightly more subtle in many-body theory

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For every time re-ordering which takes P steps, multiply result by $(-1)^P$ for Fermion Operators.

The expression for the S-matrix and Green function may be evaluated using Wick's Theorem which generates the usual Feynman diagrams. Huge reduction of terms (the disconnected diagrams) occurs due to cancellation with the denominator (phase factor) in the expression for G.The irreducible diagrams define the self-energy for which it is proved

$$G = G_0 + G_0 \Sigma G$$

The Dyson equation.

The simplest form for G is the generalised Born approximation.

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Appendix 3: finite temperature 0

This problem is also long-established in perturbation theory.
Two simplifying features:

1. The Hamiltonian $H=H_0+V$ is time-independent

2. The form of the density matrix is known

3. There is a fortuitous similarity between the grand canonical statistical density matrix and the evolution operator U in imaginary time.

The problem can be re-stated in terms of time(imaginary) evolution between $\tau=0$ and $t=ih/k_BT$.

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Appendix 3: finite temperature 1

Thermal equilibrium (known form of solution)

$$\rho = \frac{\exp[-\beta(H-\mu N)]}{Tr\{\exp[-\beta(H-\mu N)]\}} = Z^{-1}\exp[-\beta(H-\mu N)] \qquad \beta = \frac{1}{k_B T}$$

$$= \frac{\exp[\beta\mu N]\,U(-i\hbar\beta,0)}{Tr\{\exp[\beta\mu N]\,U(-i\hbar\beta,t_0)\}} = \frac{\exp[\beta\mu N]\,U(-i\hbar\beta,0)}{Z}$$

In terms of the thermal equilibrium described by H_0 we define

$$\rho_{00} = \frac{\exp[-\beta(H_0-\mu N)]}{Tr\{\exp[-\beta(H_0-\mu N)]\}} = \frac{\exp[-\beta(H_0-\mu N)]}{Z_0} \;;$$

Averages
$< .... >_0 = Tr\{\rho_{00} ...\}$

We thus separate out The free equilibrium density matrix and an evolution operator defined in complex time τ $0<\tau<-i\hbar\beta$

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Appendix 3: finite temperature 2

We may now use a modified Interaction representation in which the evolution in time is driven by evolution operators in complex time (Matsubara work).

Modified interaction picture

$$A_{I\beta}(\tau) = \exp[\tau(H_0 - \mu N)] A \exp[-\tau(H_0 - \mu N)]$$

$$V_{I\beta}(\tau) = \exp[\tau(H_0 - \mu N)]\ V\ \exp[-\tau(H_0 - \mu N)]$$

S-matrix

$$\exp[-\tau(H - \mu N)] = \exp[-\tau(H_0 - \mu N)] S_\beta(\tau)$$

$$\exp[\tau(H - \mu N)] = S_\beta^{-1}(\tau) \exp[-\tau(H_0 - \mu N)]$$

$$\frac{\partial}{\partial \tau} S_{I\beta}(\tau) = -V_{I\beta}(\tau) S_{I\beta}(\tau)$$

$$S_{I\beta}(\tau) = \mathbf{T}_\tau \exp[-\int_0^\tau d\tau' V_{I\beta}(\tau')]$$

$$Z = Tr\{\rho_{00} \mathbf{T}\{S_{I\beta}(\beta, 0)\}$$

The same Wick's theorem and Feynman diagrams work
But the averages are over the non-interacting equilibrium density matrix.

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Appendix 3: finite temperature 3

The Green function of interest is (for electrons)

$$G(\mathbf{x},\tau;\mathbf{x}',0') = -<\exp[\tau(H-\mu N)]\Psi(\mathbf{x},0)\exp[-\tau(H-\mu N)]\Psi^*(\mathbf{x}',0)> \quad \tau>0$$
$$+<\exp[\tau(H-\mu N)]\Psi^*(\mathbf{x}',0)\exp[-\tau(H-\mu N)]\Psi^*(\mathbf{x},0)> \quad \tau<0$$

$$G(\mathbf{x},\tau;\mathbf{x}',0) = \frac{<\mathbf{T}_\tau\{S_{I\beta}(\beta)\Psi_{I\beta}(\mathbf{x},\tau)\Psi_{I\beta}{}^*(\mathbf{x}',0)>_0}{<\mathbf{T}_\tau S_{I\beta}(\beta)>_0}$$

$$G_0(\mathbf{x},\tau;\mathbf{x}',0) = <\mathbf{T}_\tau\{\Psi_{I\beta}(\mathbf{x},\tau)\Psi_{I\beta}{}^*(\mathbf{x}',0)>_0$$

$$G = G_0 + G_0\Sigma G$$

The same Wick's theorem and Feynman diagrams work
But the averages are over the non-interacting equilibrium density matrix.
Dyson equation again holds

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Appendix 4: Choice of NEGF method

Zero Temperature

Use adiabatic switching from ground state to ground state

$\rho(t_0) = |\Psi_0><\Psi_0|$

time independent Hamiltonian

$H = H_0 + V.$

Expectation value

$< A >=< \Psi_0 | A | \Psi_0 >$

Switch to Interaction(Dirac)picture

If $|\Psi_{00}>=$ ground state of H_0

$$< A >= \frac{< \Psi_{00} | \mathbf{T}\{S(\infty,-\infty)A_I(t) | \Psi_{00} >}{< \Psi_{00} | S(\infty,-\infty) | \Psi_{00}>}$$

here the S-matrix is defined as

$$S(\infty,-\infty) = \mathbf{T}\exp[-(1/\hbar)\int_{-\infty}^{\infty} dt" V_I(t")]$$

Finite Temperature

Exploit known form of solution And exponential dependence on H

$$Thermal\ equilibrium\quad \beta = \frac{1}{k_B T}$$

$$\rho_0 = \frac{\exp[-\beta(H-\mu N)]}{Tr\{\exp[-\beta(H-\mu N)]\}}$$

$$= \frac{\exp[\beta\mu N]\ U(-i\hbar\beta,0)}{Tr\{\exp[\beta\mu N]\ U(-i\hbar\beta,0)\}}$$

$$< A(t) >= Tr\{\frac{\exp[\beta\mu N]U(-i\hbar\beta,t_0)U(t_0,t)AU(t,t_0)}{Tr\{\exp[\beta\mu N]U(-i\hbar\beta,t_0)\}}\}$$

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Appendix 5: The Problem of Non Equilibrium

The general zero temperature method fails because :

(i) requires a simple relation
(phase difference only) between the states at t= ± infinity

$$|\Psi_0(-\infty)\rangle = \exp[i\vartheta]\,|\Psi_0(\infty)\rangle$$

(ii) This only works because of: adiabatic switching on and off of the interactions, assumption of a non-degenerate ground state.
Not possible in non-equilibrium.

(iii) the perturbations include **applied fields that may be time dependent and long lived**.

The finite temperature method depends on knowing the form of the solution, in particular

(i) a time independent Hamiltonian
(ii) The density matrix has an exponential dependence on H
Can define perturbative evolution in complex time from t_0 to $-ih\beta = ih/k_BT$

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The Keldysh time-ordered Green Function

$$G(\mathbf{x},\tau;\mathbf{x}',\tau') = -i < \mathbf{T}_K \Psi(x,\tau)\Psi(x',\tau') >= Tr[\rho(H_0+V)\mathbf{T}_K \Psi_H(\mathbf{x},\tau)\Psi_H(\mathbf{x}',\tau')]$$

$$H = H_0 + V$$

$$Heisenberg\ representation: operators\ evolve\ under\ \ full\ \ Hamiltonian\ (H+U)$$

$\mathbf{T}_K$: Keldysh contour time ordering, put later Keldysh times to the left.
(use, fermion rules $\times(-1)$ per interchange),

$$\rho(H) = exp[-\beta(H-\mu N)]/Z$$

This Green function has the same perturbation theoretic structure as zero temperature or finite temperature theory.
In particular, G satisfies a Dyson equation.

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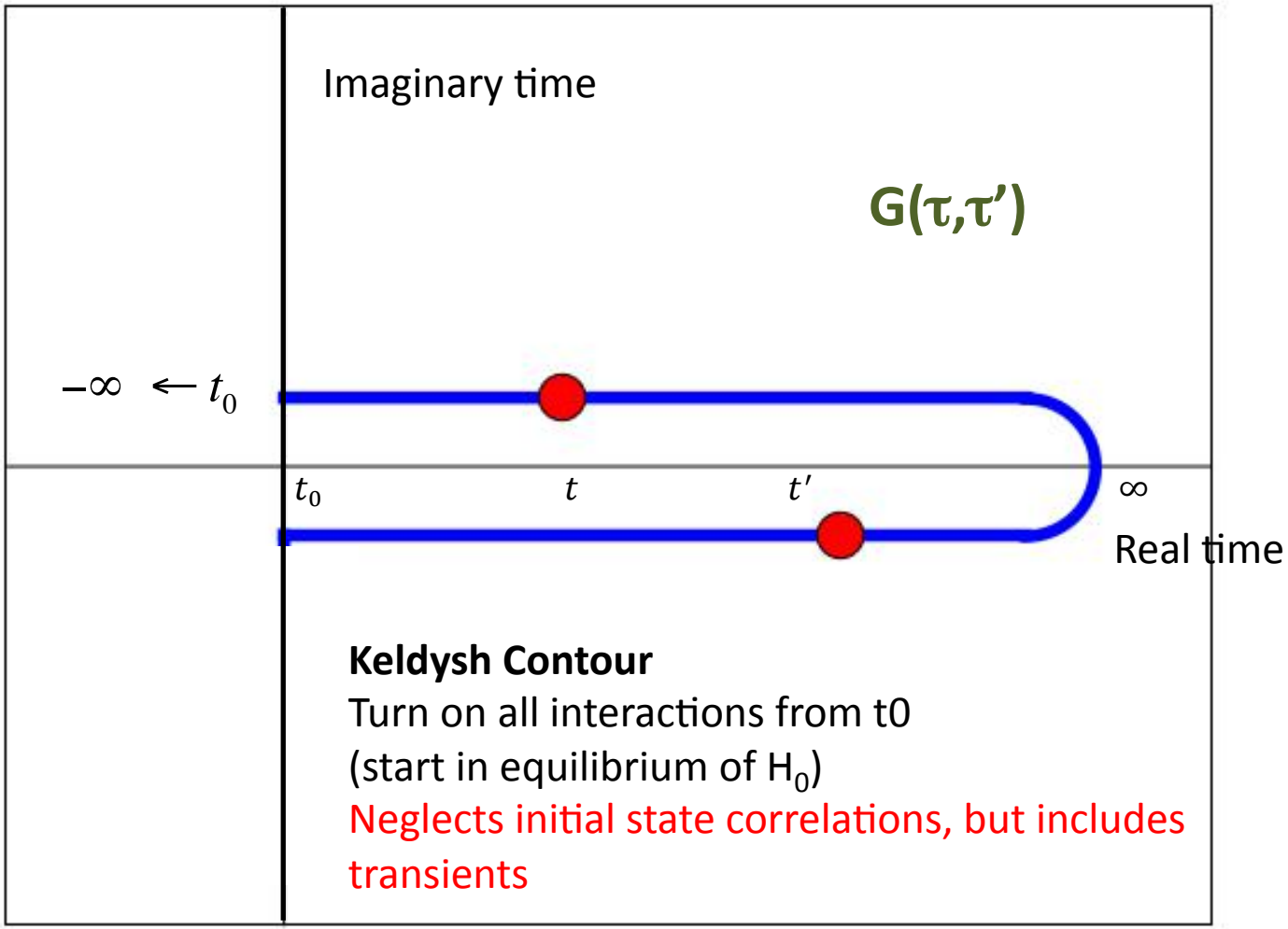
The Green Function defined on the Keldysh contour



Keldysh Contour

Turn on all interactions from t0

(start in equilibrium of H_0)

Neglects initial state correlations, but includes transients

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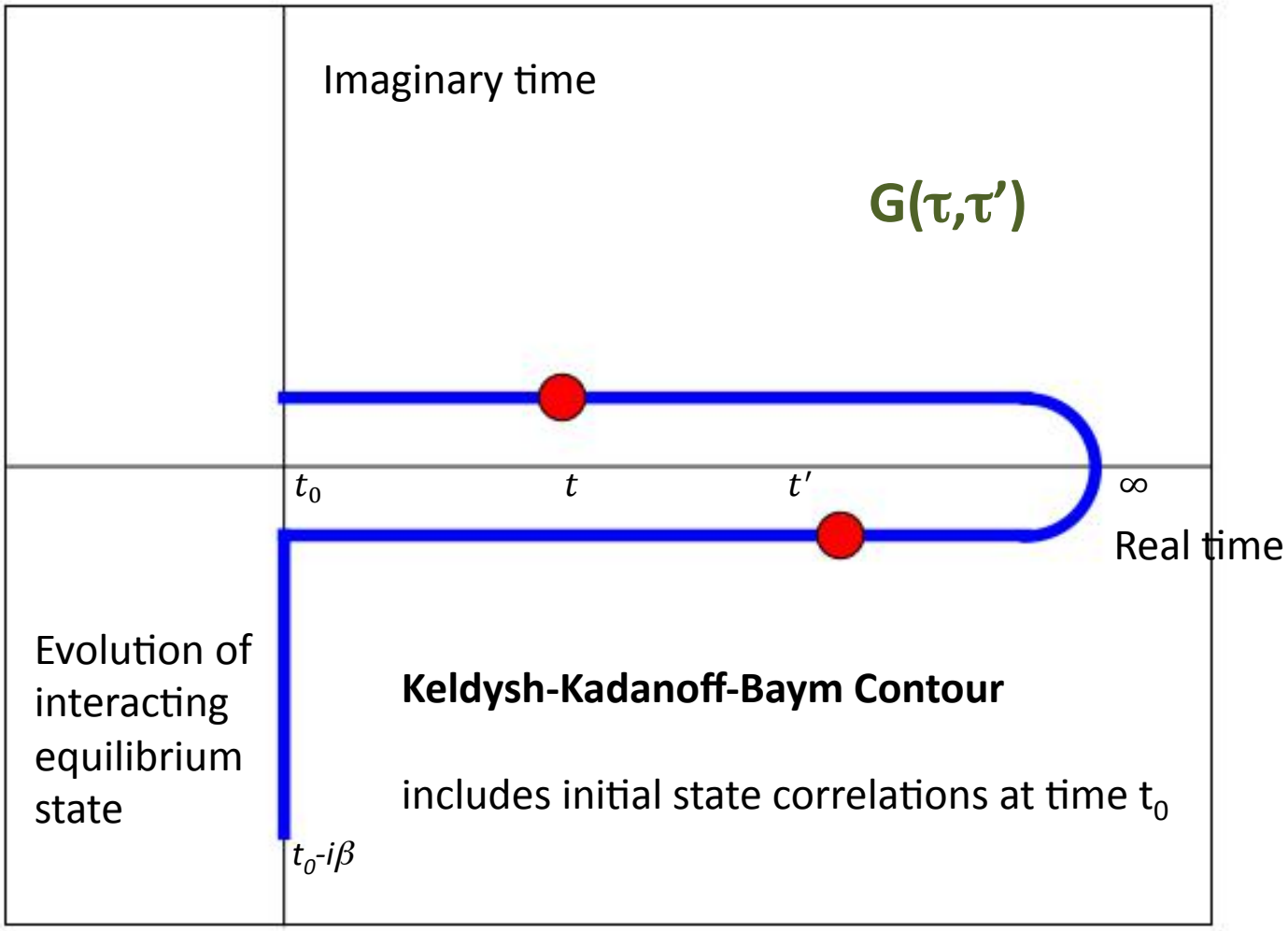
The Green Function defined on the Keldysh (Keldysh-Kadanoff-Baym) contour



