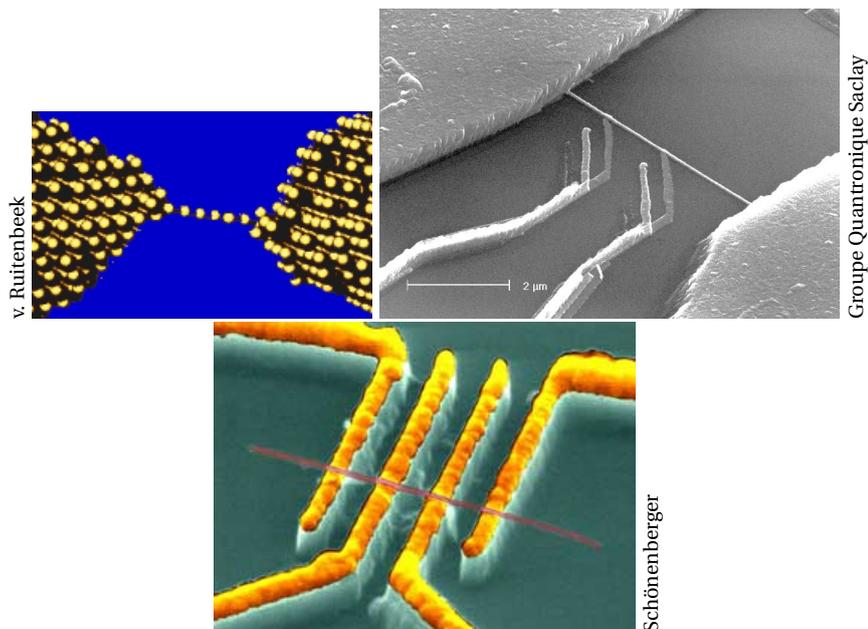




Residual conductance of correlated one-dimensional nanosystems

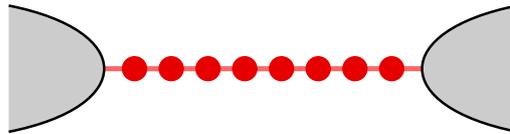
Gert-Ludwig Ingold	Uni Augsburg
Rafael A. Molina	MPIPKS Dresden
Peter Schmitteckert	Uni Karlsruhe
Dietmar Weinmann	IPCMS Strasbourg
Rodolfo A. Jalabert	IPCMS Strasbourg
Jean-Louis Pichard	CEA Saclay

Low-dimensional mesoscopic systems



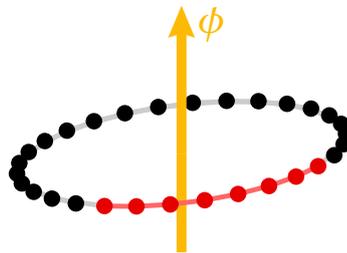
- electronic transport is **coherent**
- electronic **correlations** may become important

Transport through interacting region



difficulties:

- excitations in the interacting region possible
not for zero-bias conductance at $T = 0$
- coupling to leads \rightarrow open system
embedding method [Favand, Mila 1998]

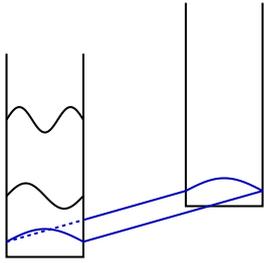


Overview



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 - Conductance of a coherent channel
 - Persistent current and conductivity
- 2 Embedding method
 - Transmission through an interacting region
 - Test of the method
- 3 Some basic aspects of transport through a correlated region
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 - Role of the contacts
 - Disorder and interaction
- 4 Application to the conductance of atomic chains
- 5 Conclusions

Conductance of a coherent channel



Conductance per open channel:

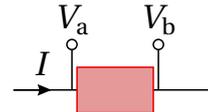
$$\frac{e^2}{h}$$



two-terminal conductance

$$G = \frac{I}{V_1 - V_2} = \frac{e^2}{h} T$$

$$G = \frac{I}{V_1 - V_2} = \frac{e^2}{h} T$$



four-terminal conductance

$$G = \frac{I}{V_a - V_b} = \frac{e^2}{h} \frac{T}{1 - T}$$

accounts for contact resistance

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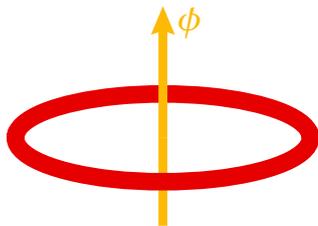
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Flux-threaded ring

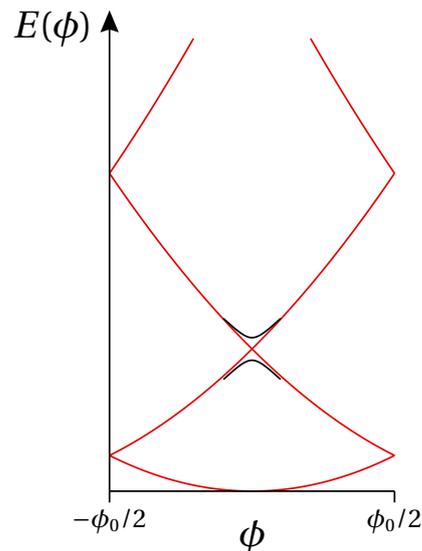


$$\Phi = \frac{\phi}{\phi_0}, \quad \phi_0 = \frac{h}{e}$$

persistent current: $J = -\frac{\partial E}{\partial \phi}$

curvature: $c = -\frac{\partial^2 E}{\partial \phi^2}$

charge stiffness: $D = (-1)^N \frac{L}{2} (E(0) - E(\pi))$



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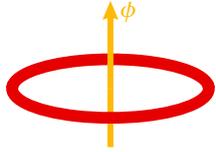
Atomic chains

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Kohn conductivity

Kohn 1964



time-dependent flux: $\phi \sim \frac{Ee^{i\omega t}}{i\omega}$

→ current response: $J = \sigma Ee^{i\omega t}$

with $\lim_{\omega \rightarrow 0} \omega \sigma''(\omega) \sim -\frac{\partial^2 E}{\partial \phi^2}$ Drude weight

- curvature is a measure of the number of extended states
- paramagnetic or diamagnetic response possible



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How and why does the embedding method work?



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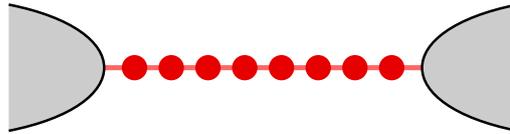
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Transport through interacting region



- are there extended states in the interacting region?
 - persistent current for interacting region, Kohn conductivity
- can we get electrons into the interacting region?
 - compressibility [Berkovits, Avishai 1996]
 - **embedding method**



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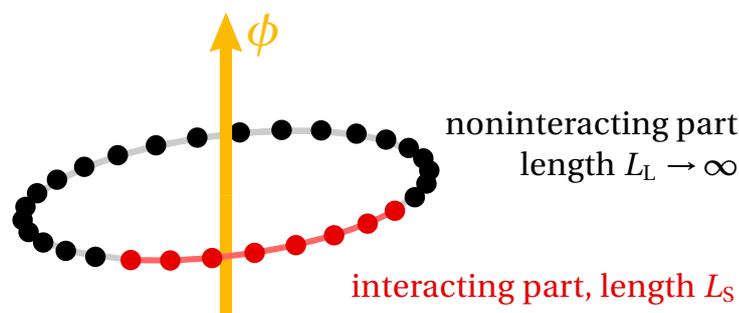
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Transmission through an interacting region



persistent current takes into account

- number of extended states
- contacts between interacting region and lead

embedding setup = tool to determine transmission

- no decoherence in the lead
- no Luttinger correlations in the noninteracting part



