*Functional RG for interacting electrons*

# Part III: Impurities in Luttinger liquids

1. Luttinger liquids
2. Impurity effects
3. Microscopic model
4. Flow equations
5. Results


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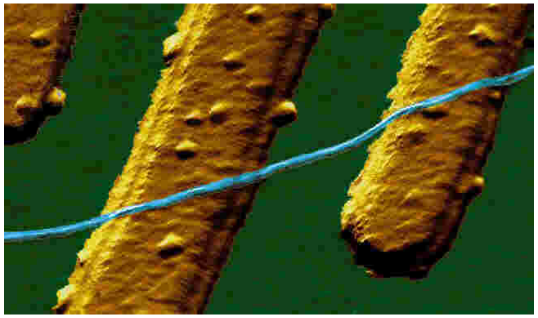
# 1. Luttinger liquids

One-dimensional interacting Fermi systems without correlation gaps
are Luttinger liquids.
(1D counterpart of Fermi liquid in 2D or 3D)

One-dimensional electron systems:

- Complex chemical compounds containing chains
- Quantum wires (in heterostructures)
- Carbon nanotubes
- Edge states



(Dekker's group)

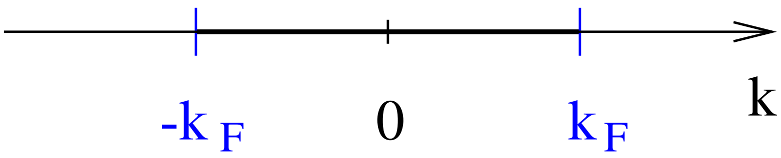
# Electronic structure of 1D systems:

Dispersion relations:

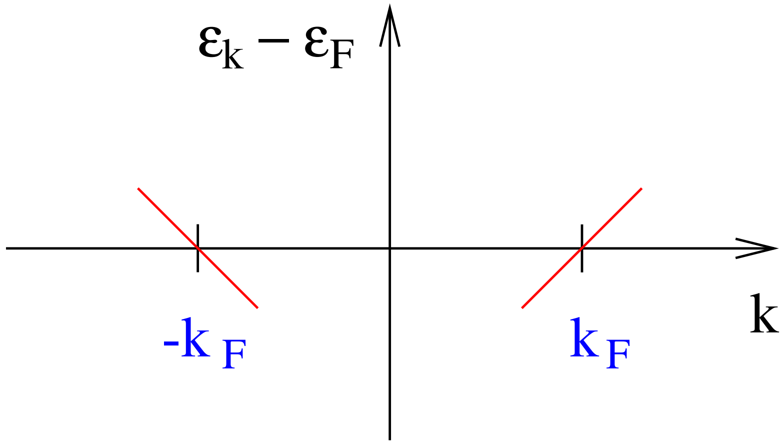
$$\epsilon_k = k^2/2m \quad \text{(low carrier density)}$$

$$\epsilon_k = -2t\cos k \quad \text{(tight binding)}$$

"Fermi surface": 2 points $\pm k_F$




Dispersion relation near Fermi points:




approx. linear:

$$\xi_k = \epsilon_k - \epsilon_F = v_F\,(|k| - k_F)$$

Electron-electron interaction:

has stronger effects than in 2D and 3D systems:

no fermionic quasi-particles, Fermi liquid theory not valid.

Fermi liquid replaced by Luttinger liquid:

- only bosonic low-energy excitations
  (collective charge/spin density oscillations)

- power-laws with non-universal exponents

$\Rightarrow$ Luttinger liquid theory

Textbook: T. Giamarchi: *Quantum physics in one dimension* (2004)

Bulk properties of Luttinger liquids:

- Bosonic low-energy excitations with linear dispersion relation

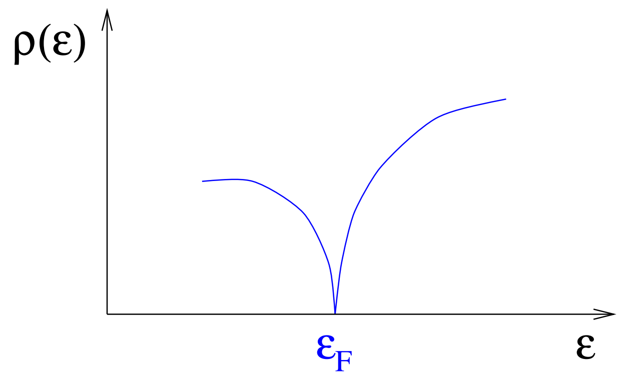
$\xi_q^c = u_c\, q$ , $\xi_q^s = u_s\, q$ (charge and spin channel)

$\Rightarrow$ specific heat $c_V \propto T$

- DOS for single-electron excitations:

$D(\epsilon) \propto |\epsilon - \epsilon_F|^{\alpha}$

vanishes at Fermi level ($\alpha > 0$)




DOS in principle observable by photoemission or tunneling.

• Density-density correlation function $N(q)$:

finite for $q \to 0$ (compressibility)

divergent as $|q-2k_F|^{-\alpha_{2k_F}}$ for $q \to 2k_F$

($\alpha_{2k_F} > 0$ for repulsive interactions)

$\Rightarrow$ enhanced back-scattering ($2k_F$) from impurity.

For spin-rotation invariant (and spinless) systems all exponents can be expressed in terms of one parameter $K_\rho$.

Asymptotic low energy behavior (power-laws) of Luttinger liquids described by Luttinger model:

$H_{\mathrm{LM}} =$ linear $\epsilon_k +$ forward scattering interactions

It is exactly solvable and scale-invariant (fixed point).

For spinless fermions only one coupling constant, parametrizing interaction between left- and right-movers:

$$H_I = g \int dx \, n_+(x) \, n_-(x)$$

# 2. Impurity effects

How does a single non-magnetic impurity (potential scatterer) affect properties of a Luttinger liquid?


