Nonequilibrium evolution of the Kondo screening cloud

Martin Nuss, Martin Ganahl, Antonius Dorda,
Hans Gerd Evertz, Enrico Arrigoni and Wolfgang von der Linden

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DPG, Dresden, 02.04.2014

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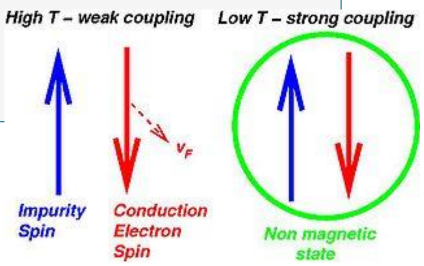
Agenda

The single impurity revisited: real time evolution

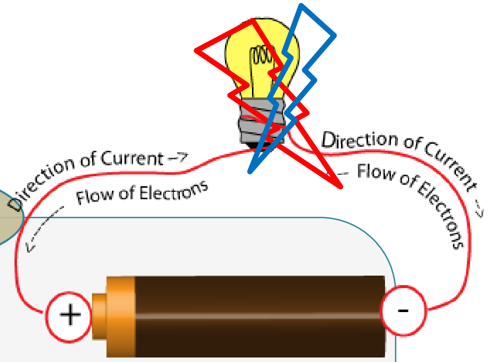
II

Non-local space-time correlations

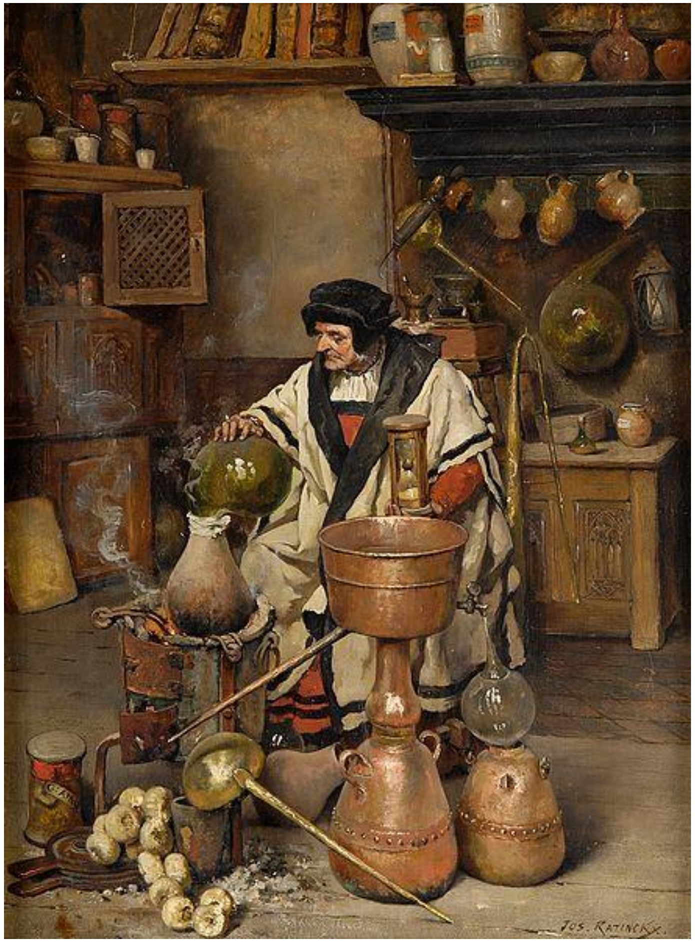


III

Correlations & bias voltage



Obtain „Gold“



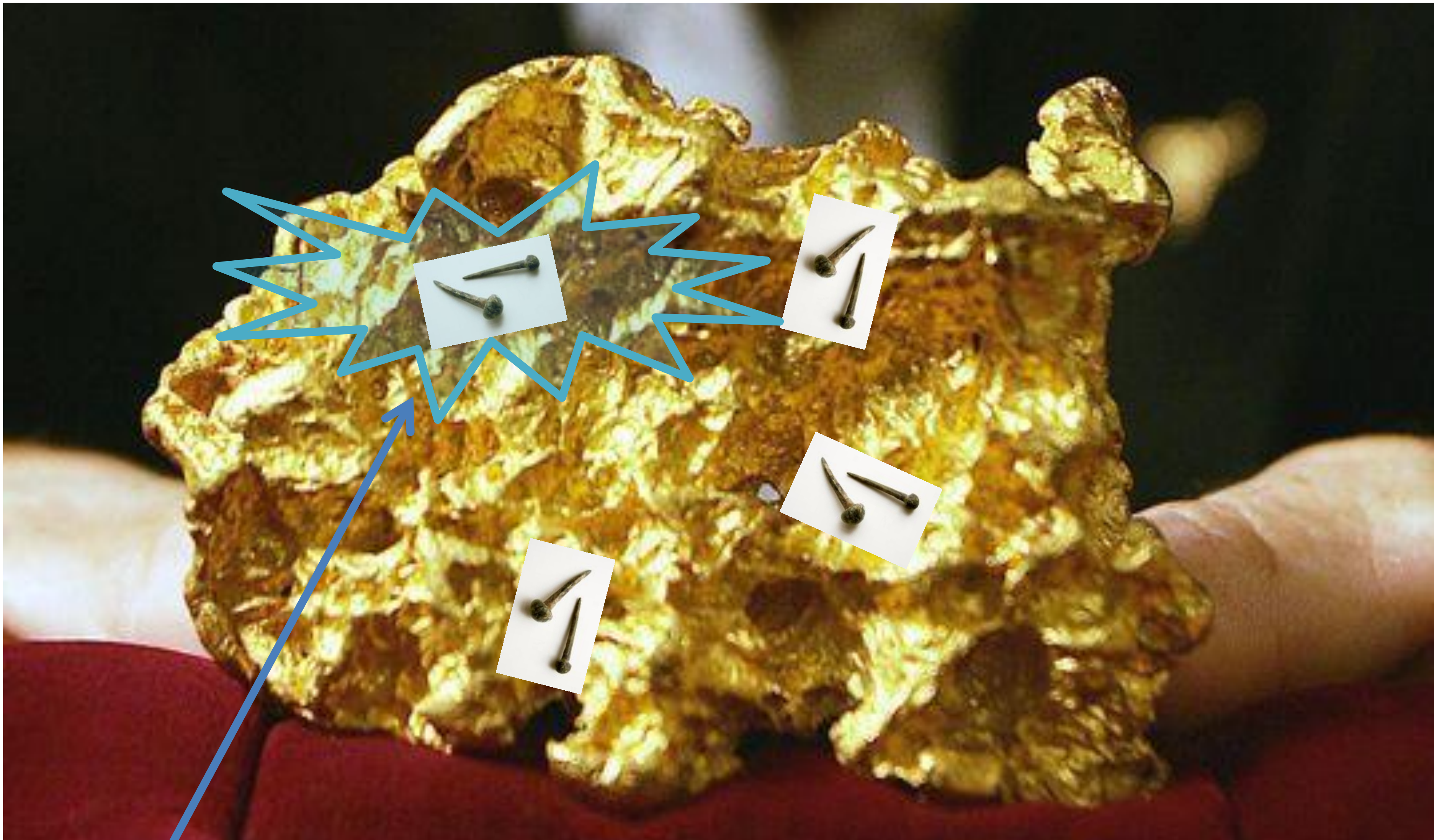
Joseph Leopold Ratinckx Der Alchemist

Put in „Iron“

TUG

Dilute Magnetic Impurities

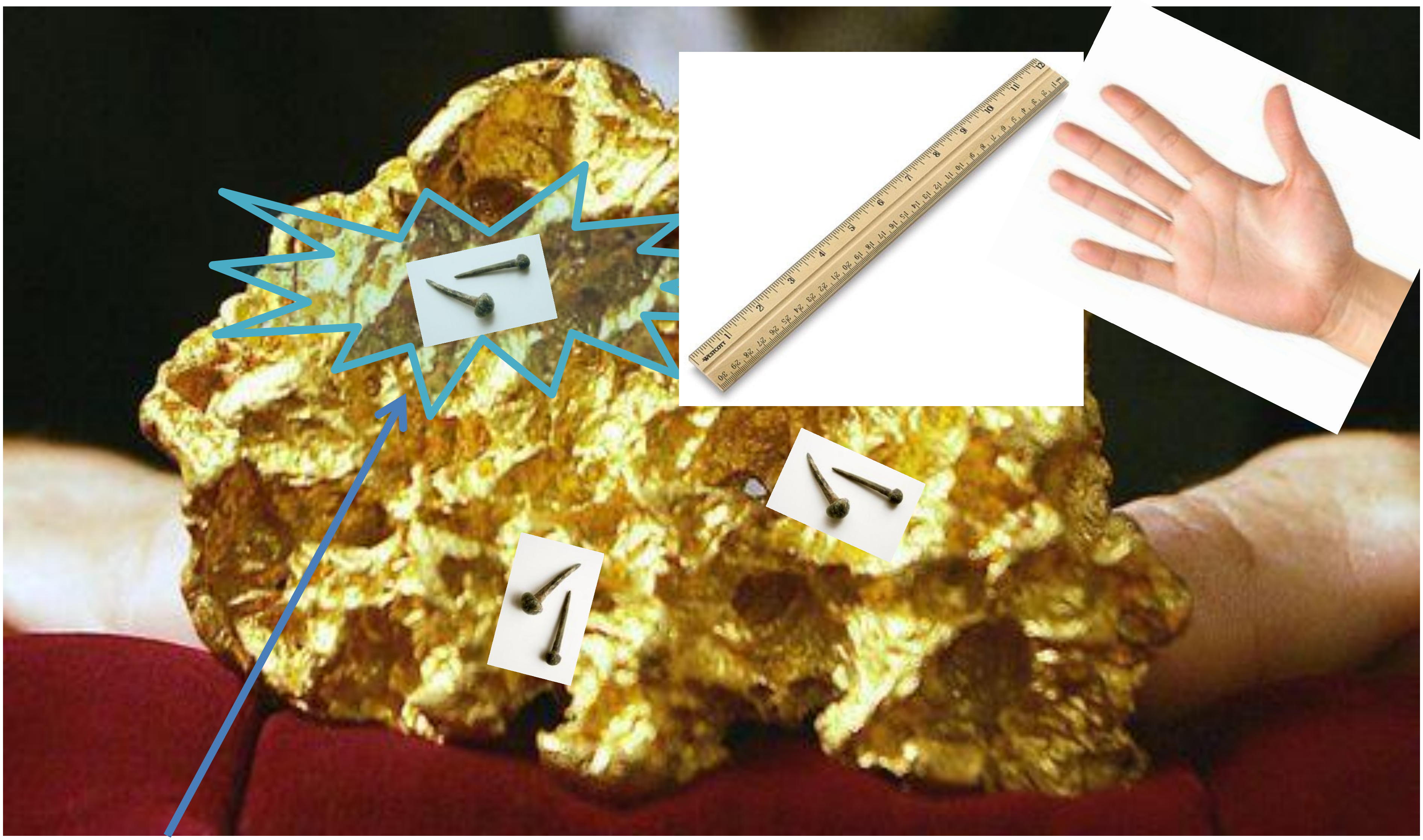
itp^cp



Singlets

A.M. Clogston, PR **125**, 541 (1962)

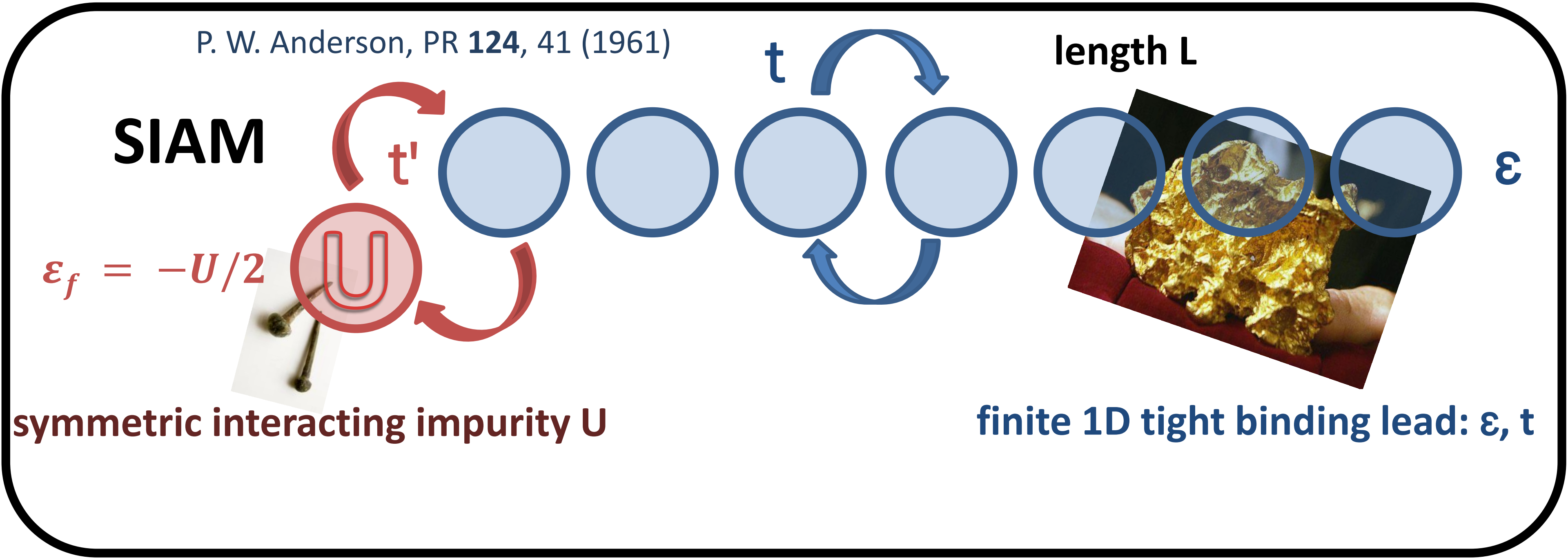
Measure Singlet Extent



Singlets

A.M. Clogston, PR **125**, 541 (1962)