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Persistent current and transmission

point scatterer with transmission t in a noninteracting ring [Gogolin, Prokof'ev 1994]

$$J(\Phi, N \text{ odd}) = -\frac{ev_F}{\pi L} \frac{\text{Arccos}(|t(E_F)| \cos(\Phi))}{\sqrt{1 - |t(E_F)|^2 \cos^2(\Phi)}} |t(E_F)| \sin(\Phi)$$

$$J(\Phi, N \text{ even}) = J(\Phi - \pi; N \text{ odd})$$

conductance:

$$g = \lim_{L \rightarrow \infty} \left(\frac{J(\pi/2)}{J^0(\pi/2)} \right)^2 \quad (J^0 : \text{persistent current of clean ring})$$

requires complex DMRG algorithm



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Charge stiffness and transmission

relation to transmission:

$$D = \frac{\hbar v_F}{2} \left[\frac{\pi}{2} - \text{Arccos}(|t(E_F)|) \right]$$

conductance:

$$g = \lim_{L \rightarrow \infty} \sin^2 \left(\frac{\pi D}{2 D^0} \right)$$

real DMRG algorithm sufficient



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A few references on the embedding method

- J. Favand, F. Mila, Eur. Phys. J. B **2**, 293 (1998)
- O. P. Sushkov, Phys. Rev. B **64**, 155319 (2001)
- R. A. Molina et al., Phys. Rev. B **67**, 235306 (2003)
R. A. Molina et al., Eur. Phys. J. B **39**, 107 (2004)
R. A. Molina et al., Europhys. Lett. **67**, 96 (2004)
- V. Meden, U. Schollwöck, Phys. Rev. B **67**, 193303 (2003)
V. Meden et al., Europhys. Lett. **64**, 769 (2003)
- T. Rejec, A. Ramšak, Phys. Rev. B **68**, 033306 (2003)
T. Rejec, A. Ramšak, Phys. Rev. B **68**, 035342 (2003)



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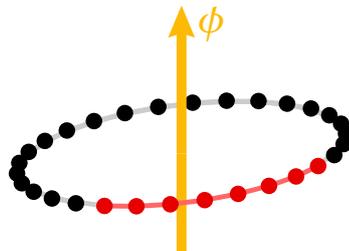
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Spinless fermions



$$H = -t \sum_{i=1}^L \left(c_i^\dagger c_{i-1} + c_{i-1}^\dagger c_i \right) + \sum_{i=2}^{L_S} U (n_i - V_+) (n_{i-1} - V_+)$$

boundary condition: $c_0 = e^{i\Phi} c_L$

- $\nu = 1/2$ $V_+ = 1/2$ (particle-hole symmetry)
- $\nu \neq 1/2$ V_+ must be determined by iteration



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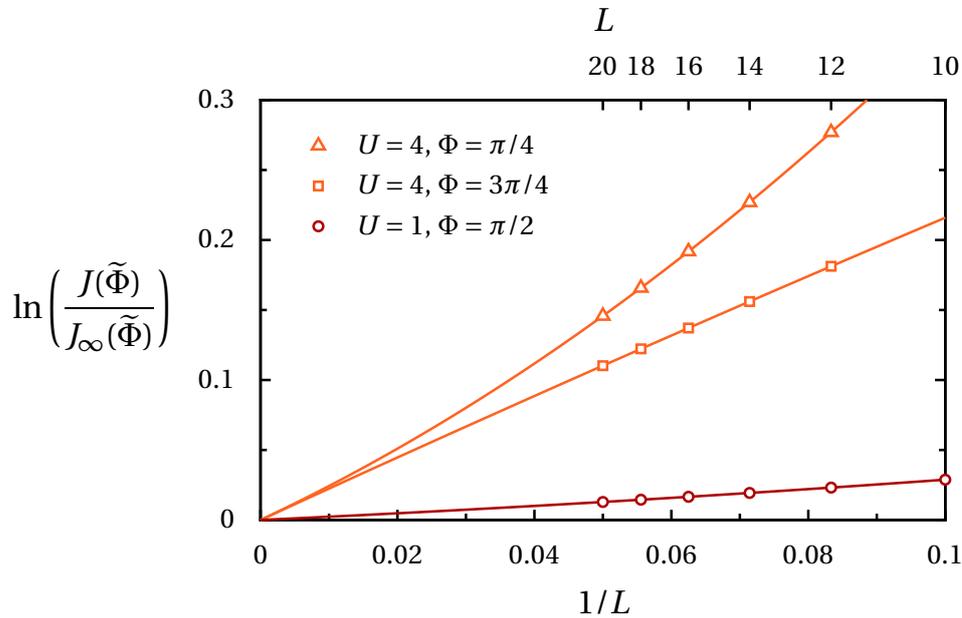
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Scaling to infinite ring length (I)

