Investigation of Luttinger liquids with DMRG and TEBD methods

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with Alex Cojuhovschi, Malcom Einhellinger, and Martin Paech

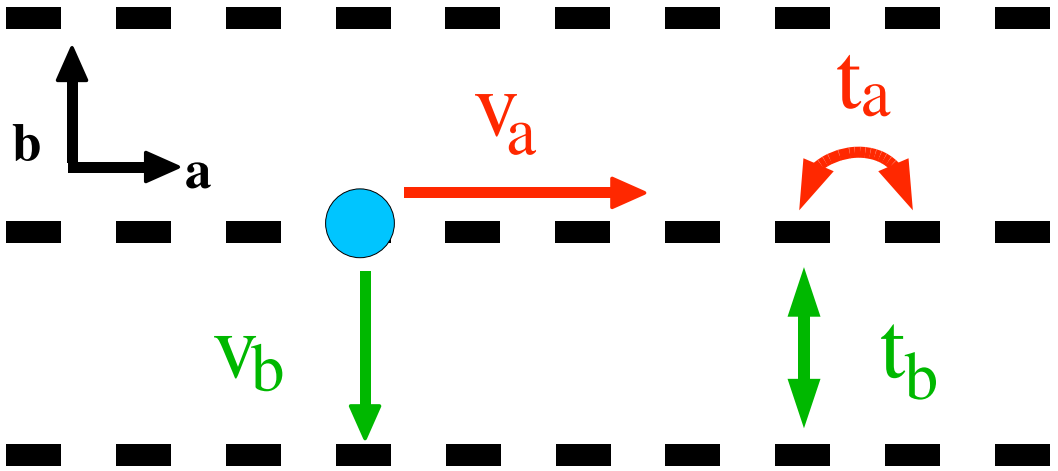
Outline

1. One-dimensional electron systems

2. Spectral properties and
   the dynamical density-matrix renormalization group
   (DDMRG) method

3. Transport properties and
   the time-evolving block decimation (TEBD) method

One-dimensional electron systems



$$\left.\begin{array}{c} \dfrac{\mathbf{b}}{\mathbf{v}_b} \gg \Delta t \gg \dfrac{\mathbf{a}}{\mathbf{v}_a} \\ \textbf{or} \\ t_b \ll \Delta E, k_B T \ll t_a \end{array}\right\} \Rightarrow \textbf{one-dimensional dynamics}$$

Separation of charge and spin dynamics

Elementary excitations

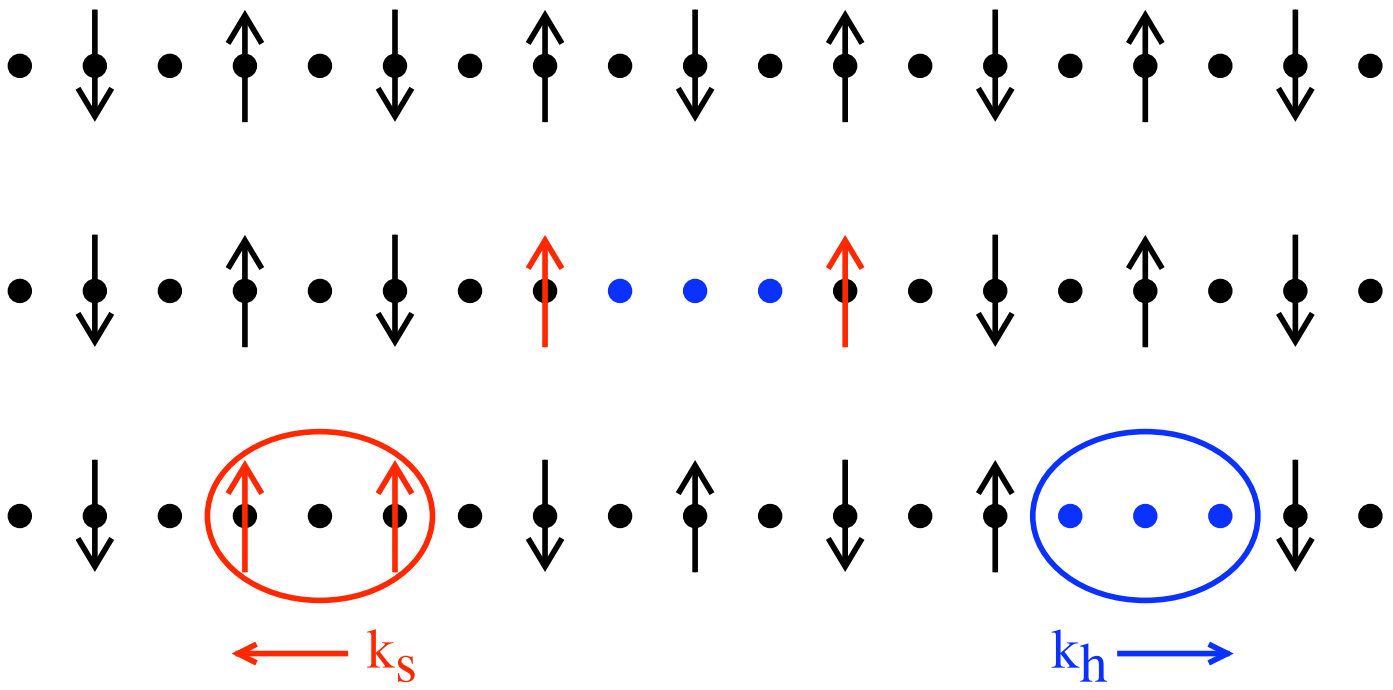
Holons $(Q = \pm e, S = 0)$: $\varepsilon_h(k_h)$

Spinons $(Q = 0, S = \frac{\hbar}{2})$: $\varepsilon_s(k_s)$

Physical excitations

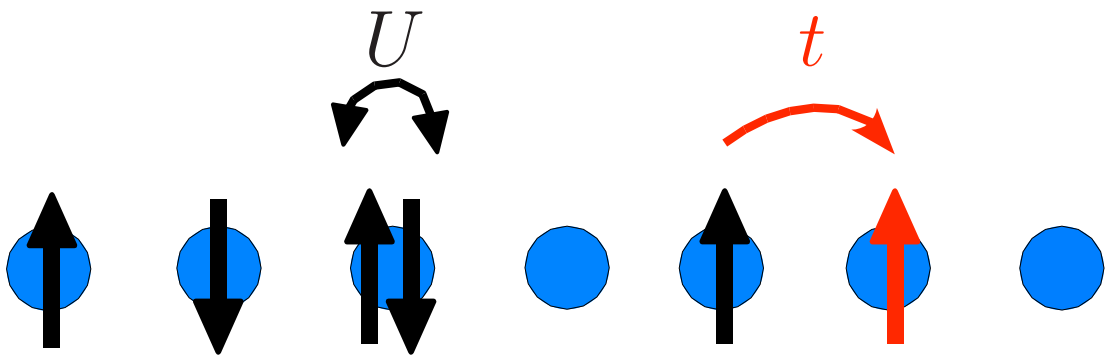
$$k = \sum_{i,j} \{k_{s,i} + k_{h,j}\}$$

$$\varepsilon(k) = \sum_{i,j} \{\varepsilon_s(k_{s,i}) + \varepsilon_h(k_{h,j})\}$$



One-dimensional Hubbard model

"Simple" model for strongly correlated electrons



Electronic density

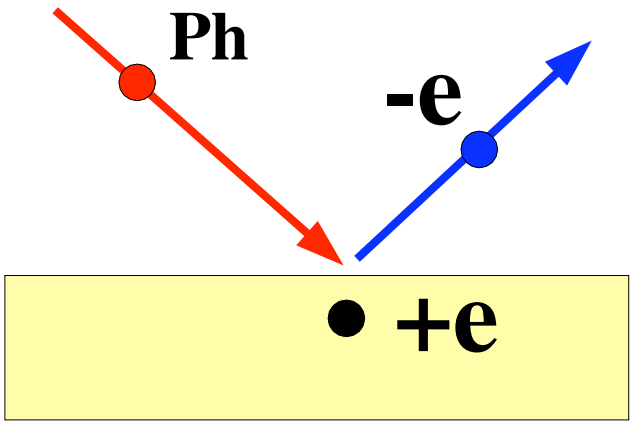
$0 < \rho < 2$

Hamiltonian

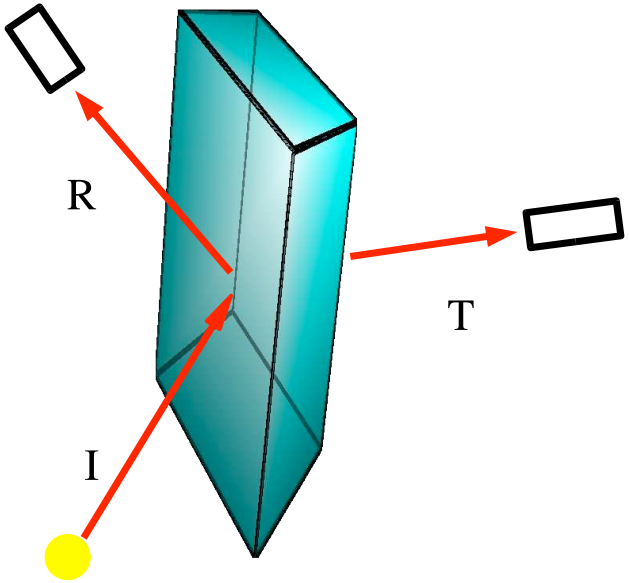
$$\hat{H} = -t \sum_{i\sigma} \left(\hat{c}^{\dagger}_{i\sigma} \hat{c}_{i+1\sigma} + \hat{c}^{\dagger}_{i+1\sigma} \hat{c}_{i\sigma} \right) + U \sum_{i} \hat{n}_{i\uparrow} \hat{n}_{i\downarrow}$$

Dynamical response functions

Photoemission



Optical absorption



ARPES spectral function $A(k,\omega)$

Conductivity $\sigma_1(\omega)$

$$A(k,\omega \leq 0) = \frac{1}{\pi}\, Im\, \langle \psi_0 | \hat{c}^{\dagger}_{k,\sigma} \frac{1}{\hat{H} - E_0 + \hbar\omega - i\eta} \hat{c}_{k,\sigma} | \psi_0 \rangle$$

$$\sigma_1(\omega \geq 0) = \frac{1}{N\omega}\, Im\, \langle \psi_0 | \hat{J} \frac{1}{\hat{H} - E_0 - \hbar\omega - i\eta} \hat{J} | \psi_0 \rangle$$

Dynamical DMRG

[E. Jeckelmann, PRB **66**, 045114 (2002)]