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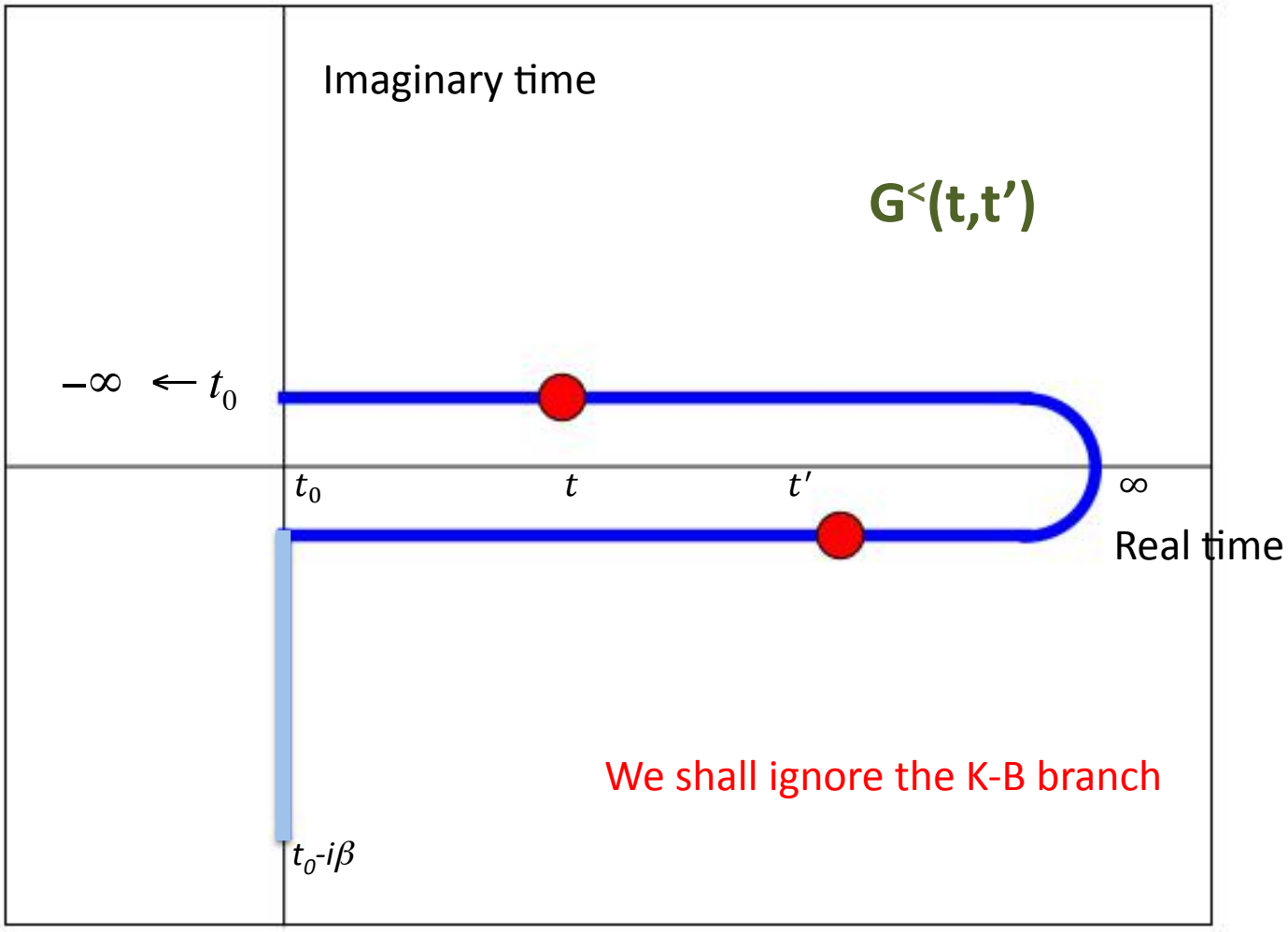
The Green Function Zoo:
distinguished by ordering on the Keldysh contour

Example 1: $G(\tau,\tau') = G^{<}(t,t')$; $\tau<\tau'$; $\tau \Rightarrow t$, $\tau' \Rightarrow t'$; $t<t'$



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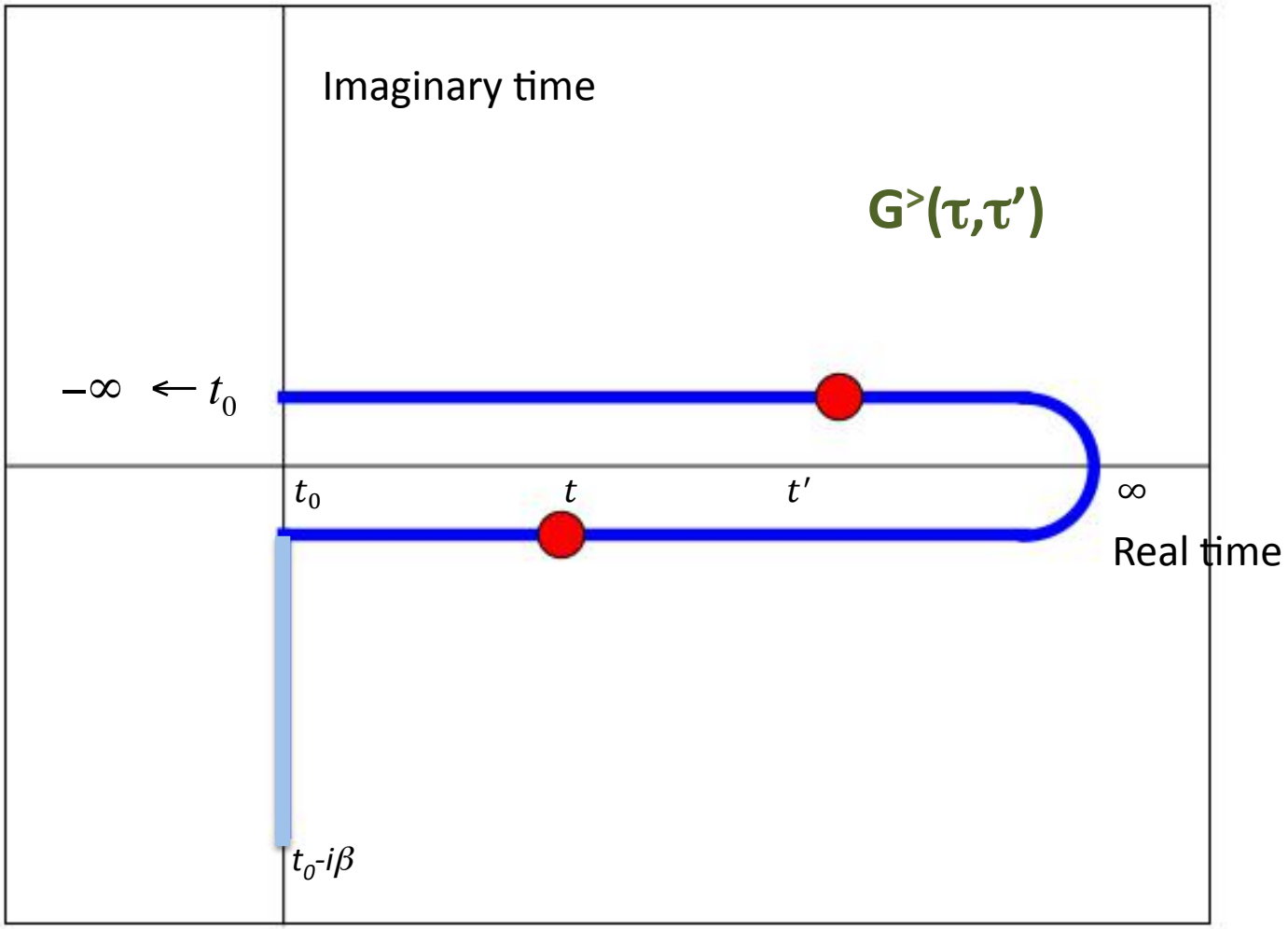
The Green Function Zoo:
distinguished by ordering on the Keldysh contour

Example 2: $G(\tau,\tau') = G^{>}(t,t')$; $\tau > \tau'$; $\tau \Rightarrow t$, $\tau' \Rightarrow t'$; $t < t'$



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The Green Function Zoo: distinguished by ordering on the Keldysh contour

$$G(\mathbf{x},\tau;\mathbf{x}',\tau') \equiv <\mathbf{x}\,|\,G(\tau,\tau')\,|\,\mathbf{x}'>$$

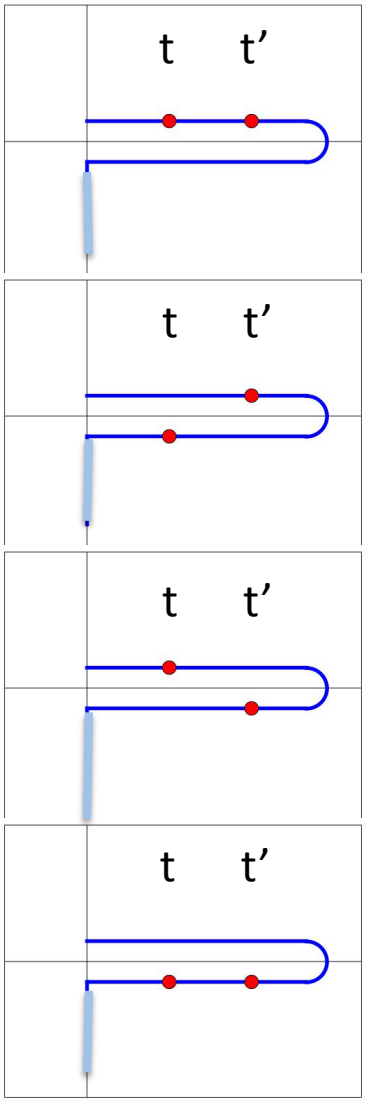
$$= -i\hbar <T_K \psi_h(\mathbf{x},\tau)\psi_h^+(\mathbf{x}',\tau')$$

$$= G_T(\mathbf{x},\tau;\mathbf{x}',\tau') \quad t,t' \text{ on upper contour}$$

$$= G^>(\mathbf{x},\tau;\mathbf{x}',\tau') \quad t \text{ on lower contour},\ t' \text{ on upper contour}$$

$$= G^<(\mathbf{x},\tau;\mathbf{x}',\tau') \quad t \text{ on upper contour},\ t' \text{ on lower contour}$$

$$= G_{T^*}(\mathbf{x},\tau;\mathbf{x}',\tau') \quad t,t' \text{ on lower contour}$$



G_T

$G^>$

$G^<$

G_{T^*}

< Less Than; > Greater Than; T time-ordered, T* anti-time ordered

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Identities

$$G^R = G_T - G^< = G^> - G_{T*}$$

Retarded Green Function

$$G^R(\mathbf{x},t;\mathbf{x}',t') = -i\hbar\vartheta(t-t') < \{\psi(\mathbf{x},t),\psi^*(\mathbf{x}',t')\} >$$

$$G^A = G_T - G^> = G^< - G_{T*}$$

Advanced Green Function

$$G^A(\mathbf{x},t;\mathbf{x}',t') = i\hbar\vartheta(t'-t) < \{\psi(\mathbf{x},t),\psi^*(\mathbf{x}','t)\} >$$

$$G_K = G^> + G^< = G_T + G_{T*}$$

Keldysh Green Function

$$G_K(\mathbf{x},t;\mathbf{x}',t') = -i\hbar < [\psi(\mathbf{x},t),\psi^*(\mathbf{x},t)] >$$

Spectral Function

$$A = G^R - G^A = G^> - G^<$$

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Three independent Non-Equilibrium Green Functions

Only 3 independent Green functions typical choice:

$G^{<,} \quad and \quad G^{A}, \quad G^{R}$

G$^{<}$ statistics
initial state

G^{R}, G^{A} dynamics

Advanced Green function

$$G^{A}(\mathbf{x},t;\mathbf{x}',t') \equiv \; < \mathbf{x} \,|\, G^{A}(t,t') \,|\, \mathbf{x}' >$$

$$G^{A}(t,t') = \; \theta(t'-t)\{G^{<}(t,t') - G^{>}(t,t')\}$$

Retarded Green Function

$$G^{R}(\mathbf{x},t;\mathbf{x}',t') \equiv \; < \mathbf{x} \,|\, G^{R}(t,t') \,|\, \mathbf{x}' >$$

$$G^{R}(t,t') = \; \theta(t-t')\{G^{>}(t,t') - G^{<}(t,t')\}$$

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G^R and $G^<$

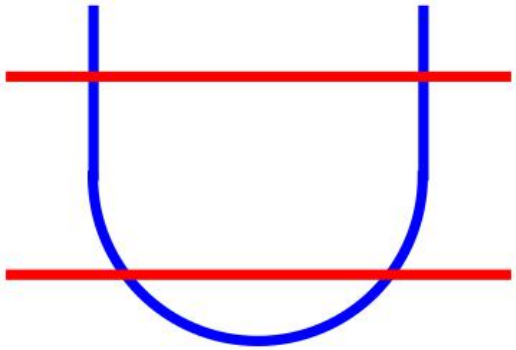
The Retarded Green Function G^R
Describes the Electronic States
(DYNAMICS)