half filling ($\nu = 1/2$), $L_S = 6$



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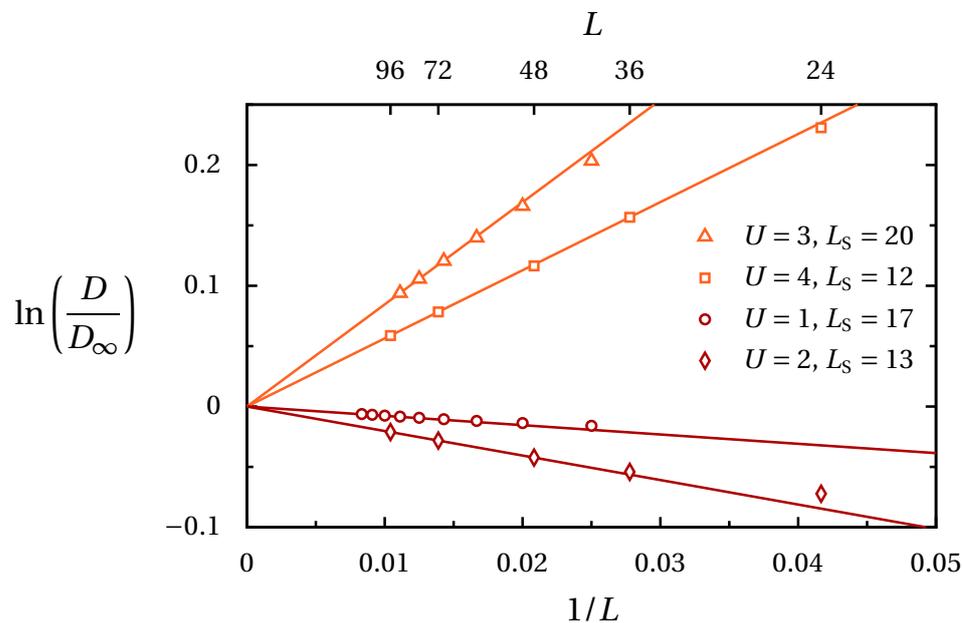
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Scaling to infinite ring length (II)