Non-interacting system:

Impurity induces Friedel oscillations (density oscillations with wave vector $2k_F$)

DOS near impurity finite at Fermi level

Conductance reduced by a finite factor (transmission probability)

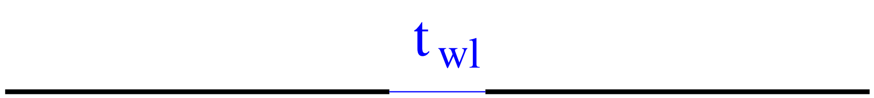
**Kane, Fisher '92: impurity in interacting system** (spinless Luttinger liquid)

- Weak impurity potential:

Backscattering amplitude $V_{2k_F}$ generated by impurity grows as $\Lambda^{K_\rho - 1}$
for decreasing energy scale $\Lambda$.
($K_\rho < 1$ for repulsive interactions; $V_{2k_F}$ is "relevant" perturbation of pure LL)

$\Rightarrow$ Low energy probes see high barrier even if (bare) impurity potential is weak!

- Weak link:




DOS at boundary of LL vanishes as $|\epsilon - \epsilon_F|^{\alpha_B}$ $\Rightarrow$

Tunneling amplitude $t_{\mathrm{wl}}$ between two weakly coupled
chains scales to zero as $\Lambda^{\alpha_B}$ with $\alpha_B = K_\rho{}^{-1} - 1 > 0$ at low energy scales.
($t_{\mathrm{wl}}$ is "irrelevant" perturbation of split chain)

Hypothesis (Kane, Fisher):

Any impurity effectively "cuts the chain" at low energy scales and physical properties obey weak link or boundary scaling. $\Rightarrow$

DOS near impurity:

$D_i(\epsilon) \propto |\epsilon - \epsilon_F|^{\alpha_B}$ for $\epsilon \to \epsilon_F$ at $T = 0$

Conductance through impurity:

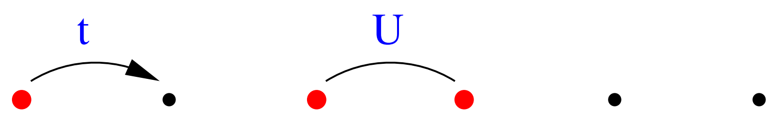
$G(T) \propto T^{2\alpha_B}$ for $T \to 0$

supported within effective bosonic field theory by:

refermionization (Kane, Fisher '92)
QMC (Moon et al. '93; Egger, Grabert '95)
Bethe ansatz (Fendley, Ludwig, Saleur '95)

# 3. Microscopic model

Spinless fermion model:




nearest neighbor hopping $t$

nearest neighbor interaction $U$

$$H_{\rm sf} = -t \sum_j \left( c_{j+1}^\dagger c_j + c_j^\dagger c_{j+1} \right) + U \sum_j n_j n_{j+1}$$

Properties (without impurities):

- exactly solvable by Bethe ansatz
- Luttinger liquid except for $|U| > 2t$ at half-filling
- charge density wave for $U > 2t$ at half-filling

Impurity potential added to bulk hamiltonian $H_{\mathrm{sf}}$:

general form: $$H_{\mathrm{imp}} = \sum_{j,j'} V_{j'j}\, c^\dagger_{j'} c_j$$

"site impurity":

$$H_{\mathrm{imp}} = V n_{j_0}$$ ($j_0$ impurity site)

"hopping impurity":

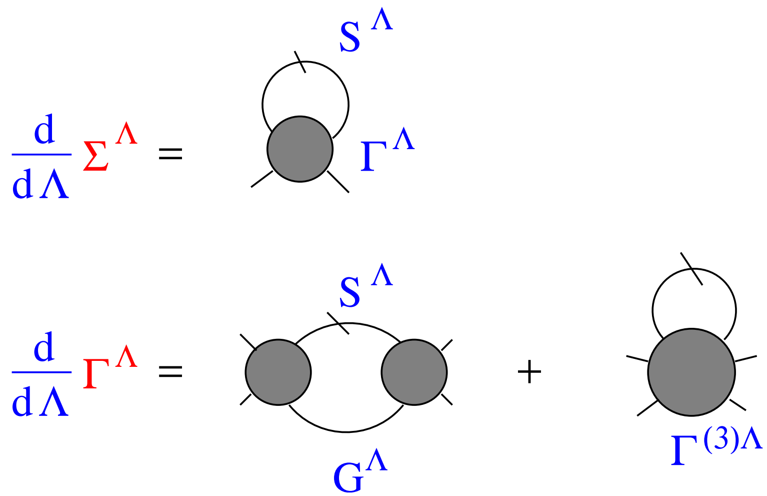
$$H_{\mathrm{imp}} = (t - t')\left(c^\dagger_{j_0+1} c_{j_0} + c^\dagger_{j_0} c_{j_0+1}\right)$$

Later also double barrier (two site or hopping impurities)

# 4. Flow equations

Starting point (for approximations):

Exact hierarchy of differential flow equations for 1-particle irreducible vertex functions with infrared cutoff $\Lambda$:




etc. for $\Gamma^{(3)\Lambda}$, $\Gamma^{(4)\Lambda}$, ...

where

$$G^{\Lambda} = \left[(G_0^{\Lambda})^{-1} - \Sigma^{\Lambda}\right]^{-1} \qquad S^{\Lambda} = \left[1 - G_0^{\Lambda}\Sigma^{\Lambda}\right]^{-1} \frac{dG_0^{\Lambda}}{d\Lambda} \left[1 - \Sigma^{\Lambda}G_0^{\Lambda}\right]^{-1}$$

Cutoff:

At $T = 0$ sharp frequency cutoff: $G_0^\Lambda = \Theta(|\omega| - \Lambda)\, G_0$

At finite $T$ (discrete Matsubara frequencies) soft cutoff with width $2\pi T$

$G_0$ bare propagator without impurities and interaction

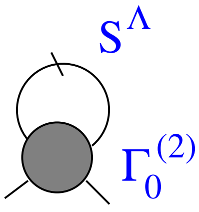
## Approximations:

Scheme 1 (first order):

Approximate $\Gamma^\Lambda \approx \Gamma^{\Lambda^0}$ (ignore flow of 2-particle vertex)

$\Rightarrow$ $\Sigma^\Lambda$ tridiagonal matrix in real space

$$\frac{\mathrm{d}}{\mathrm{d}\Lambda}\Sigma^\Lambda =$$




Flow equation very simple; at $T = 0$:

$$\frac{d}{d\Lambda}\Sigma^\Lambda_{j,j} = -\frac{U}{2\pi}\sum_{s=\pm 1}\sum_{\omega=\pm\Lambda}\tilde{G}^\Lambda_{j+s,j+s}(i\omega) \qquad \frac{d}{d\Lambda}\Sigma^\Lambda_{j,j\pm 1} = \frac{U}{2\pi}\sum_{\omega=\pm\Lambda}\tilde{G}^\Lambda_{j,j\pm 1}(i\omega)$$

where $\tilde{G}^\Lambda(i\omega) = [G_0^{-1}(i\omega) - \Sigma^\Lambda]^{-1}$.