Single Impurity

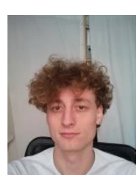


- **DMRG**
  - **T=0**

  S. R. White, PRB **48**, 10345 (1993)

see talk by F. Heidrich-Meisner: TT2.1, Sun

- **massively *parallel* code**
  - **Martin Ganahl**

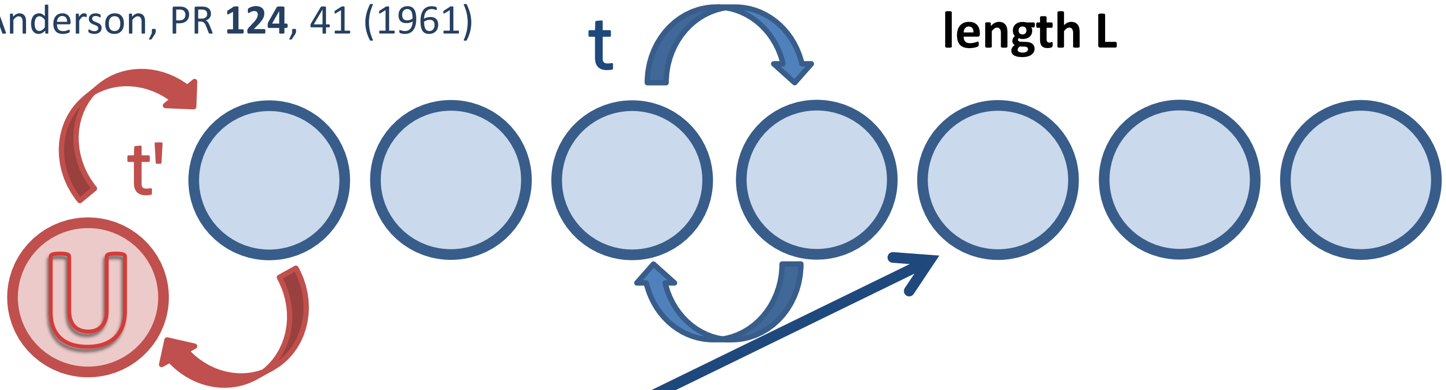


Spin-Spin Correlations

P. W. Anderson, PR **124**, 41 (1961)

length L

SIAM



$\varepsilon_f = -U/2$

symmetric interacting impurity U

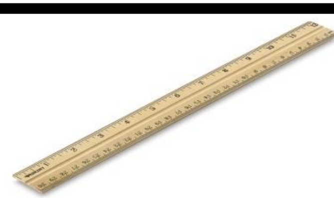
finite 1D tight binding lead: ε, t

r

0

looking for Kondo Singlet

$$< S_0 S_r > \propto TK$$



experimentally difficult

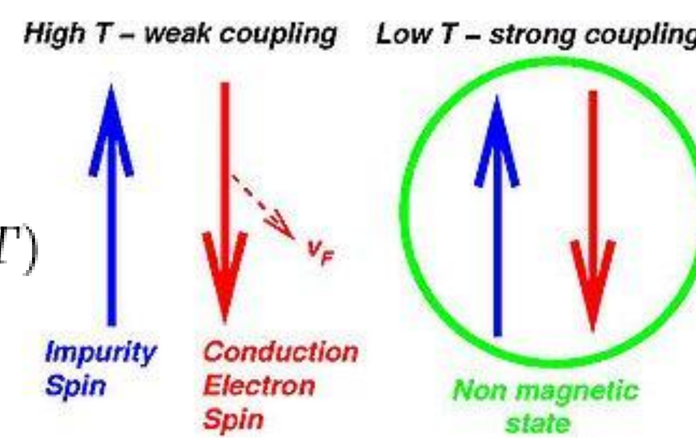
- **NMR (bulk)**

$$\chi(r) - \nu/2 \to \frac{\cos 2k_F r}{4\pi r^3} f(r/\xi_K)\chi(T)$$

- **persistent currents (nano)**

I. Affleck, arXiv:**0911.2209** (2010)

J. Park etal. PRL **110**, 246603 (2013)



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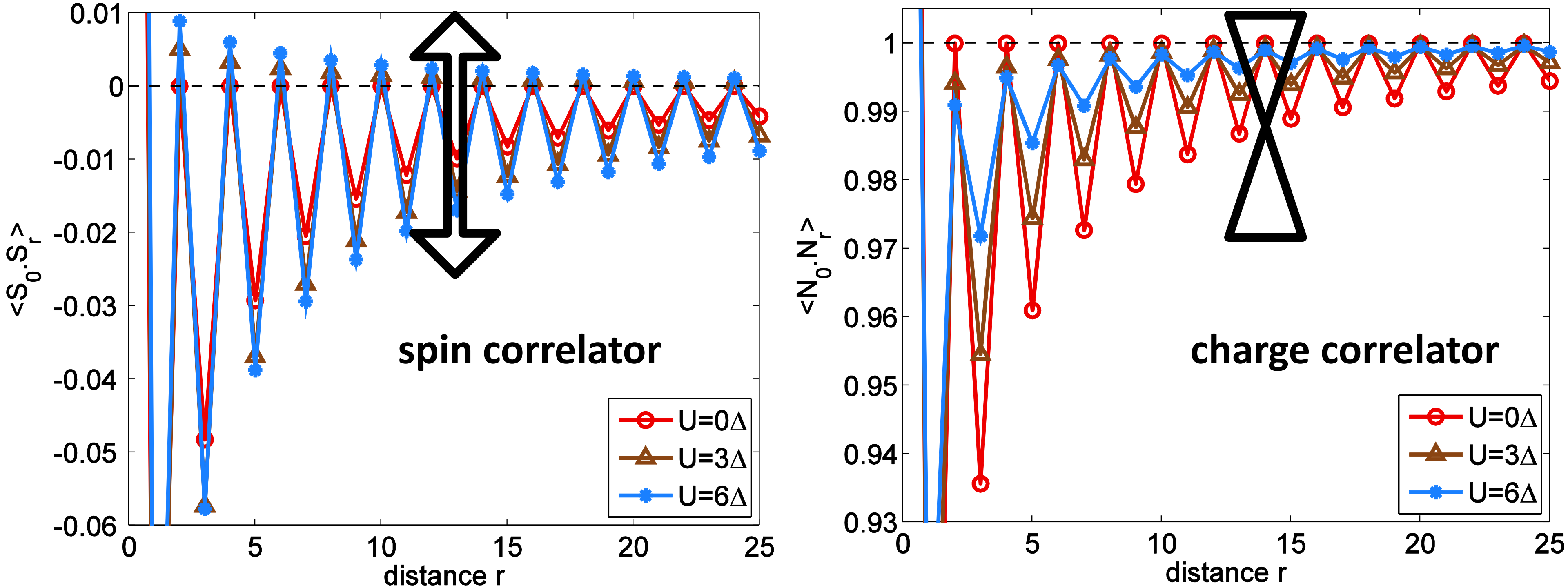
Spin & Charge Correlators

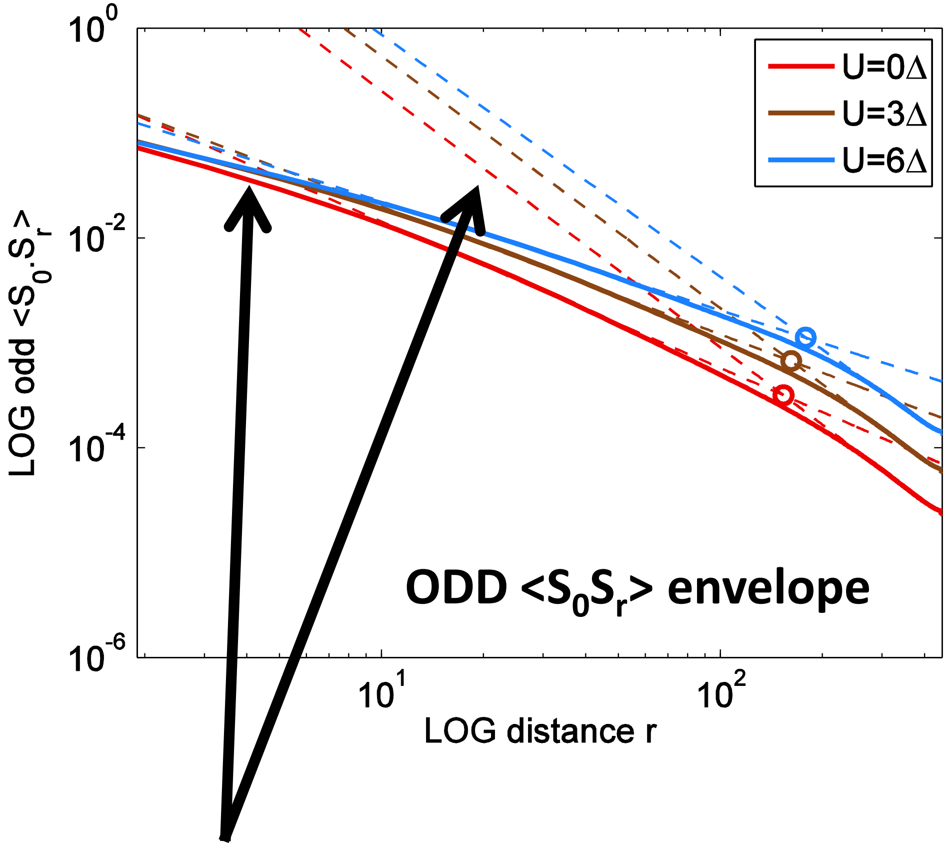
itp^cp

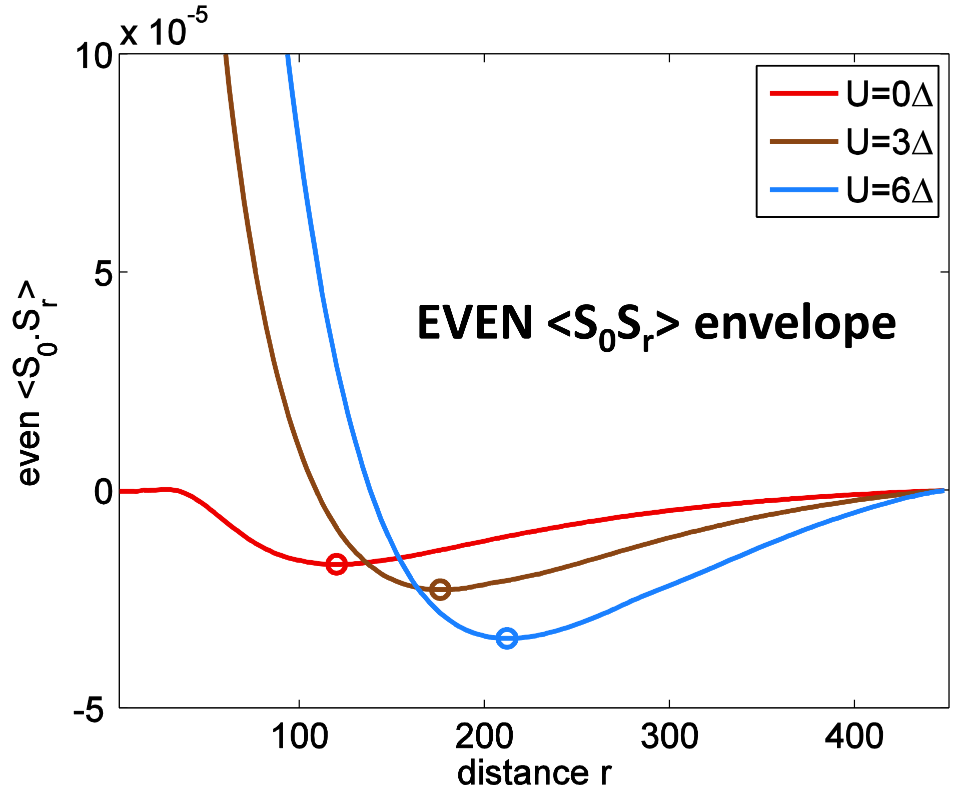


- **U=0** H. Ishii, JLTP **32**, 457 (1978)
  - $C = \frac{4}{3} S + < n >$
  - $\xi \propto 1/\Delta$
- **U induces „ferromagnetic“ sites**
  - $\xi \propto 1/T_K$
- **U>0** F. Mezei etal. PRL **29**, 1465 (1972)
  - **Fridel-like oscillations suppressed**
  - **recover at long distances**

see also QMC & tDMRG: J. E. Gubernatis, etal. RB **35**, 8478 (1987), A. Holzner etal. PRB **80**, 205114 (2009)

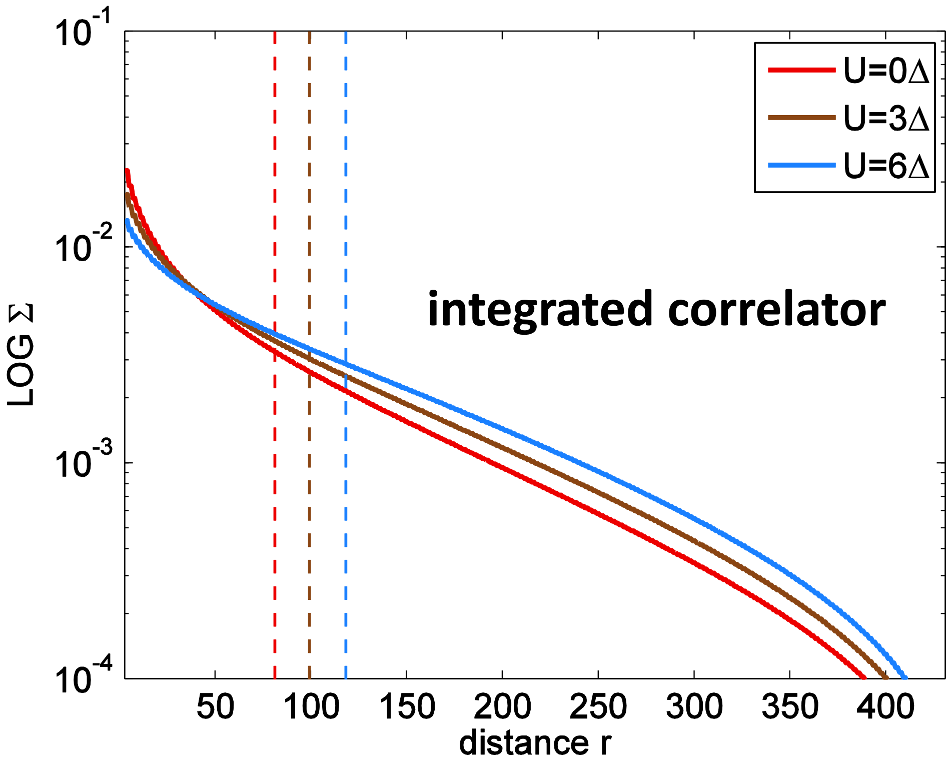
Characteristic Length

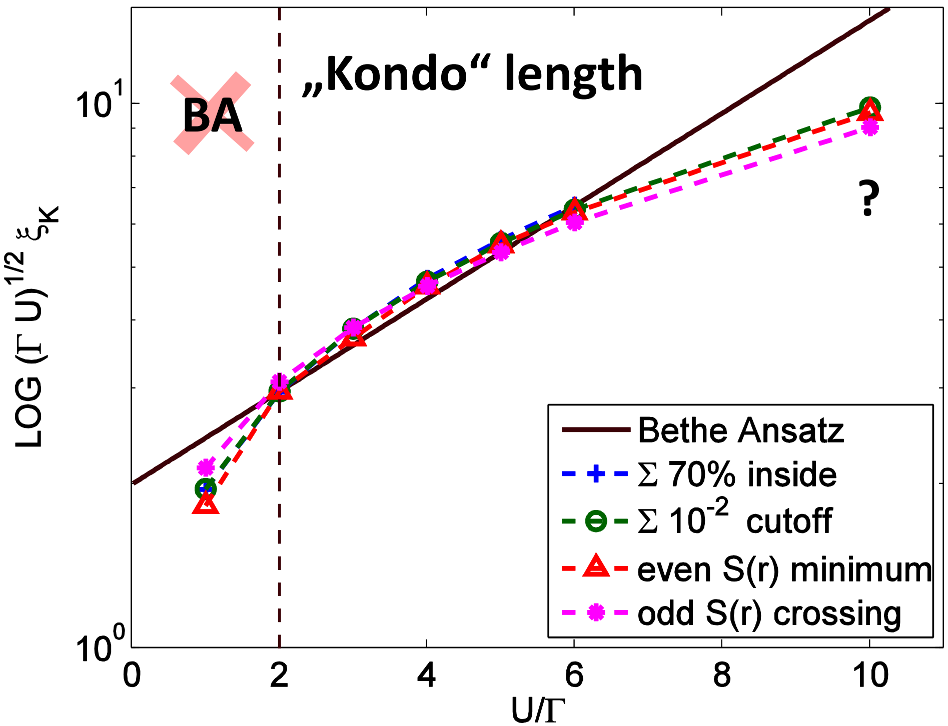




- **2 power laws, exponents:**
  - $\sim 1.4 - U/2$
  - $\sim 2.4 - U/3$
- **follow minima**

Characteristic Length





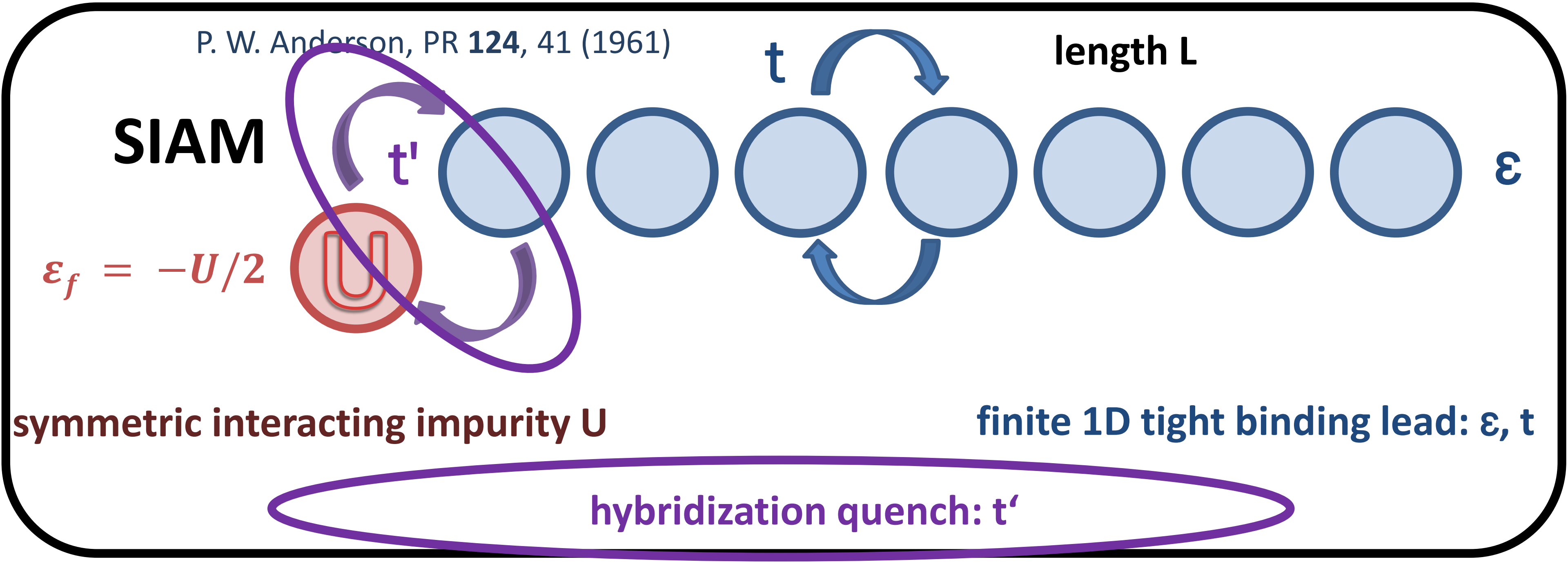
- $\sum(r) = \sum_{r'=0}^{r} \frac{S(r)}{S(0)}$