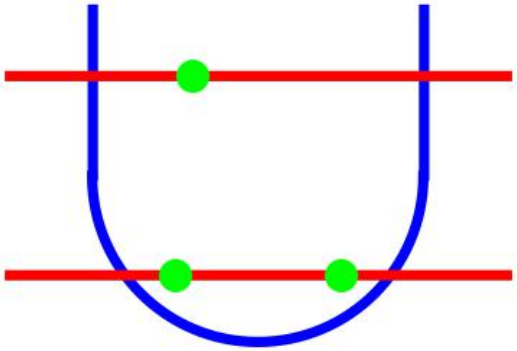
Confinement-sub bands et
Applied field shifts
Resonances
Bound states
Lifetime of states

$$\{E - H_0 - e\varphi - \Sigma^R\}G^R = 1$$

The Lesser than Green Function $G^<$
Describes the Occupancy of States
(STATISTICS)

$$\mathbf{G}^< = G^R \Sigma^< G^A$$





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Equations of Motion

Start from the Dyson equation on Keldysh contour

$$G = G_0 + G_0 \Sigma G$$

$$G(\mathbf{x}\tau;\mathbf{x}'\tau' = G_0(\mathbf{x}\tau;\mathbf{x}'\tau') +$$

$$\int dx'' dx''' \int_K d\tau'' \int_K d\tau''' G_0(\mathbf{x}\tau,\mathbf{x}''\tau'')\Sigma(\mathbf{x}''\tau'',\mathbf{x}'''\tau''')G(\mathbf{x}'''\tau''';\mathbf{x}'\tau')$$

Transform to Real Times

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Equations of Motion

We encounter products such as AB and triple products such as ABC along the Keldysh contour. For example: $D^<(t,t') = \int_K d\tau_1 \; A(t,\tau'')B(\tau'',t')$

$$D^<(t,t') = \int_K d\tau_1 \; A(t,\tau'')B(\tau'',t') =$$

$$\int_{-\infty}^{\infty} dt'' \; A_T(t,t'')B^<(t'',t') + \int_{-\infty}^{\infty} dt'' \; A^<(t,t'')B_{T*}(t'',t') =$$

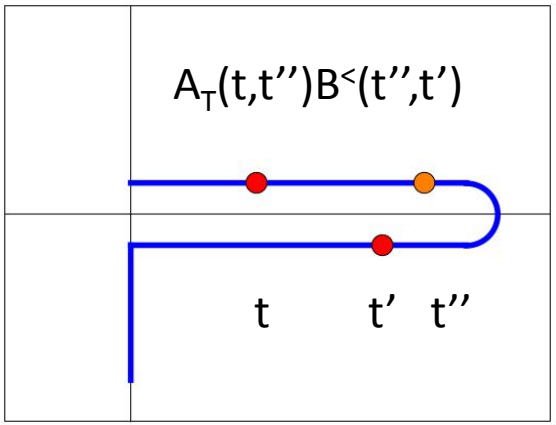
$$\int_{-\infty}^{\infty} dt''\{ \; A_T(t,t'')B^<(t'',t') + \; A^<(t,t'')B_{T*}(t'',t')\}$$

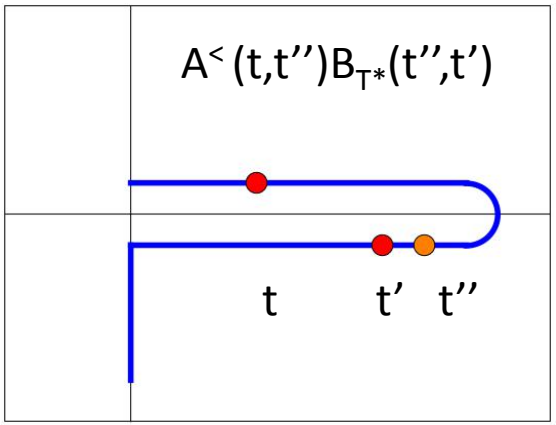
$$C^< = A_T B^< + A^< B_{T*}$$

$$A^T = A^R + A^<; \;\; B_{T*} = B^< - B^A$$

$$\therefore C^< = A^R B^< + A^< B^A$$

$$\int_{-\infty}^{\infty} dt''\{ \; A^R(t,t'')B^<(t'',t') + \; A^<(t,t'')B^A(t'',t')\}$$





Products of two and three Keldysh objects-> access a whole zoo of Green Functions

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Langreth Rules

$D \sim A\ B$	$D \sim A\ B\ C$
$(A\ B)^{<} \sim A^{R}B^{<} + A^{<}B^{A}$	$(A\ B\ C)^{<} \sim A^{R}B^{R}C^{<} + A^{<}B^{A}C^{A} + A^{R}B^{<}C^{A}$
$(A\ B)^{>} \sim A^{R}B^{>} + A^{>}B^{A}$	$(A\ B\ C)^{>} \sim A^{R}B^{R}C^{>} + A^{>}B^{A}C^{A} + A^{R}B^{>}C^{A}$
$(A\ B)^{R} \sim A^{R}B^{R}$	$(A\ B\ C)^{R} \sim A^{R}B^{R}C^{R}$
$(A\ B)^{A} \sim A^{A}B^{A}$	$(A\ B\ C)^{A} \sim A^{A}B^{A}C^{A}$

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Equations of Motion

Project the Dyson equation from Keldysh contour to real time :
Keep U explicitly as a perturbation here

$$G = G_0 + G_0(U + \Sigma)G$$

Dyson equation on Keldysh contour

$$G^R = G_0^R + G_0^R U G^R + G_0^R \Sigma^R G^R = \{G_0^{R\ -1} - U - \Sigma^R\}^{-1}$$

First Keldysh equation

$$G^< = G_0^< + G_0^R U G^< + G_0^< U G^A + G_0^R \Sigma^R G^< + G_0^R \Sigma^< G^A + G_0^< \Sigma^A G^A$$

$$G^< = \{1 + G^R(U + \Sigma^R)\} G_0^< \{1 + (U + \Sigma^A)G^A\} + G^R \Sigma^< G^A$$

Vanishes in steady state, no ISCs

Second Keldysh equation

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Equations of Motion

$$\left\{ i\hbar\left(\frac{\partial}{\partial\tau}\right) - H_0(\mathbf{x}; -i\hbar\nabla') \right\} G_0(\mathbf{x},\tau;\mathbf{x}',\tau') = \delta(x-x')\delta(\tau,\tau')$$

In real time domain

$$\left\{ i\hbar\frac{\partial}{\partial t} + \frac{\hbar^2\nabla^2}{2m} \right\} G_0^R(\mathbf{x},t;\mathbf{x}',t') = \delta(\mathbf{x}-\mathbf{x}')\delta(t-t')$$

$$\left\{ i\hbar\frac{\partial}{\partial t} + \frac{\hbar^2\nabla^2}{2m} \right\} G_0^<(\mathbf{x},t;\mathbf{x}',t') = 0$$

$+conjugate\ \ equations\ \ in\ \ x',t'$

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Equations of Motion: stationary case

The stationary case is determined by transforming to the time variables T_1= (t-t'); setting T_2=(t+t')/2 and setting time derivatives in d/dT_2 to zero. Finally introduce energy-dependent NEGF by Fourier transforming over T_1.

$$G^<(\mathbf{x},\mathbf{x}';E) = \lim_{T_2 \to 0} \int_{-\infty}^{\infty} dT_1 \exp(iET_1/\hbar)\, G^<(\mathbf{x},\mathbf{x}';T_1,T_2)$$

$$G^R = \{G_0^{R\ -1} - U - \Sigma^R\}^{-1}$$

$$G_0^{R\ -1} = \{E + i\eta - H_0\}$$

$$G^< = G^R \Sigma^< G^A$$

Huge simplification
IF self-energies
Are diagonal

$$\{E + \hbar^2 \frac{\nabla^2}{2m} - U(\mathbf{x})\} G^R(\mathbf{x},\mathbf{x}';E) = \delta(\mathbf{x}-\mathbf{x}') + \int d\mathbf{x}''\ \Sigma^R(\mathbf{x},\mathbf{x}'';E) G^R(\mathbf{x}'',\mathbf{x}';E)$$

$$\{E + \hbar^2 \frac{\nabla^2}{2m} - U(\mathbf{x})\} G^<(\mathbf{x},\mathbf{x}';E) = \int d\mathbf{x}''\ \Sigma^<(\mathbf{x},\mathbf{x}'';E) G^A(\mathbf{x}'',\mathbf{x}';E) + \int d\mathbf{x}''\ \Sigma^R(\mathbf{x},\mathbf{x}'';E) G^<(\mathbf{x}'',\mathbf{x}';E)$$

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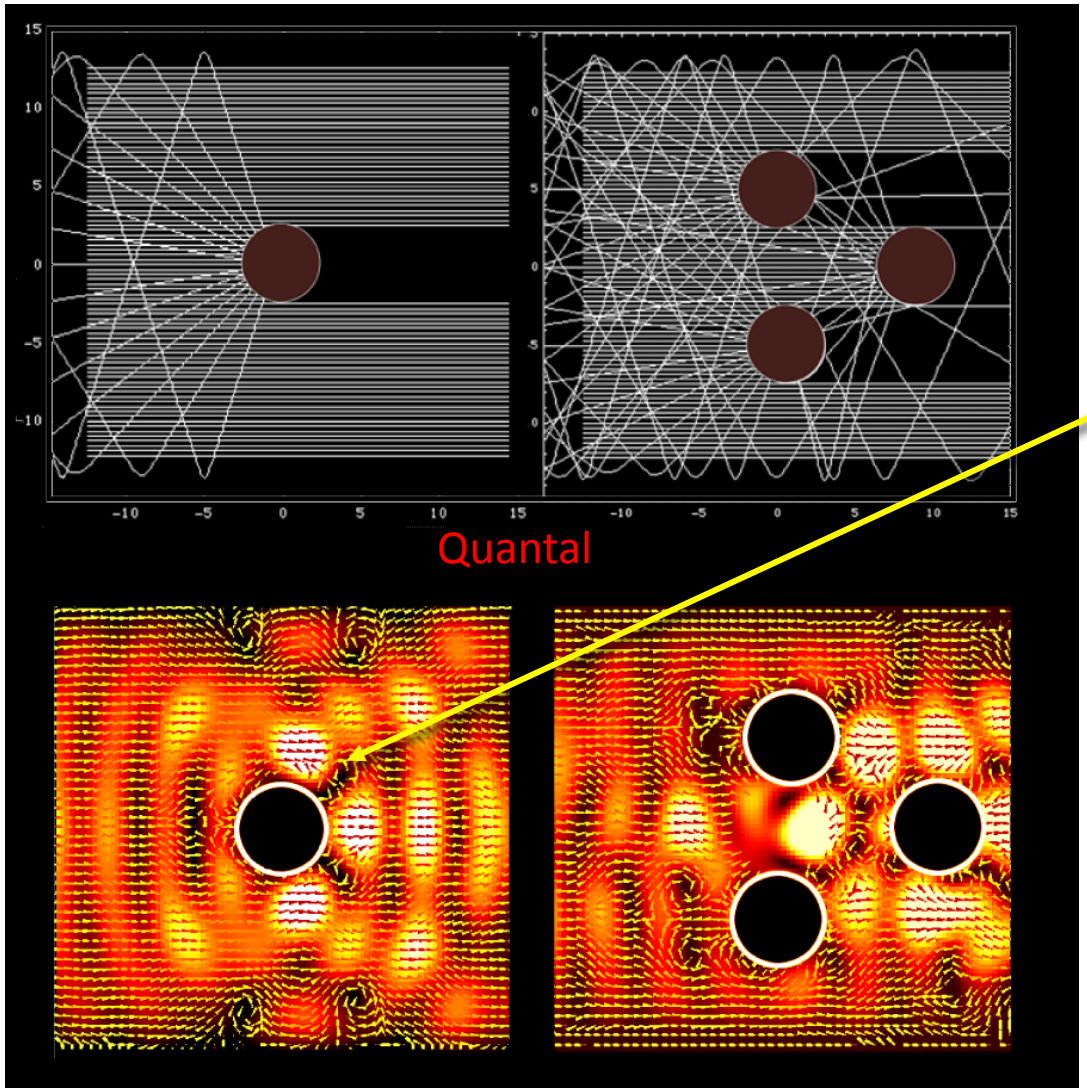
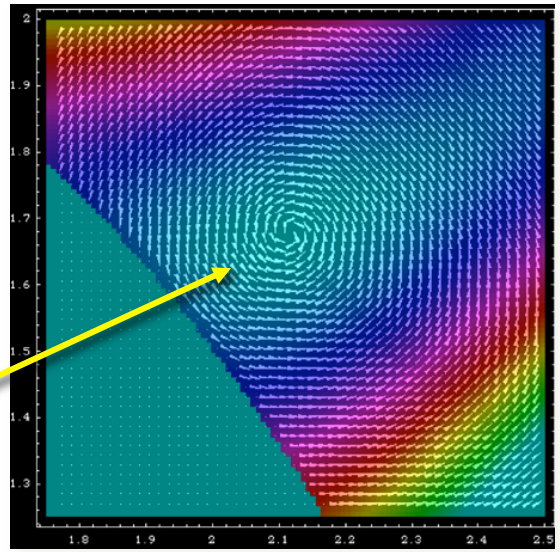
Appendix 6: Visualisation of Vortex flows (analytical Green functions)