linear scaling for charge stiffness

$$D(U, L_S, L_L) = D_\infty(U, L_S) \exp\left(\frac{C(U, L_S)}{L}\right)$$



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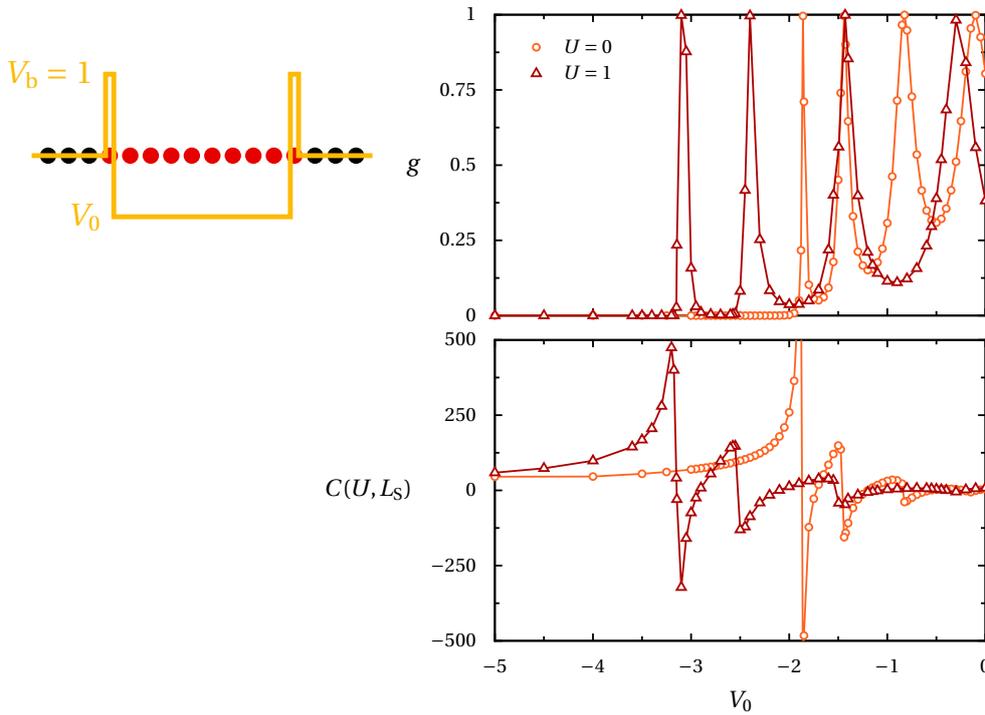
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Resonances



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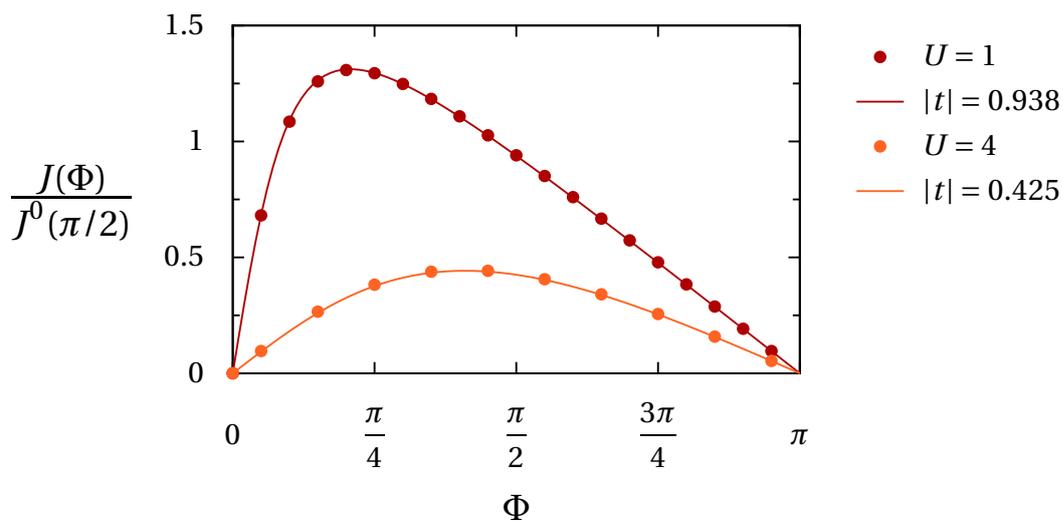
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Flux dependence of persistent current



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→ interacting region can be described by an effective point scatterer with transmission t