Kane/Fisher physics already qualitatively captured !

Scheme 2 (second order):

Neglect $\Gamma^{(3)\Lambda}$; approx. $\Gamma^{\Lambda}$ by flowing nearest neighbor interaction $U^{\Lambda}$

$\Rightarrow$ 1-loop flow for $U^{\Lambda}$; flow of $\Sigma^{\Lambda}$ as in scheme 1 with renormalized $U^{\Lambda}$

$$\frac{d}{d\Lambda}\Sigma^{\Lambda}_{j,j} = -\frac{U^{\Lambda}}{2\pi}\sum_{s=\pm 1}\sum_{\omega=\pm\Lambda}\tilde{G}^{\Lambda}_{j+s,j+s}(i\omega) \qquad \frac{d}{d\Lambda}\Sigma^{\Lambda}_{j,j\pm 1} = \frac{U^{\Lambda}}{2\pi}\sum_{\omega=\pm\Lambda}\tilde{G}^{\Lambda}_{j,j\pm 1}(i\omega)$$

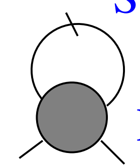
Works quantitatively even for rather big $U$

## Derivation of flow equation (scheme 1):

Flow equation for self-energy:

$$\frac{d}{d\Lambda}\Sigma^\Lambda(1',1) = T\sum_{2,2'} e^{i\omega_2 0^+}\, S^\Lambda(2,2')\,\Gamma_0(1',2';1,2)$$

$\frac{\mathrm{d}}{\mathrm{d}\,\Lambda}\,\Sigma^\Lambda$ =




Single-scale propagator

$$S^\Lambda = -G^\Lambda[\partial_\Lambda (G_0^\Lambda)^{-1}]G^\Lambda = \frac{1}{1-G_0^\Lambda\Sigma^\Lambda}\,\frac{\partial G_0^\Lambda}{\partial\Lambda}\,\frac{1}{1-\Sigma^\Lambda G_0^\Lambda}$$

Self-energy and propagator diagonal in frequency: $\omega_1 = \omega_{1'}$ and $\omega_2 = \omega_{2'}$.

$\Gamma_0$ freqency-independent $\Rightarrow$ $\Sigma$ frequency-independent.

Sharp frequency cutoff ($T = 0$): $G_0^\Lambda(i\omega) = \Theta(|\omega| - \Lambda)\, G_0(i\omega) \quad \Rightarrow$

$$S^\Lambda(i\omega) = -\frac{1}{1 - \Theta(|\omega|-\Lambda) G_0(i\omega) \Sigma^\Lambda}\, \delta(|\omega|-\Lambda) G_0(i\omega)\, \frac{1}{1 - \Theta(|\omega|-\Lambda) \Sigma^\Lambda G_0(i\omega)}$$

$\delta(.)$ meets $\Theta(.)$: ill defined!

Consider regularized (smeared) step functions $\Theta_\epsilon$ with $\delta_\epsilon = \Theta'_\epsilon$,
then take limit $\epsilon \to 0$, using

$$\int dx\, \delta_\epsilon(x - \Lambda)\, f[x, \Theta_\epsilon(x - \Lambda)] \xrightarrow{\epsilon \to 0} \int_0^1 dt\, f(\Lambda, t)$$

proof:
substitution $t = \Theta_\epsilon$

Integration can be done analytically, yielding

$$\frac{d}{d\Lambda} \Sigma^\Lambda_{j'_1, j_1} = -\frac{1}{2\pi} \sum_{\omega = \pm\Lambda} \sum_{j_2, j'_2} e^{i\omega 0^+}\, \tilde{G}^\Lambda_{j_2, j'_2}(i\omega)\, \Gamma^0_{j'_1, j'_2; j_1, j_2}$$

where $\tilde{G}^\Lambda(i\omega) = [G_0^{-1}(i\omega) - \Sigma^\Lambda]^{-1}$

Insert real space structure of bare vertex for spinless fermions with nearest neighbor interaction $U$:

$$\Gamma^0_{j_1',j_2';j_1,j_2} = U_{j_1,j_2}\left(\delta_{j_1,j_1'}\delta_{j_2,j_2'} - \delta_{j_1,j_2'}\delta_{j_2,j_1'}\right)$$

$$U_{j_1,j_2} = U\left(\delta_{j_1,j_2-1} + \delta_{j_1,j_2+1}\right)$$

$\Rightarrow$ Flow equations

$$\frac{d}{d\Lambda}\Sigma^\Lambda_{j,j} = -\frac{U}{2\pi}\sum_{s=\pm 1}\sum_{\omega=\pm\Lambda} e^{i\omega 0^+}\,\tilde{G}^\Lambda_{j+s,j+s}(i\omega)$$

$$\frac{d}{d\Lambda}\Sigma^\Lambda_{j,j\pm 1} = \frac{U}{2\pi}\sum_{\omega=\pm\Lambda} e^{i\omega 0^+}\,\tilde{G}^\Lambda_{j,j\pm 1}(i\omega)$$

Convergence factor $e^{i\omega 0^+}$ matters only for $\Lambda \to \infty$

Initial condition at $\Lambda = \Lambda_0 \to \infty$:

$$\Sigma^{\Lambda_0}_{j_1,j_1'} = V_{j_1,j_1'} + \frac{1}{2}\sum_{j_2} \Gamma^0_{j_1',j_2;j_1,j_2}$$

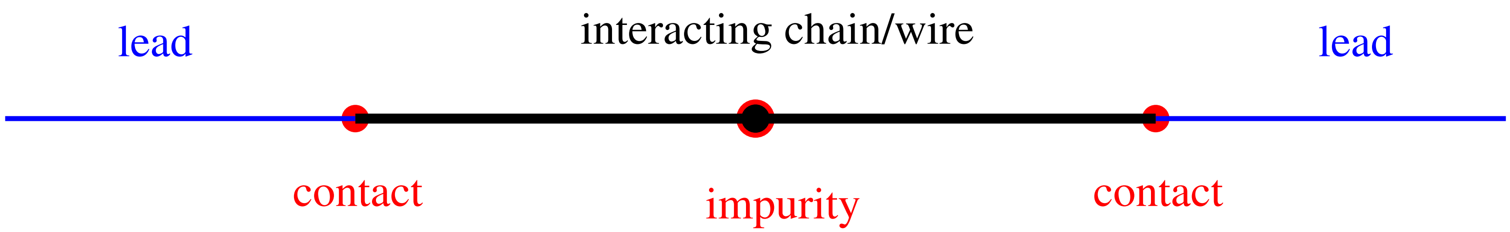
where $V_{j_1,j_1'}$ is the bare impurity potential and
the second term is due to the flow from $\infty$ to $\Lambda_0$ (!)