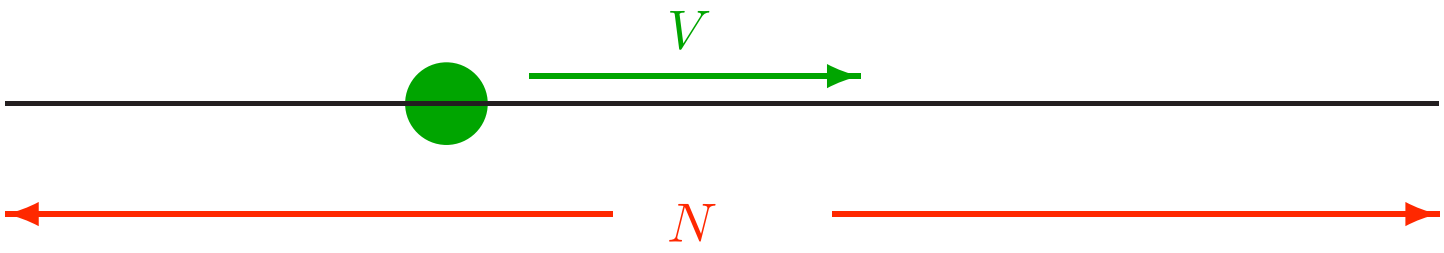
Minimization of

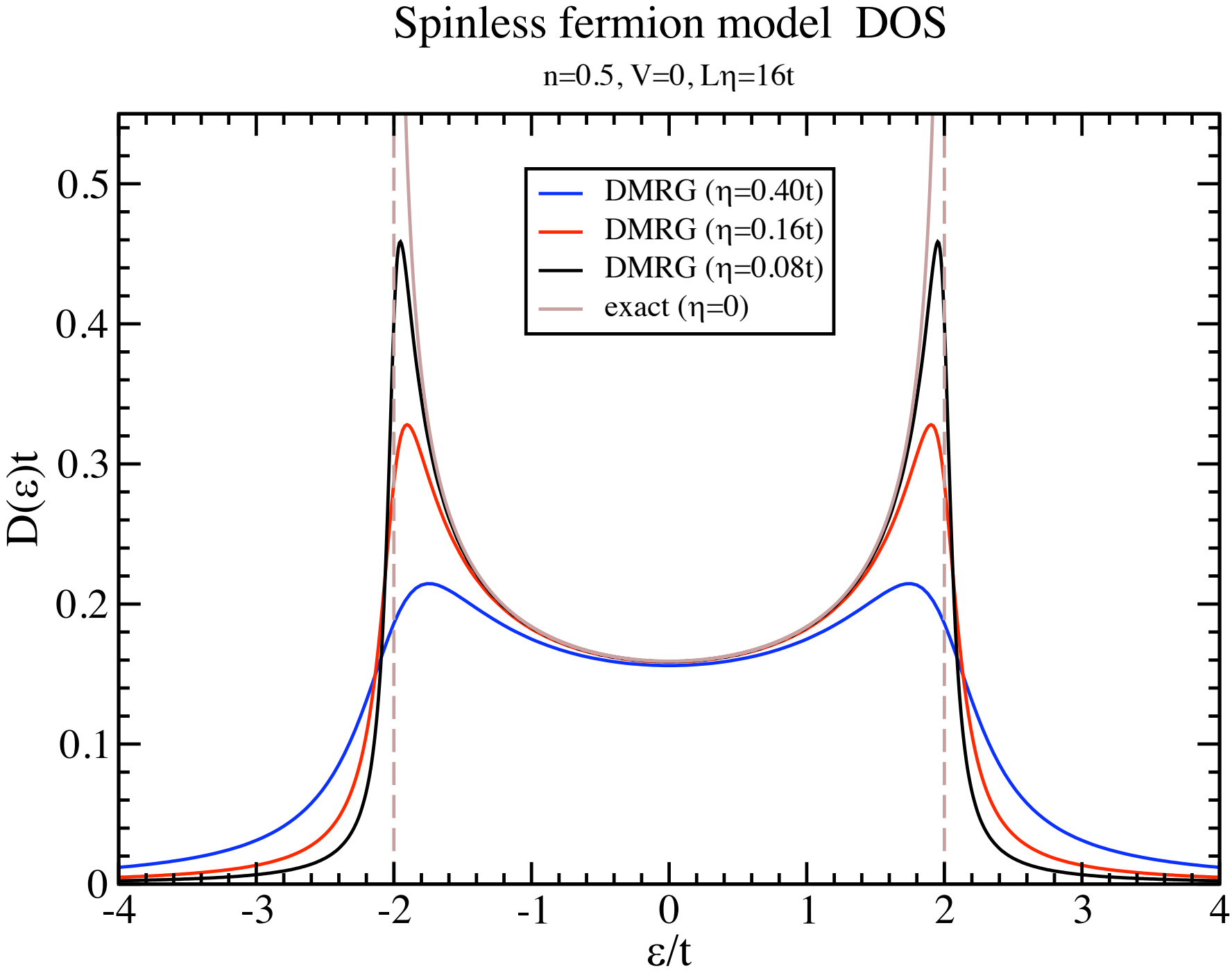
$$W_{k,\omega,\eta}(\psi) = \langle\psi| \left(\hat{H} + \omega - E_0\right)^2 + \eta^2 |\psi\rangle + \eta\langle\psi|\hat{c}_{k,\sigma}|\psi_0\rangle + \eta\langle\psi_0|\hat{c}^\dagger_{k,\sigma}|\psi\rangle$$

yields

$$\begin{aligned} W_{k,\omega,\eta}(\psi_{\min}) &= -\pi\eta A^\eta_\sigma(k,\omega) \\ A^\eta_\sigma(k,\omega) &= \frac{1}{\pi}\int_{-\infty}^{\infty} d\omega' A_\sigma(k,\omega') \frac{\eta}{(\omega-\omega')^2+\eta^2} \end{aligned}$$

Extrapolation $N \sim (\frac{1}{\eta}$ band width$) \to \infty \quad \Rightarrow V\frac{1}{\eta} < N$




Spinless fermion model DOS
n=0.5, V=0, Lη=16t
DMRG (η=0.40t)
DMRG (η=0.16t)
DMRG (η=0.08t)
exact (η=0)
D(ε)t
ε/t
0
0.1
0.2
0.3
0.4
0.5
-4
-3
-2
-1
0
1
2
3
4

Deconvolution

In principle, minimization of

$$S(\{A_\sigma(k,\omega)\}) = \int_{-\infty}^{\infty} d\omega' \left(A_\sigma^\eta(k,\omega') - \frac{1}{\pi} \int_{-\infty}^{\infty} d\omega A_\sigma(k,\omega) \frac{\eta}{(\omega-\omega')^2+\eta^2} \right)^2$$

Ill-conditioned problem

Usual method: Linear regularization

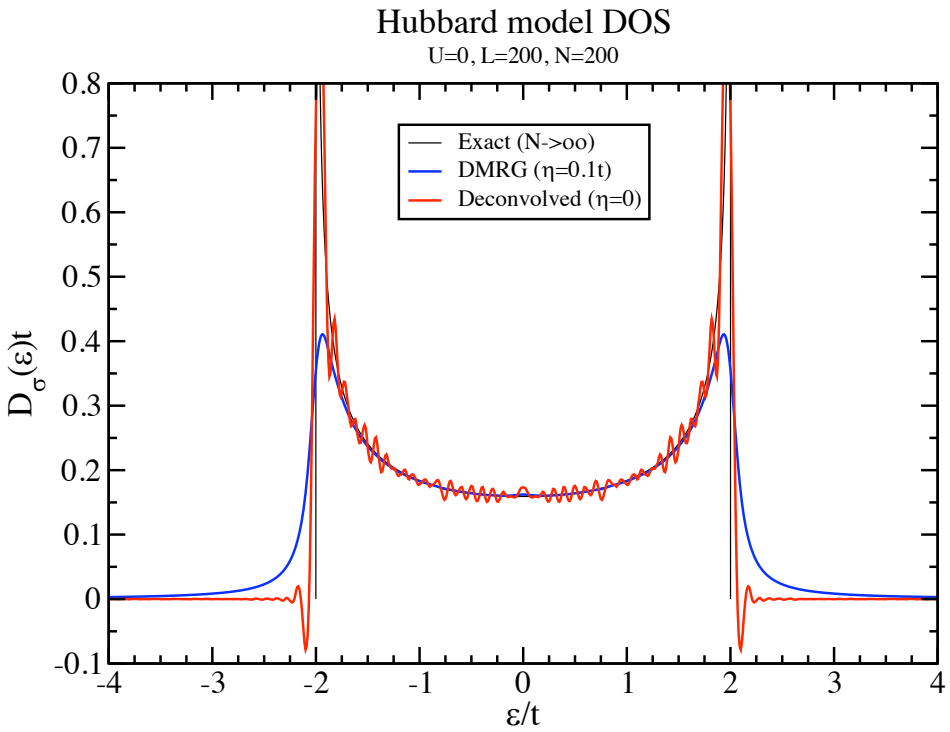
$$\tilde{S}(\{A_\sigma(k,\omega)\}) = S(\{A_\sigma(k,\omega)\}) + \lambda \int_{-\infty}^{\infty} d\omega \left(\frac{dA_\sigma(k,\omega)}{d\omega} \right)^2$$

New method: Nonlinear inequality constraints

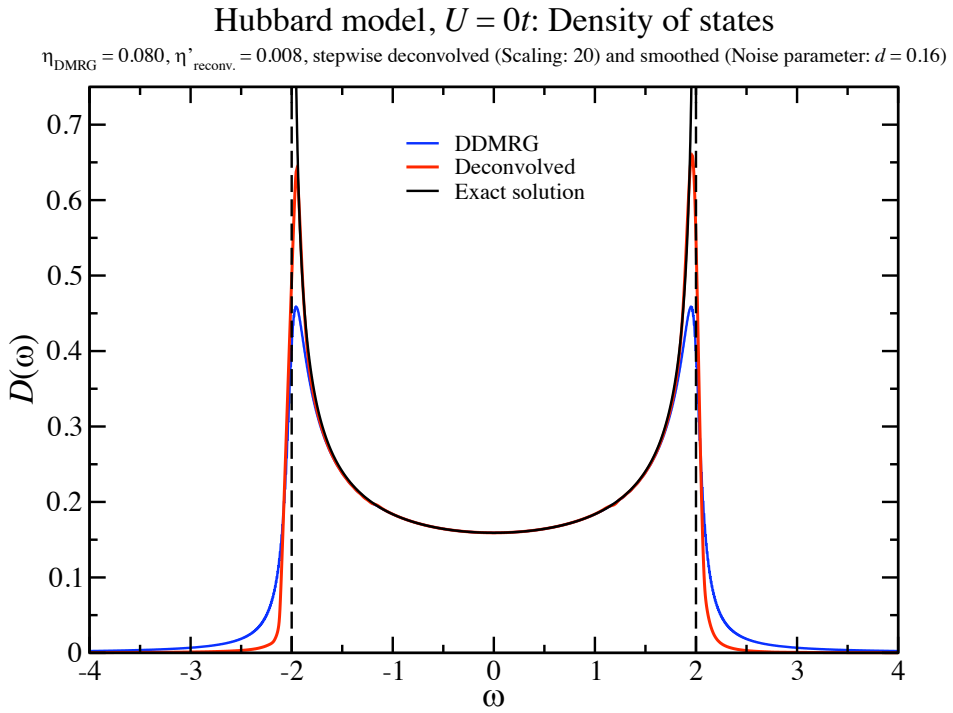
- $A_\sigma(k,\omega) \geq 0$
- Smoothness: Distance between extrema $> d \sim \eta$

Deconvolution of non-interacting fermion DOS

Linear regularization



New method



Quasi-momentum for open boundary conditions

[H. Benthien, F. Gebhard, and E. Jeckelmann, Phys. Rev. Lett. **92**, 256401 (2004)]
[E.J. and H. Benthien, *Computational Many Particle Physics*, H. Fehske *et al.*, Springer]

Periodic boundary conditions

$\Rightarrow$ Bloch wavefunctions for momenta (wavevectors)

$$\hat{c}_{k\sigma} = \sqrt{\frac{1}{N}} \sum_n e^{ikn}\, \hat{c}_{n\sigma} \qquad k = \frac{2\pi}{N} z \quad \text{with} \quad z = 0, \pm 1, \pm 2, \ldots, \frac{N}{2}$$

Open boundary conditions

$\Rightarrow$ particle-in-the-box wavefunctions for quasi-momenta

$$\hat{c}_{k\sigma} = \sqrt{\frac{2}{N+1}} \sum_n \sin(kn)\, \hat{c}_{n\sigma}\ , \qquad k = \frac{\pi}{N+1}\, j \quad \text{with} \quad j = 1, 2, \ldots, N$$

Spectral functions of a Luttinger liquid

[V. Meden and K. Schönhammer, PRB **46**, 15753 (1992); V. Meden, PRB **60**, 4571 (1999)]

Tomonaga-Luttinger model

Holon branches $\varepsilon_h(q_h) = v_\rho |q_h|$ Spinon branches $\varepsilon_s(q_s) = v_\sigma |q_s|$

Interaction parameters: $\alpha = \frac{1}{4}(K_\rho + K_\rho^{-1} - 2) > 0$ and $K_\sigma = 1$

Universal properties: DOS, Fermi points, . . .

$$\lim_{\omega \to 0} \int dk \; A(k, \omega < 0) \quad \sim \quad (-\omega)^{\alpha}$$

$$\lim_{\omega \to 0} A(\pm k_F, \omega < 0) \quad \sim \quad (-\omega)^{\alpha - 1}$$