- **Bethe Ansatz**

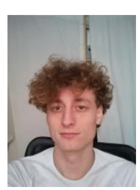
$$\xi_K \propto \frac{v_F}{k_B T_K} \propto 2t\sqrt{\frac{2}{\Delta U}}\, e^{\frac{\pi}{8\Delta}U}$$

see also QMC & tDMRG: J. E. Gubernatis, etal. RB **35**, 8478 (1987), A. Holzner etal. PRB **80**, 205114 (2009)

Real Time Evolution

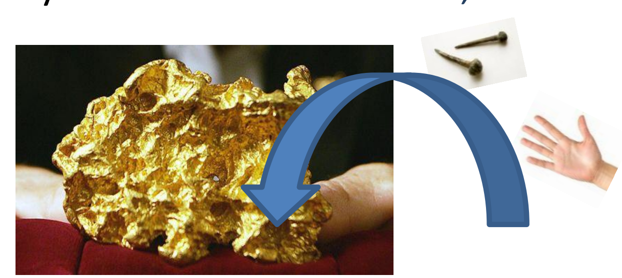


- Suzuki-Trotter *real* time evolution using MPS
  - DMRG + TEBD
    S. R. White, PRB **48**, 10345 (1993)
    G. Vidal, PRL **93**, 040502 (2004)
- *unitary*: finite time + finite size
- massively *parallel* code
  - Martin Ganahl



see talk by F. Heidrich-Meisner: TT2.1, Sun

see talk by P. Schmitteckert: TT9.1, Mon



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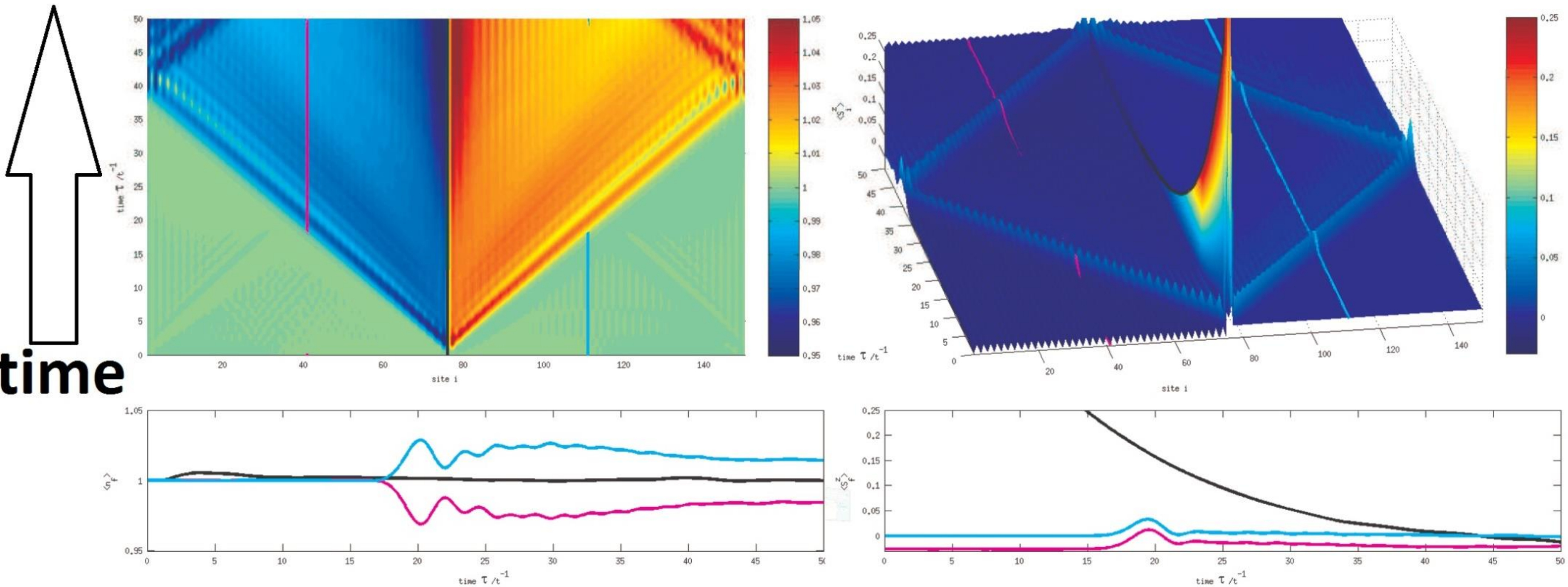
Local Densities

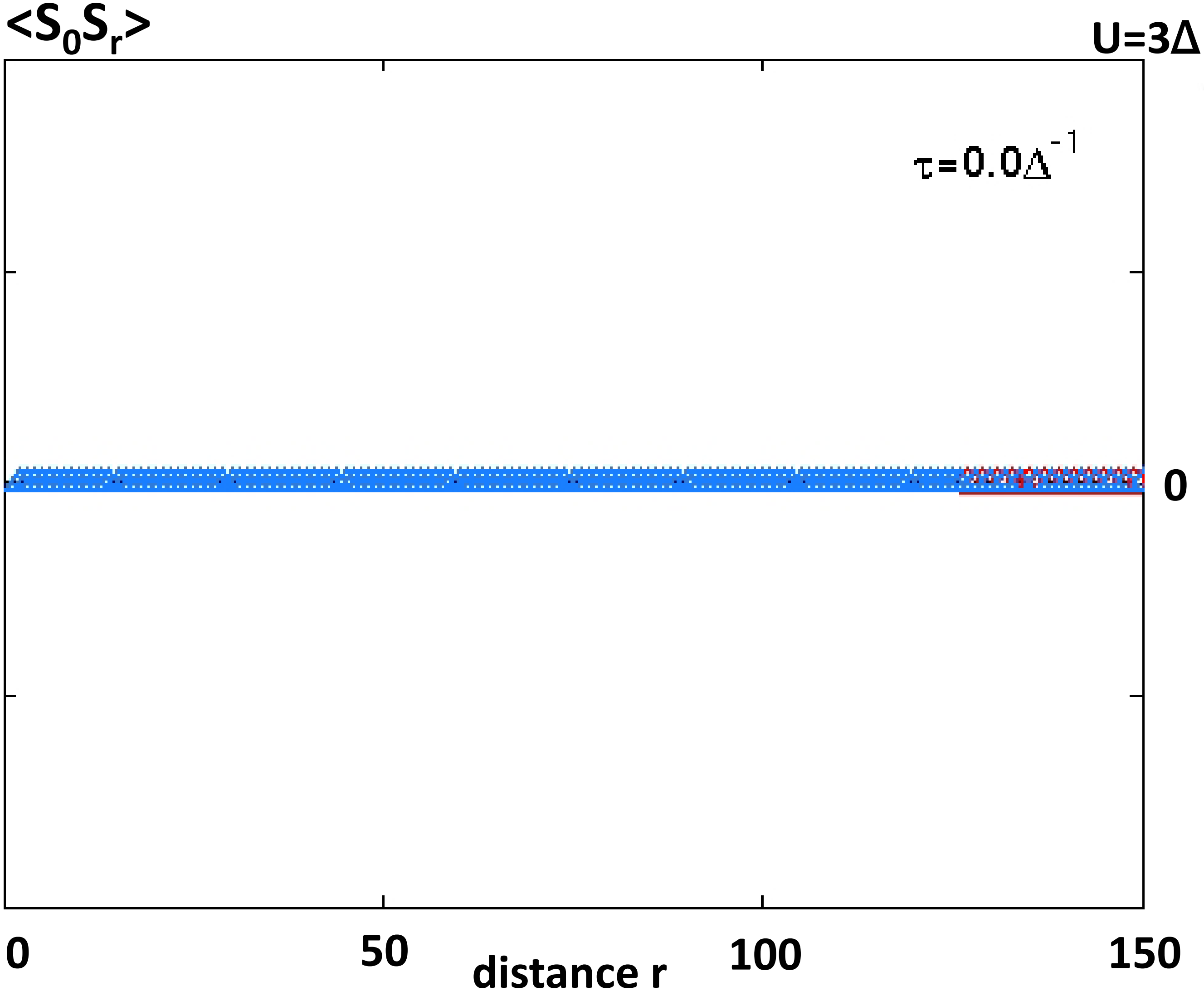
itp^cp

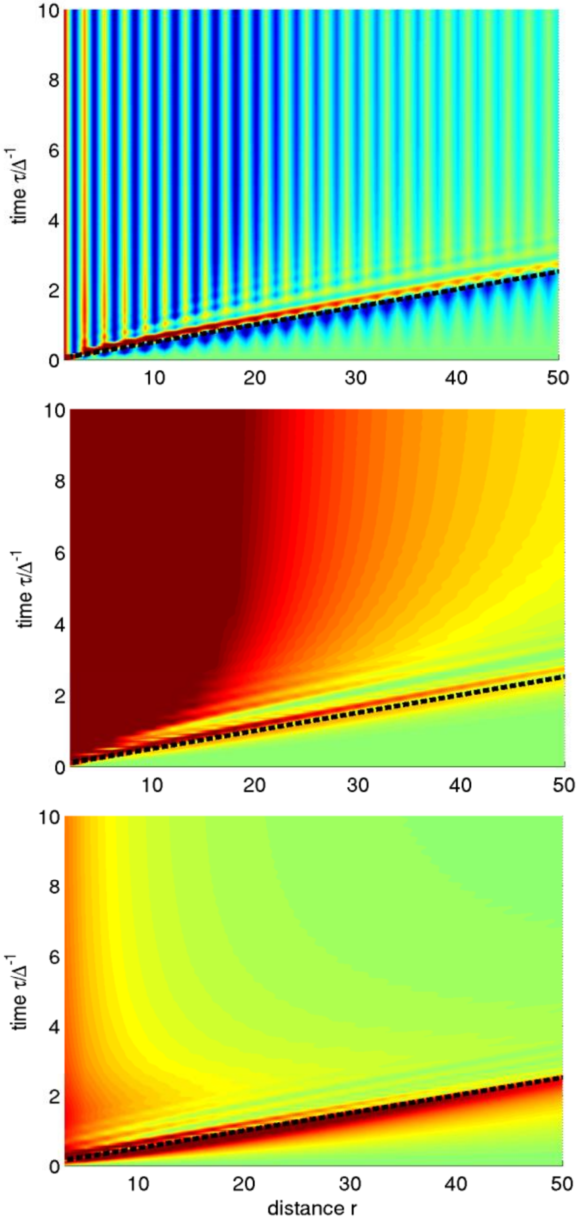


<n> <S_z>

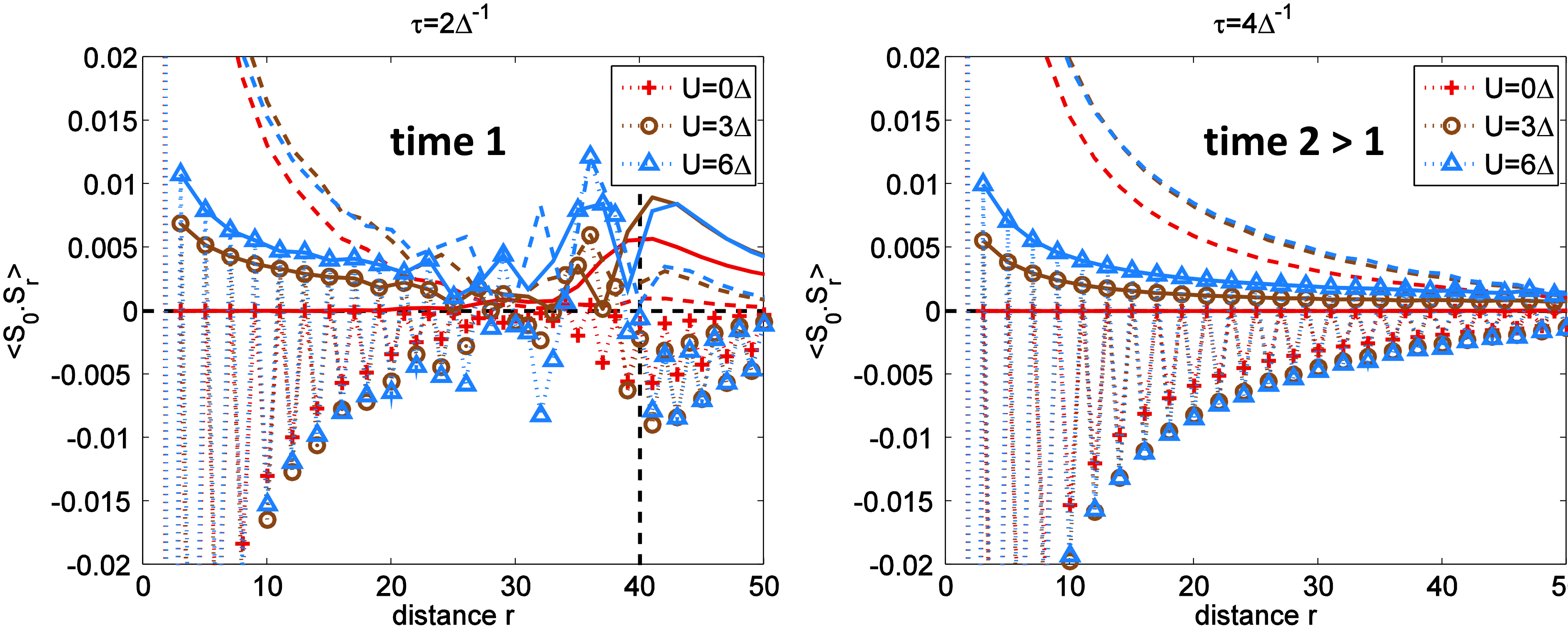
- **quench – transients**
- **travelling signal (Lieb Robinson)**
  Lieb and Robinson, CMP. **28**, 251 (1972)
- **eventually: (local) steady-state**
- **finite size (reflections)**
- **finite time (entanglement growth)**

$\langle S_0 S_r \rangle$ (time)





$<S_0 S_r>$ (time)



time →

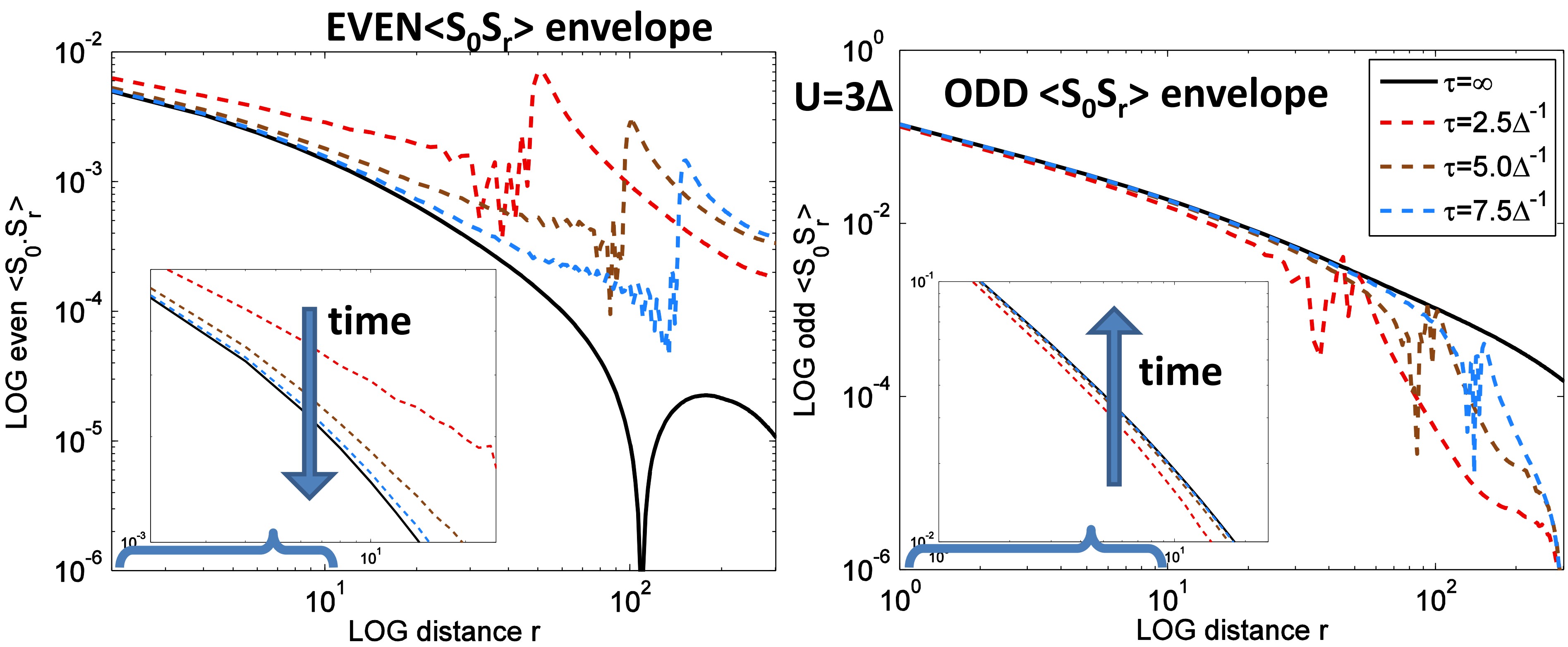
- **Toulouse limit (bosonization + refermionization)**