Flow equations at finite temperatures $T > 0$:

Replace $\omega = \pm\Lambda$ by $\omega = \pm\,\omega_n^\Lambda$ in flow equations,
where $\omega_n^\Lambda$ is the Matsubara frequency most close to $\Lambda$.

**Calculation of conductance:**

Interacting chain connected to semi-infinite non-interacting leads via smooth or abrupt contacts




Conductance $\quad G(T) = -\frac{e^2}{h}\int d\epsilon\, f'(\epsilon)\,|t(\epsilon)|^2 \quad$ with $\quad |t(\epsilon)|^2 \propto |G_{1,N}(\epsilon)|^2$

Propagator $G_{1,N}(\epsilon)$ calculated in presence of leads, which affect the interacting region only via boundary contributions $\Sigma_{1,1}(\epsilon)$ and $\Sigma_{N,N}(\epsilon)$ to the self-energy

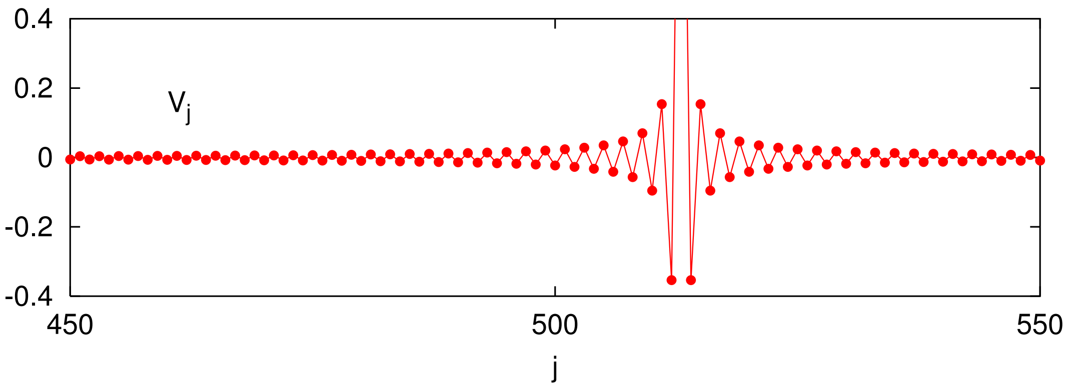
Vertex corrections vanish within our approximation (no inelastic scattering) (see Oguri '01)

**fRG features:**

- perturbative in $U$ (weak coupling)
- non-perturbative in impurity strength
- arbitrary bare impurity potential (any shape)
- full effective impurity potential
  (cf. Matveev, Yue, Glazman '93: only $V_{2k_F}$)
- cheap numerics up to $10^5$ sites for $T > 0$ and $10^7$ sites at $T = 0$.
- captures all scales, not just asymptotics.

# 5. Results

Renormalized impurity potential (from self-energy $\Sigma_{jj}$ at $\Lambda = 0$):

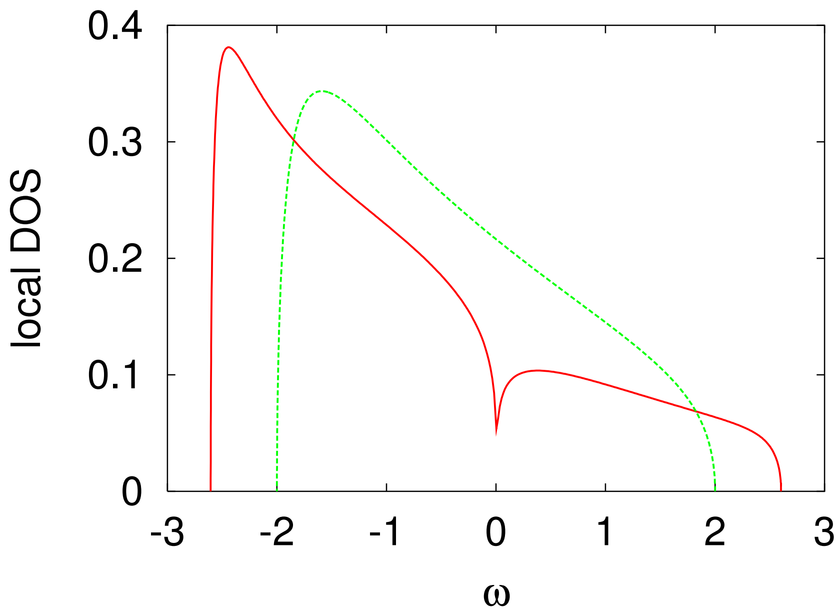



long-range $2k_F$-oscillations ! (associated with Friedel oscillations of density)

$2k_F$-oscillations also in renormalized hopping amplitude around impurity

Results for local DOS near impurity site:

(half-filling, ground state, $U = 1$, $V = 1.5$, 1000 sites)




red: Lutt. liquid

green: Fermi gas

Strong suppression of DOS near Fermi level

Power law with boundary exponent $\alpha_B$ for $\omega \to 0$, $N \to \infty$

Spectral weight at $\omega = 0$ in good agreement with DMRG for $U < 2$.