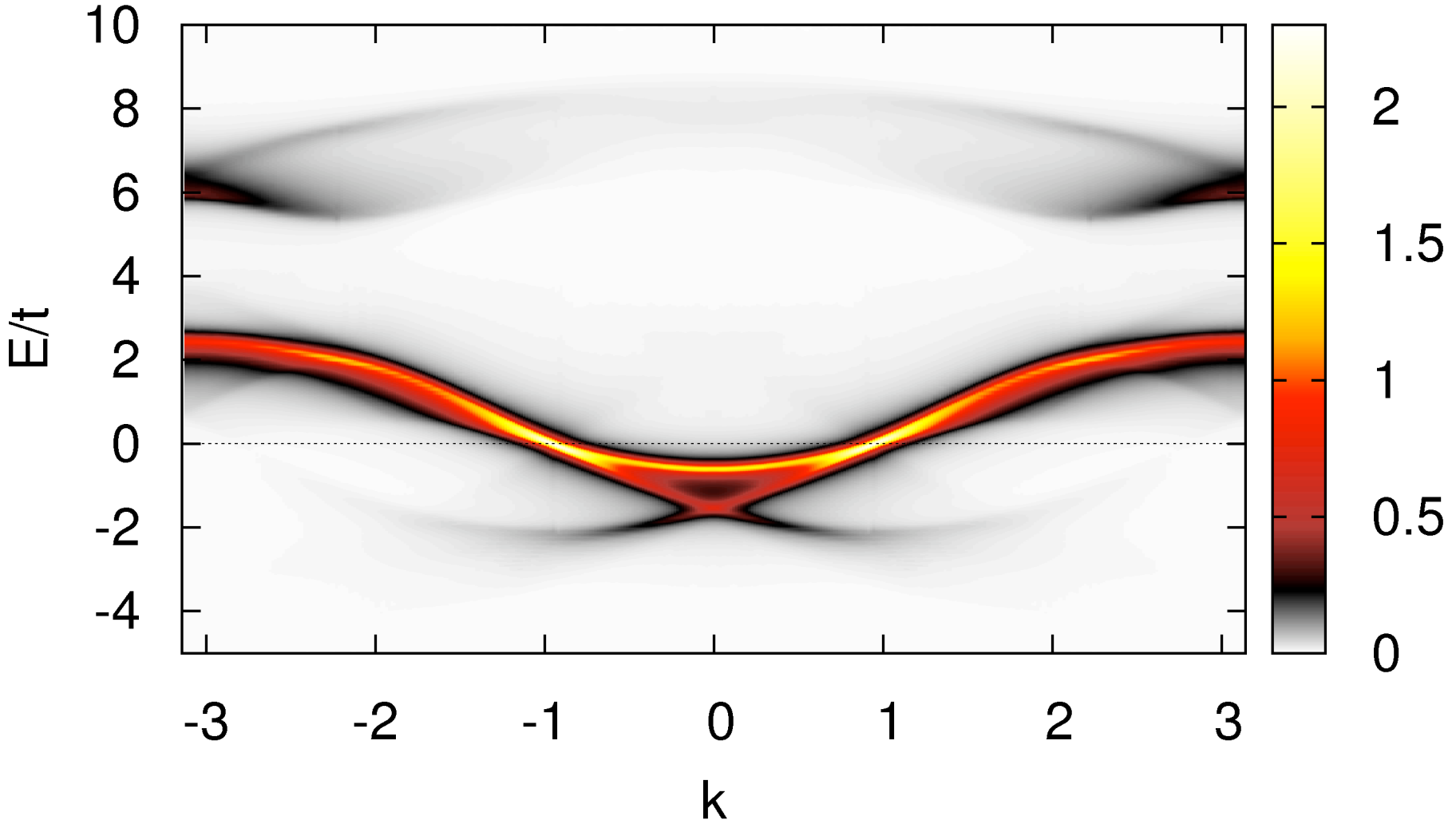
Non-universal properties: Spinon and holon branches

$$\lim_{\omega \to v_\rho q} A(\pm(k_F + q), \omega < 0) \quad \sim \quad |\omega - v_\rho q|^{(\alpha-1)/2}$$

$$\lim_{\omega \to v_\sigma q} A(\pm(k_F + q), \omega < 0) \quad \sim \quad \theta(v_\sigma q - \omega) |\omega - v_\sigma q|^{\alpha - 1/2}$$

Spectral funtions of a Luttinger liquid

Hubbard model, $U = 4.9t, \rho = 0.59, L = 200, \eta = 0.1t$



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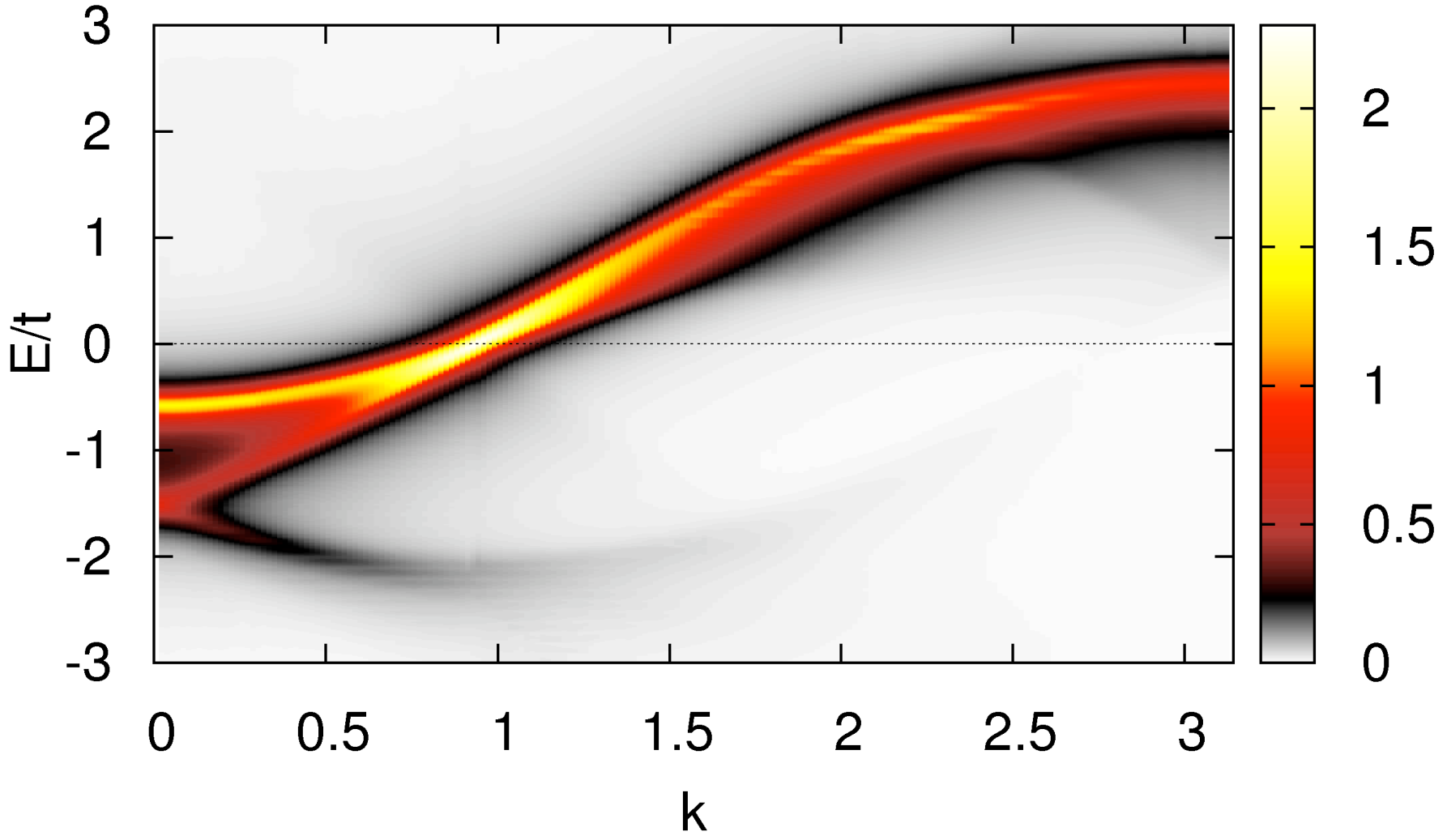
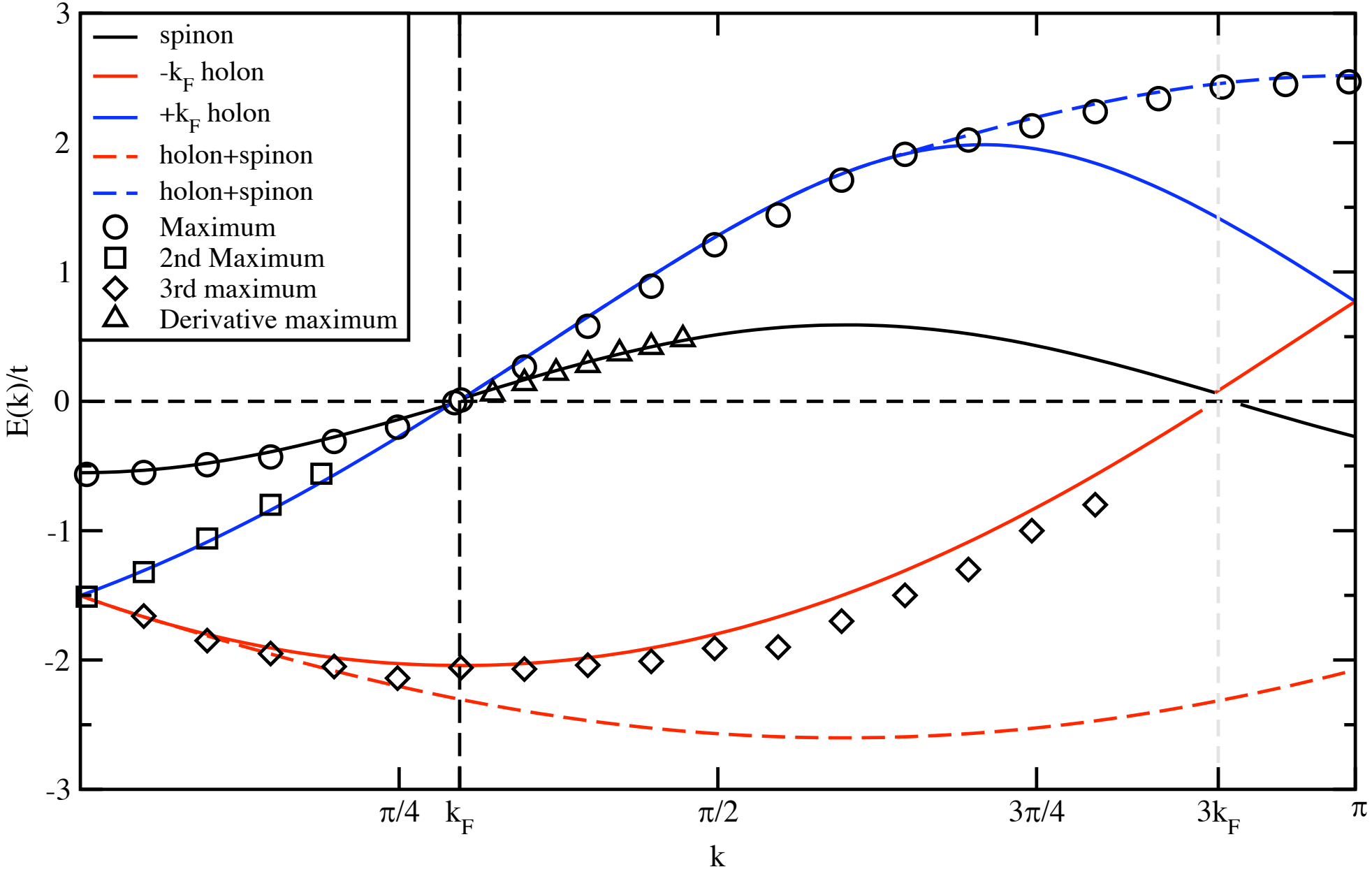
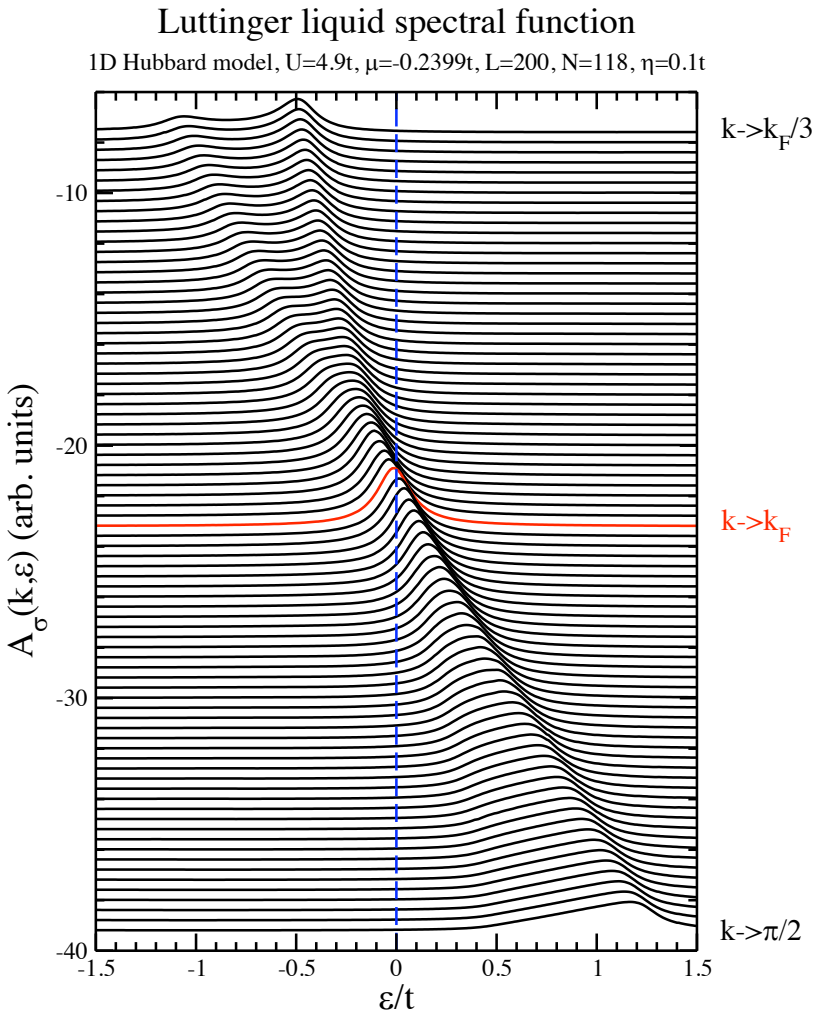