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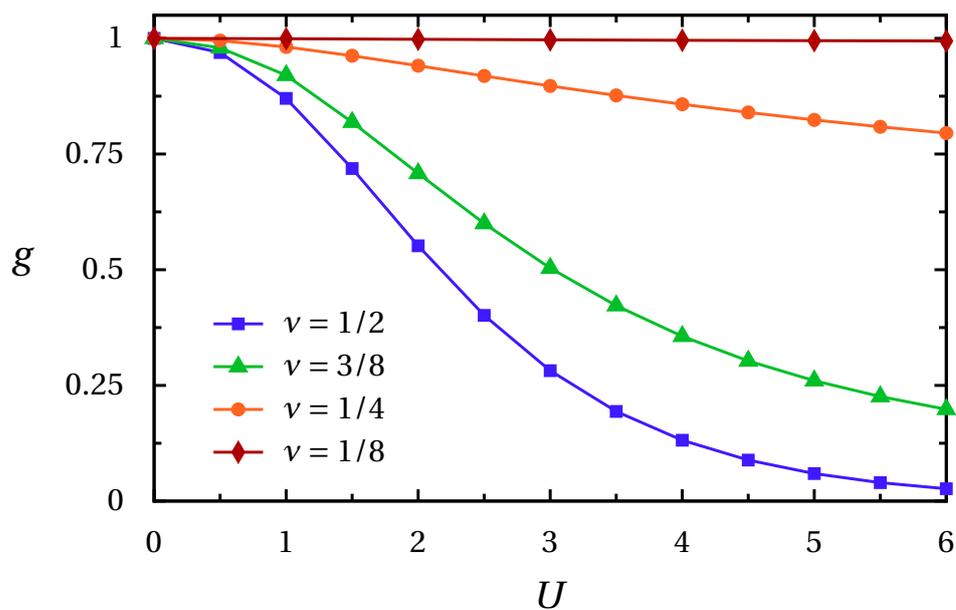
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Some basic aspects of transport through a correlated region

Outside half filling



- signature of Mott transition
- suppression of the conductance is most effective at half filling



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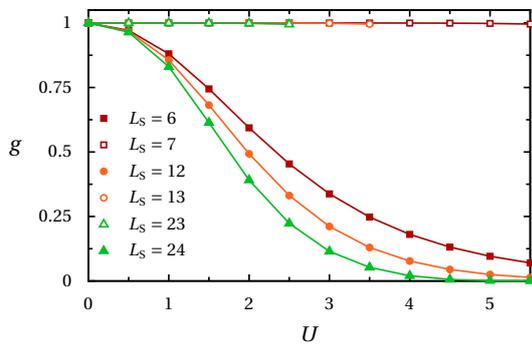
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Even-odd effects



even number of lattice sites: ●●●●●● ●●●●●●

→ additional electron costs energy U ●●●●●●

odd number of lattice sites: ●●●●●● ●●●●●●

→ transfer of electrons does not cost energy

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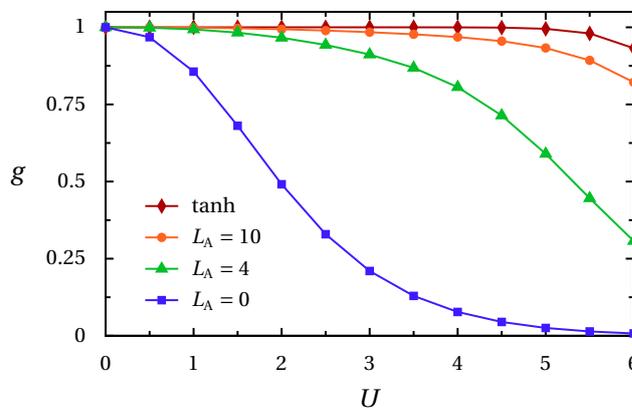
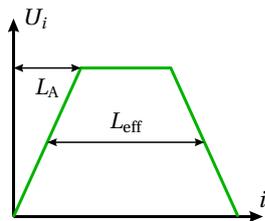
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Influence of contacts