Classical





Open meandering flow between vortices and impurities

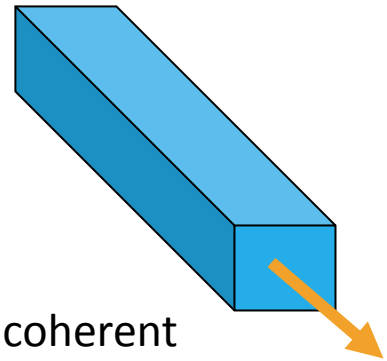
Hard sphere model

J R Barker 2003

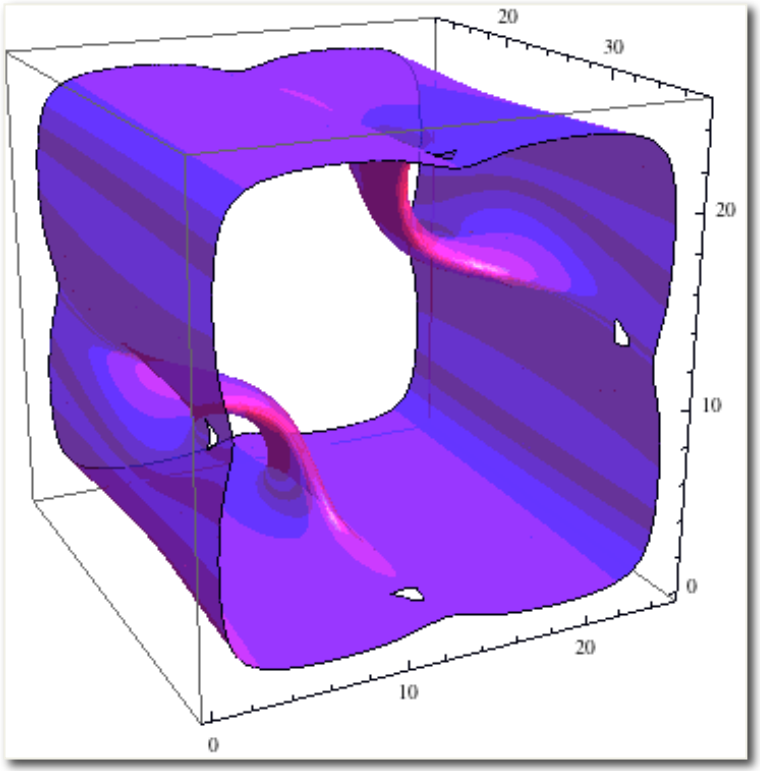
John R Barker
2013 IWCE

Time dependent vortex flow in 3D nanowire: vortex tubes

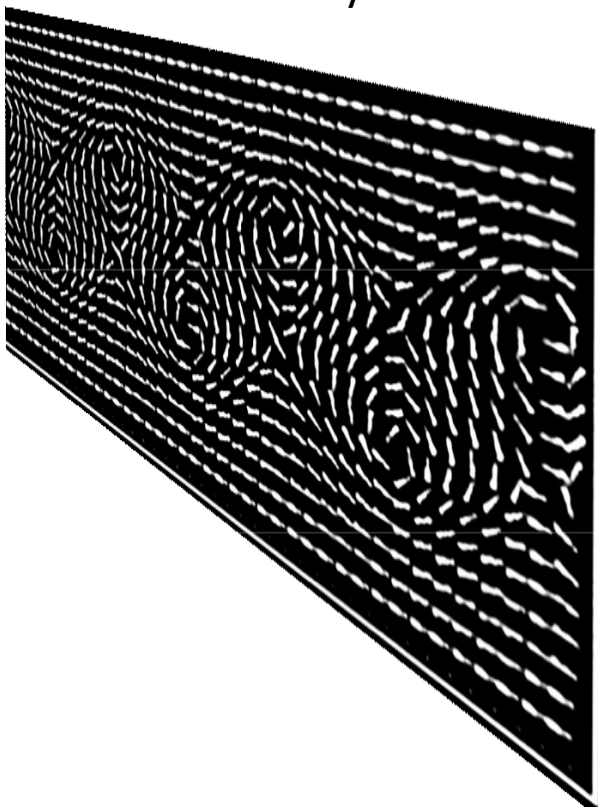
silicon nanowire



coherent time-dependent flow



Velocity field

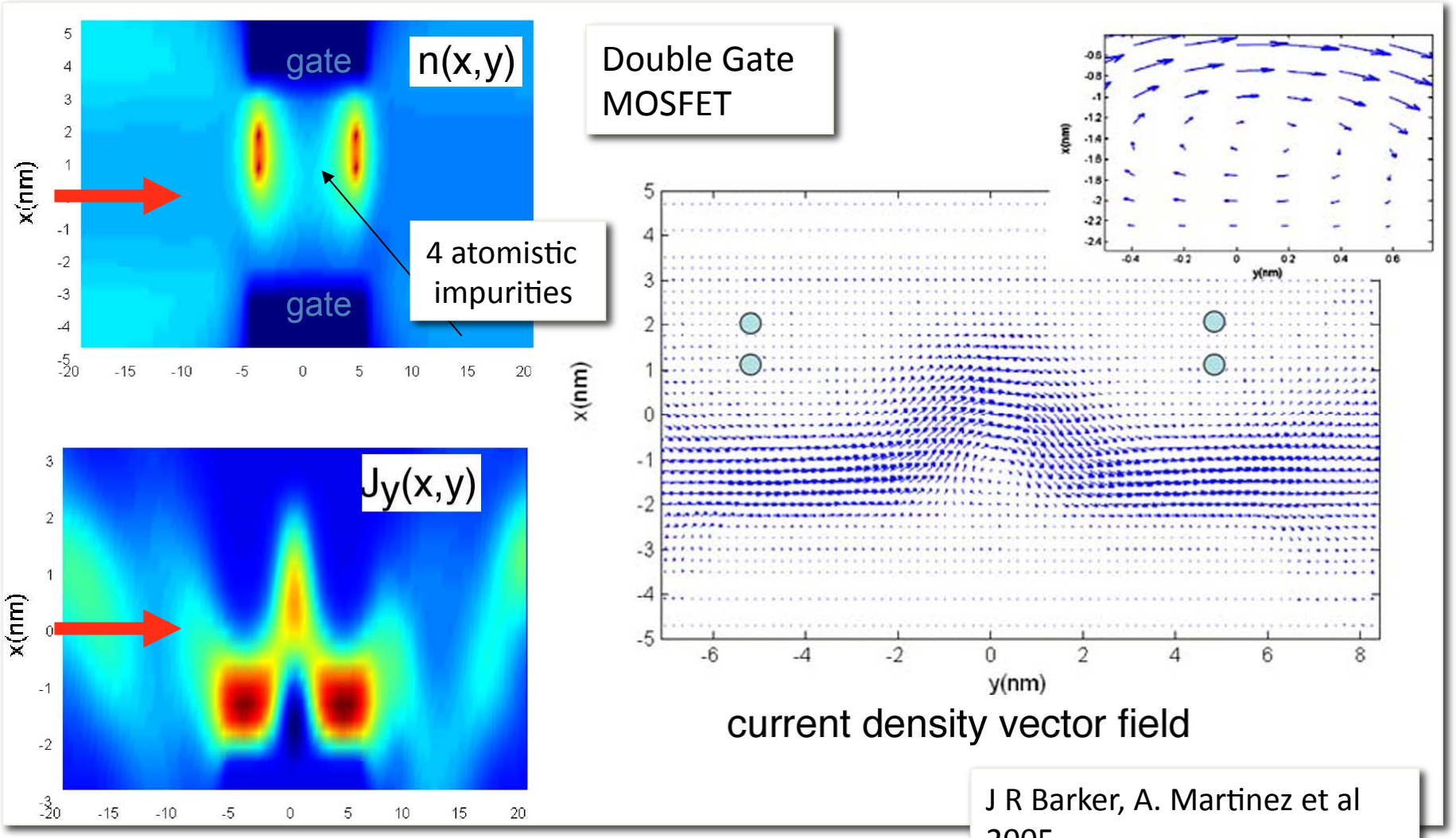


Arises from superposition of 2 different travelling Waves in 2 different transverse (confined) states

J R Barker
1998

John R Barker
2013 IWCE

Exotic effects: quantized vortices from quantum ballistic flow at room temperature shows even in macroscopic current.



J R Barker, A. Martinez et al 2005

John R Barker
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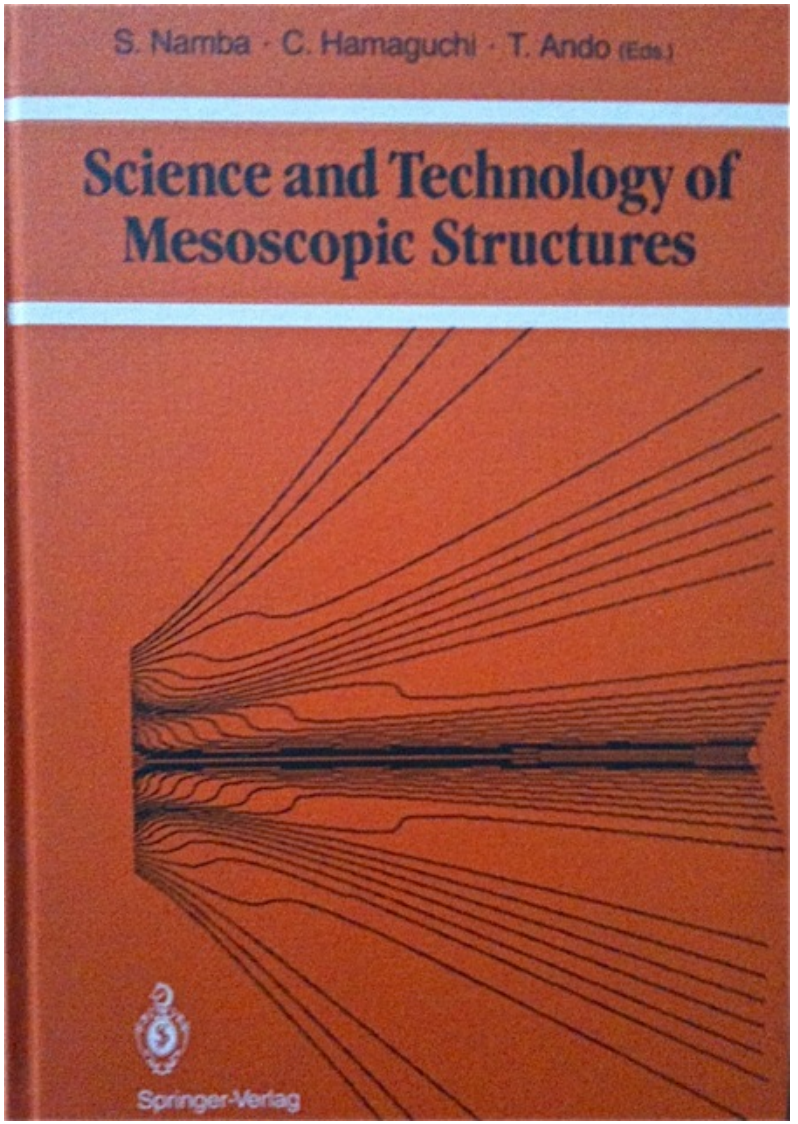
Particle “Trajectories” from velocity field - 2 slit experiment

Velocity flow fields were discussed in:

BARKER, J.R. ”On the pilot-field representation of quantum transport theory”,
Semiconductor Sci.Tech. 9 911-917 (1994).

BARKER, J.R., ROY, S., BABIKER, S. “Trajectory representations, fluctuations and stability of single electron devices”,
Science and Technology of Mesoscopic Structures’,
Namba, S., Hamaguchi, C., Ando, T., eds.,
(London:Springer Verlag, Ch 22, 213-231 (1992)



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Experimental Observation of Photon "flow fields or Trajectories"- 2 slit experiment

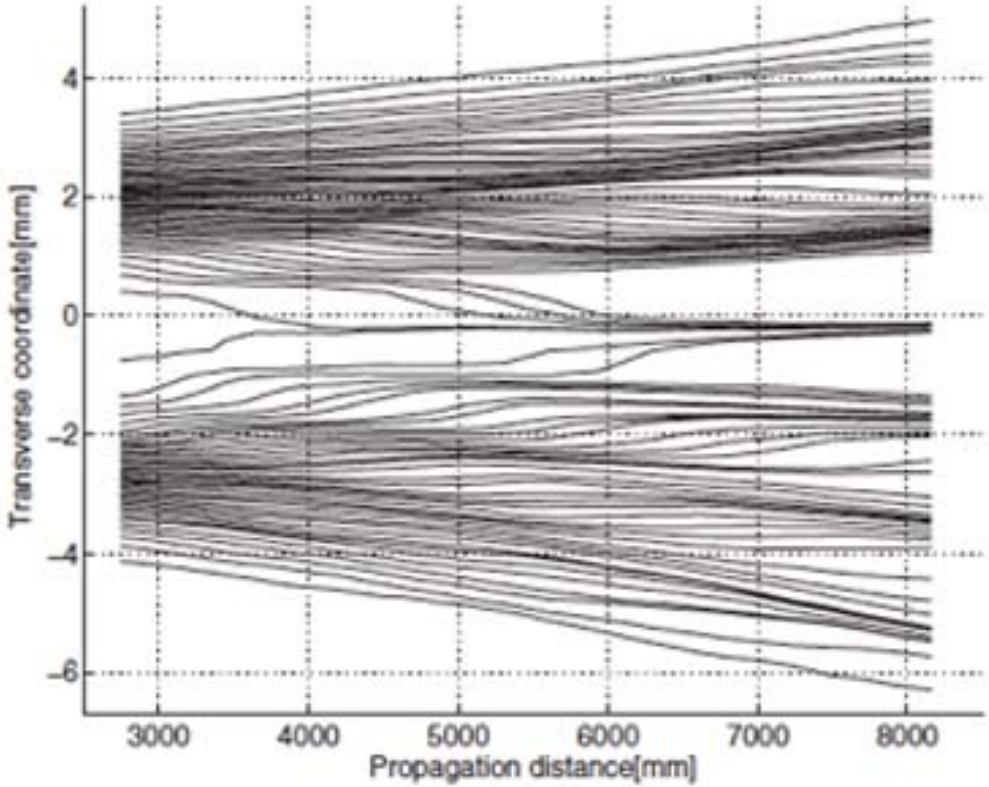

Fig. 3. The reconstructed average trajectories of an ensemble of single photons in the double-slit apparatus. The trajectories are reconstructed over the range 2.75 ± 0.05 to 8.2 ± 0.1 m by using the momentum data (black points in Fig. 2) from 41 imaging planes. Here, 80 trajectories are shown. To reconstruct a set of trajectories, we determined the weak momentum values for the transverse x positions at the initial plane. On the basis of this initial position and momentum information, the x position on the subsequent imaging plane that each trajectory lands is calculated, and the measured weak momentum value k_x at this point found. This process is repeated until the final imaging plane is reached and the trajectories are traced out. If a trajectory lands on a point that is not the center of a pixel, then a cubic spline interpolation between neighboring momentum values is used.