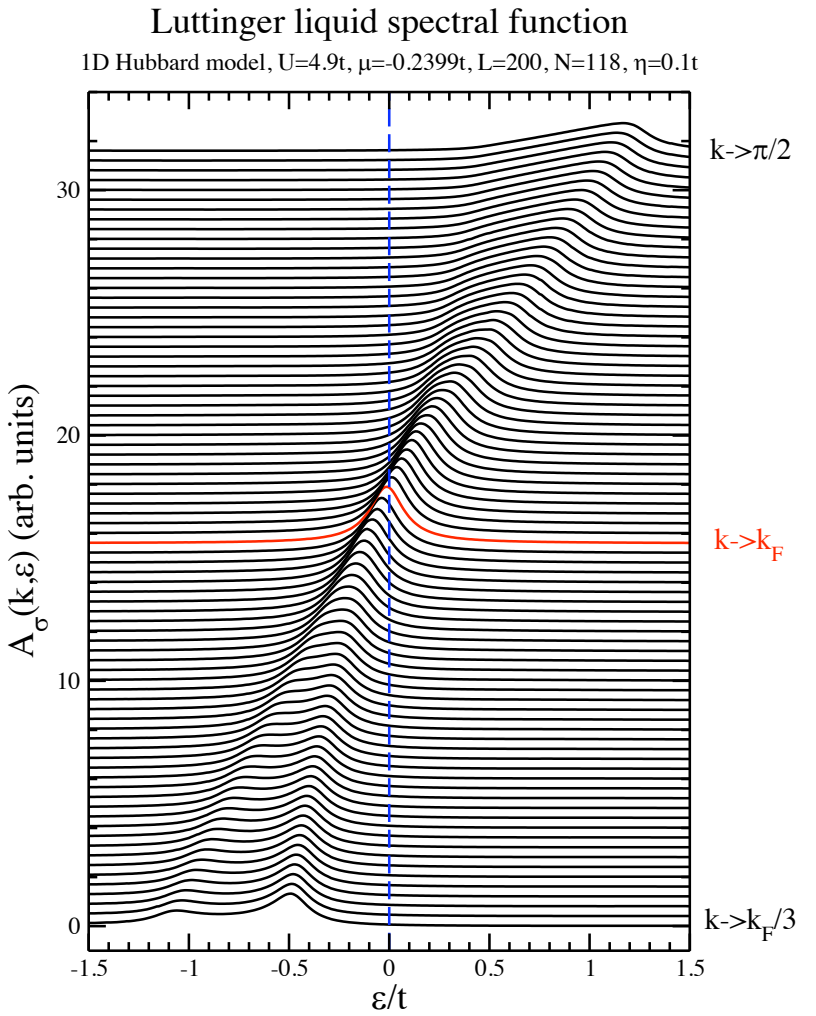
Single hole and electron excitations in the 1D Hubbard model

L=200, N=118 , U=4.9t, Bethe Ansatz (PBCs, μ=0.24220t) vs. DMRG (OBCs, -0.2399t)



Spectral weight of holon and spinon lines



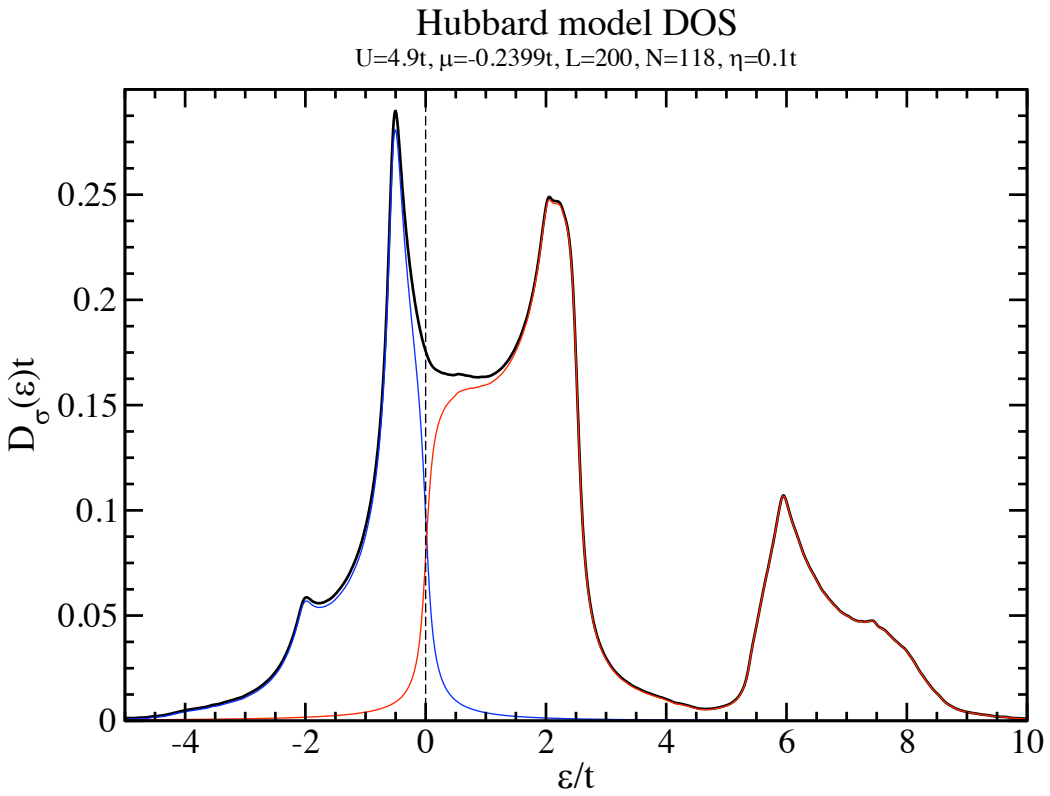


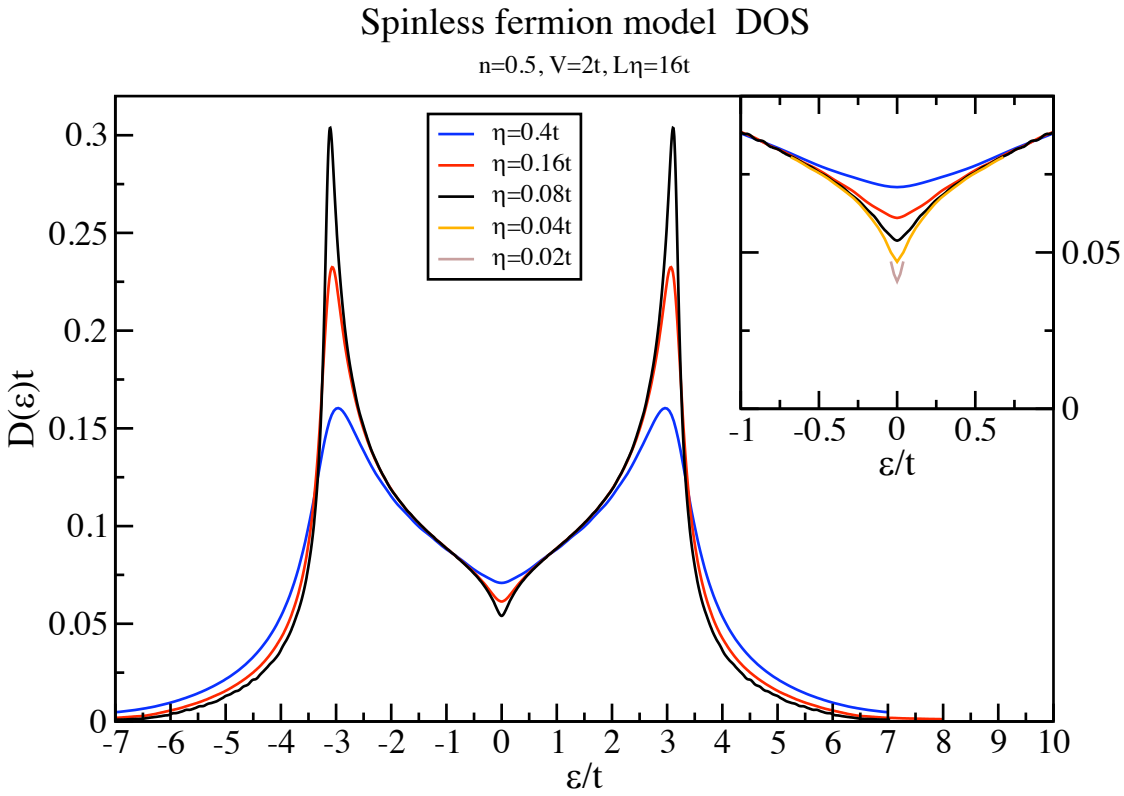
Non-universal behavior of $A(k,\omega)$ on the spinon branch:

For $n < 1$ peak in $A(|k| < k_F, \omega < 0)$ and shoulder/cusp in $A(|k| > k_F, \omega > 0)$

For $n > 1$ peak in $A(|k| > k_F, \omega > 0)$ and shoulder/cusp in $A(|k| < k_F, \omega < 0)$

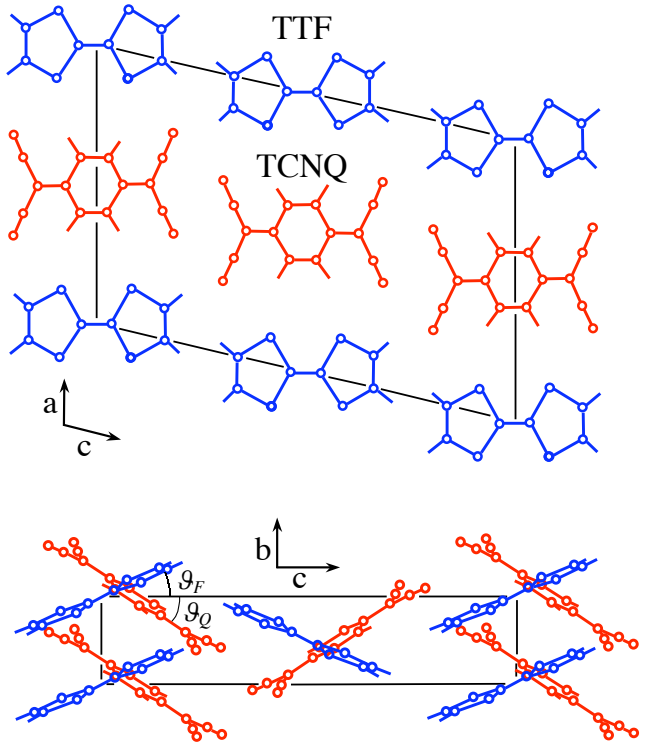
DOS of a Luttinger liquid





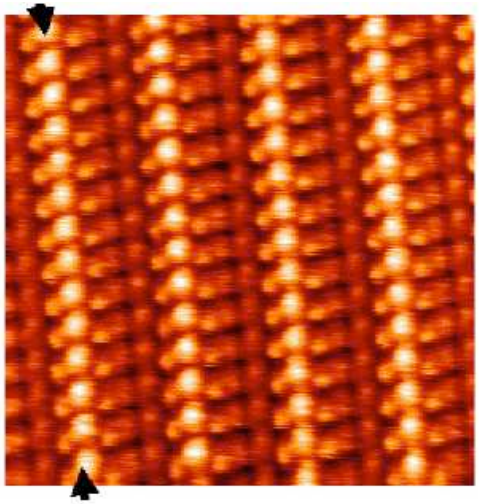
TTF-TCNQ

Lattice structure



[R. Claessen *et al.*, PRL **88**, 096402 (2002)]

Surface (STM)

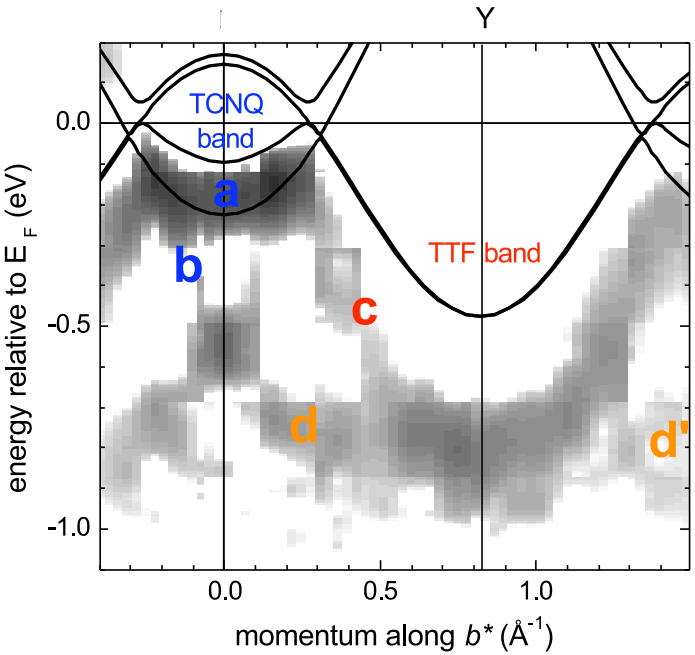


[Wang *et al.*, PRB 2003]