→ smoothing of the contacts increases the conductance



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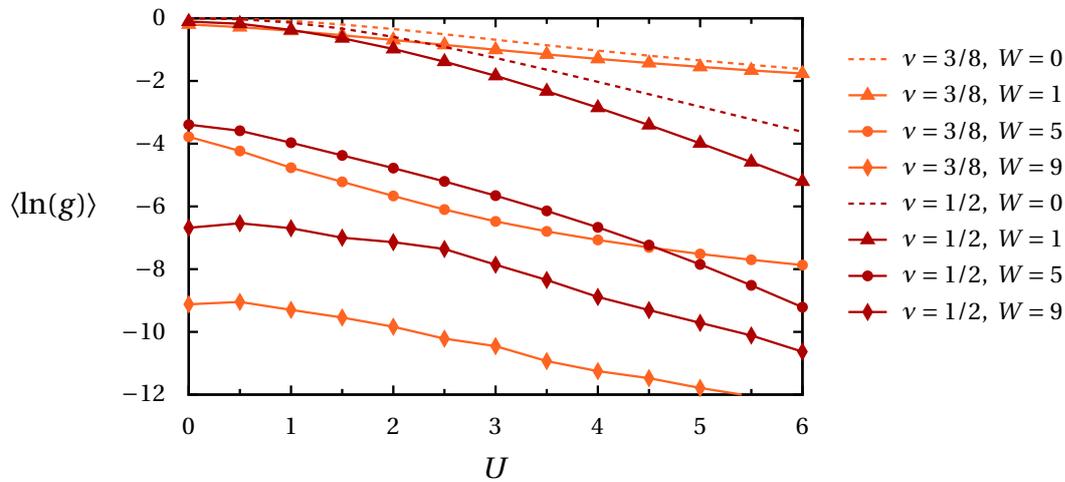
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Disorder and interaction



→ repulsive interaction can increase the conductance for sufficiently strong disorder



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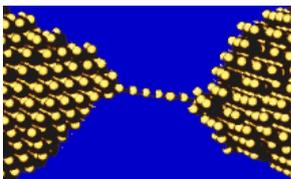
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Application to the conductance of atomic chains



possible explanation of conductance oscillations as a function of length in break junction contacts

[R. A. Molina, D. Weinmann, J.-L. Pichard, *Europhys. Lett.* **67**, 96 (2004)]



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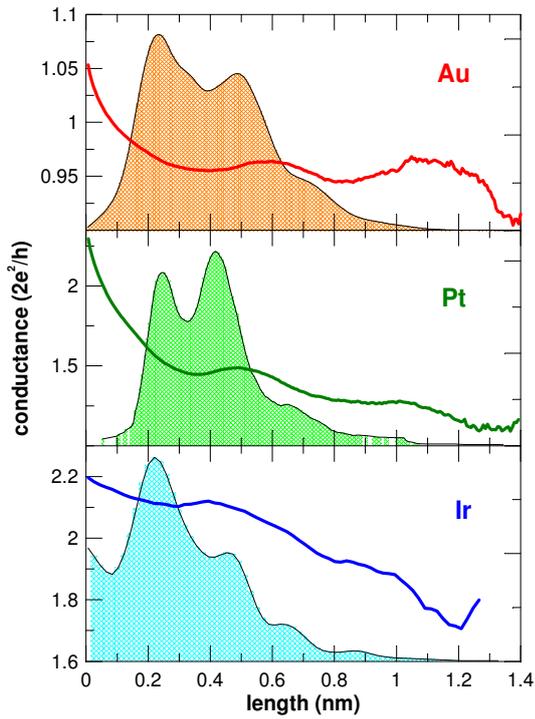
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Even-odd effects in atomic chains