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Appendix 7: Selected Application

The variability problem: short channel double-gate Si MOSFETs

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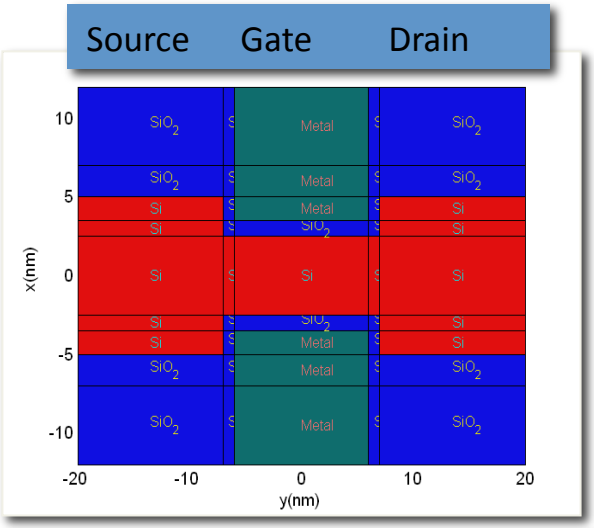
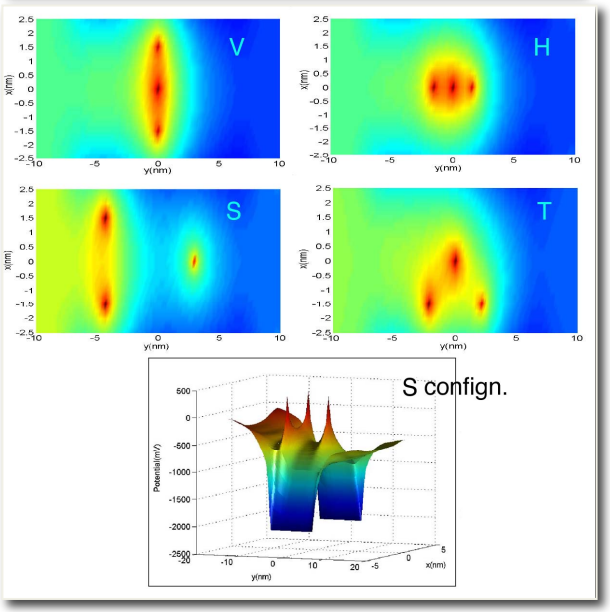
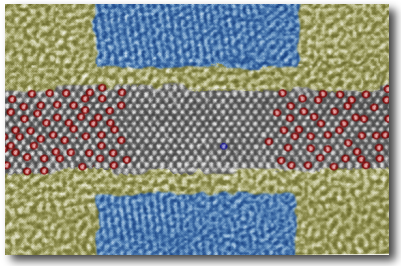
Atomistic effects





atomistic
impurity distribution

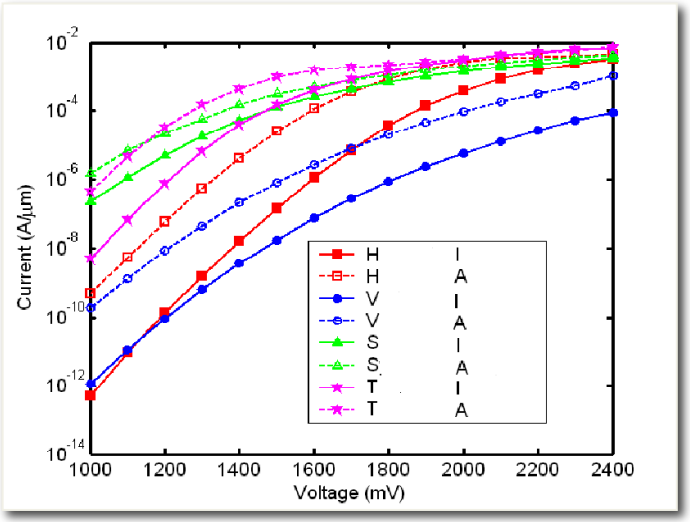


2D NEGF
simulations

Martinez and Barker et al

IEDM 2005
NPMS-7/SIMD5
J. Phys. Conf . **38**
192-195 (2006)

treat impurities exactly

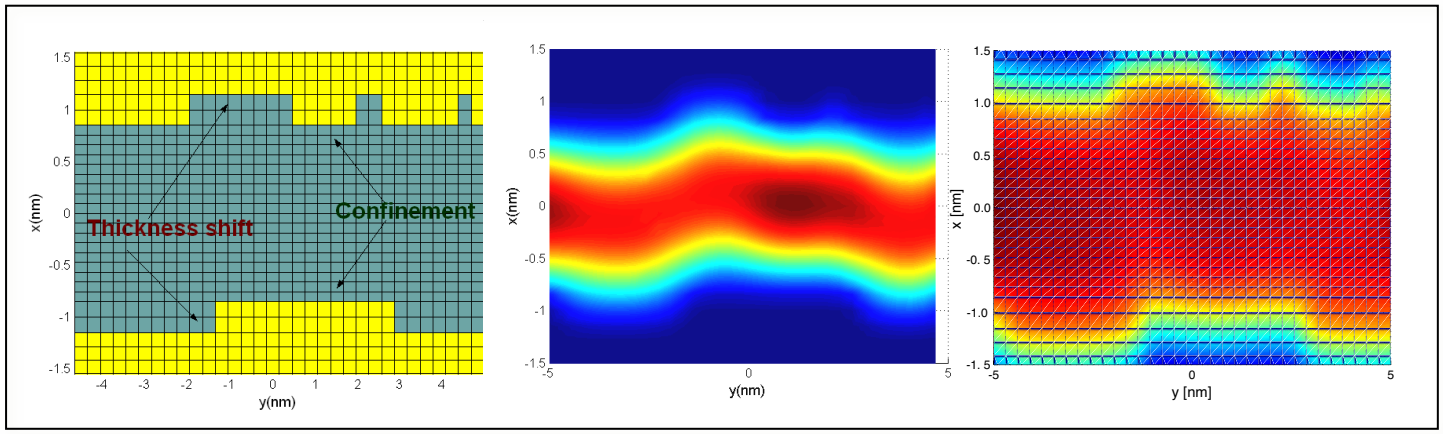


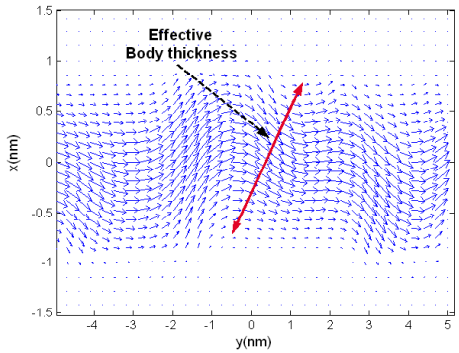
Large shifts in threshold voltage and conductance due to micro-distribution of impurity atoms

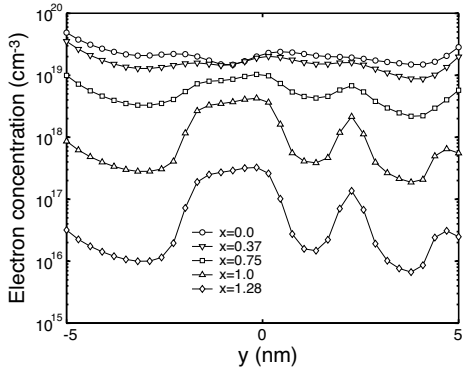
Interface roughness

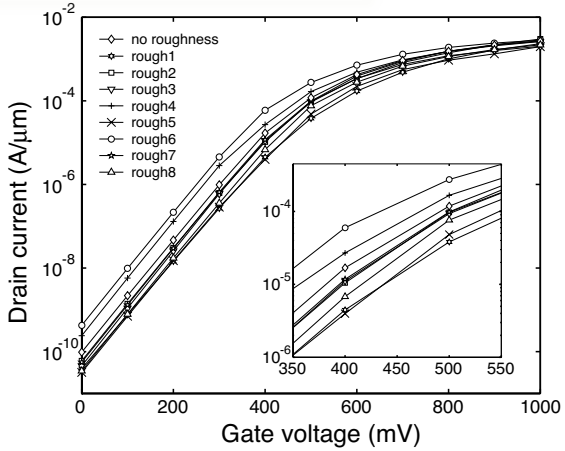
MARTINEZ, A., SVIZHENKO, A., ANANTRAM, M.P., BARKER, J.R., BROWN, A.R., and ASENOV, A.,
'A study of the effect of the interface roughness on a DG-MOSFET using a full 2D NEGF technique'
The International Electronic Devices Meeting IEDM 2005, San Francisco, December, 2005.

2D NEGF simulations









Electron and current density landscapes show strong inhomogeneity for rough interfaces.
Devices with different generated randomly generated roughness patterns have been compared.
At nano-scales the effects of the specific profile of the surface roughness do not self-average.
The total macroscopic current pattern follows the microscopic detail of the roughness.
While the related threshold voltage fluctuations of the order of 100mV on average,
the subthreshold slope remains quite similar between the different devices.

Random dopant aggregation in source-drain extensions in double gate MOSFETs

John R Barker
2013 IWCE

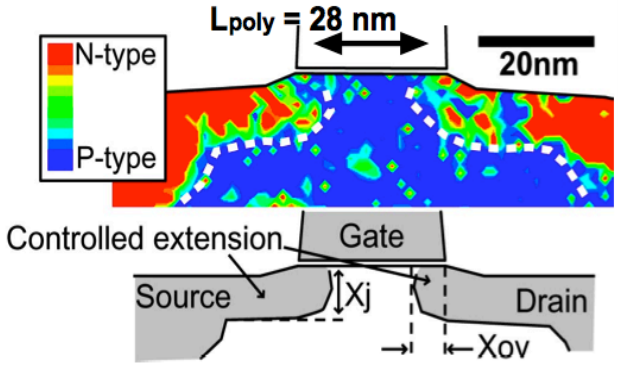
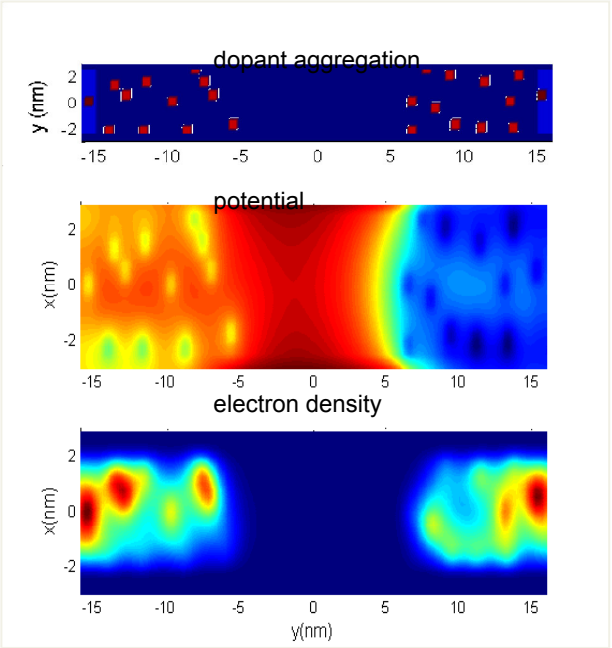
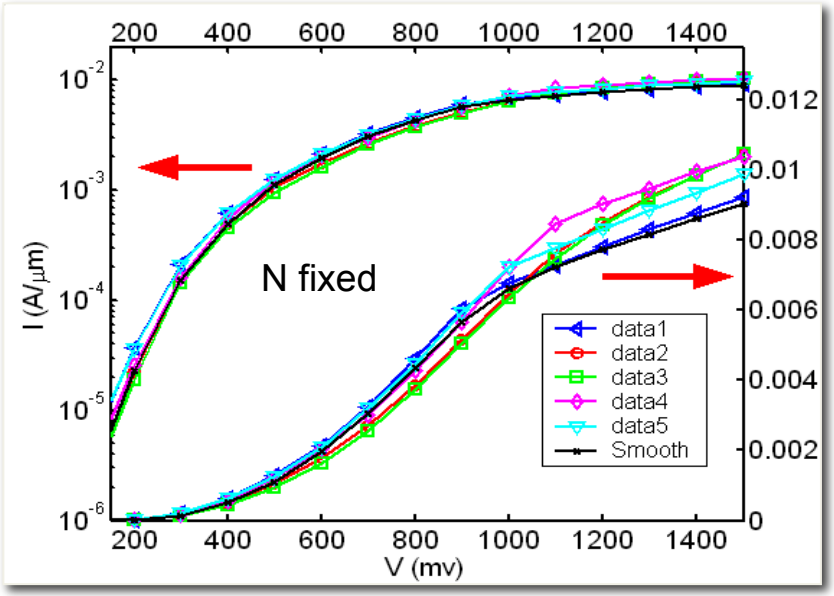


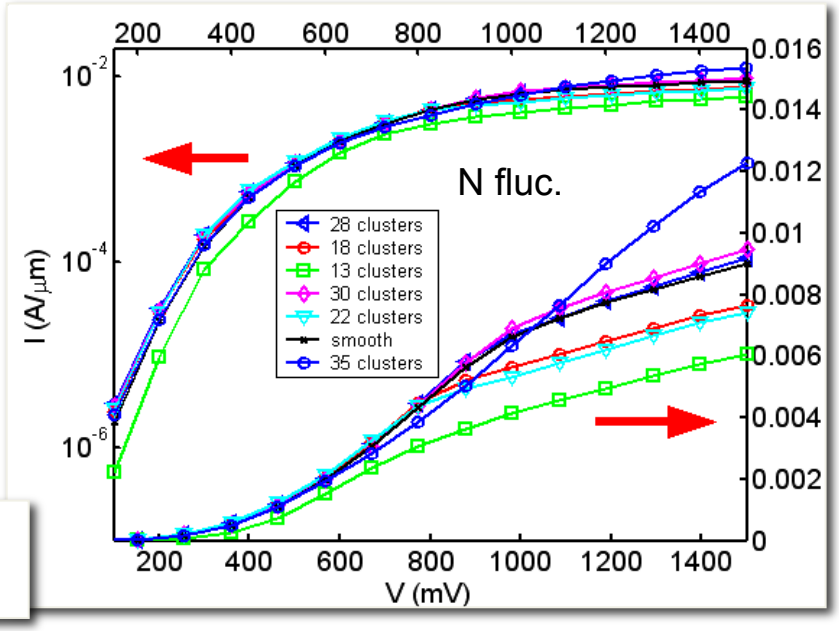
Fig. 9 Carrier profile around S/D extension region in n-MOSFET with gate length of 28 nm. This image was taken at negative gate bias voltage and under measuring conditions sensitive to n-type region. Overlap length of S/D extension region (X_{ov}) is about 6 nm.

From: H.Fukotome, Y. Momiyama, E. Yoshida, M. Okuno, T.Itakura and T. Aoyama
IEDM Technical Digest (2005)



Fluctuations in total number of dopants has a stronger effect (50% fluctuation in on-current) than purely positional fluctuations (10%). The computed on-current fluctuations are significantly larger than the classical predictions.