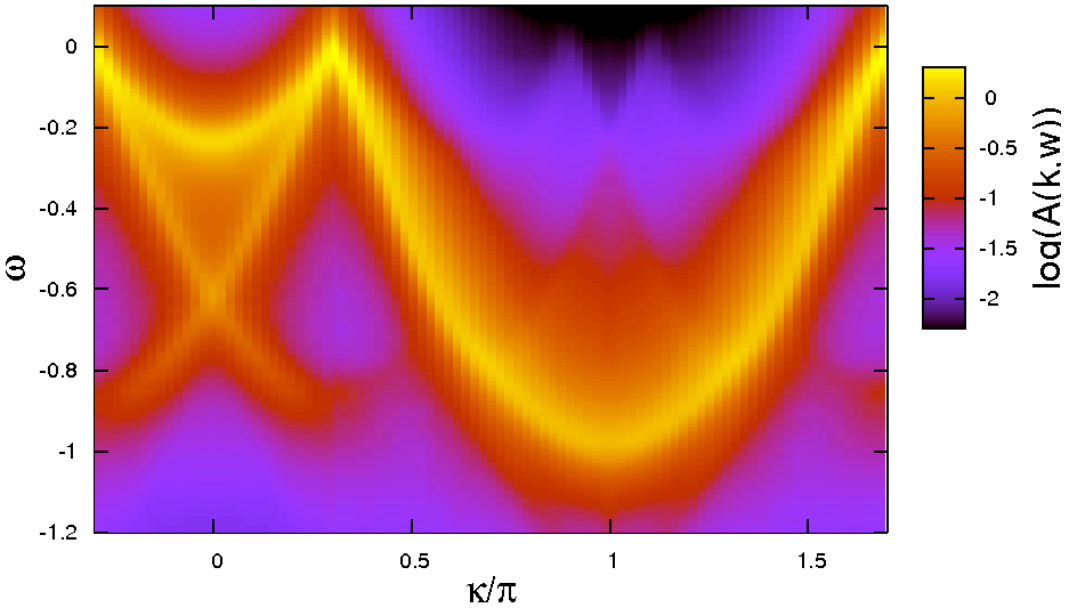
ARPES spectrum of TTF-TCNQ

[R. Claessen *et al.*, PRL **88**, 096402 (2002); M. Sing *et al.*, PRB **68**, 125111 (2003)]
[Benthien, Gebhard, and Jeckelmann, PRL **92**, 256401 (2004)]

Experiment



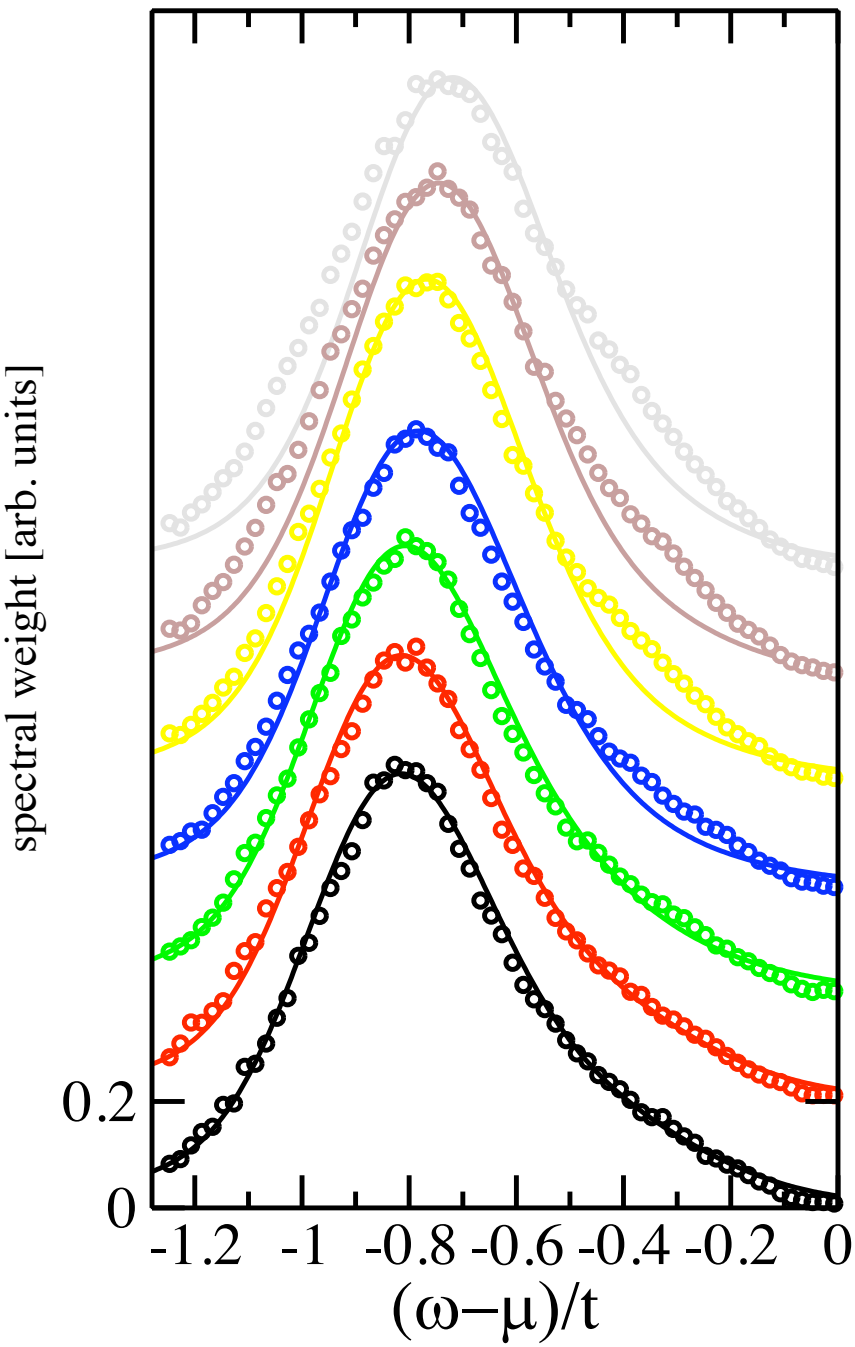
Hubbard model



Two independent chains with
$\rho = 0.6$ and 1.4, $U = 4.9t$, $t = 0.4$ eV

U/t=7, σ=0.2eV, t=0.39eV

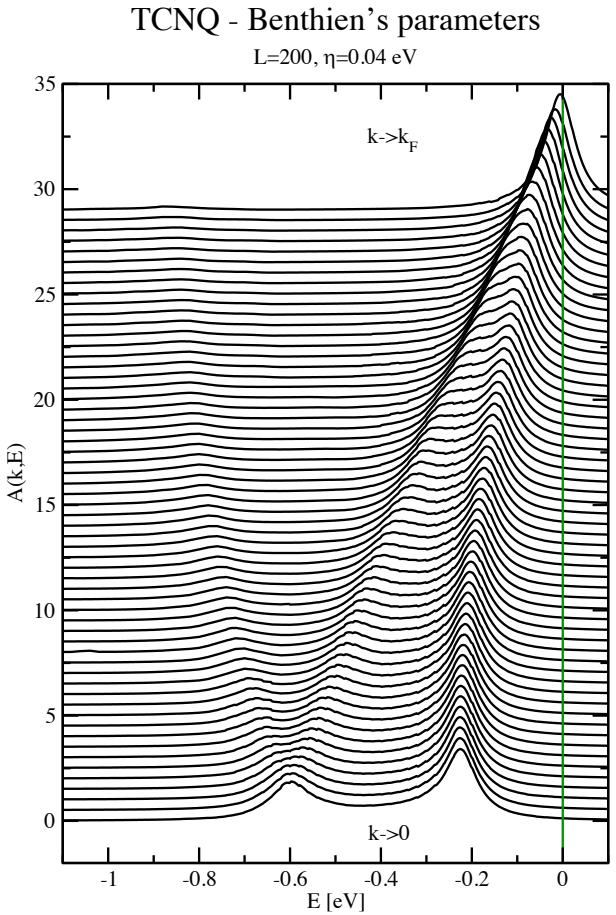
only the peak height is a free fit parameter

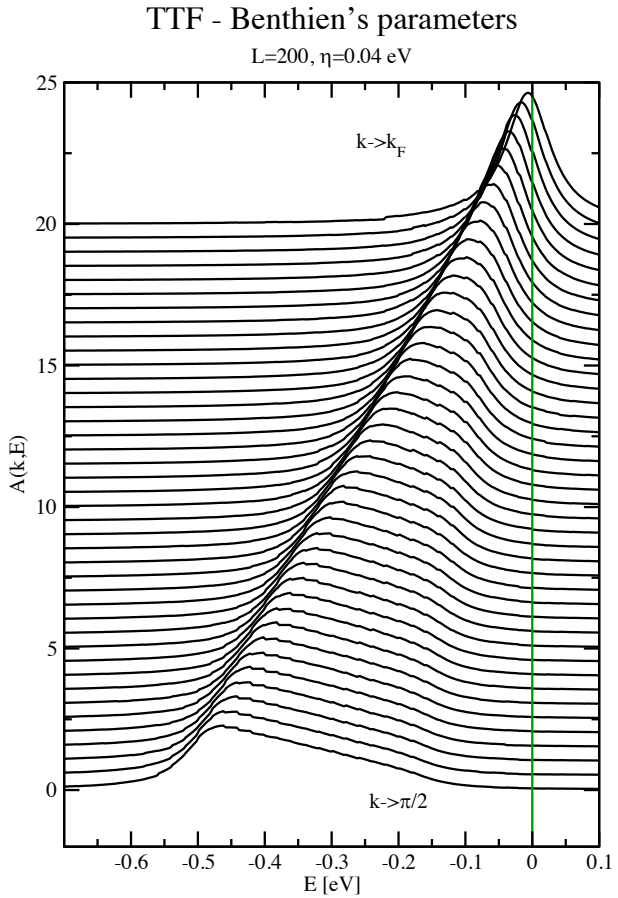


22.8°: sh5_EF_nb_TTFK10A055.txt
22.3°: sh5_EF_nb_TTFK10A054.txt
21.3°: sh5_EF_nb_TTFK10A052.txt
19.8°: sh5_EF_nb_TTFK10A049.txt
18.8°: sh5_EF_nb_TTFK10A047.txt
17.8°: sh5_EF_nb_TTFK10A045.txt
16.8°: sh5_EF_nb_TTFK10A043.txt

all experimental data * 0.03

Influence of band filling in Luttinger liquids





Non-universal behavior of $A(k,\omega)$ on the spinon branch:
Peak for band-filling $n < 1$ but only a shoulder or cusp for $n > 1$

Problems with Hubbard chain model for TTF-TCNQ

- Two-band system, interchain coupling, and three-dimensional structure
- *Ab initio* or bulk parameters: $V_1 \approx \frac{U}{2}, V_2, V_3 \gg |t| \approx 0.15 - 0.18$ eV
  [Cano-Cortes *et al.*, EPJB **56**, 173 (2007)]
- Peierls insulator for $T < 54$ K $\Rightarrow$ phonons
- Lineshapes
- DOS $\sim \omega$ and $A(k_F, \omega) \sim \omega$
- Temperature dependence

Extended one-dimensional Hubbard model

$$\begin{aligned}\hat{H} \;=\; & -t\sum_{i\sigma}\left(\hat{c}^{\dagger}_{i\sigma}\hat{c}_{i+1\sigma}+\hat{c}^{\dagger}_{i+1\sigma}\hat{c}_{i\sigma}\right)+U\sum_{i}\hat{n}_{i\uparrow}\hat{n}_{i\downarrow} \\ & +V_1\sum_{i}\hat{n}_i\hat{n}_{i+1}+V_2\sum_{i}\hat{n}_i\hat{n}_{i+2}+V_3\sum_{i}\hat{n}_i\hat{n}_{i+3}\;+\;J\sum_{i}\hat{\mathbf{S}}_i\hat{\mathbf{S}}_j\end{aligned}$$

Parameters [eV] for the TTF band ($n = 1.41$)

Fit (Hubbard): $t = 0.4$, $U = 2.8$, $V_j = 0$, $J = 0$

Ab initio: $t = 0.15$, $U = 2$, $V_1 = 1$, $V_2 = 0.55$, $V_3 = 0.4$, $J = 0$

Fit (EHM): $t = 0.15$, $U = 2$, $V_1 = 0.75$, $V_2 = V_3 = 0$, $J = 0.3$

Parameters [eV] for the TCNQ band ($n = 0.59$)