  M. Medvedyeva etal. PRB **88**, 094306 (2013)

- **RLM (exact diagonalization)**

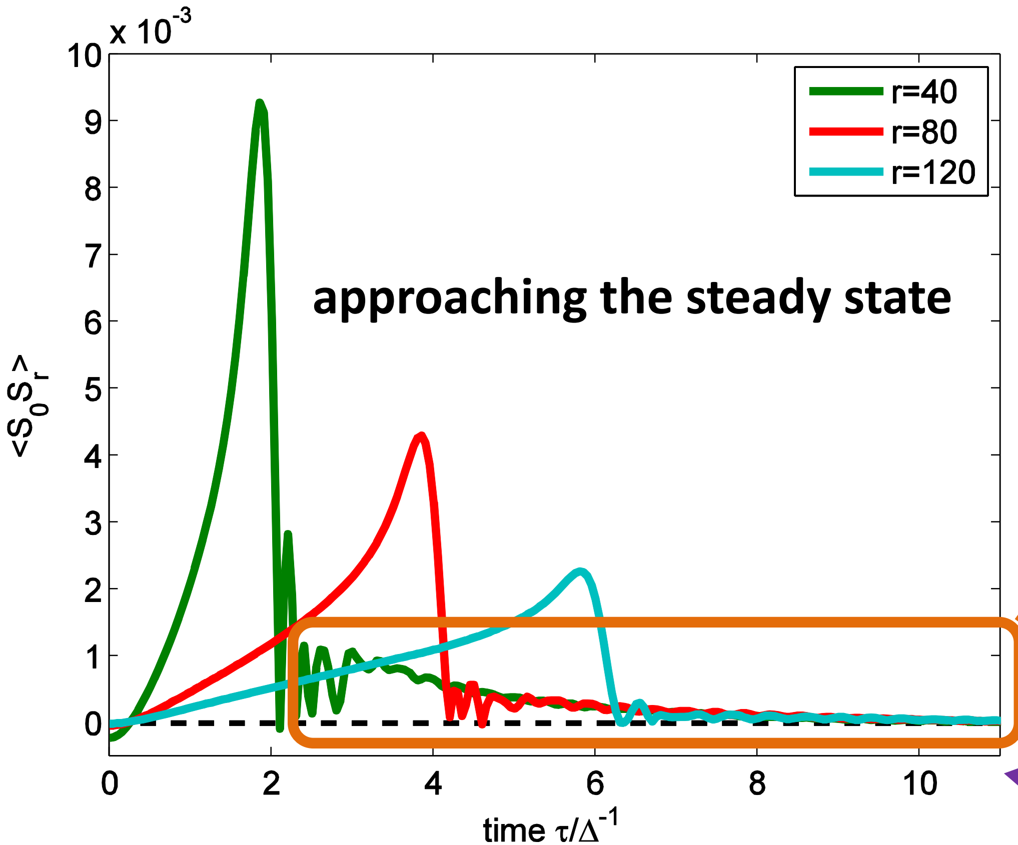
  S. Ghosh etal. arXiv:**1309.0027**v1 (2013)

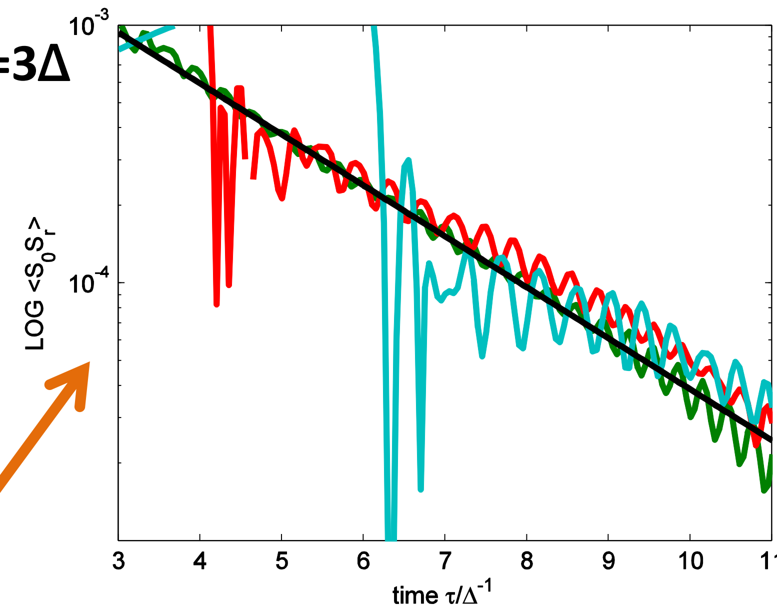
$<S_0 S_r>$(time) envelope

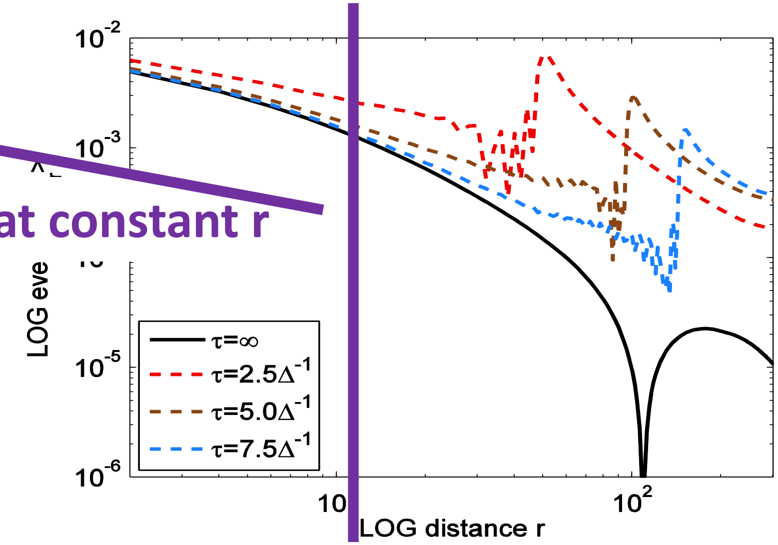


- time to infinity data = equilibrium simulation!

$<S_0S_r>$(time) envelope







- **single exponential decay:**

$$< S_0 S_r > (t) = 0.0037 e^{-0.4555\, t\, [\frac{1}{\Delta}]}$$

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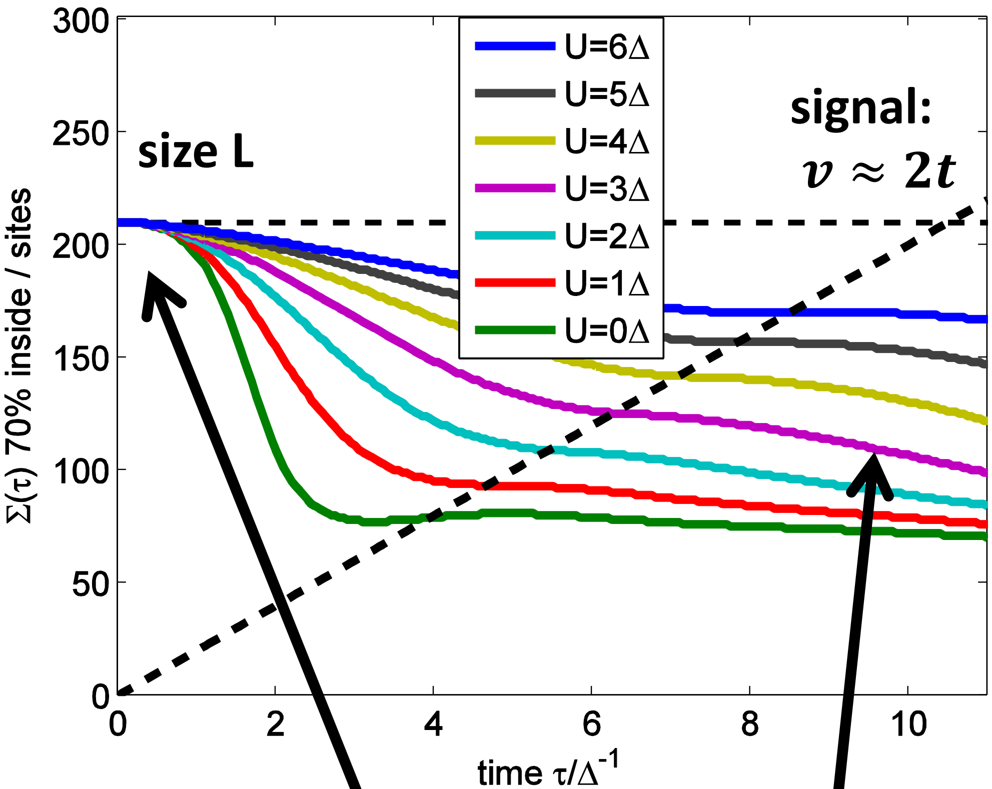
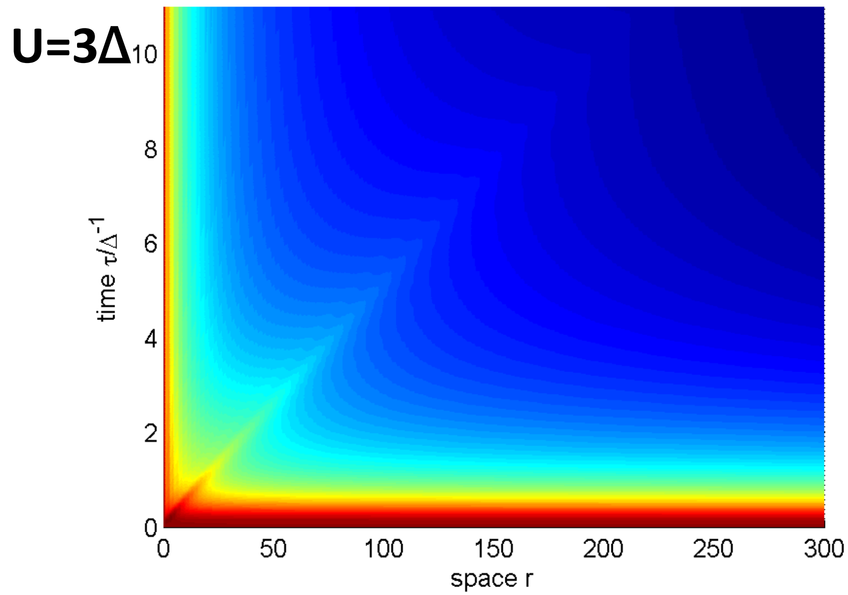
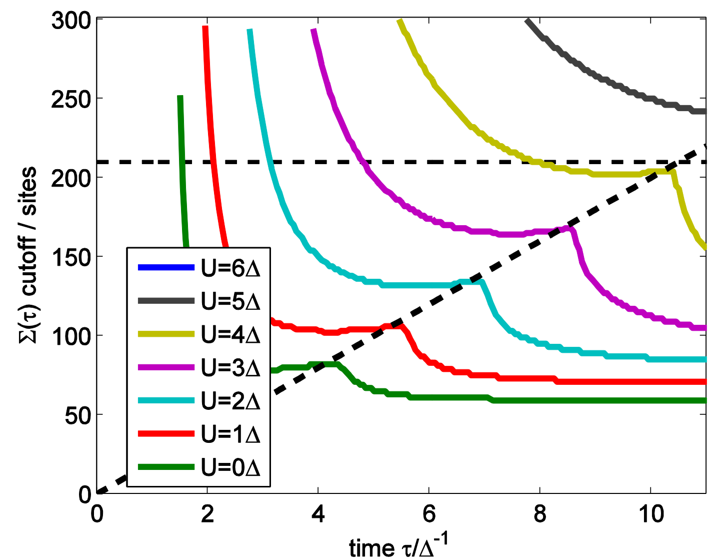
itp[cp]

Integrated Correlator

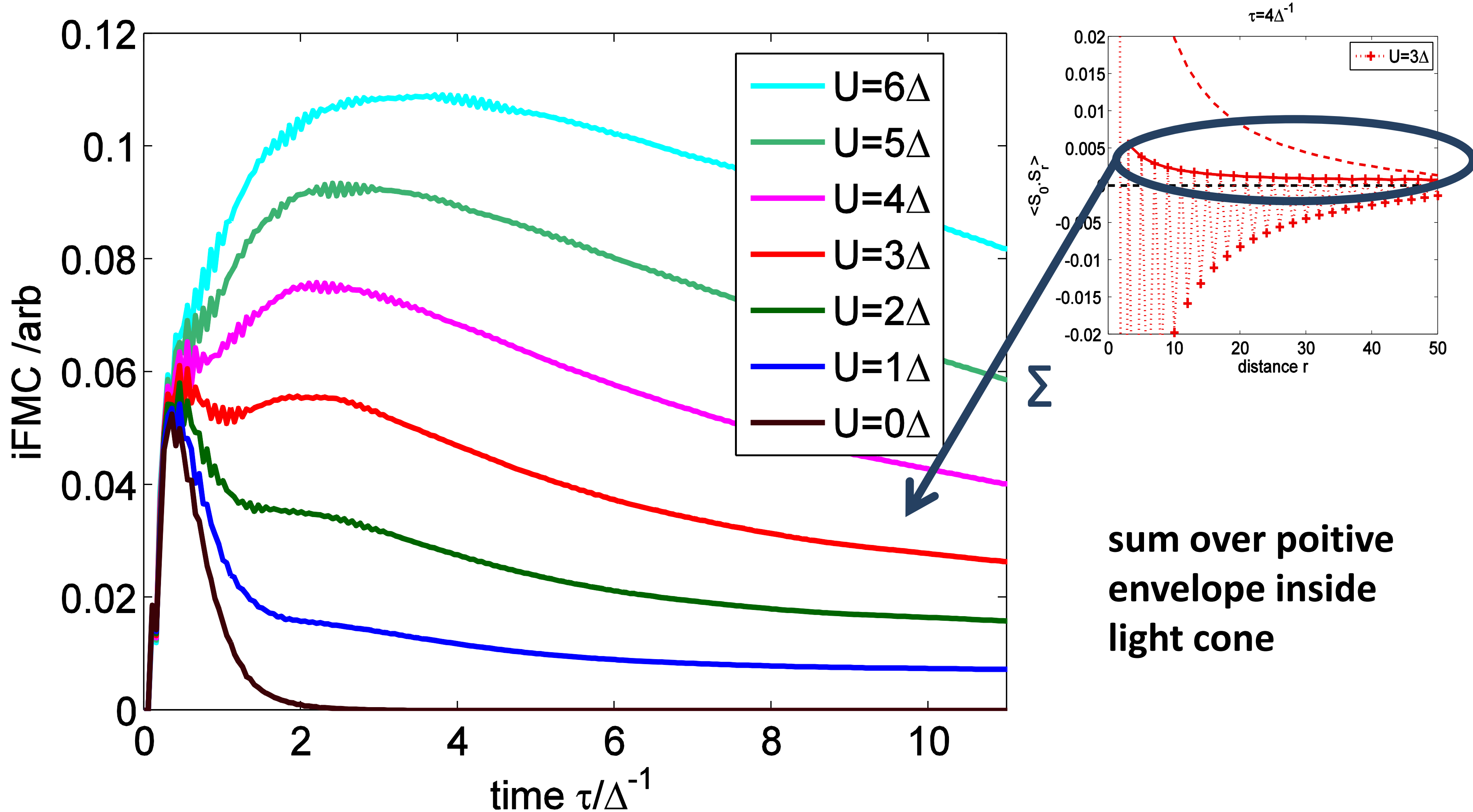






- **small times** ✗
- **general trend of Kondo buildup**
  - **convergence at long times?**
- **lattice velocity builds up singlet**
  - **larger time scale?**