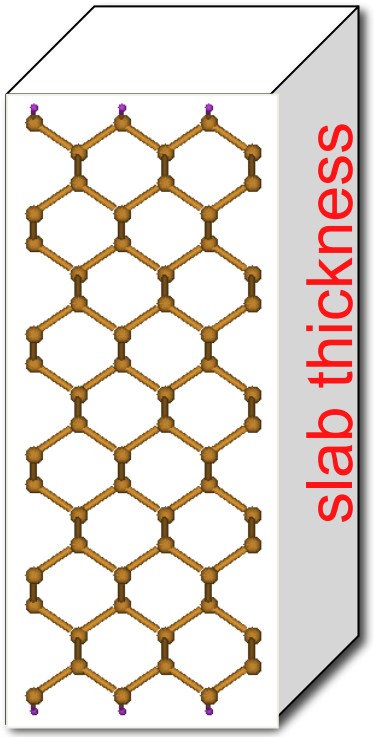


Martinez , Barker et al
IEEE Trans Nanotechnology
6 438-445 (2007).

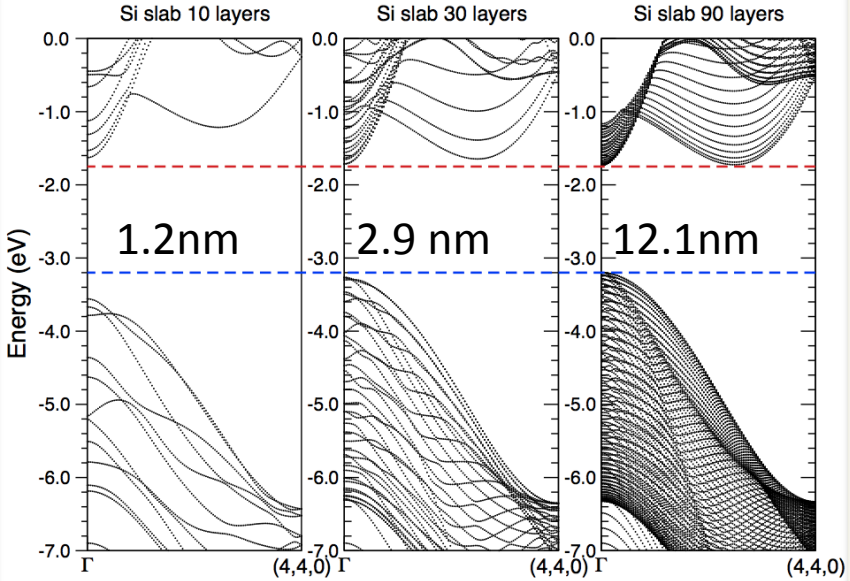
Atomistic treatment of silicon channel

John R Barker
2013 IWCE

University of Glasgow



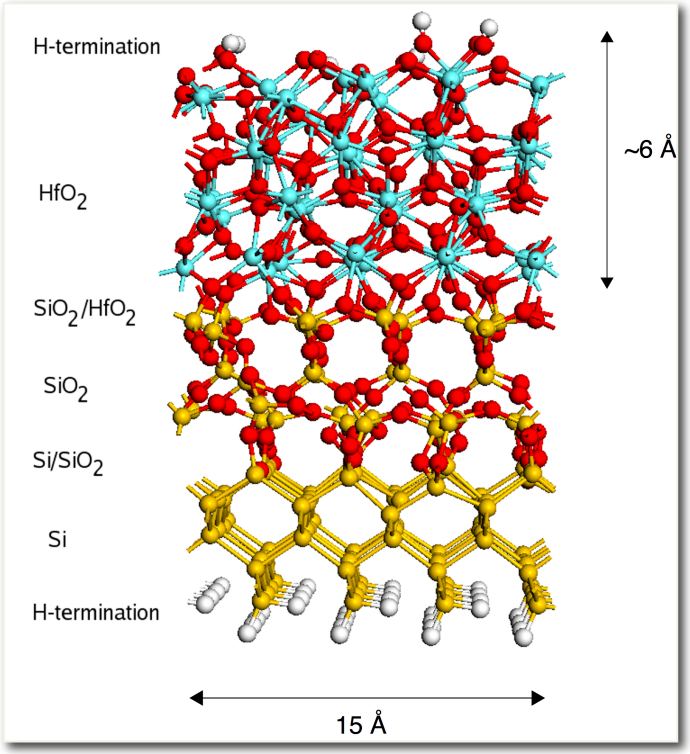
Si Slab



Energy levels

Shrinking slab

DFT calculations



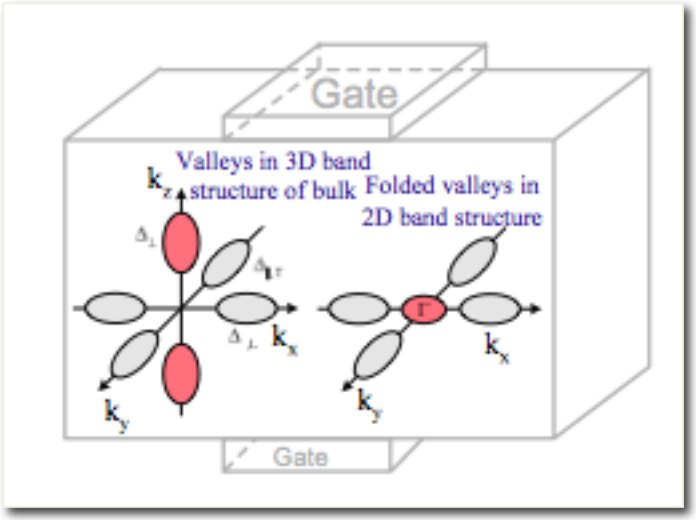
Complex interface

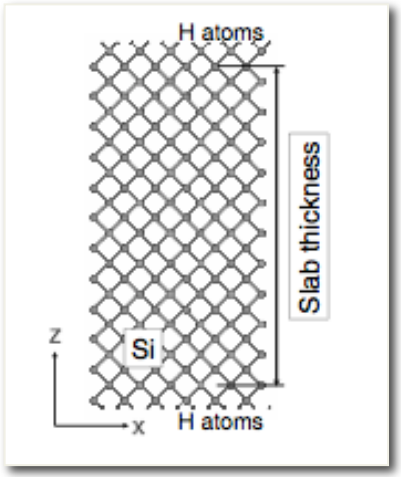
IEEE TRANSACTIONS ON NANOTECHNOLOGY (2008)

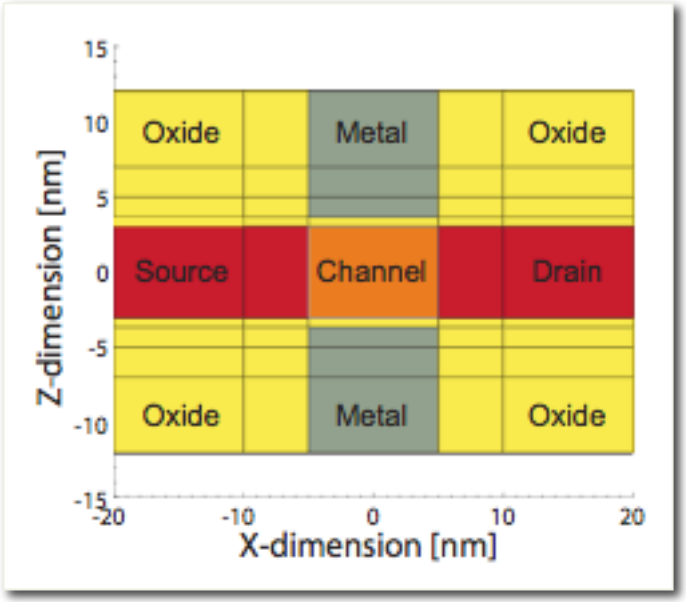
Impact of Body-Thickness-Dependent Bandstructure on Scaling of Double Gate MOSFETs: a DFT/NEGF study

A. Martinez, K. Kalna, P. V. Sushko, A. L. Shluger, J. R. Barker, and A. Asenov, Senior Member IEEE

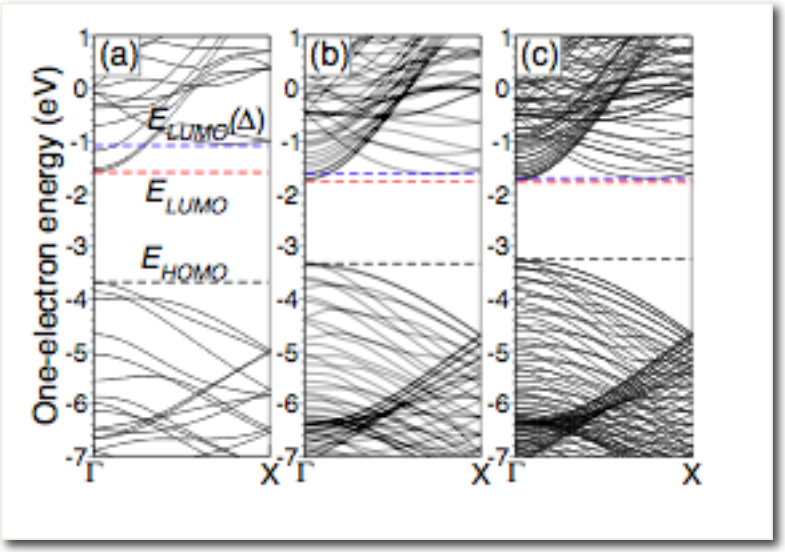
University of Glasgow
John R Barker
2013 IWCE







***Abstract*—First principles density functional theory has been used to calculate the 2D bandstructure of Si slabs with different thicknesses. From the calculated 2D bandstructure, electron longitudinal and transverse effective masses have been extracted as a function of the slab thickness. These thickness dependent electron effective masses have then been used to simulate I_D-V_G characteristics of scaled, sub-10 nm double gate (DG) MOSFETs and to compare them with the results obtained using bulk masses. The channel thickness dependence of the Si bandstructure starts to affect noticeably DG MOSFET performance at channel lengths below 10 nm, lowering the on-current by approximately 10% for transistors with a body thickness of 2.6 nm, and by 20% for transistors with a body thickness of 1.3 nm. On the other hand, the subthreshold swing is improved by 10% in the 6 nm gate length DG MOSFET and by 15% in the 4 nm gate length device. Finally, the impact of thickness dependent effective masses has been related to the behaviour of the transmission coefficients.**



The Data!

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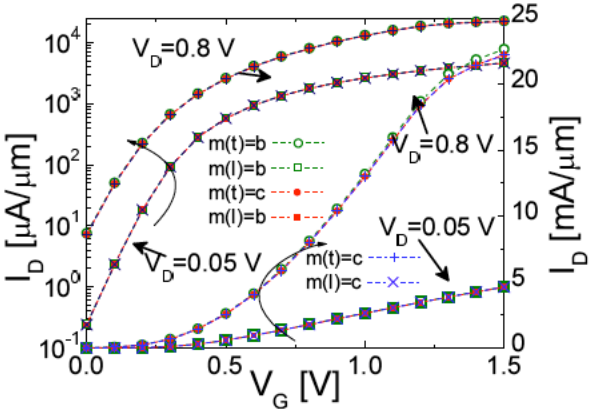

Fig. 8. I_D-V_G characteristics at indicated drain voltages for the 10 nm gate length, 6.1 nm thick body DG MOSFET obtained from the 2D NEGF simulations assuming a ballistic transport along the channel. The behaviour of the on-current is shown on linear scale while the subthreshold behaviour is presented on logarithmic scale opposite. The impact of confined (c) masses in transverse [m(t)] and longitudinal [m(l)] transport directions is compared with that of bulk (b) masses.

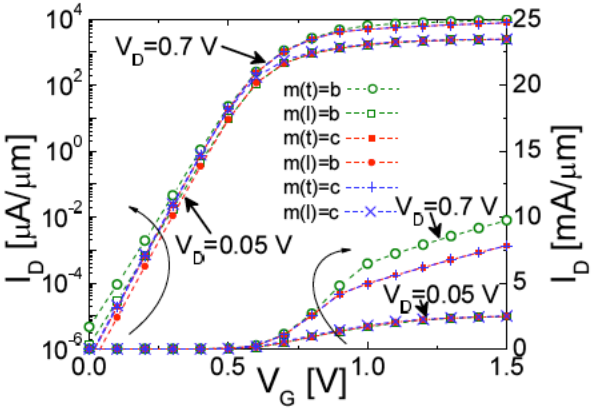

Fig. 10. I_D-V_G characteristics at indicated drain voltages for the 6 nm gate length, 1.3 nm thick body DG MOSFET are plotted on linear scale for the on-current regions and on logarithmic scale for the subthreshold region comparing the effect of progressive replacement of transverse (t) and longitudinal (l) bulk (b) Si masses with their respective confined (c) values.

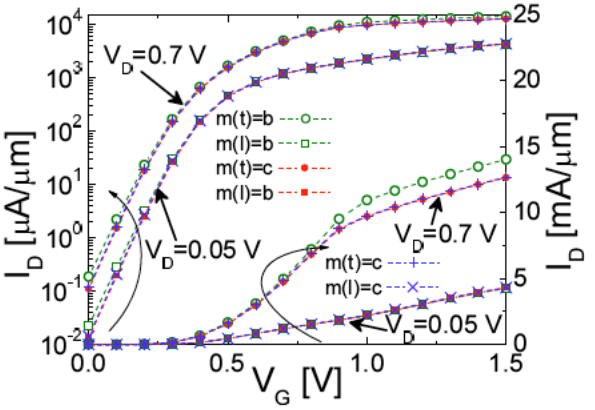

Fig. 9. I_D-V_G characteristics at a low drain bias of 0.05 V and a high drain bias of 0.7 V for the 6 nm gate length, 2.6 nm thick body DG MOSFET shown on linear and logarithmic scales, respectively. The effect of confined (c) and bulk (b) Si masses in transverse [m(t)] and longitudinal [m(l)] transport directions is compared.