Fit (Hubbard): $t = 0.4$, $U = 2.0$, $V_j = 0$, $J = 0$

Ab initio: $t = 0.18$, $U = 1.7$, $V_1 = 0.9$, $V_2 = 0.4$, $V_3 = 0.3$, $J = 0$

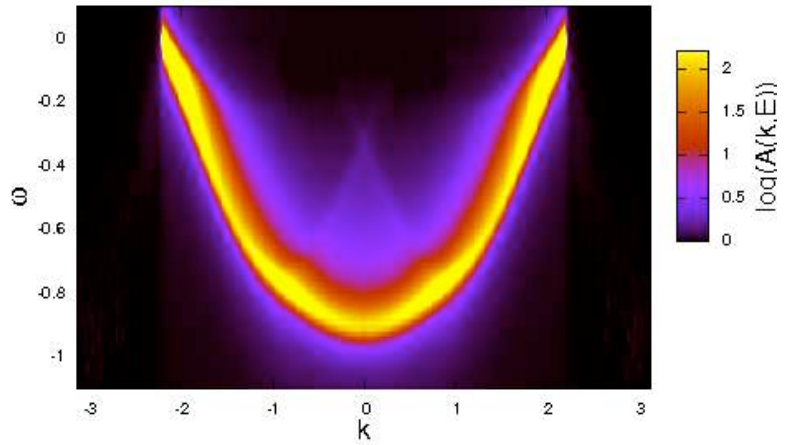
Fit (EHM): $t = 0.18$, $U = 1.7$, $V_1 = 0.72$, $V_2 = V_3 = 0$, $J = 0.25$

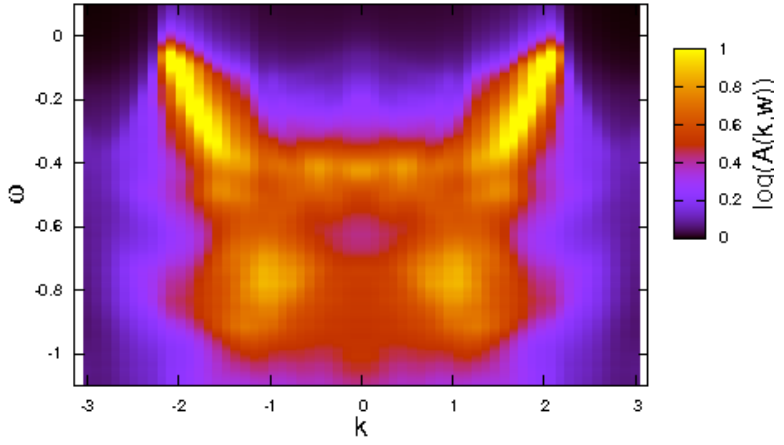
Ab initio parameters / Long-range Coulomb interactions

[L. Cano-Cortés et al., EPJB 56, 173 (2007)]

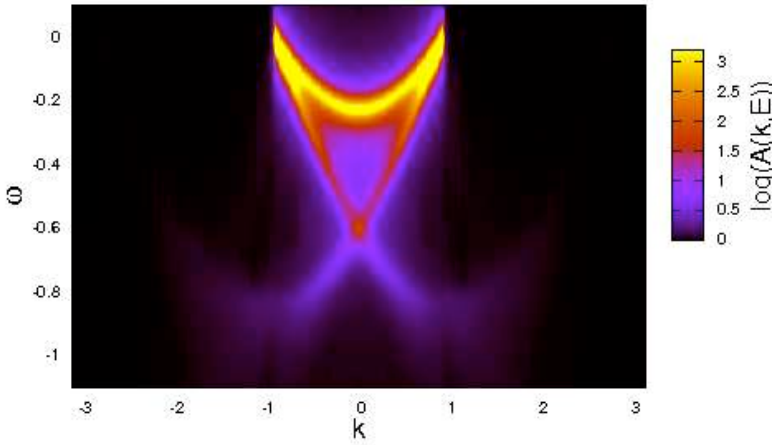
Fit (Hubbard model) | Ab initio parameters

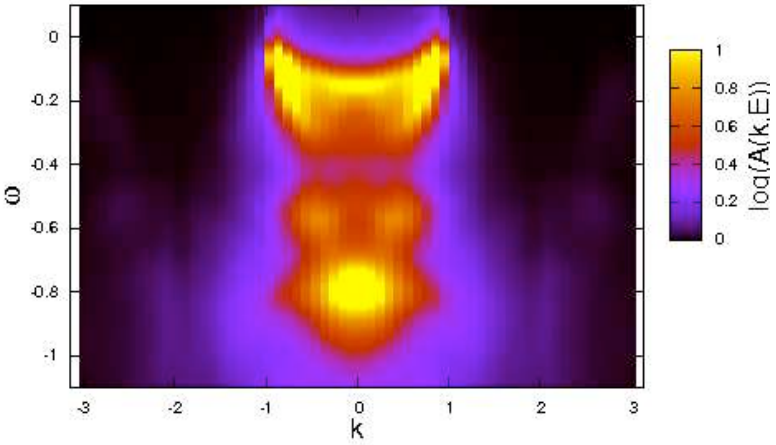
TTF





TCNQ





- Spinon band width in TCNQ is too small (0.1 vs. 0.2 eV)
- Strong structure at high-binding energy in TTF
- Complicated line shapes $\Leftrightarrow$ difficult interpretation

Optimal parameters for TTF-TCNQ

- TCNQ (Γ): Spinon band width 0.2 eV, holon crossing 0.6 eV

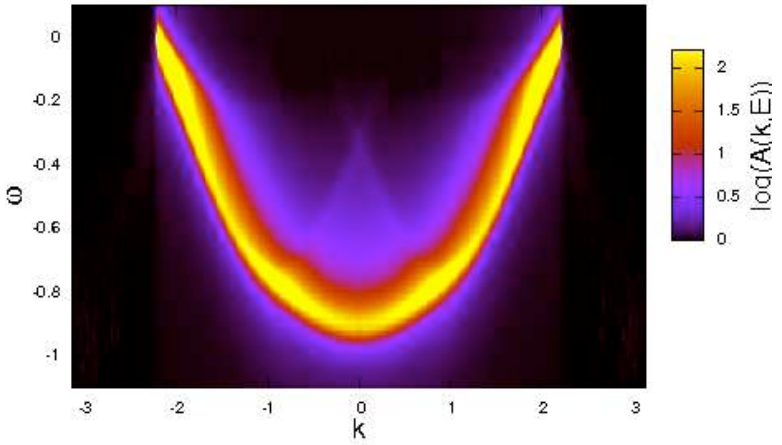
$\Rightarrow$ EHM with $t = 0.18$, $U = 1.7$, $V_1 = 0.72$, $J = 0.25$ [eV]

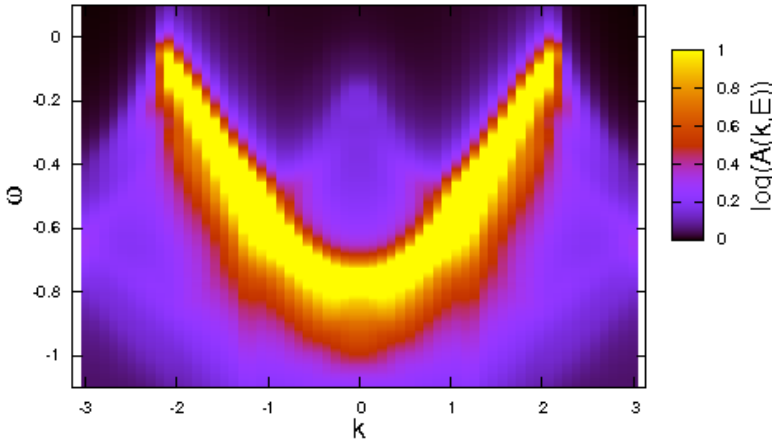
- TTF (Z): Band width 0.8 eV, onset 0.1 eV

$\Rightarrow$ EHM with $t = 0.15$, $U = 2$, $V_1 = 0.75$, $J = 0.3$ [eV]

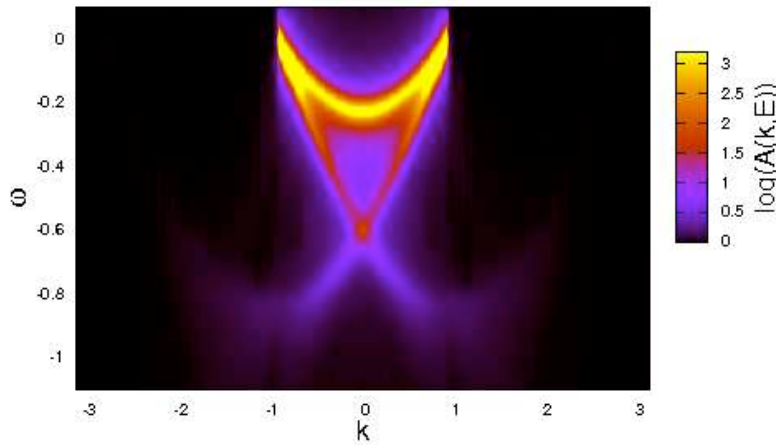
Fit (Hubbard model) Fit (EHM)

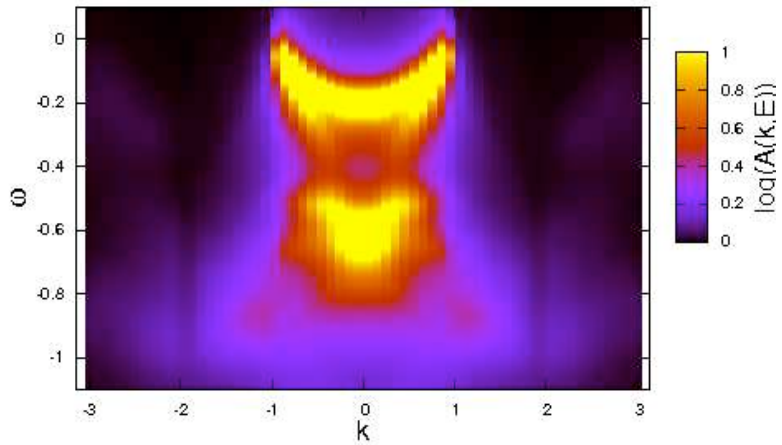
TTF





TCNQ





Summary

- Momentum- and frequency-resolved spectra
  with dynamical density-matrix renormalization group

- Non-universal spectral functions in Luttinger liquids

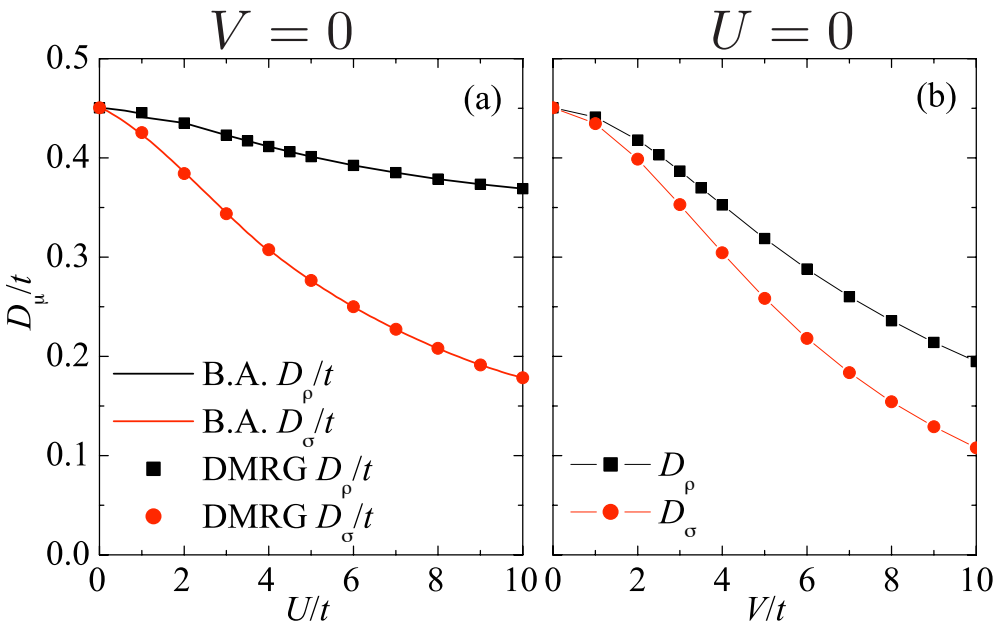
- ARPES spectrum of TTF-TCNQ for 0.1 eV $< \hbar\omega <$ 1 eV