R. H. M. Smit et al.,
Phys. Rev. Lett. **91**, 076805 (2003)

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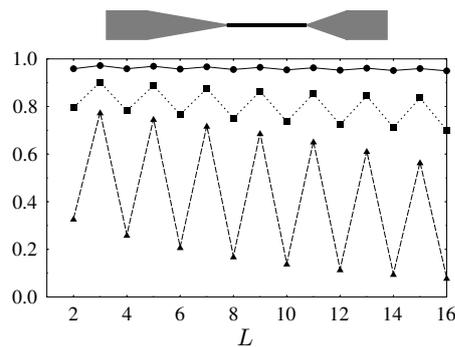
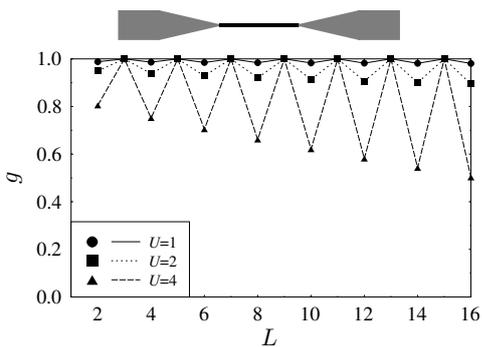
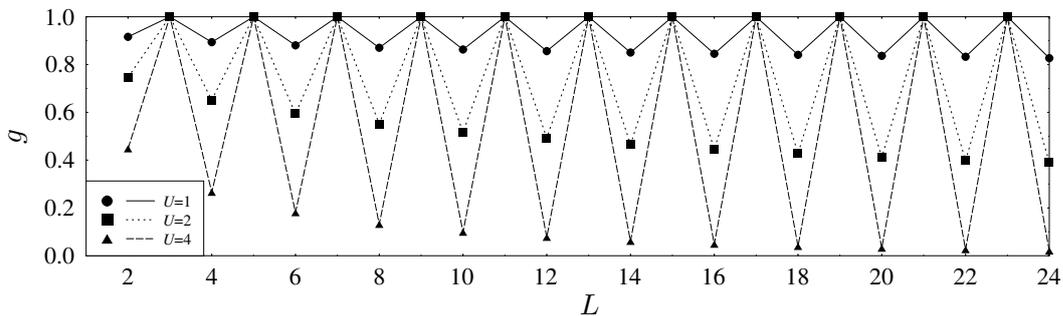
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Length-dependent oscillations



R. A. Molina et al., Europhys. Lett. **67**, 96 (2004)



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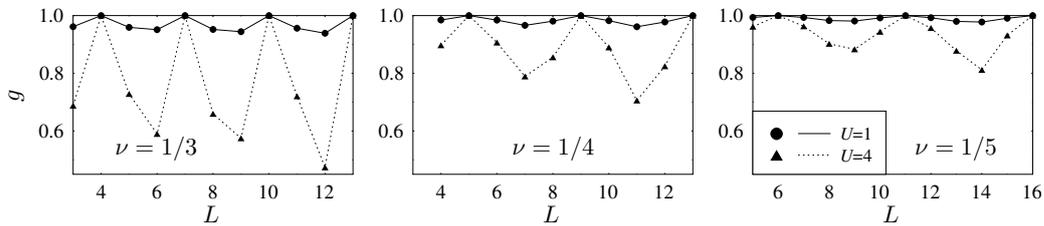
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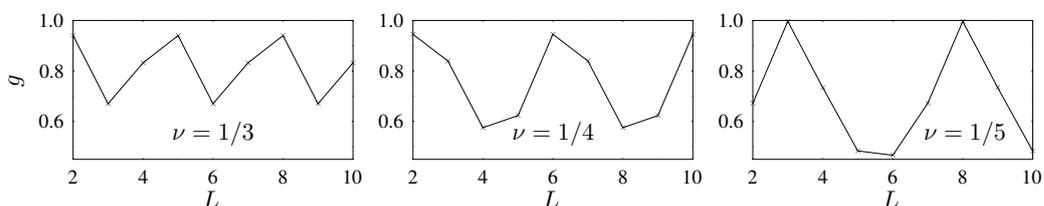


Period of oscillation

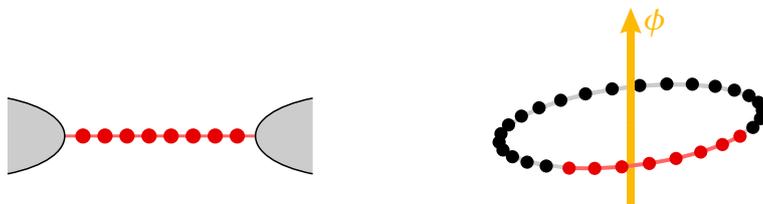
finite interaction:



non-interacting:



Conclusions



embedding method

- ✗ close an interacting system to a ring by means of a noninteracting lead
- ✗ interacting region can be described by an effective point scatterer
- ✗ residual conductance can be obtained from the persistent current or charge stiffness

■ Phys. Rev. B **67**, 235306 (2003)

■ Eur. Phys. J. B **39**, 107 (2004)



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