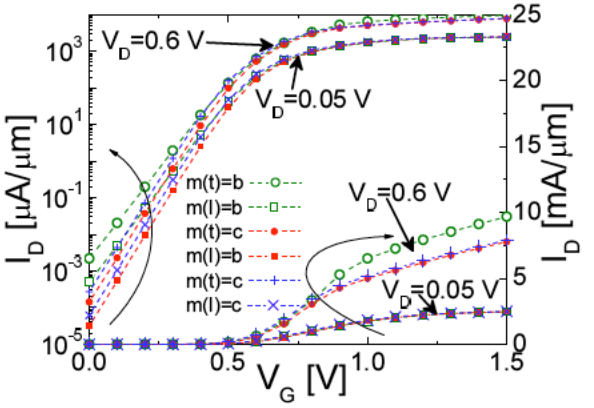

Fig. 11. I_D-V_G characteristics at a low drain bias of 0.05 V and at an expected operational bias of 0.6 V for the 4 nm gate length, 1.3 nm body DG MOSFET. Again, results are plotted on linear and logarithmic scales in order to evaluate the on-current and subthreshold regions, respectively. The bulk (b) values of transverse [m(t)] and longitudinal [m(l)] electron effective masses are replaced with their confined (c) values as indicated.

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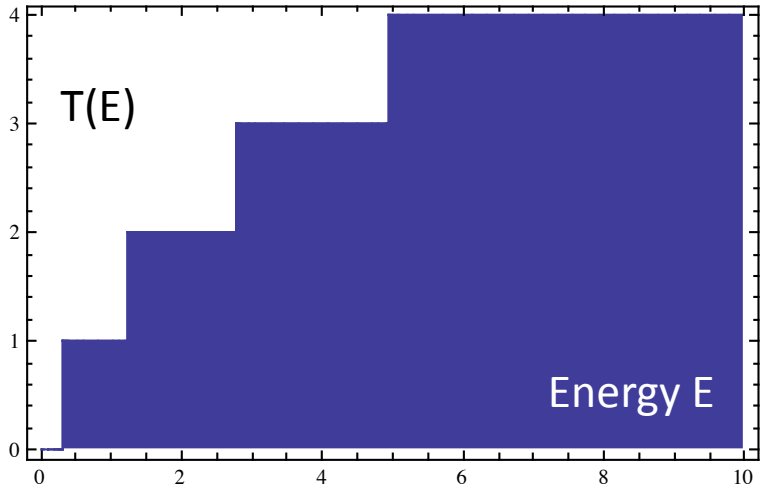
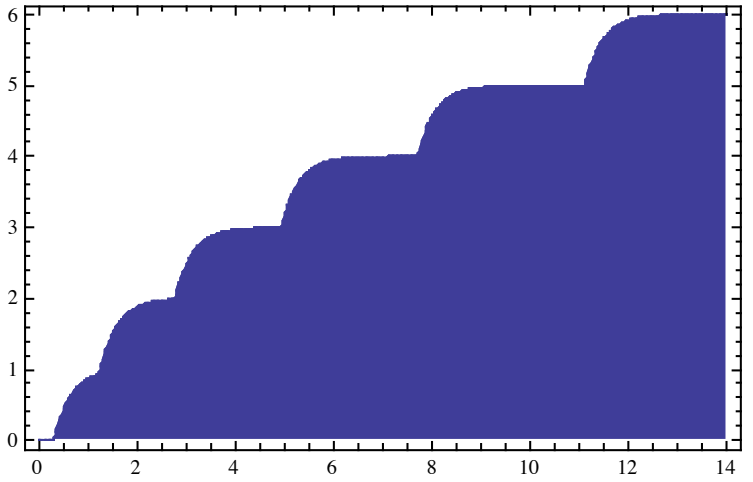
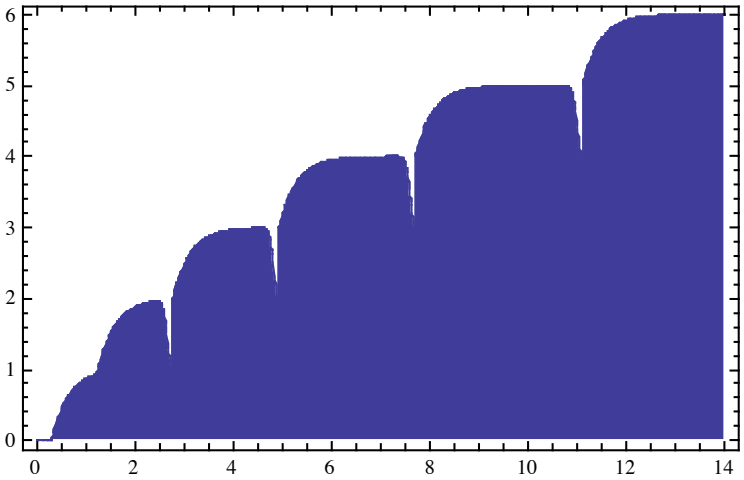
Appendix 8: Transmission curves and atomistic dopants
What to expect



no charged dopants in channel



repulsive potential

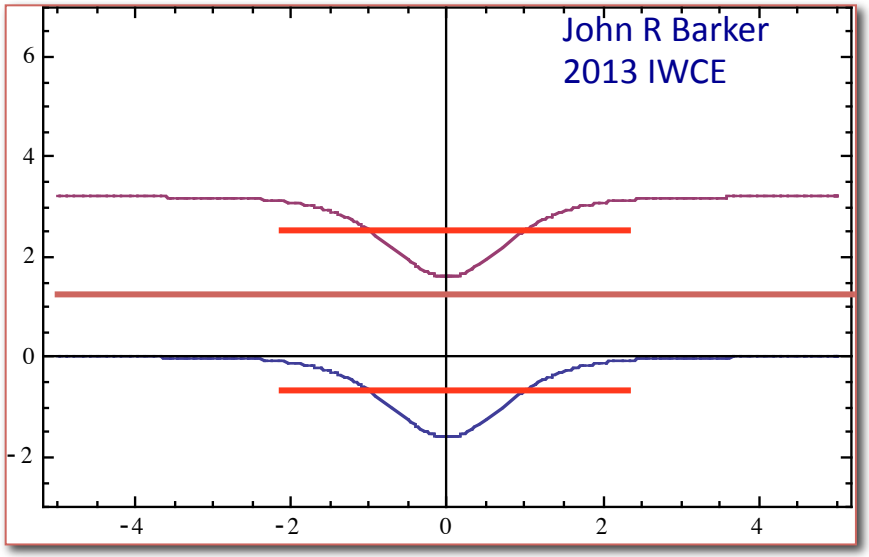


simple attractive potential

Transmission function T(E)

Special case $E_1<E<E_2$

first mode propagates,
second mode evanescent



Energies of bound states

$$E = E^*_N = E_2 - \left(\alpha^2 \frac{\hbar^2}{2m}\right)\left\{-(1+2N) + \sqrt{1+\frac{8mW_{22}}{(\alpha\hbar)^2}}\right\}$$

$$W_{mn} = -\left(\frac{\gamma\hbar^2}{2m}\right)V^{mn}{}_{trans}$$

$$N = 0,1,2,\ldots$$

Transmission coefficient

$$T(E) = |t|^2 \frac{(E - E^*_N)^2}{(E - E^*_N - \Delta_N)^2 + \Gamma_N^2}$$

background transmission

generalised Fano resonances

Transmission function T(E)

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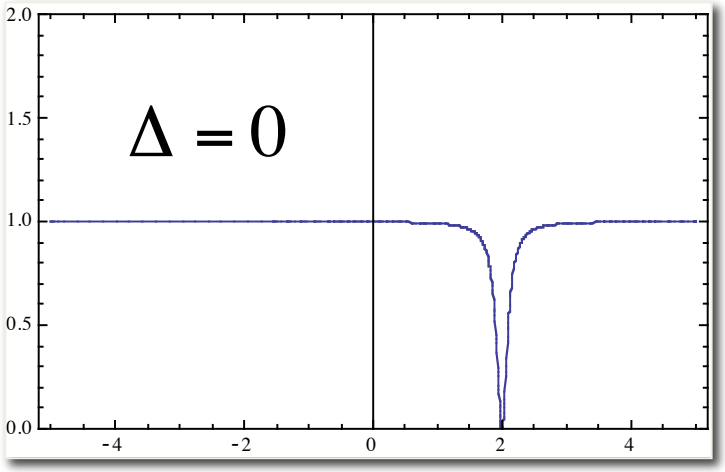
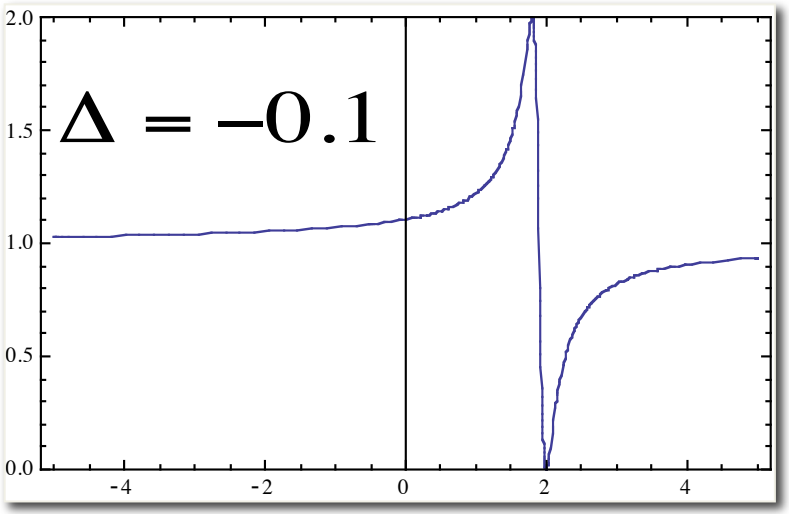
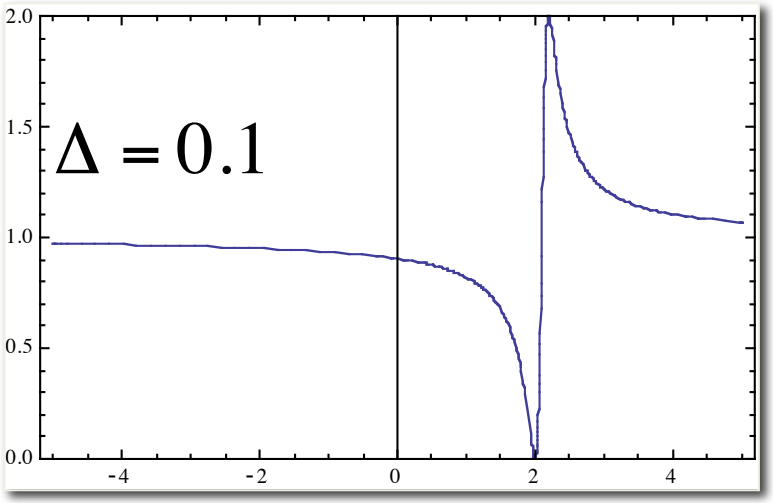
case t=1



Breit-Wigner resonance





Asymmetric Fano Resonances

Transmission function T(E)

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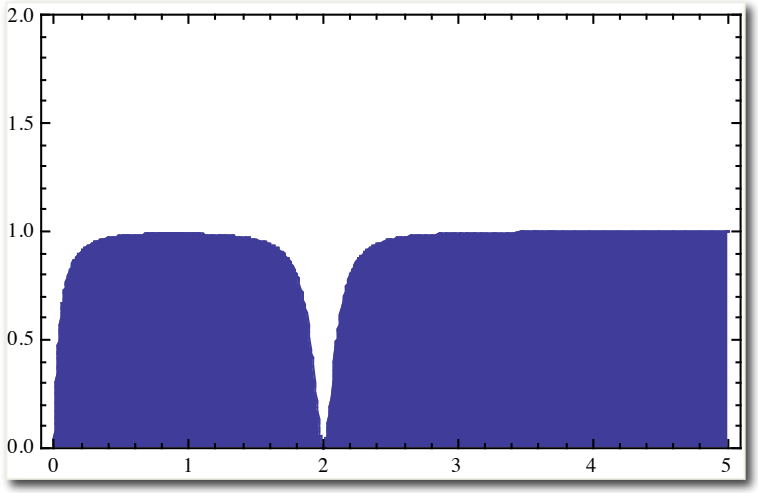
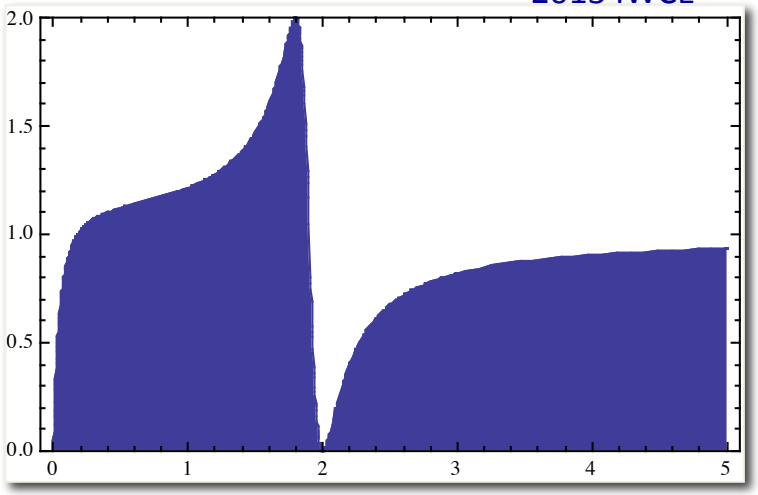
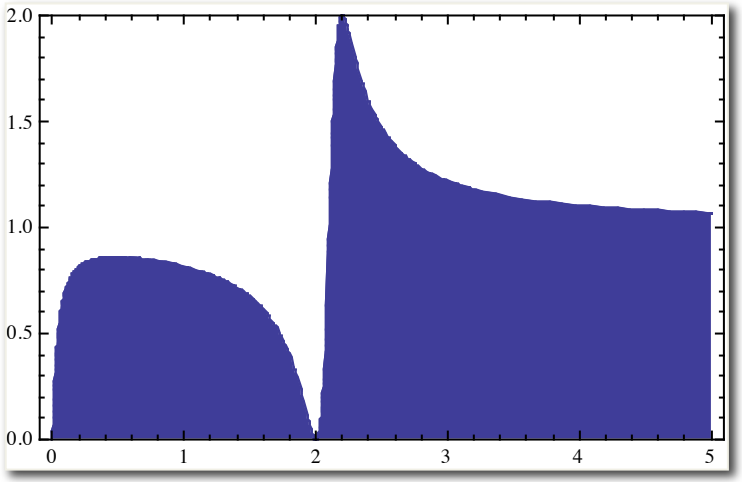
realistic t