Log. derivative of spectral weight

at Fermi level as fct. of system size:

- near boundary (*solid lines*)
- near hopping impurity (*dashed lines*)

*circles:* quarter-filling, $U = 0.5$

*squares:* quarter-filling, $U = 1.5$

*open symbols:* fRG

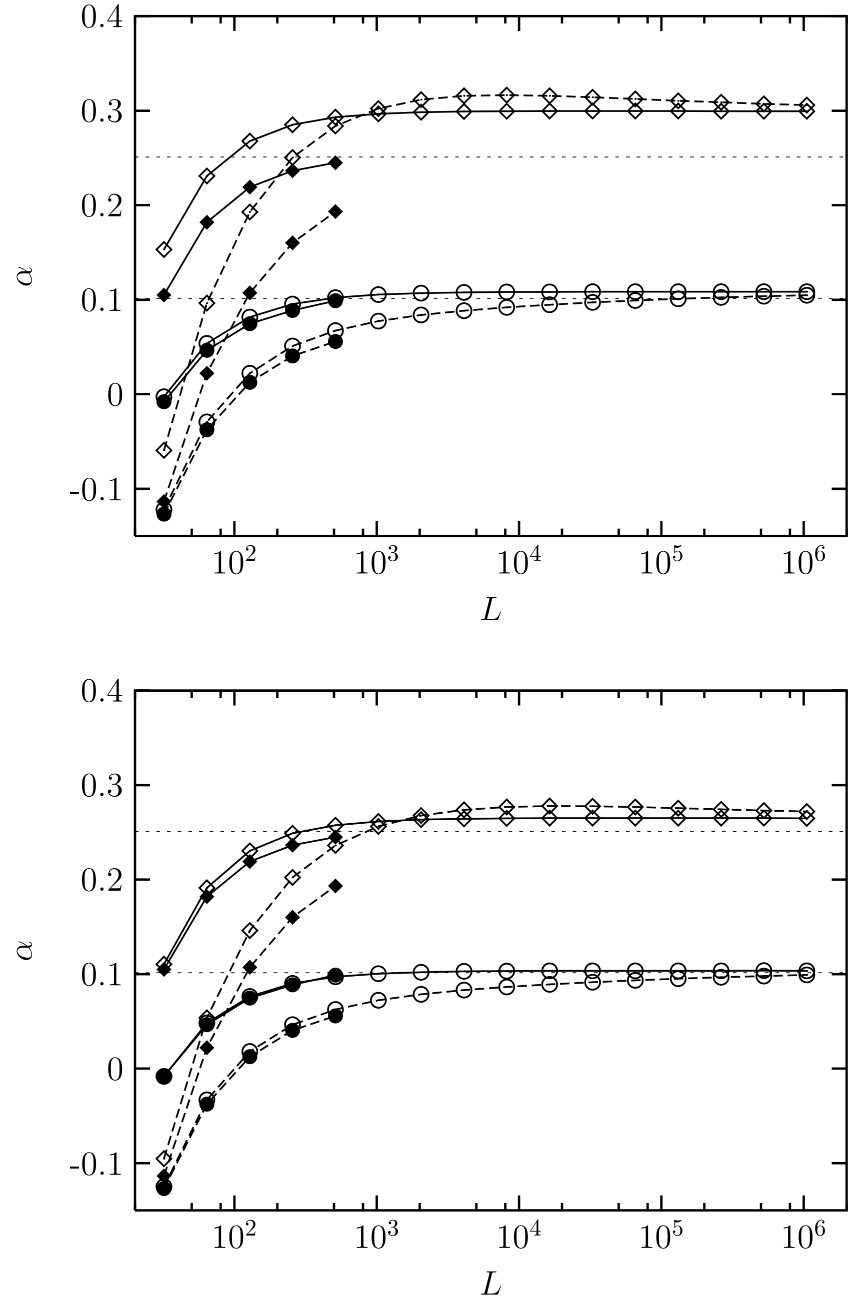
*filled symbols:* DMRG

*top panel:* without vertex renorm.

*bottom panel:* with vertex renorm.

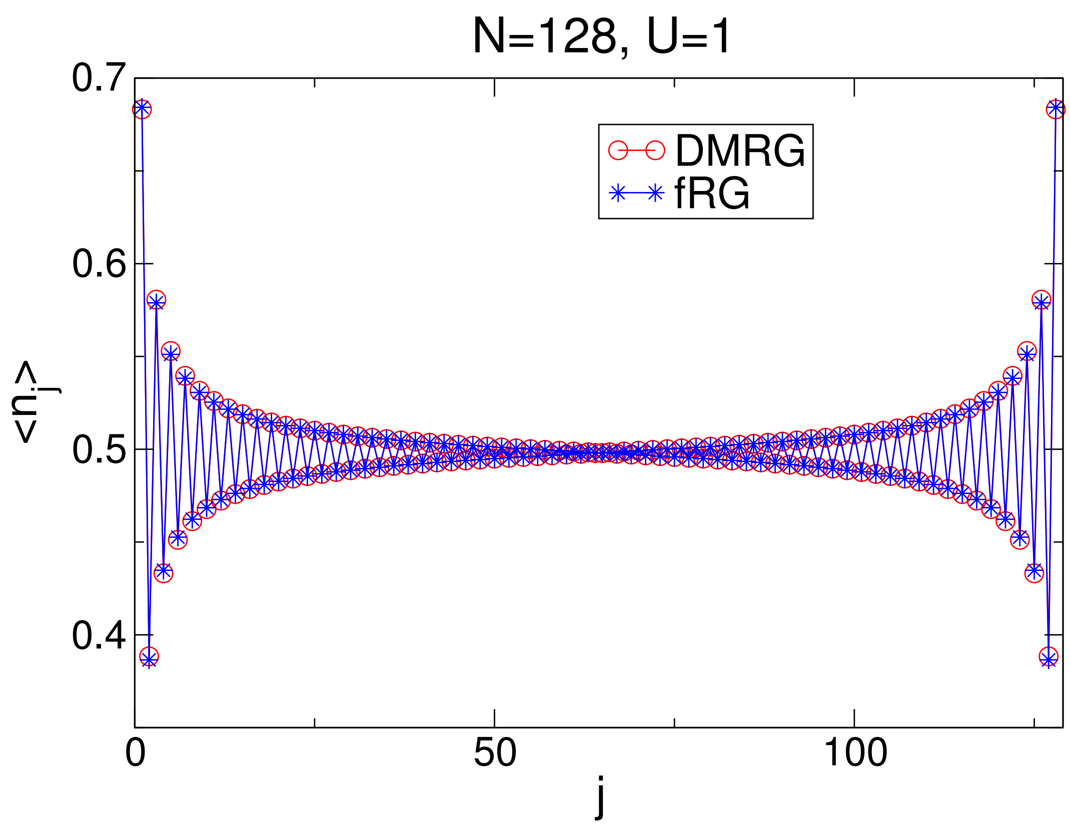
*horizontal lines:*

exact boundary exponents



Friedel oscillations from open boundaries:

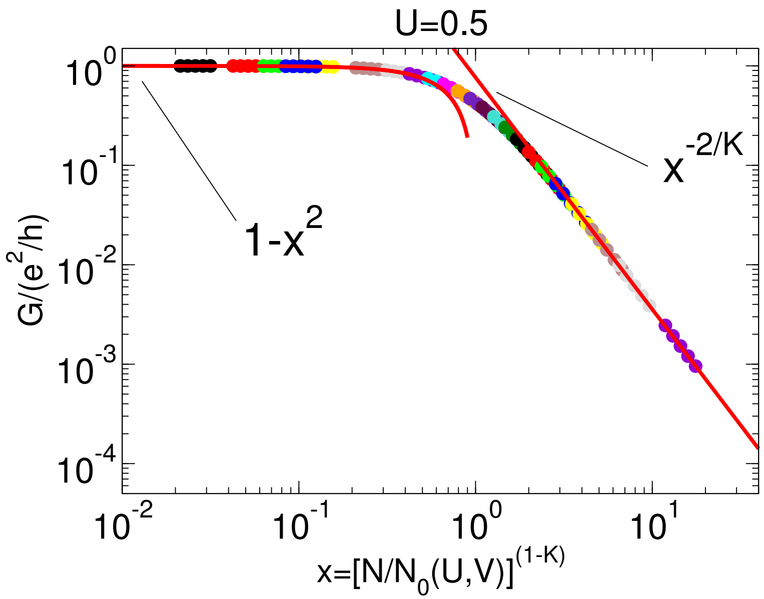
(half-filling, ground state)

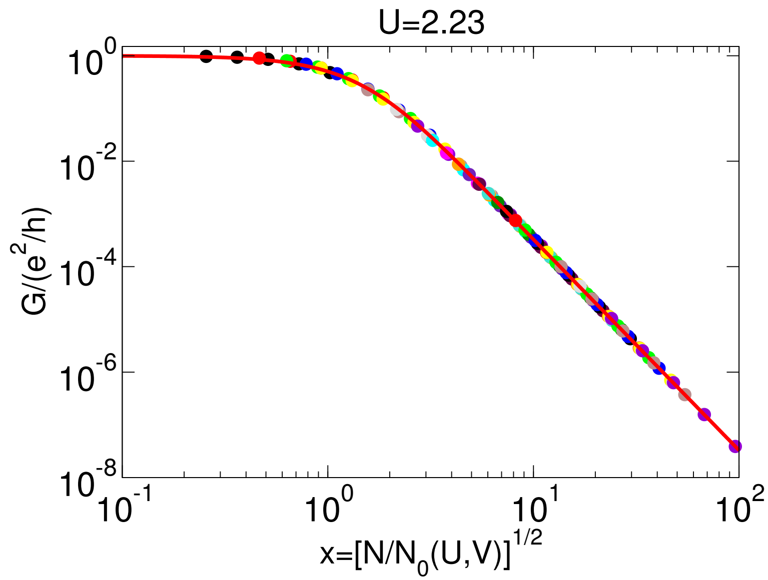



Excellent agreement between fRG and DMRG

One parameter scaling of conductance ($T = 0$):

Single impurity, smooth contacts: $G(N) = \frac{e^2}{h} \tilde{G}_K(x)$ , $x = [N/N_0(U,V)]^{1-K}$