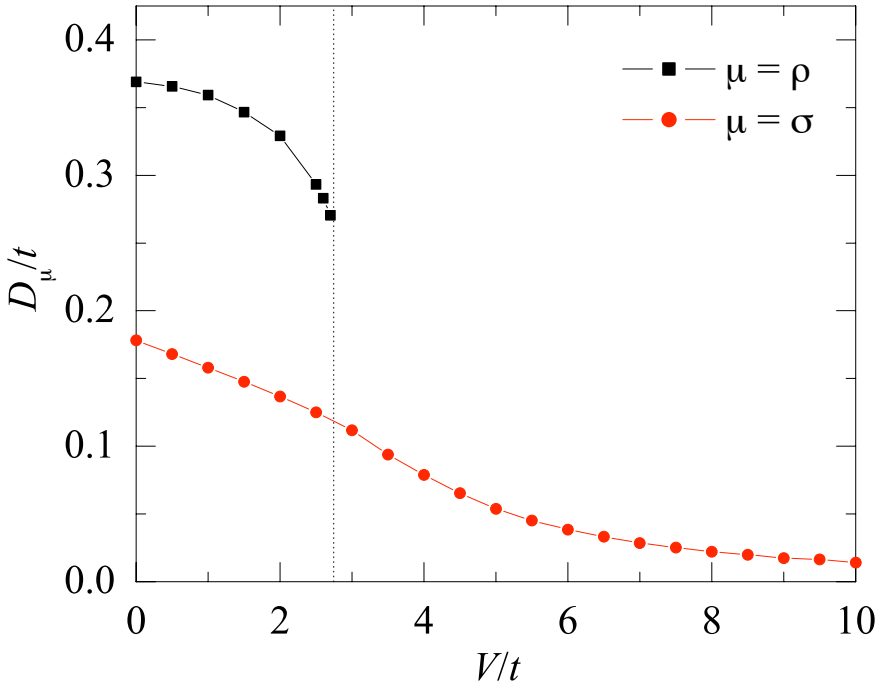
- Current works: Deconvolution, phonons, coupled chains, and ladders

Drude weights in quarter-filled extended Hubbard model

T. Shirakawa and E. Jeckelmann, Phys. Rev. B 79, 195121 (2009)]

$$\text{Re } \sigma_\mu(\omega) = \pi D_\mu \delta(\omega) + \sigma_\mu^{\text{reg}}(\omega)$$



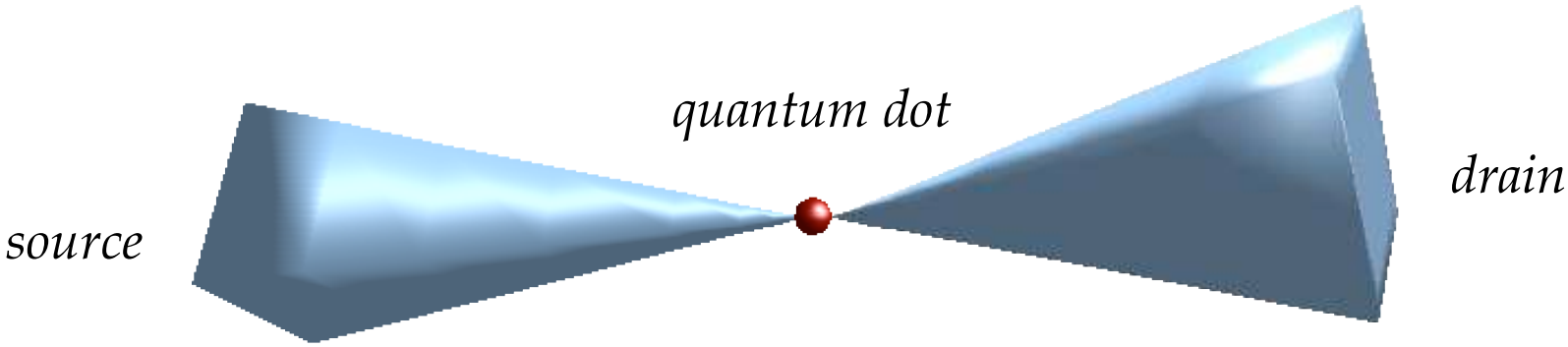


$U = 10$

- Tomonaga-Luttinger liquids: $D_\mu = v_\mu K_\mu/\pi$
- Jump in charge Drude weight at (Kosterlitz-Thouless?) metal-insulator transition
- Gapless spin excitations in CDW phase
- Spin-charge separation in all four regions

Problem: Electronic transport in nanostructures

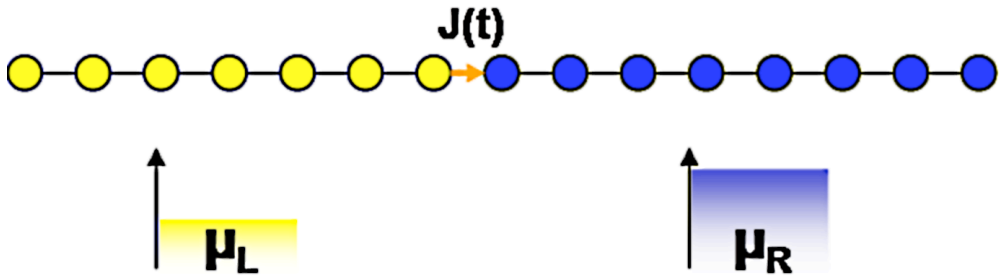
Goal: Transport in nanostructures connected to interacting leads



- Electron-electron interaction in *narrow* leads
- Electron-phonon interaction in *large* reservoirs

Test systems: Luttinger liquids

Two semi-infinite interacting chains with a potential bias



- Spinless fermion model ($0 \leq V \leq 2t_H, n = \frac{1}{2}$)

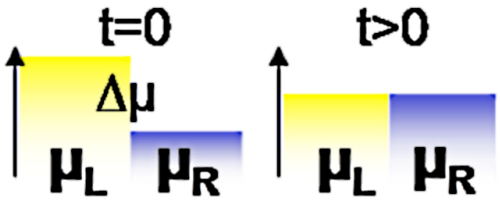
$$H = -t_H \sum \left(c_j^\dagger c_{j+1} + c_{j+1}^\dagger c_j \right) + V \sum n_j n_{j+1} - \sum \mu_j(t) n_j$$

- Hubbard model ($U \geq 0, n \neq 1$)

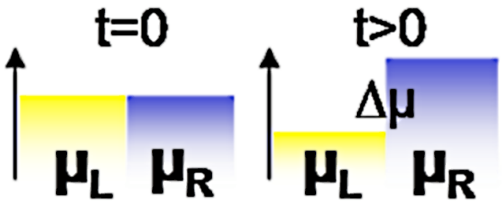
$$H = -t_H \sum \left(c_{j\sigma}^\dagger c_{j+1\sigma} + c_{j+1\sigma}^\dagger c_{j\sigma} \right) + U \sum n_{j\uparrow} n_{j\downarrow} - \sum \mu_j(t) n_{j\sigma}$$

Setups for transport calculations

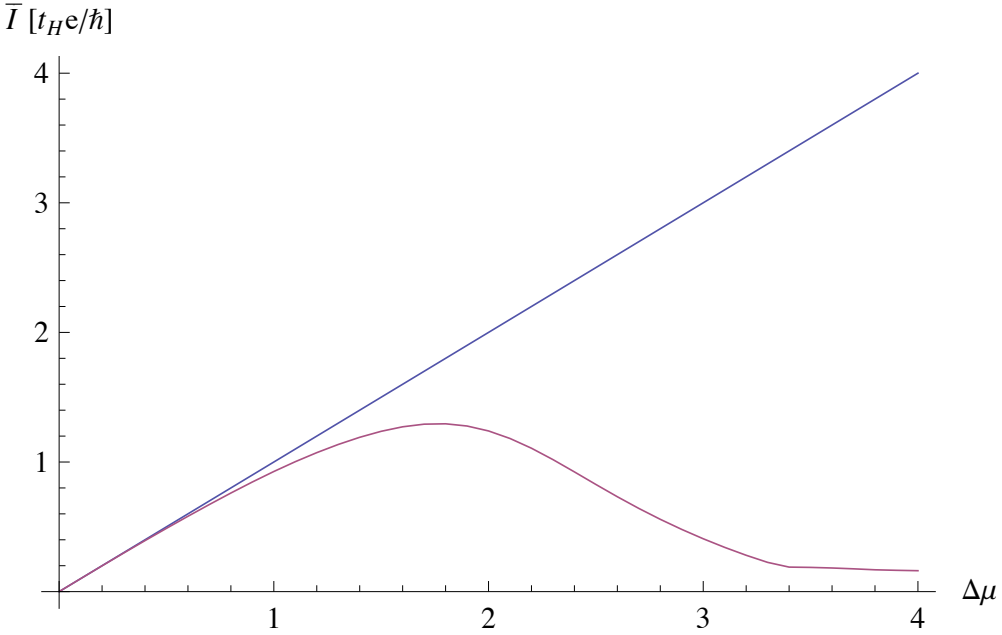
Setup 1: Reservoir discharge



Setup 2: Voltage source



Different steady-state currents



Nonequilibrium quantum many-body dynamics for long time scales

Method: Time-evolving block decimation (TEBD)

Vidal, PRL **91**, 147902 (2002); **93**, 040502 (2004)

Vidal's matrix product state

- $|\psi\rangle = \sum_{\{s_j\}} \psi(s_1, \ldots, s_N)|s_1, \ldots, s_N\rangle$

  $\psi(s_1, \ldots, s_N) = \Gamma_1[s_1]\ \lambda_1\ \Gamma_2[s_2] \ldots \lambda_{N-1}\ \Gamma_N[s_N]$

- Nn "orthonormalized" matrices $\Gamma_j[s]$
  $N-1$ diagonal matrices λ_j
  Matrix dimensions $\leq m$

Reduced density matrices

- $\rho_{L,k} = \mathrm{Tr}_{\{k+1,\ldots,N\}}|\psi\rangle\langle\psi| \ = \ \Gamma_k[s_k]\ \lambda_{k-1}^2\ \Gamma_k[s_k]\ \lambda_k^2$
- Truncation: At most m density matrix eigenstates are kept

Method: Time-evolving block decimation (TEBD)

Vidal's algorithm

- Time evolution $|\psi(t+\tau)\rangle = \exp(-i\tau H)|\psi(t)\rangle$
- 1D nearest neighbor Hamiltonian $H = \sum_j H_{j,j+1}$

  Trotter-Suzuki decomposition
  $\exp(-i\tau H) \approx \prod_{\text{even } j} U_{j,j+1} \prod_{\text{odd } j} U_{j,j+1}$

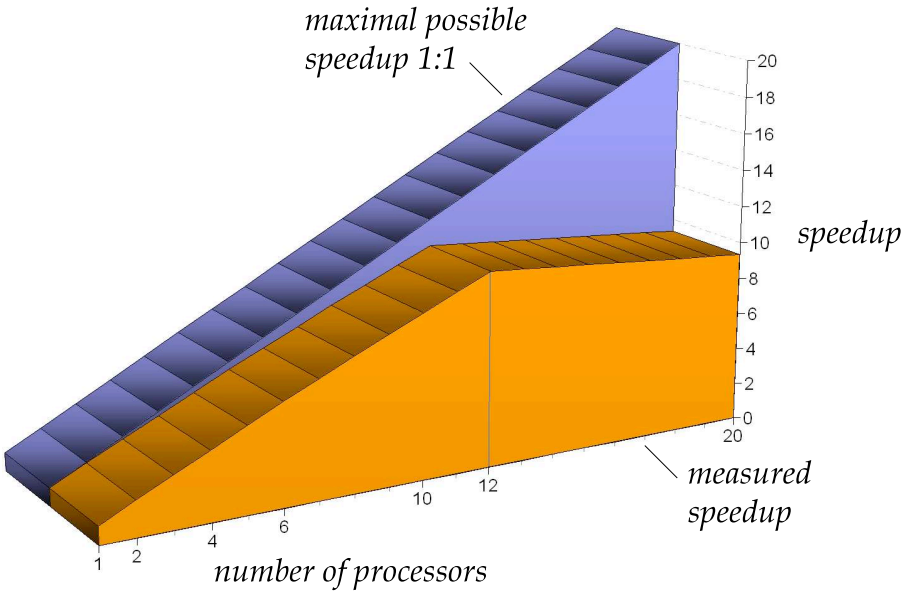
  two-bit gates $U_{j,j+1} = \exp(-i\tau H_{j,j+1})$
- Only λ_j, Γ_j and Γ_{j+1} change in new state $|\psi'\rangle = U_{j,j+1}|\psi\rangle$

  Truncation after each application of $U_{j,j+1}$
- Computational cost: CPU $\propto Nm^3 T/\tau$, memory $\propto Nm^2$

Parallelization of TEBD

Easy parallelization

- Simultaneous computation for all even (odd) bonds
- Advantage over time-dependent DMRG