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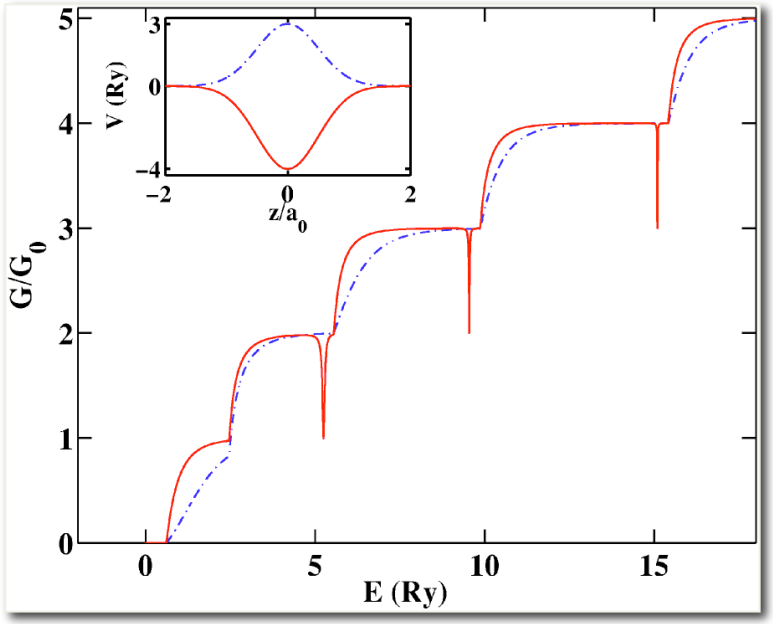
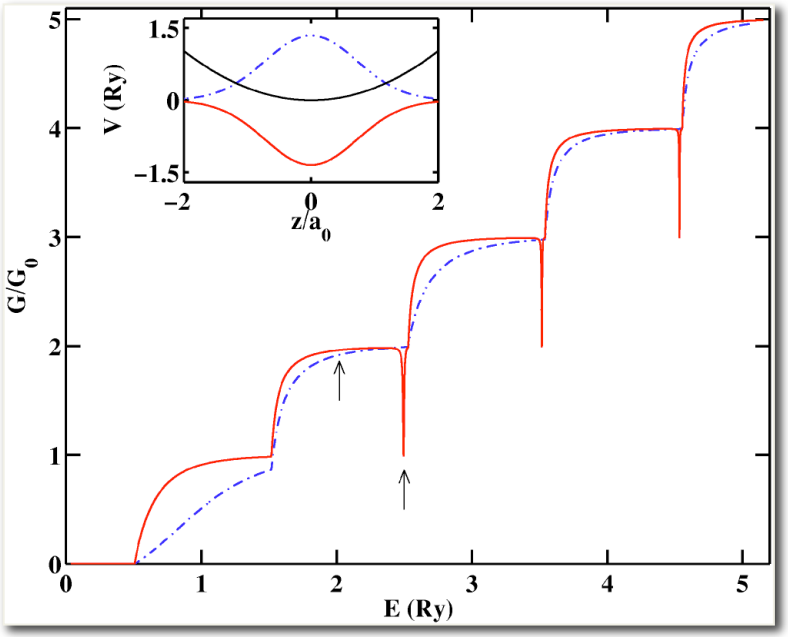
PHYSICAL REVIEW B **70**, 245308 (2004)

Coherent electronic transport in a multimode quantum channel with Gaussian-type scatterers

Jens Hjorleifur Bardarson,[1] Ingibjorg Magnusdottir,[1] Gudny Gudmundsdottir,[1] Chi-Shung Tang,[2] Andrei Manolescu,[1] and Vidar Gudmundsson[1]



hard walled



parabolic wall

2D, numerical non self-consistent potential T(E) only

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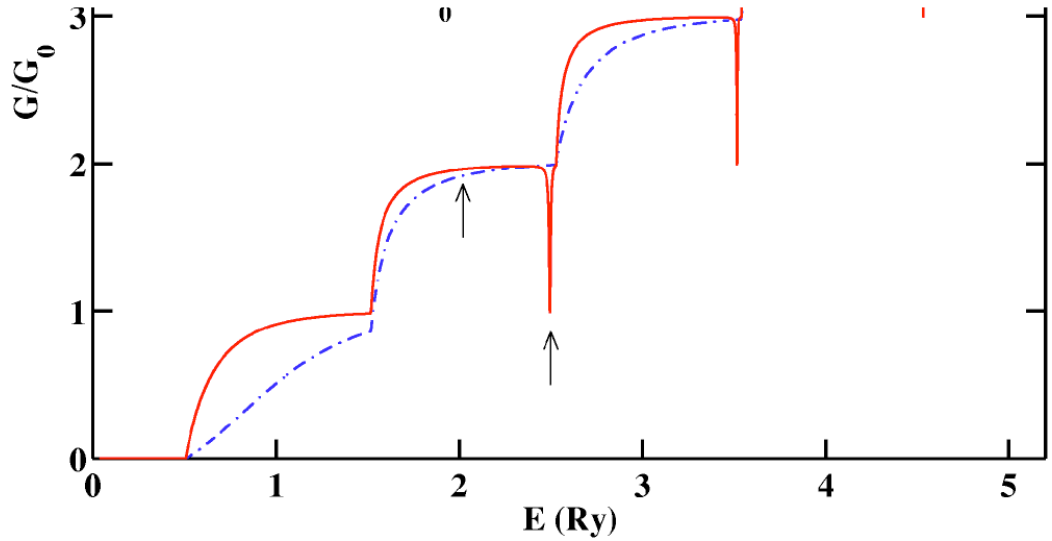
Minima in transmission just before next mode.
Back-scattering by a quasi-bound state originating from an evanescent mode in next energy sub-band.



2D model

Coupled mode interpretation of lack of minimum in first sub band
Coupling between first propagating mode and quasi-bound state in the first evanescent mode gives a zero matrix element because wave functions for the first and second transverse modes are even and respectively: thus no minimum in transmission.

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PHYSICAL REVIEW B 72, 195333 (2005)

Resonances in electronic transport through a quantum wire with impurities and variable cross-sectional shape

Vassilios Vargiamidis* and Hariton M. Polatoglou

Detailed discussion of Fano resonances

for 3D analytical model based on

Poschl-Teller potentials.

Non-self consistent

Only computes transmission

No device profile

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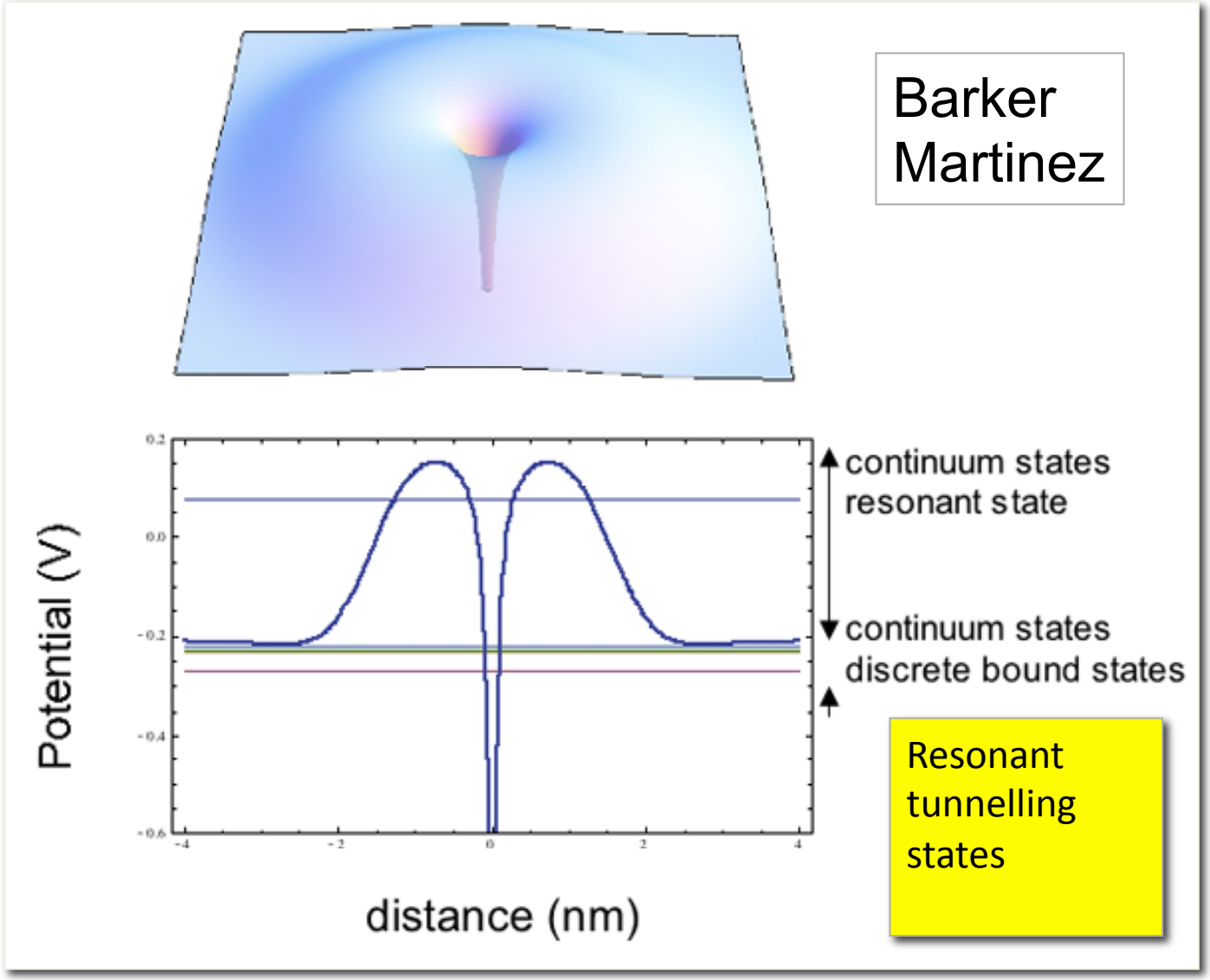
Attractive Coulombic impurity in channel centre +
gate potential: realistic nanowire device-self consistent



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M. ALDEGUNDE, A. MARTINEZ and J. R. BARKER
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2.*Study of Discrete Doping Induced Variability in Junctionless Nanowire MOSFETs using Dissipative Quantum Transport Simulations*
M. ALDEGUNDE, A. MARTINEZ and J. R. BARKER
IEEE Electron Device Letters, Vol. 33, 194 (2012)

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MARTINEZ, A.; ALDEGUNDE, M.; KALNA, K.; BARKER, J. R.
IEEE Publication: Proceedings 15th International Workshop on ComputationalElectronics (2102)
IEEE Catalog Number: CFP12462-PRT (ISBN: 978-1-4673-0705-5), pp 102-105 (2012)

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J R BARKER, A MARTINEZ and M ALDEGUNDE
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A. MARTINEZ, N. SEOANE, M. ALDEGUNDE, A. R. BROWN,
J. R. BARKER and A. ASENOV
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MARTINEZ, M. ALDEGUNDE, N. SEOANE, A. R. BROWN, J. R. BARKER, A. ASENOV
IEEE Colloquium on Humanities, Science and Engineering Research (CHUSER 2011), Dec 5-6, 2011, Penang (2011)
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A. MARTINEZ, N. SEONE, M. ALDEGUNDE, A. ASENOV and J.R. BARKER
2011 International Conference on Simulation of Semiconductor Processes and Devices, Osaka, Japan, 8-10 September, 2011 Proc. SISPAD 2011, pages 95-98 IEEE Cat. No. (2011).
8.*A new approach to modelling quantum distributions and quantum trajectories for density matrix and Green Function simulation of nano-devices*
J. R. BARKER
J. Computational Electronics, Vol. 9, 243-251 (2010)
9.Variability in Si Nanowire MOSFETs Due to the Combined Effect of Interface Roughness and Random Dopants: A Fully 3D NEGF Simulation Study,
A. MARTINEZ, N. SEONE, A. R. BROWN, J. R. BARKER and A. ASENOV,
IEEE Transactions on Electron Devices, Vol. 57, 1626-1635 (2010)
10.Quantum phase space distributions with compact support
J.R. BARKER
Physica E 42, 491-496 (2010).
10.Dopants and Roughness induced Resonances in thin Si Nanowire transistors: A self-consistent NEGF-Poisson study
A. MARTINEZ, N. SEOANE, A. BROWN, J. BARKER, and A. ASENOV
Progress in Nonequilibrium Green's Functions IV, Journal of Physics: Conference Series Vol. 220, 012009 (2010)

11.*3-D Non-Equilibrium Green's Function Simulation of Non-Perturbative Scattering from Discrete Dopants in the Source and Drain of a Silicon Nanowire Transistor,*
A. MARTINEZ, N. SEONE, A. R. BROWN, J. R. BARKER and A. ASENOV
IEEE Transactions on Nanotechnology, vol. 8, no. 5, 603-610 (2009)

12.*Current variability in Si nanowire MOSFETS due to random dopants in the source/ drain regions: a fully 3-D NEGF Simulation study*
N. SEOANE, A. MARTINEZ, A.R. BROWN, J.R. BARKER, A. ASENOV
IEEE Transactions on Electron Devices,vol. 56, No.7, pp. 1388-1395 (2009).
13.*Impact of Body Thickness Dependent Bandstructure on Scaling of Double Gate MOSFETs: a DFT/NEGF study*
A. MARTINEZ, K.KALNA, P.V.SUSHKO, A.L. SCHLUGER, J.R. BARKER and A. ASENOV
IEEE Transactions on Nanotechnology, vol. 8, 159-166 (2009).
14.*Ballistic Quantum Simulators for Studying Variability in Nanotransistors*
A. MARTINEZ, J.R. BARKER, A. SVIZHENKO, M.P. ANANTRAM, M. BESCOND, A. ASENOV.
Journal of Computational and Theoretical Nanoscience, Volume **5**, 2289 (2008)
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A. MARTINEZ, M. BESCOND, A. R. BROWN, J. R. BARKER and A. ASENOV,
Journal of Computational Electronics, Vol.7, No.3, pp.359-362 (2008)
17.*Performance variability in wrap-round gate silicon nano-transistors: a 3D self-consistent NEGF study of ballistic flows for atomistically-resolved source and drain*
A MARTINEZ, J R BARKER, M BESCOND, A R BROWN and A ASENOV
Journal of Physics: Conference Series 109, 012026 (2008)
18.*NEGF simulations of the effect of strain on scaled double gate nanoMOSFETs*
K.KALNA , A. MARTINEZ, A. SVIZHENKO, M. P. AANATRAM, J. R. BARKER
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