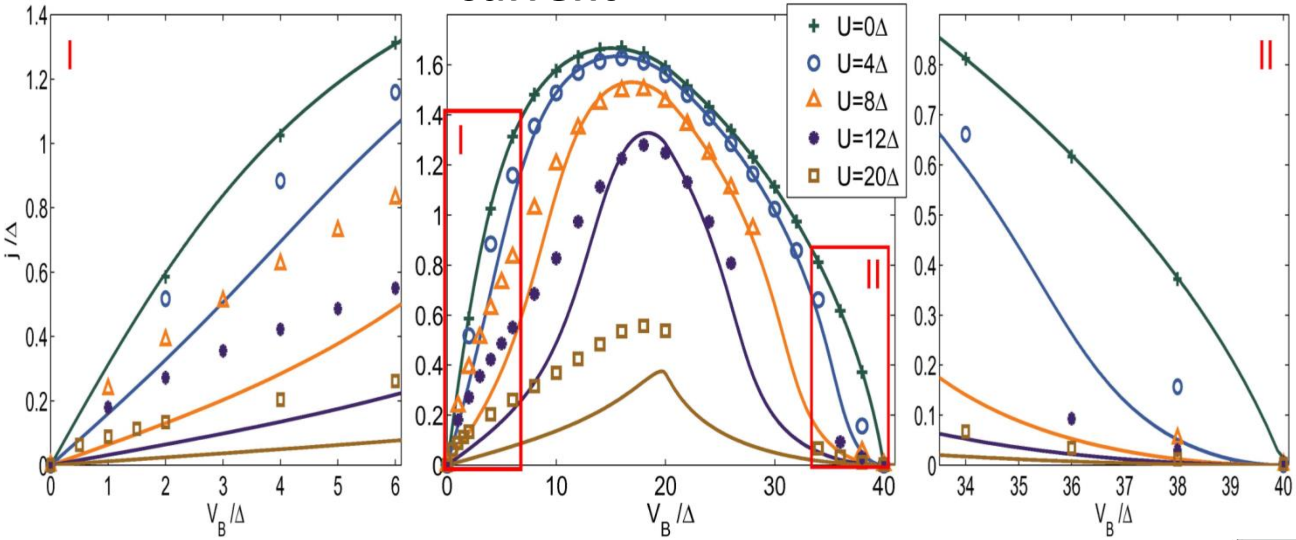
„Ferromagnetic“ Component

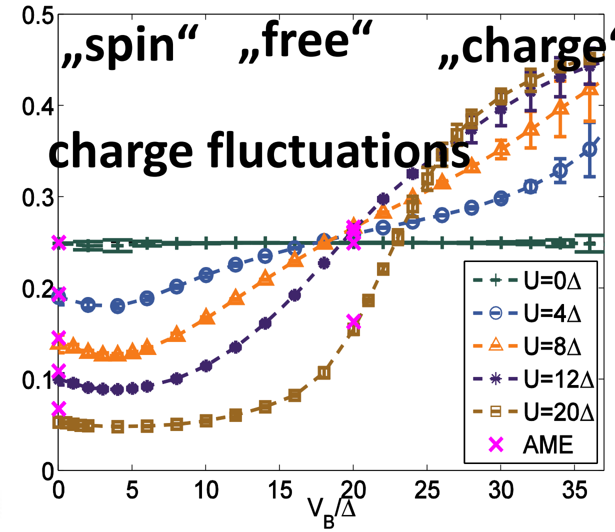


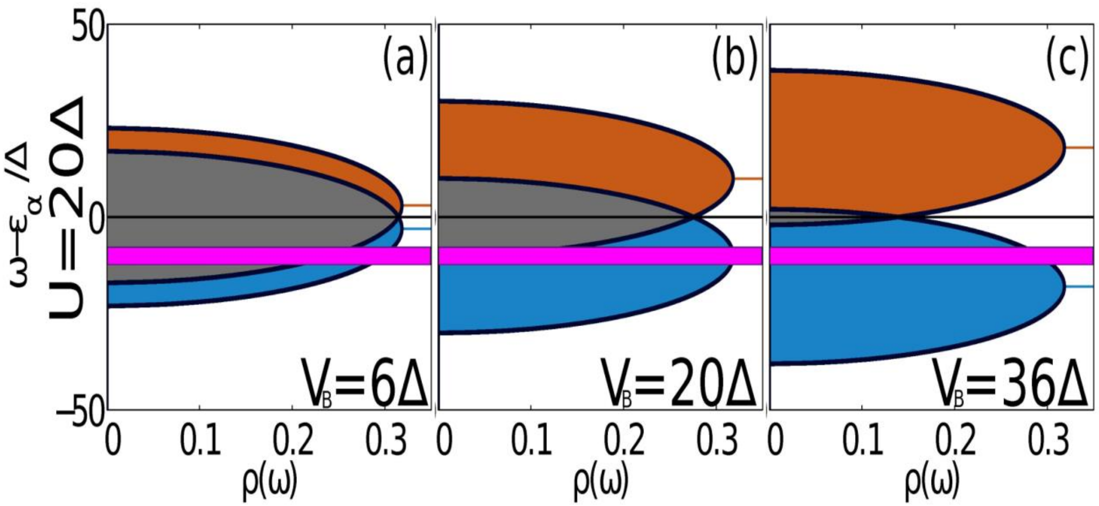
sum over poitive envelope inside light cone

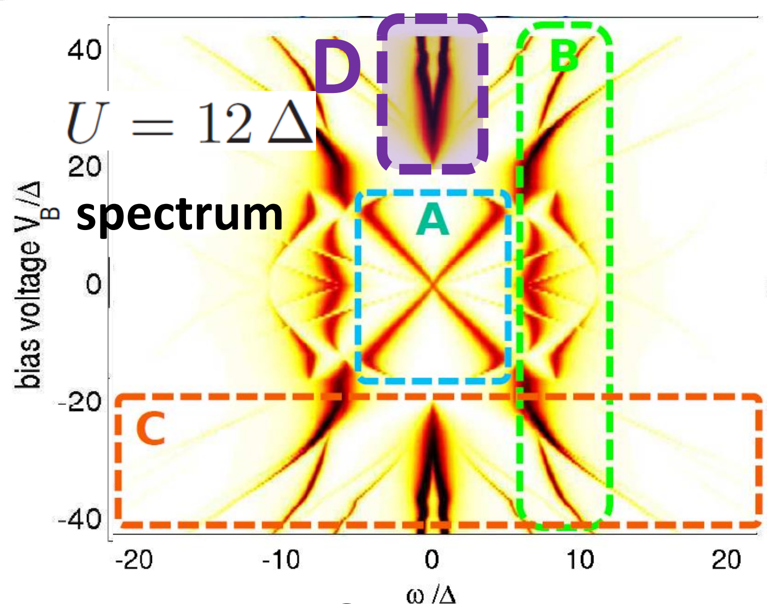
Correlations & Bias

current









data from MPS, AME & nVCA

Conclusions + Outlook

- **1) real time evolution up to steady state**

MN, M. Ganahl, H. G. Evertz, E. Arrigoni, W. von der Linden, PRB **88**, 045132 (2013)
MN, E. Arrigoni, W. von der Linden, AIP Conf. Proc. 1485, ISBN: 978-0-7354-1097-8 (2012)

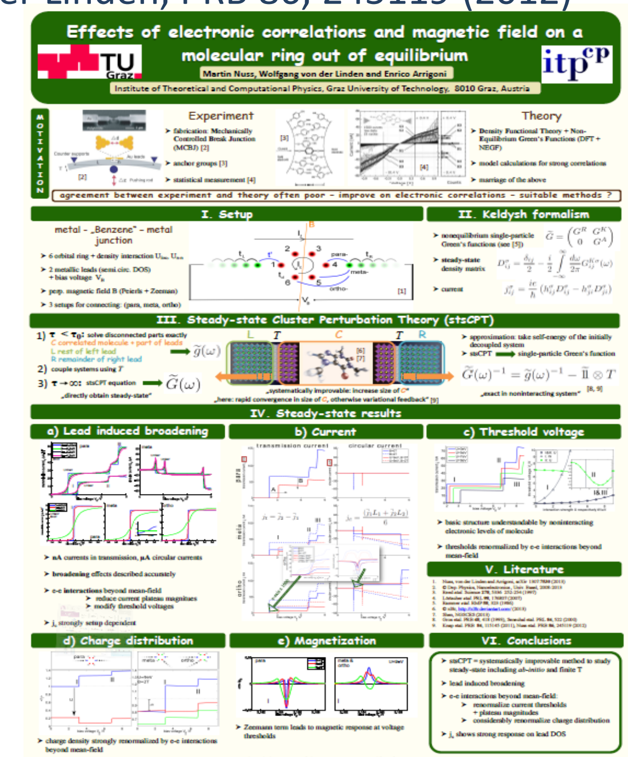
- **2) correlations + bias voltage**

MN, C. Heil, M. Ganahl, M. Knap, H. G. Evertz, E. Arrigoni, W. von der Linden, PRB 86, 245119 (2012)

- **3) Kondo singlet**

MN, M. Ganahl, A. Dorda, H. G. Evertz, E. Arrigoni, W. von der Linden, (2014)

- **whats to come**
  - **Kondo singlet under bias**
  - **Reverse quench**



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our work on molecular junctions:
TT 101.14 „Transport“, Thu 15:00

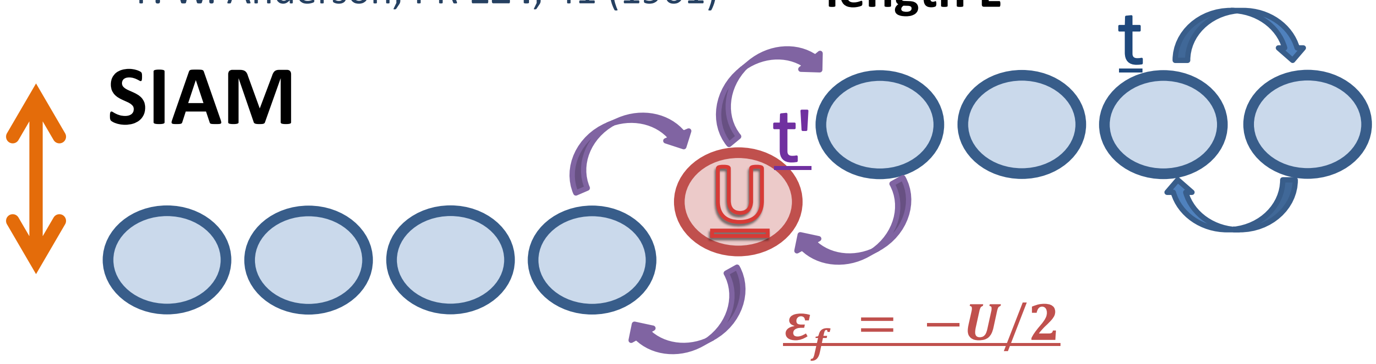
MN, W. von der Linden, E. Arrigoni, arXiv:**1307.7530**, **PRB** in press (2014)

Real Time Evolution

P. W. Anderson, PR **124**, 41 (1961)

length L

bias Voltage V_B



symmetric interacting impurity U

2 finite 1D tight binding leads: ε, t

hybridization quench: t'

- Suzuki-Trotter *real* time evolution using MPS
  - DMRG + TEBD
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    G. Vidal, PRL **93**, 040502 (2004)

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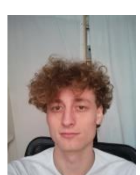
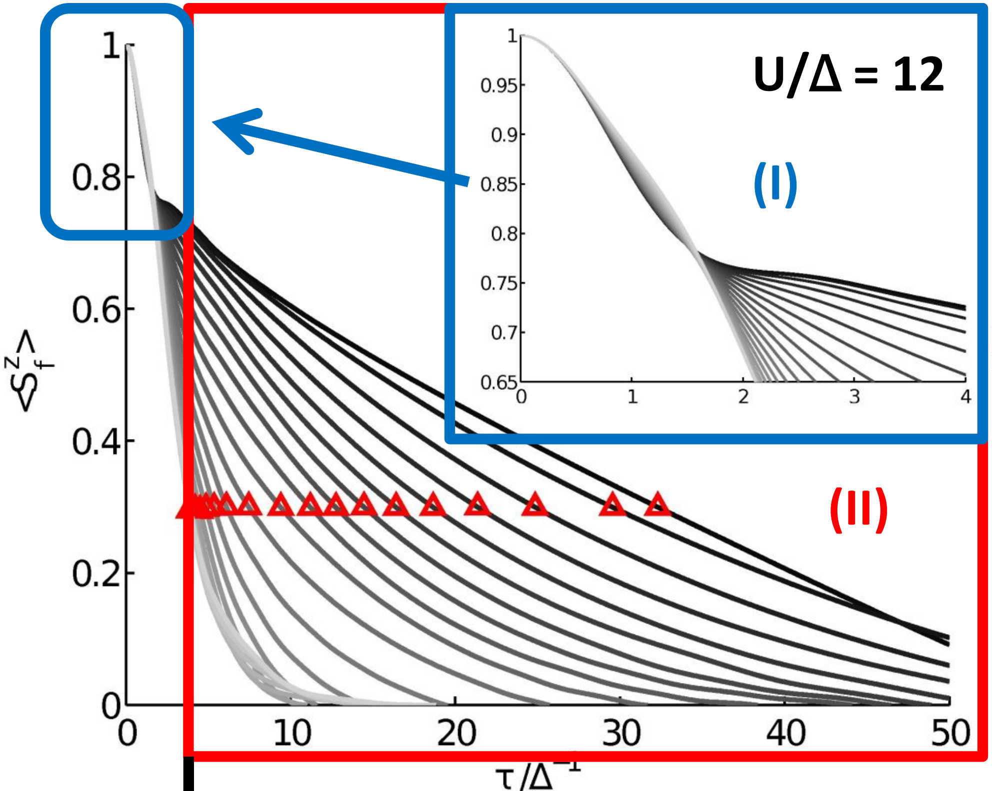
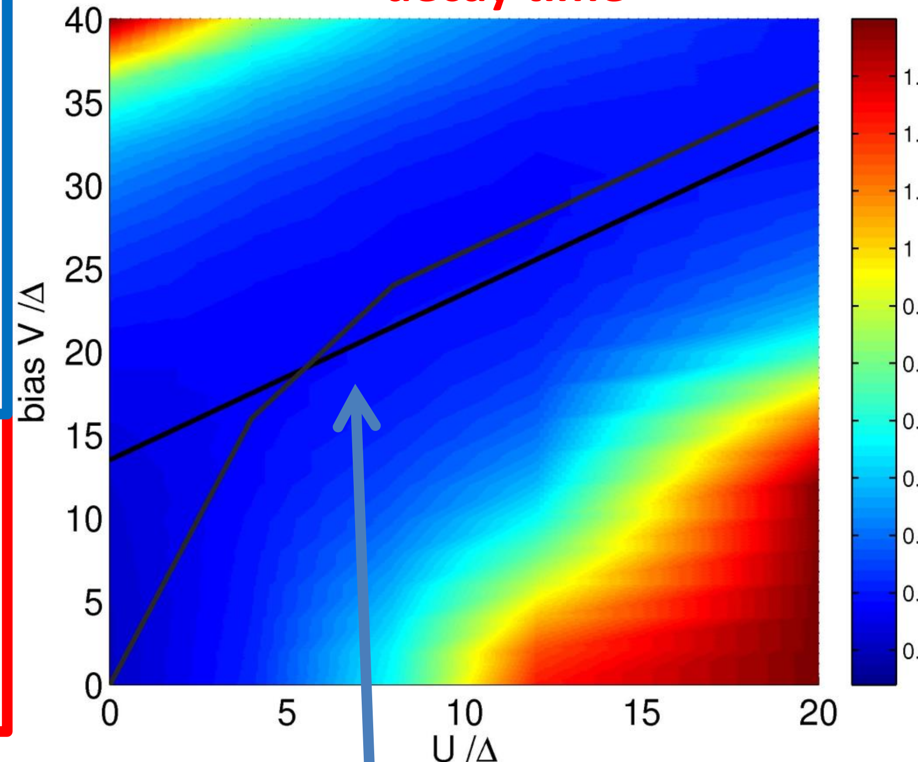
- massively *parallel* code
  - Martin Ganahl