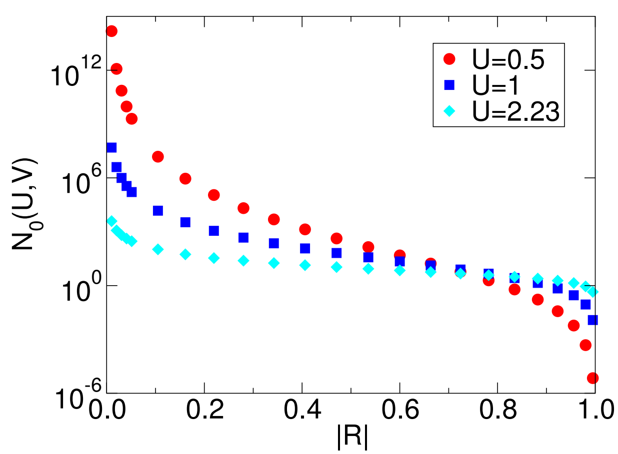


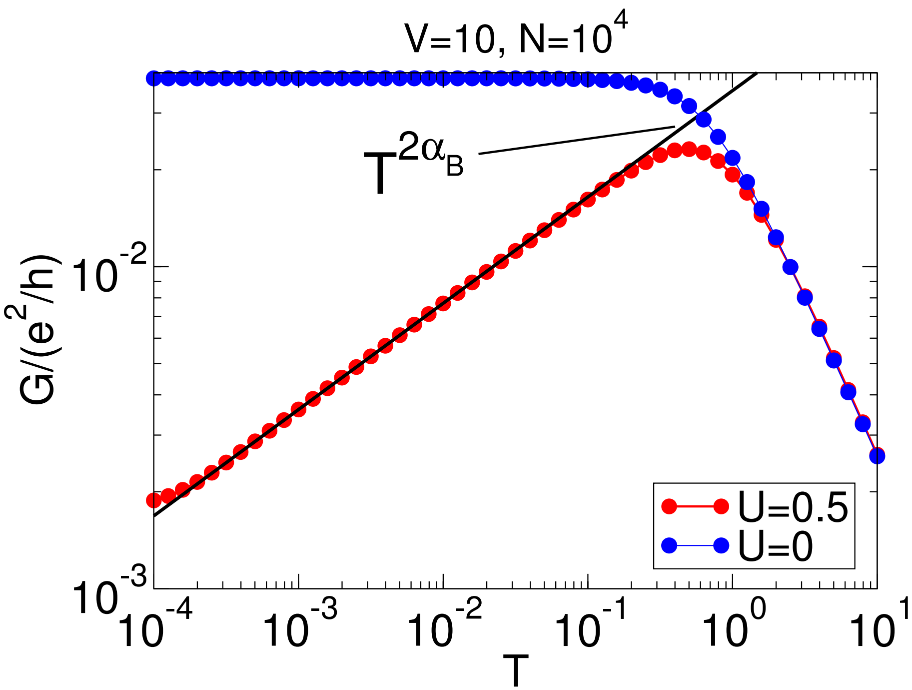

Crossover size

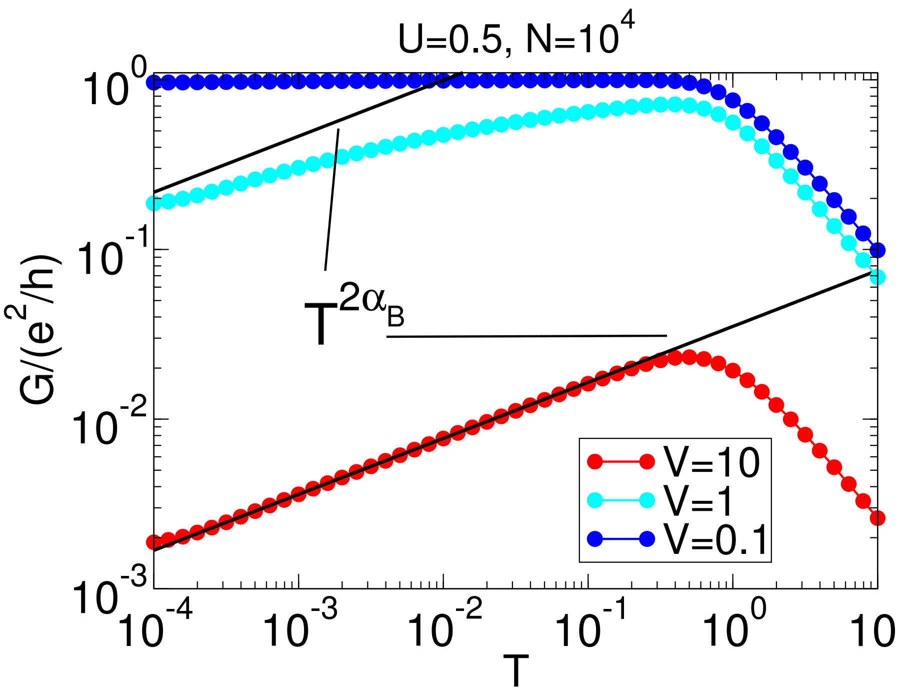
as function of bare

reflection amplitude



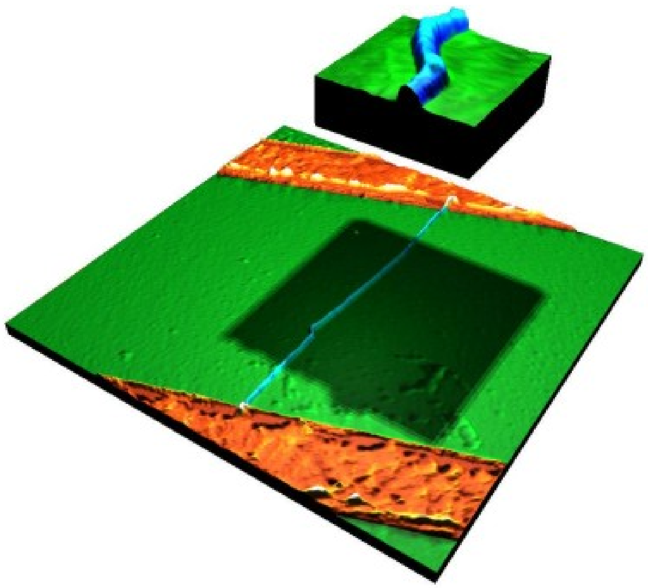
Conductance at $T > 0$ — smooth contacts

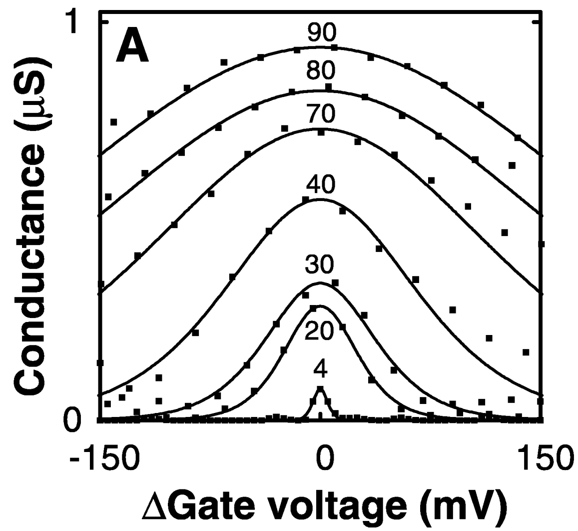



Asymptotic power law $G(T) \propto T^{2\alpha}$ reached on accessible scales only for sufficiently strong impurities