Spin Relaxation



decay time



(I) complex $\tau_s \approx 1.7\,\Delta^{-1}$ (II) single exponential

optimal relaxation: $V_c[\Delta] \approx 1.35(U[\Delta]+1)$

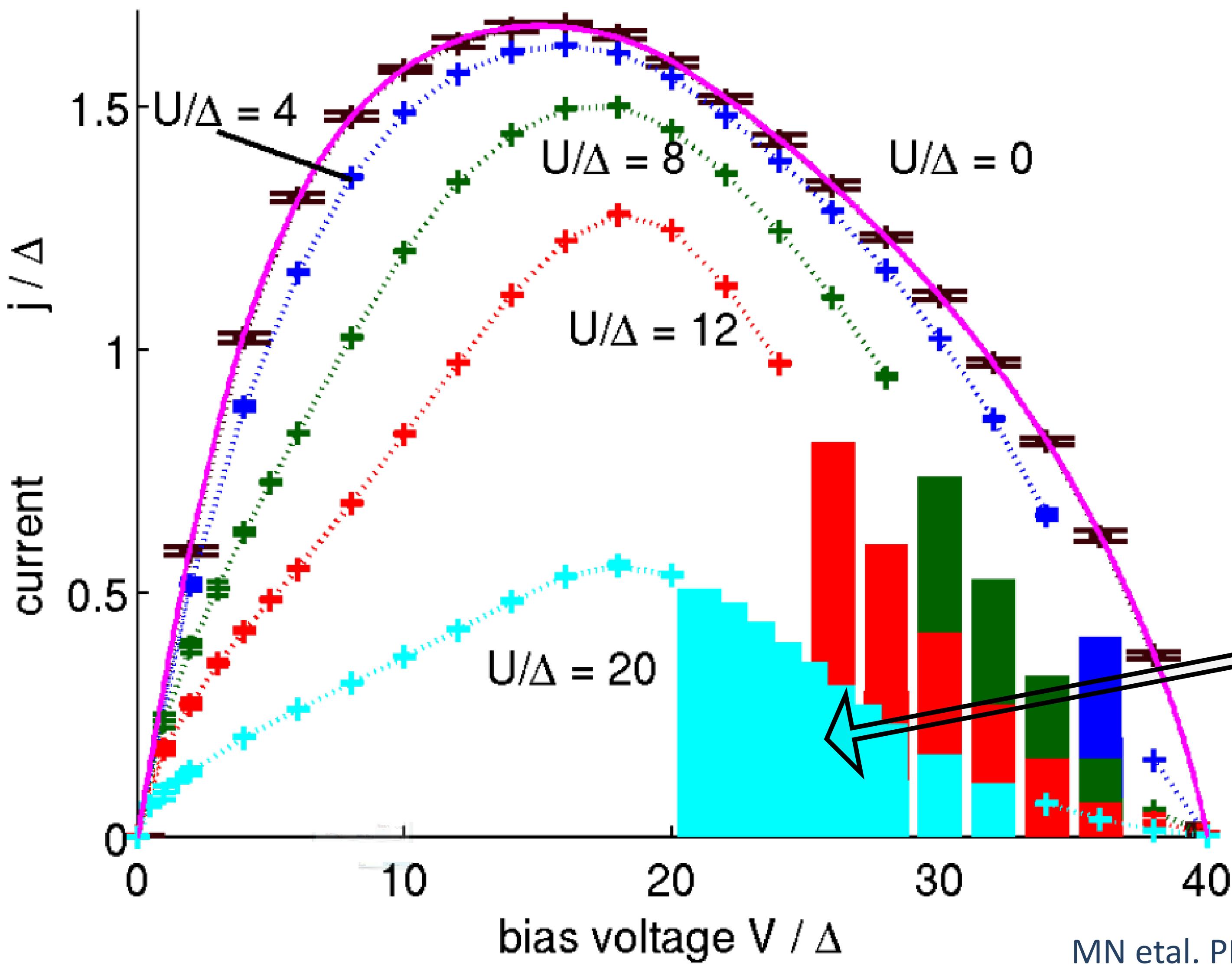
$T \approx (V - U - c)^4$

low bias voltage → high bias voltage

see also bold-line QMC:

G. Cohen, etal. PRB **87**, 195108 (2013)

Current - Voltage



see also tDRMG

F. Heidrich-Meisner, etal. PRB **79**, 235336 (2009)

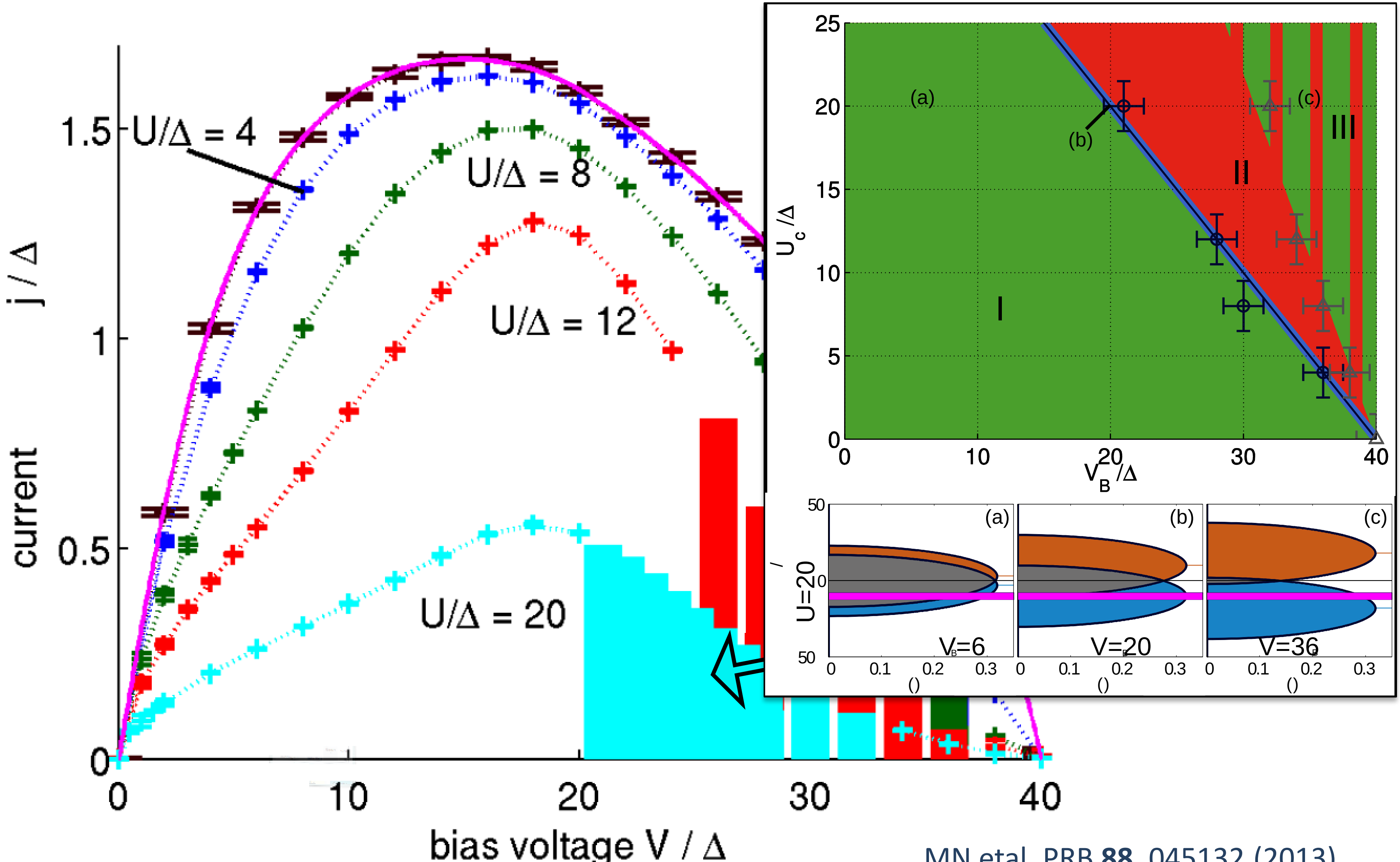
QMC

P. Werner etal. PRB **81**, 035108 (2010)

...

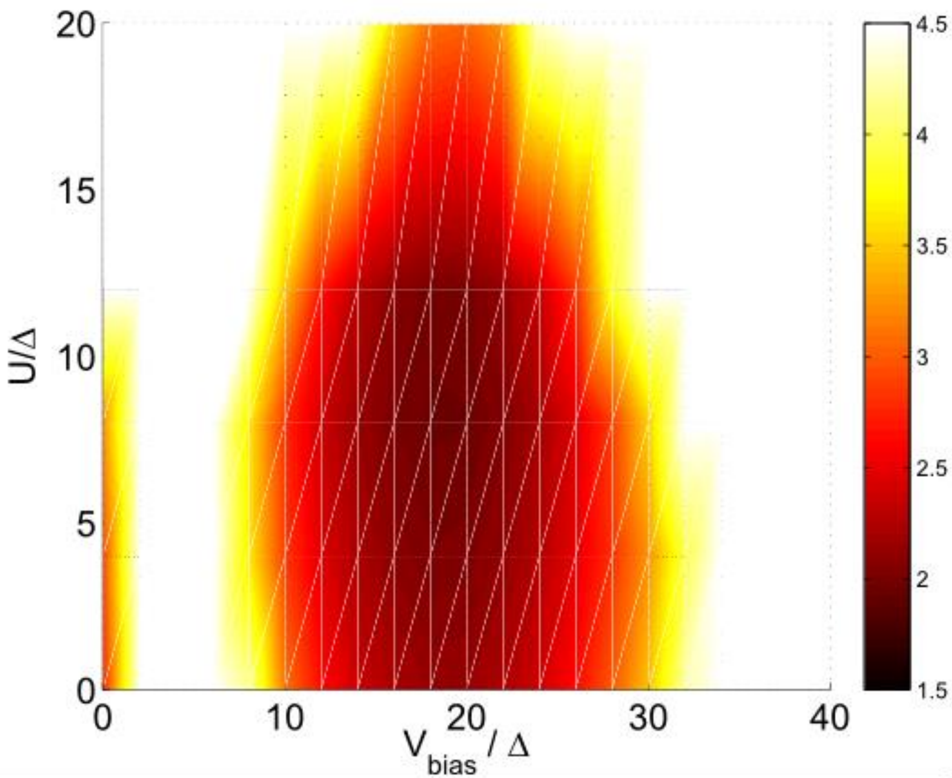
MN etal. PRB **88**, 045132 (2013)

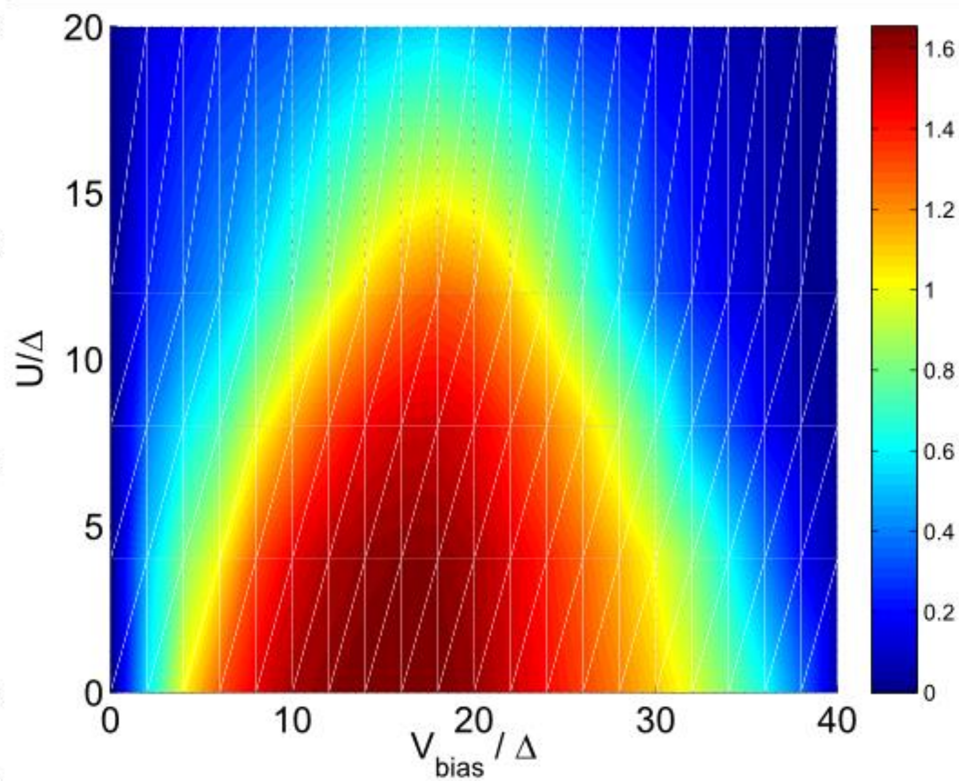
Current - Voltage



MN etal. PRB **88**, 045132 (2013)

Entanglement vs Current

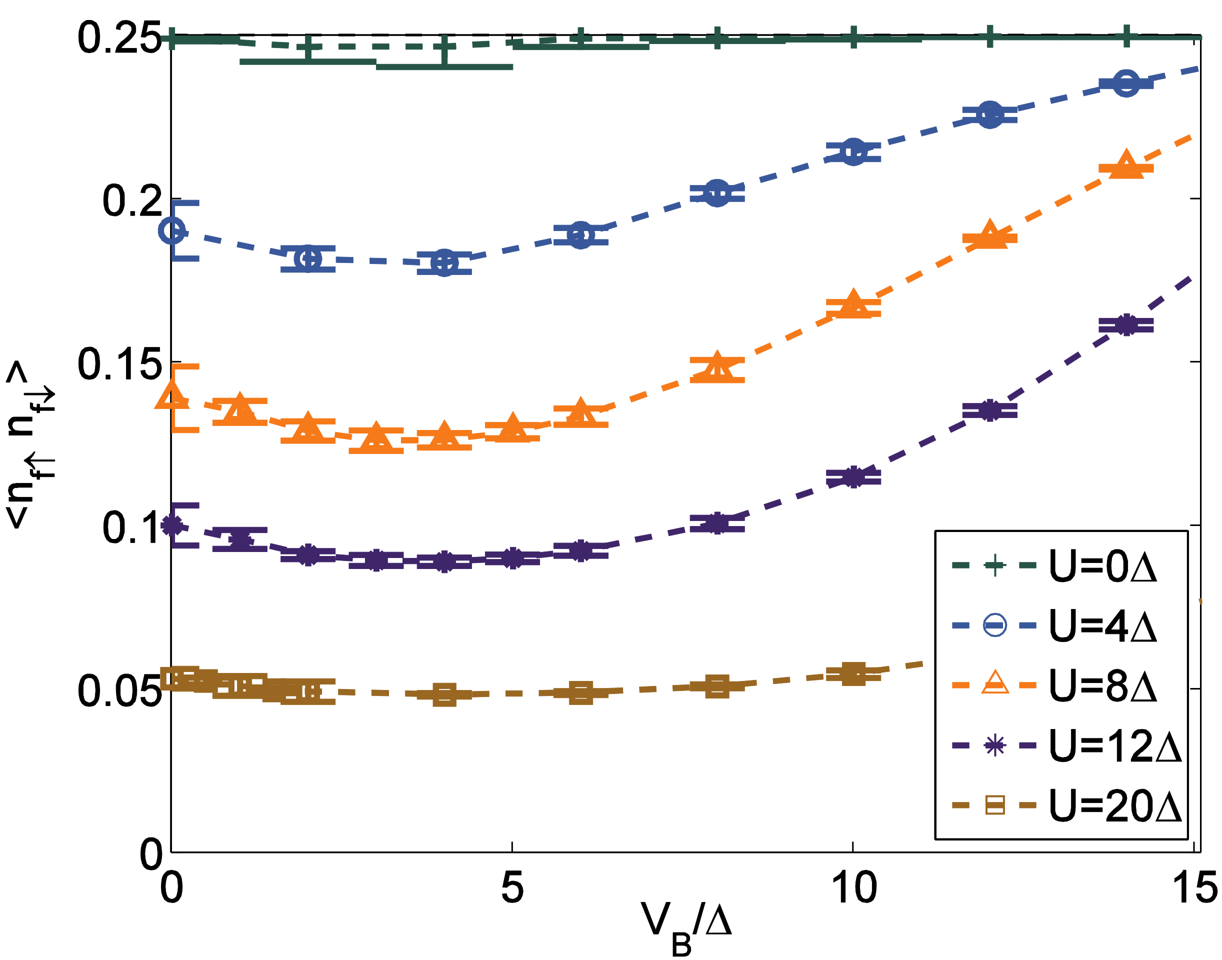




$$S_i = -\mathrm{tr}\left(\hat{\rho}_L \ln\left(\hat{\rho}_L\right)\right)$$

$$\hat{j}_{ij}(\tau) = \imath\, t_{ij} \sum_{\sigma} \left(a^{\dagger}_{i\sigma}\, a_{j\sigma} - a_{i\sigma}\, a^{\dagger}_{j\sigma} \right)$$

Double Occupancy



bias voltage ⇨

- **charge fluctuations**

$$\langle n_f \rangle = 1 \quad \langle m_f \rangle = 0$$

$$D = \langle n_{f\uparrow} n_{f\downarrow} \rangle = \frac{1}{2}\left(\langle n_f^2 \rangle - \langle n_f \rangle^2\right)$$

$$M = \tfrac{1}{4}\,(1 - 2\,D)$$

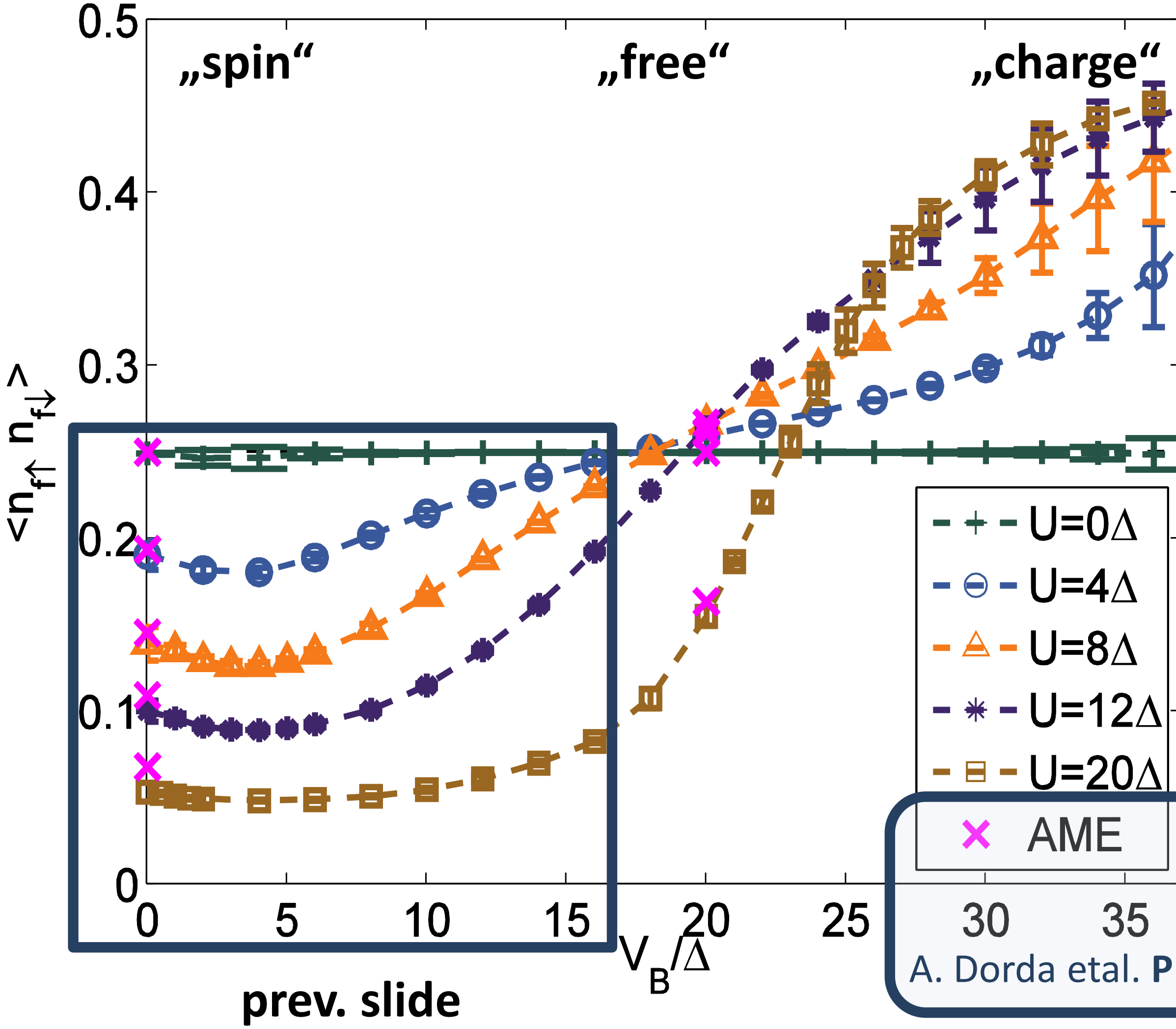
- **noninteracting limit**
  - **D = 0.25**

- **for MV-QMC, RT-QMC, SNRG see**

A. Dirks etal EPL **102** 37011 (2013)

TUG itp^cp

Double Occupancy



correl.	D	2M
„spin“	0 … ¼	½ … ¼
„free“	¼	¼
„charge“	¼ … ½	¼ … 0

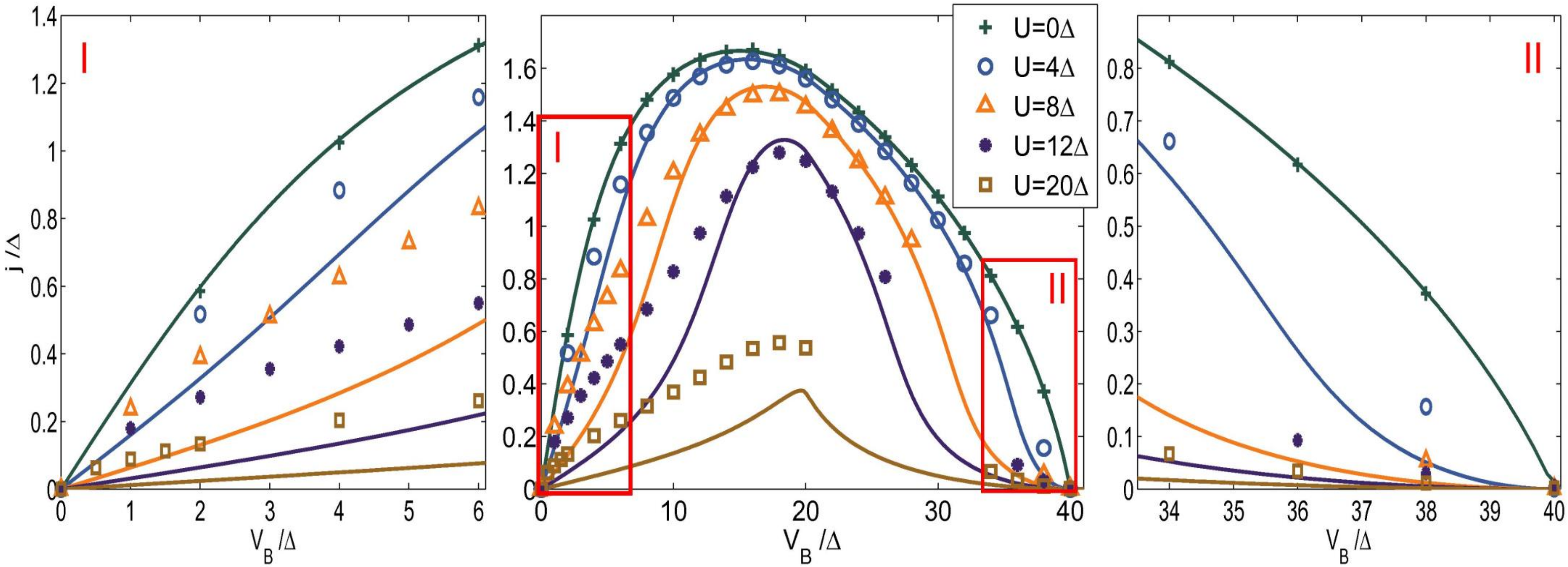
implications for transport?

$$|\Psi^{>}\rangle \sim \sum \left(c_{\uparrow\downarrow}\,|\uparrow\downarrow\rangle_f - c_0\,|0\rangle_f\right)\otimes|L\rangle\otimes|R\rangle$$

see talk by A. Dorda
TT96.5, Thu 16:00

A. Dorda etal. **PRB** in press (2014), arXiv:**1312.4586**

Current - Voltage



non interacting

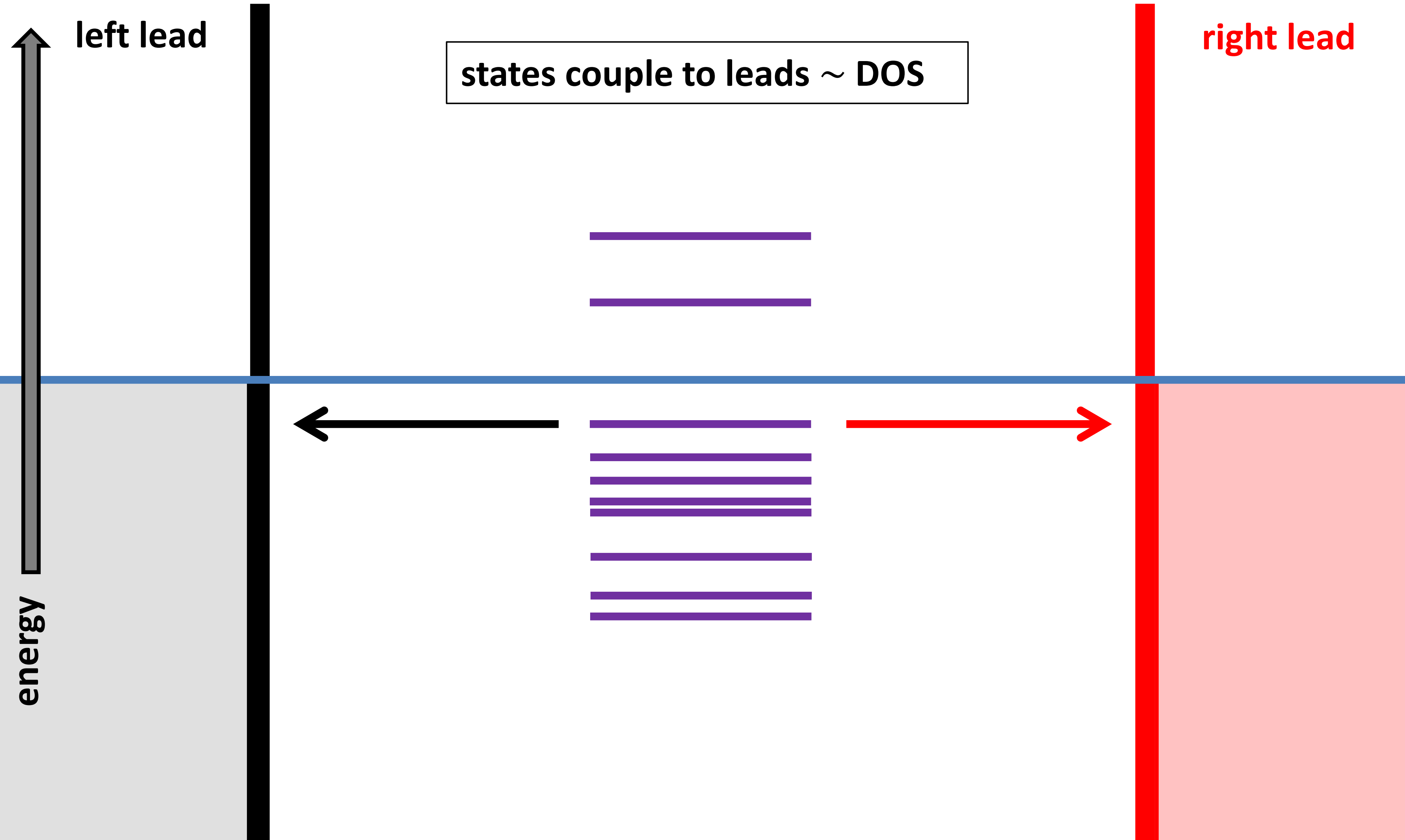
interacting

$$j = i \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} \left(\left(\gamma_L(\omega) - \gamma_R(\omega)\right) G^<(\omega) + \left(p_{\mathrm{F},L}(\omega)\gamma_L(\omega) - p_{\mathrm{F},R}(\omega)\gamma_R(\omega)\right) \left(G^R(\omega) - G^A(\omega)\right) \right)$$

Meir and Wingreen, PRL **68**, 2512 (1992)
Haug and Jauho, **Springer**, (1998)

Dynamics ?

Wide Band



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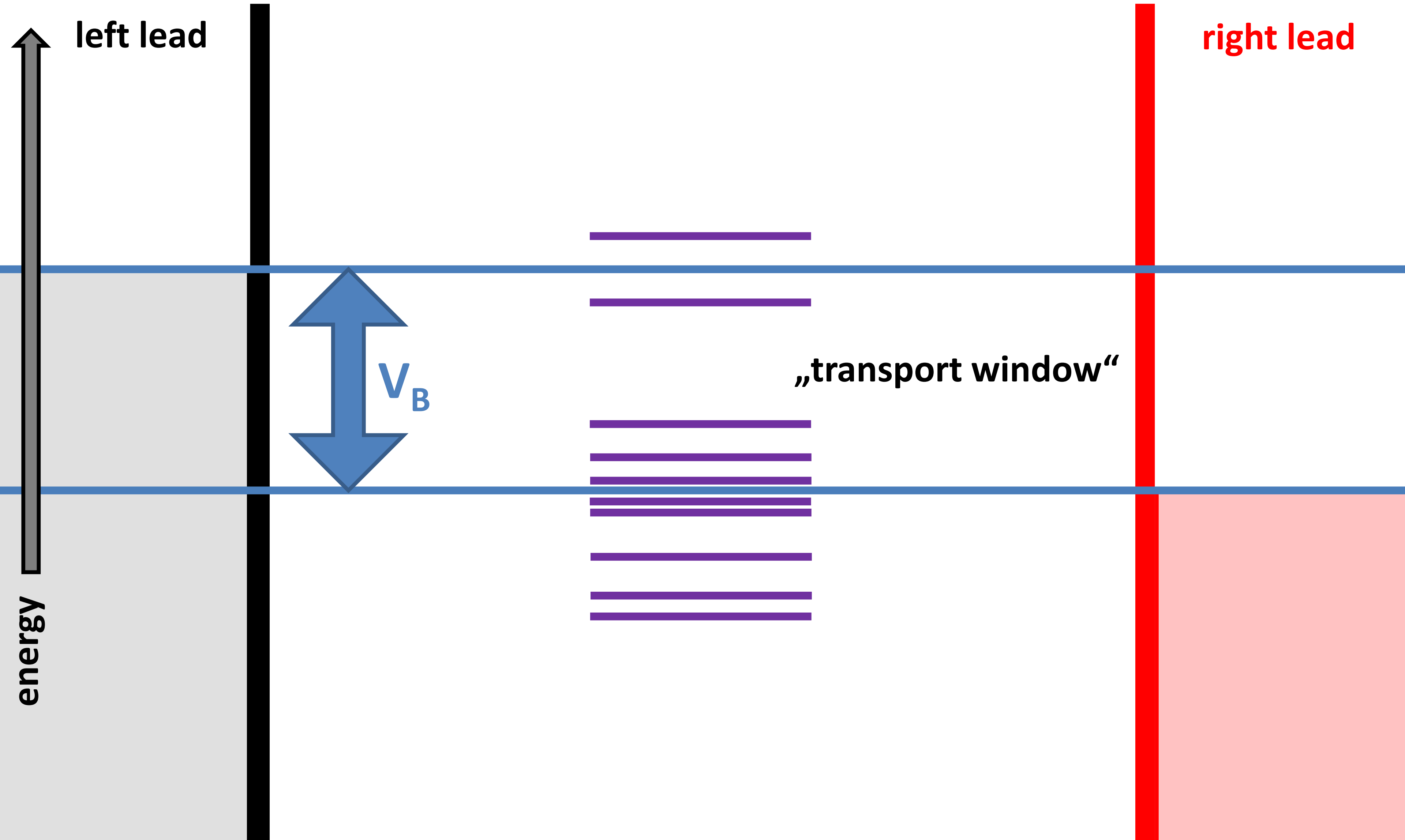
Wide Band