## Resonant tunneling through double barrier:

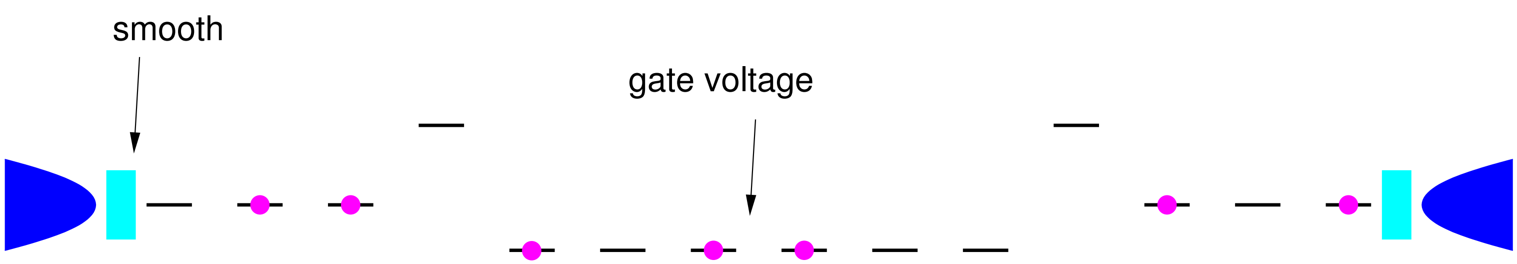




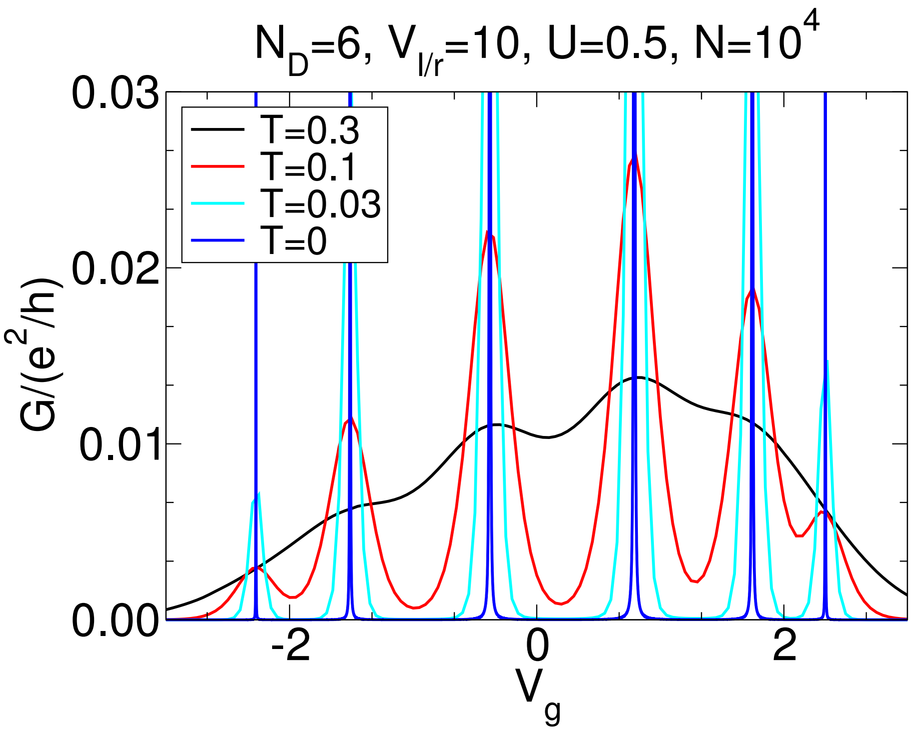

(Dekker's group '01)

Treated theoretically by many groups; controversial results !

Model setup:

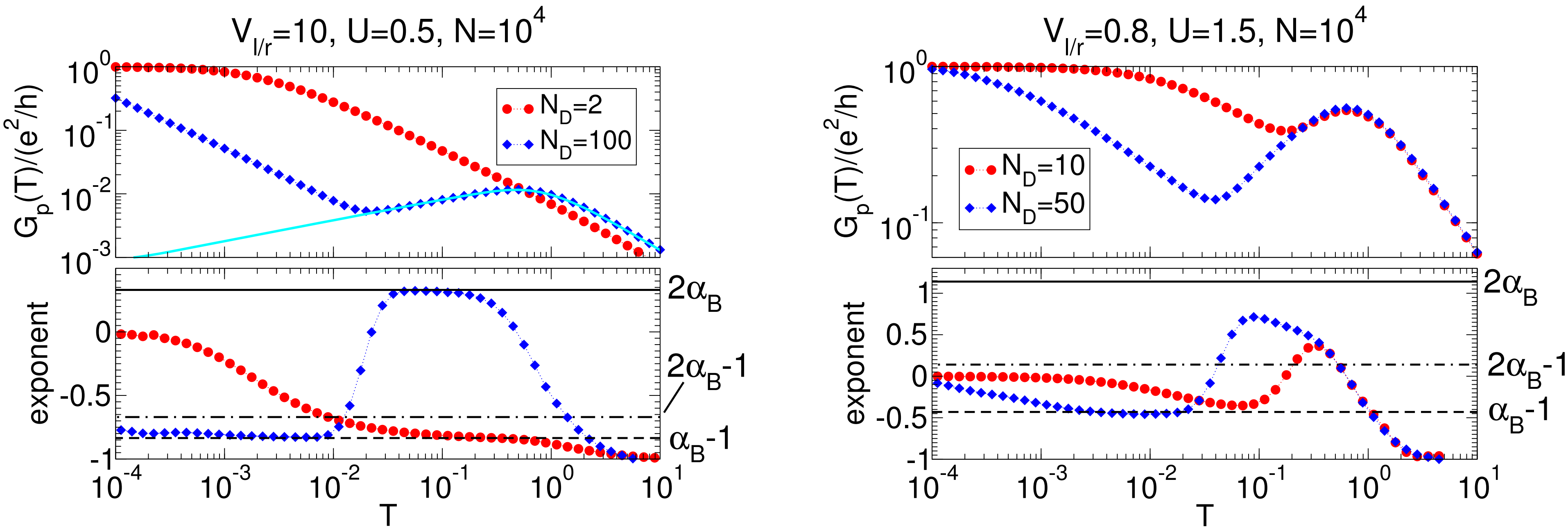


Resonance peaks in conductance as a function of gate voltage:




At $T = 0$, width $w \sim N^{K-1}$

$T$-dependence of $|t(\epsilon)|^2$ important fRG results for $G_p(T)$ (symmetric double barrier):




Various distinctive power laws, in particular (Furusaki, Nagaosa '93,'98):

- exponent $2\alpha_B$ (looks like independent impurities in series)
- exponent $\alpha_B - 1$ (*"uncorrelated sequential tunneling"*)

No indications of exponent $2\alpha_B - 1$ (*"correlated sequential tunneling"*)

## Summary

- fRG is reliable and flexible tool to study Luttinger liquids with impurities
- can be applied to microscopic models, restricted to "weak" coupling
- provides simple physical picture
- interplay of contacts, impurities, and correlations
- method covers all energy scales
- resonant tunneling: universal behavior and crossover captured

# Extensions

- include spin
  (extended Hubbard model: Andergassen et al., PRB **73**, 045125 (2006))

- more complex geometries
  (Y-junctions: Barnabé-Thériault et al., PRL **94**, 136405 (2005))