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„Wide Band“ Limit

itp^{cp}

"perturbing" energy scale V_B

~ effective temperature T

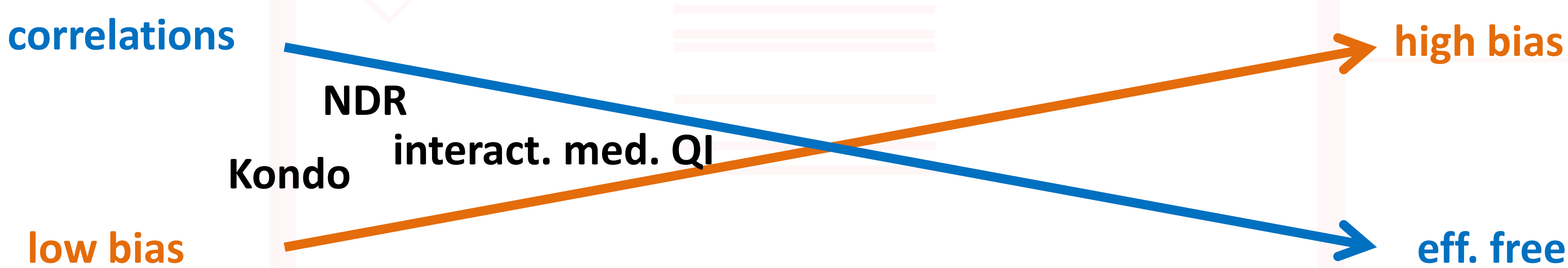
L. Mühlbacher etal. PRB **83**, 075107 (2011)
M. Pletyukhov etal, PRL **108**, 260601 (2012)
A. V. Kretinin etal.PRB **85**, 201301 (2012)

~ effective magnetic field B

A. V. Kretinin etal. PRB **84**, 245316 (2011)

M. Pletyukhov etal. PRL **104**, 106801 (2010)

suppressing electronic correlations



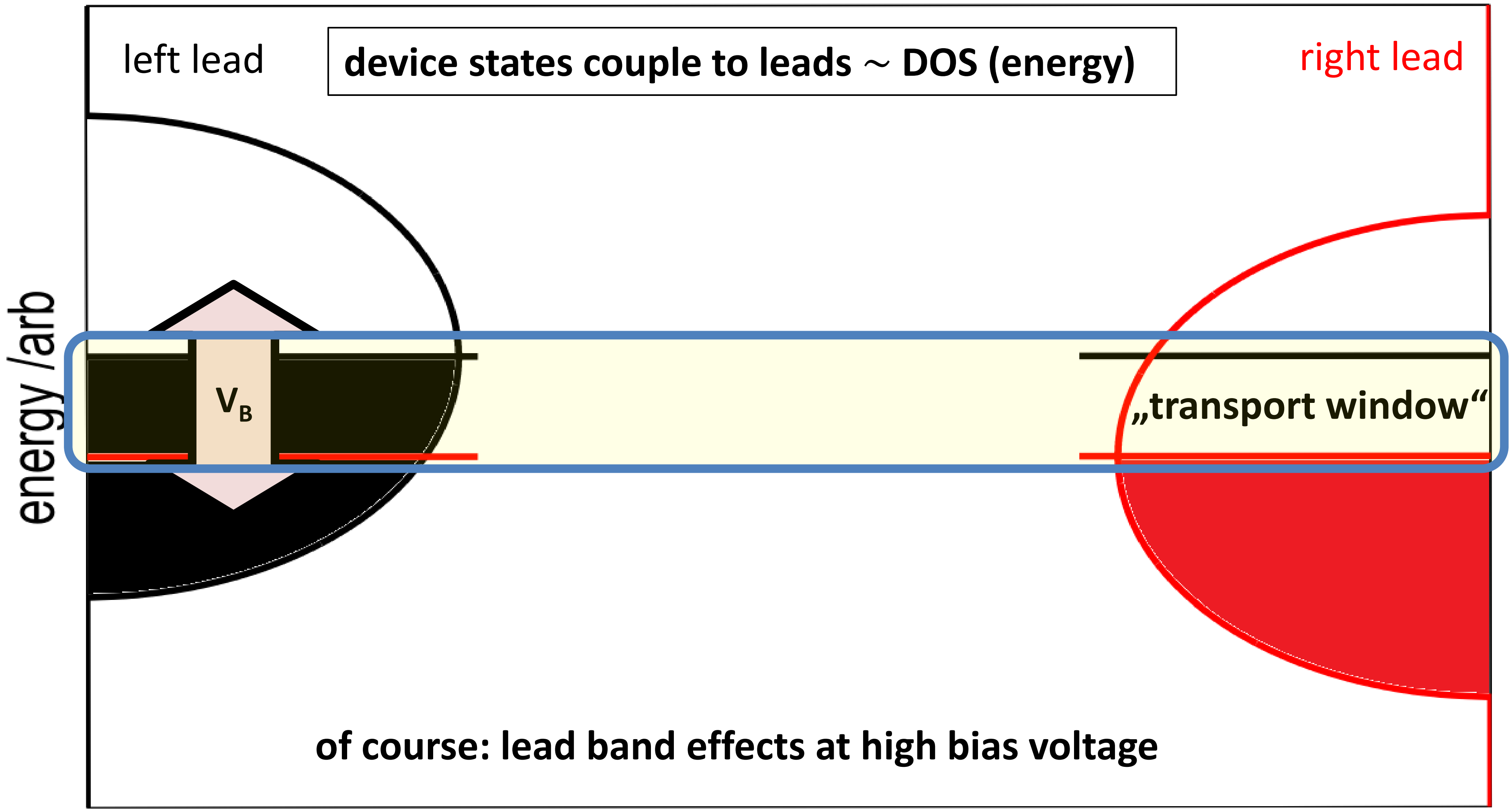
nothing interesting at high bias voltages? NO: Lead induced NDR:

Bâldea and Köppel, PRB **81**, 193401 (2010)

TUG

itp[cp]

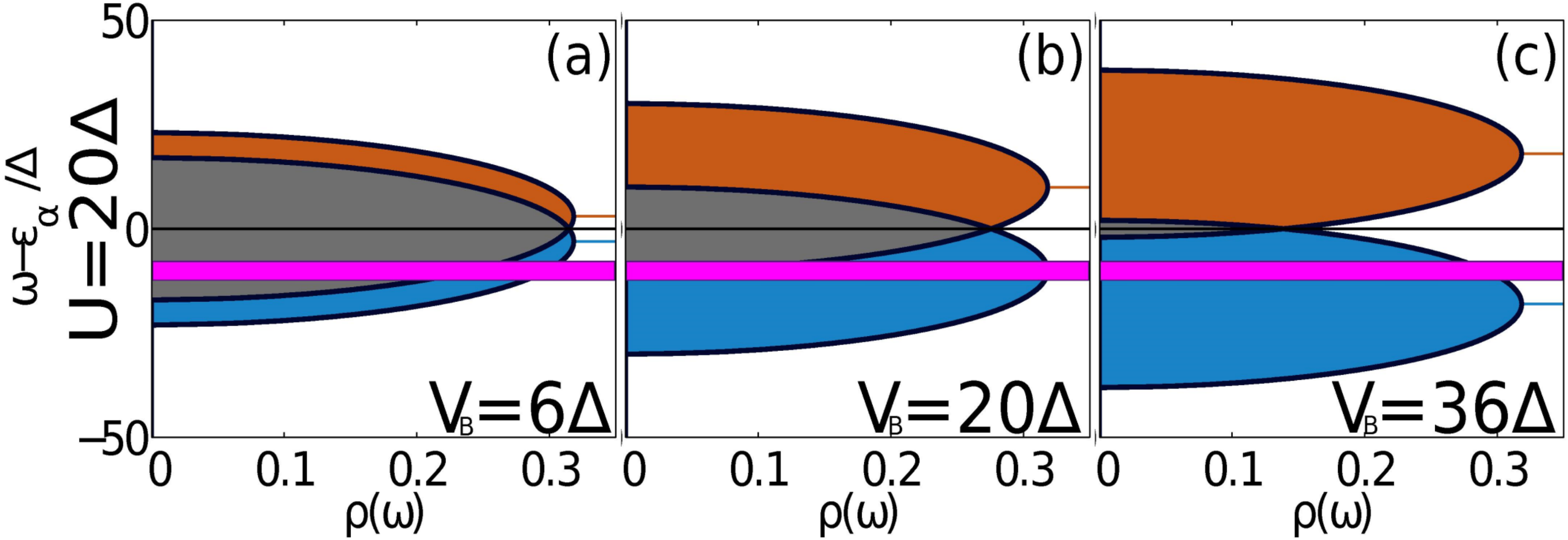
Lead DOS effects



TUG

Lead DOS effects

itp^cp

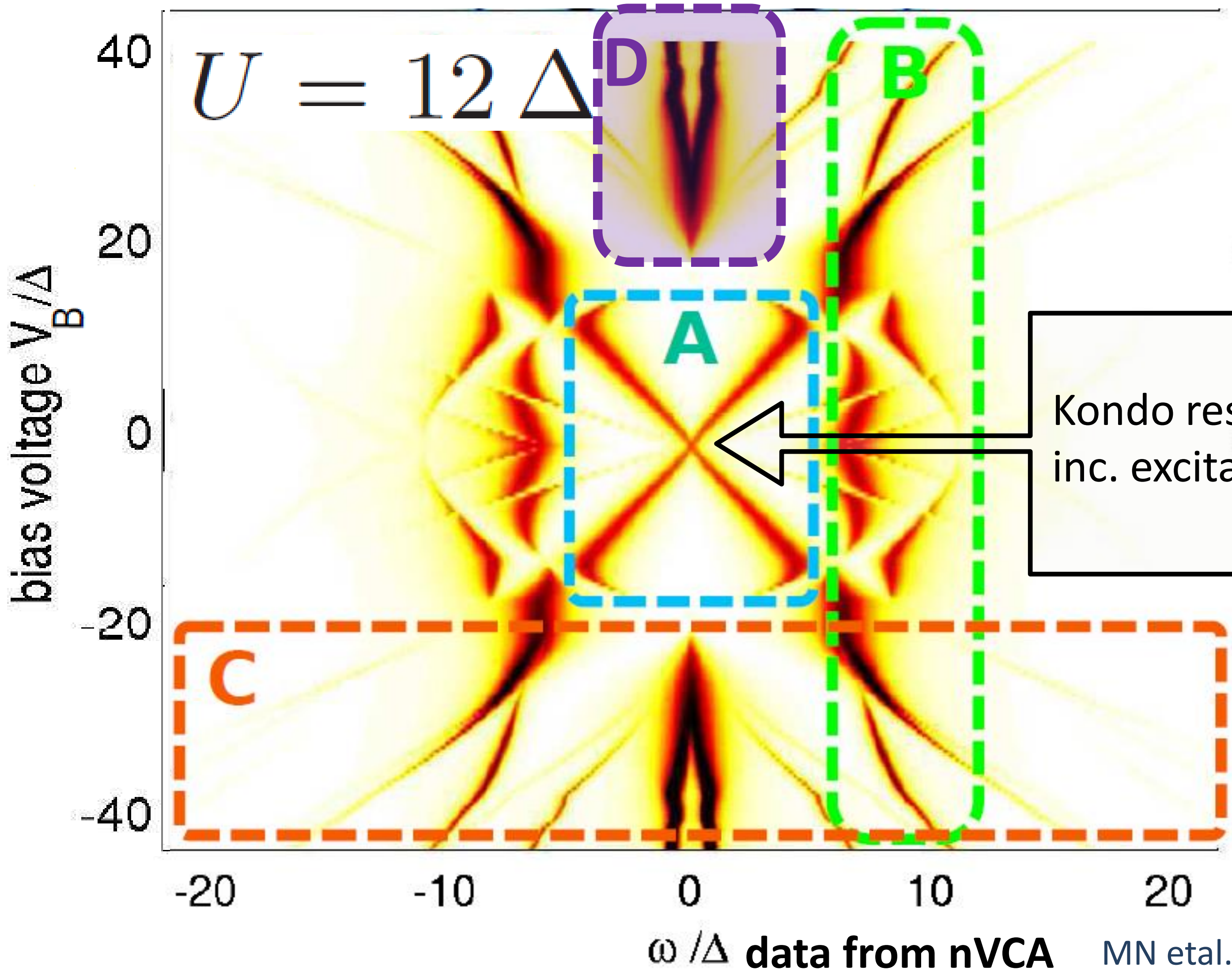


bias voltage

transport window **single particle state** **left lead** **right lead**

structured lead DOS can promote electronic correlations also at high bias voltage

Non Equilibrium Spectral Function



data from nVCA

A: „Kondo“

D: High bias resonance

Equilibrium

Kondo resonance @ $\omega \approx 0$

inc. excitations @ $\omega \approx \pm\frac{U}{2}$

B: Hubbard band

C: lead-band

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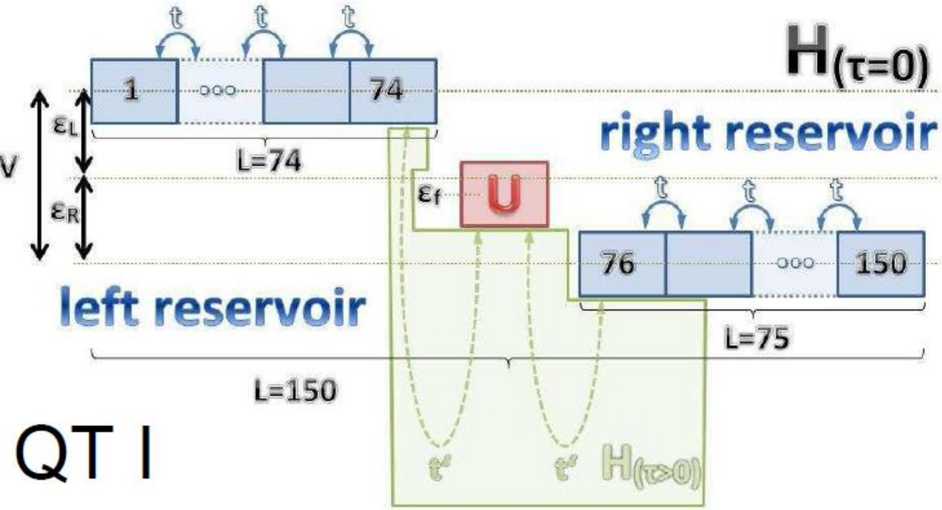
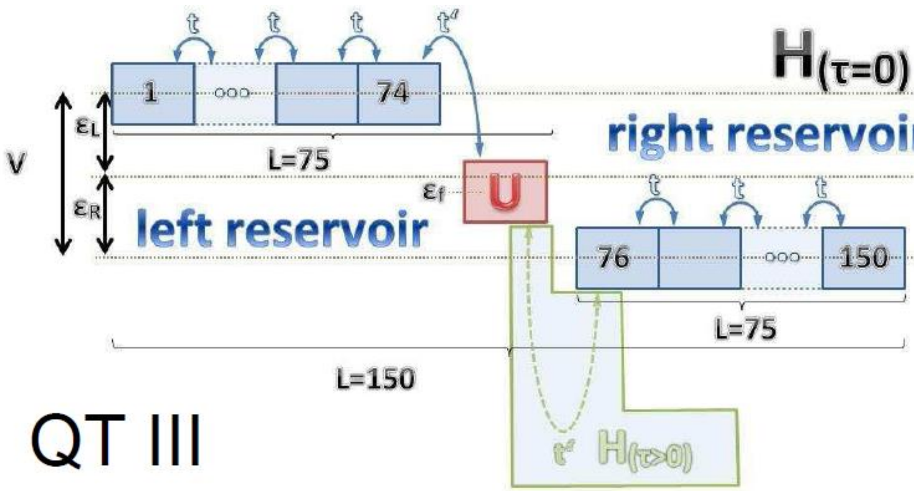
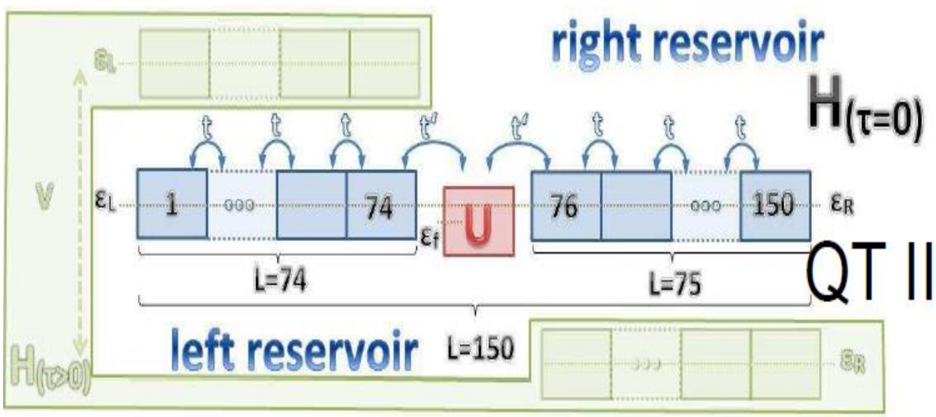
3 Queneches



QT I



QT III



QT II

comparison of short time quench dynamics
+ quasi-steady-state

Time evolution of Current