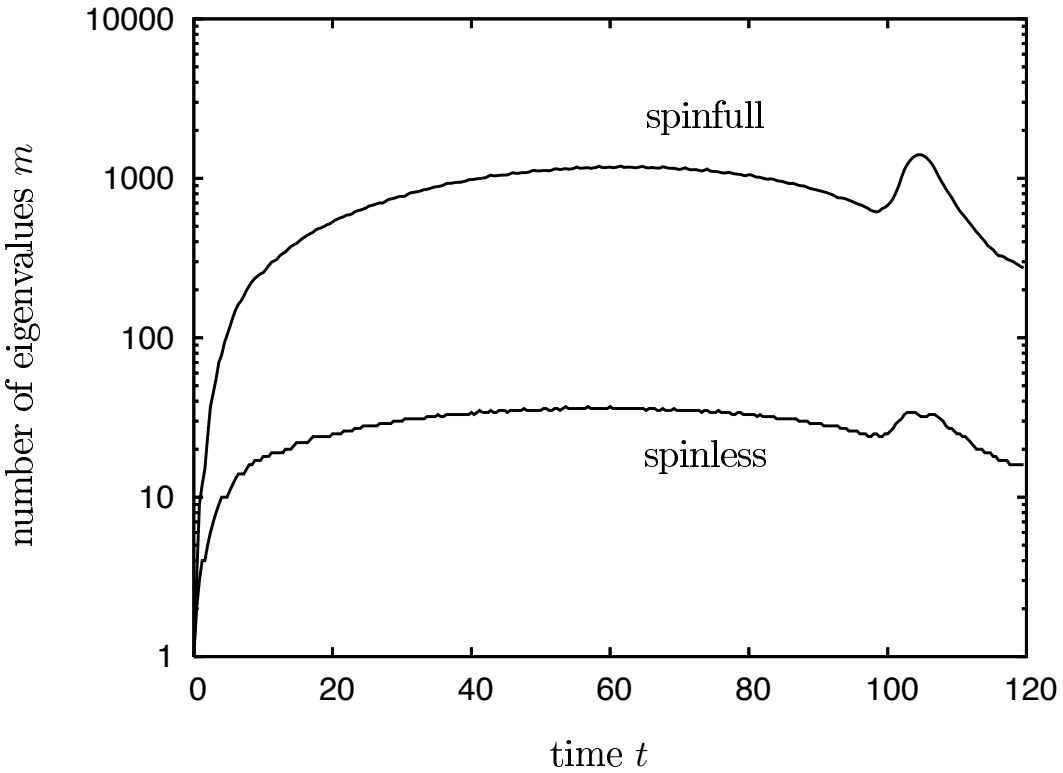
- Theoretical speedup $N/2$
- Optimal speedup with up to 12 processors
- Communication bottleneck in our cluster

Accuracy of TEBD: Truncation error

Estimation of truncation errors

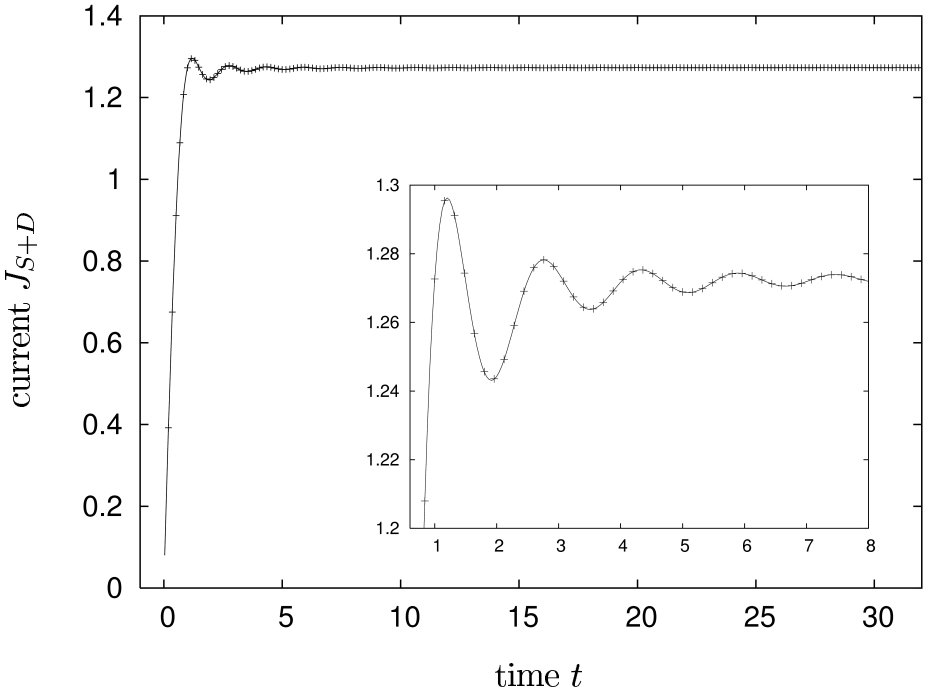
- Discarded weight $D(m) = 1 - \sum_{\alpha=1}^{m} w_\alpha$
- Entanglement entropy $S = \sum_\alpha w_\alpha \ln(w_\alpha)$
- Constant m or D

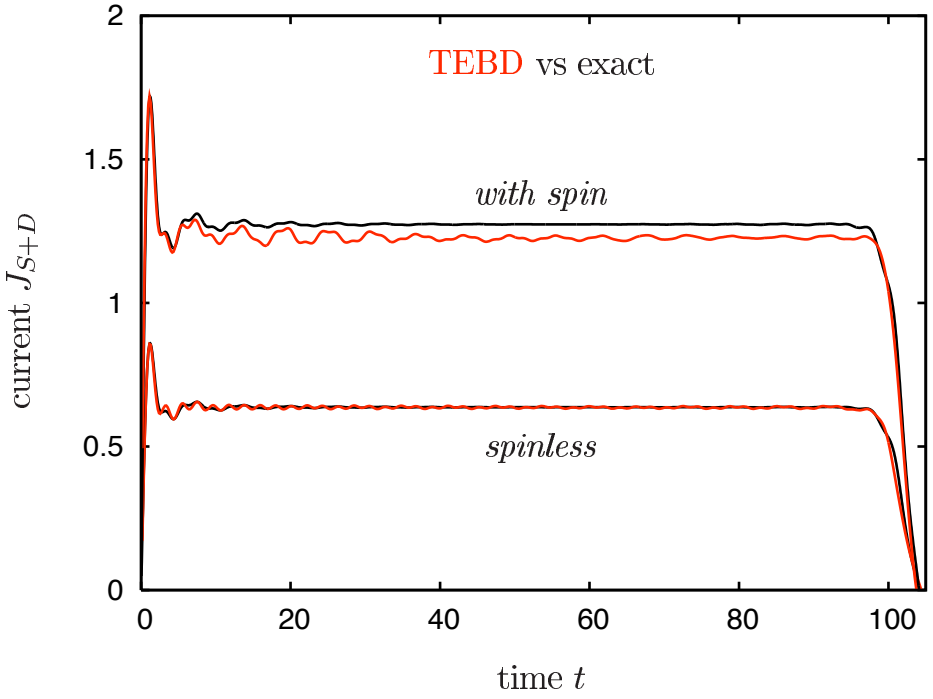
m vs time for fixed $D = 10^{-2}$



Accuracy of TEBD: Comparison with exact results

Tight-binding model for non-interacting fermions





Relative error

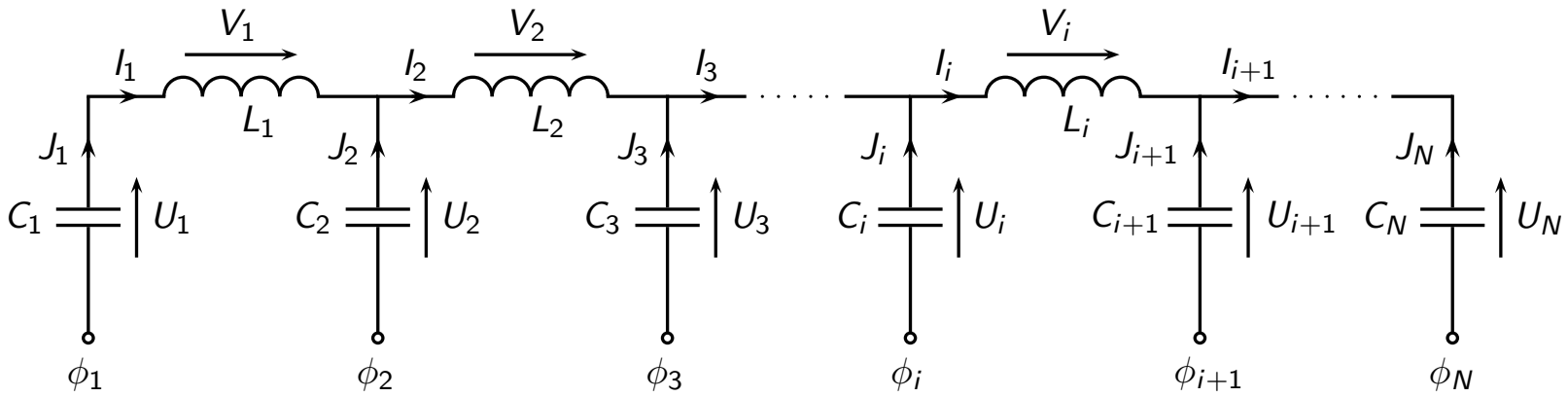
- Spinless fermions: $\sim 0.1\%$
- Spin $\frac{1}{2}$ fermions: $\sim 1\%$

Computational effort

- Spinless fermions: 400 hours
- Spin $\frac{1}{2}$ fermions: 2000 hours

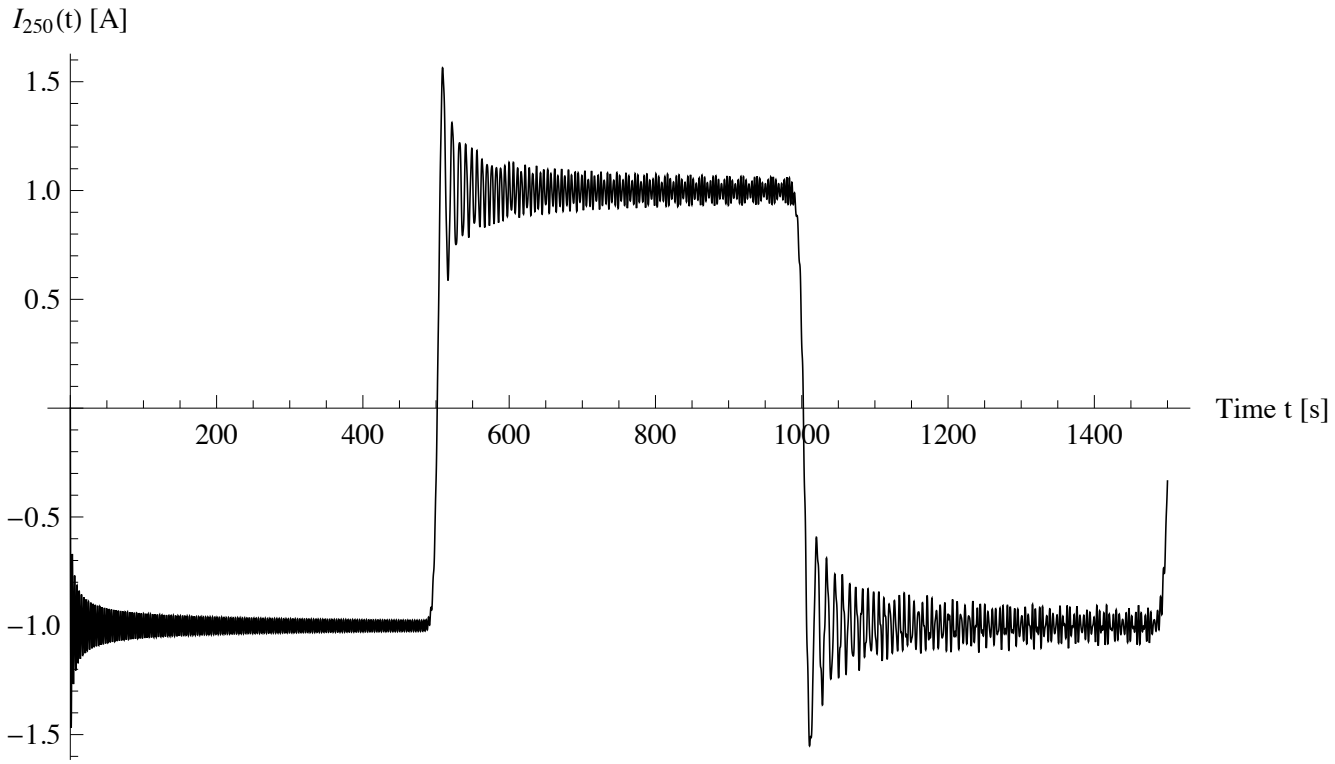
Model for finite-size effects: Classical LC-line

- Extrapolation to steady state $\Leftrightarrow$ Understanding finite-system dynamics
- Finite-size effects: Classical electrical network $\approx$ Quantum system



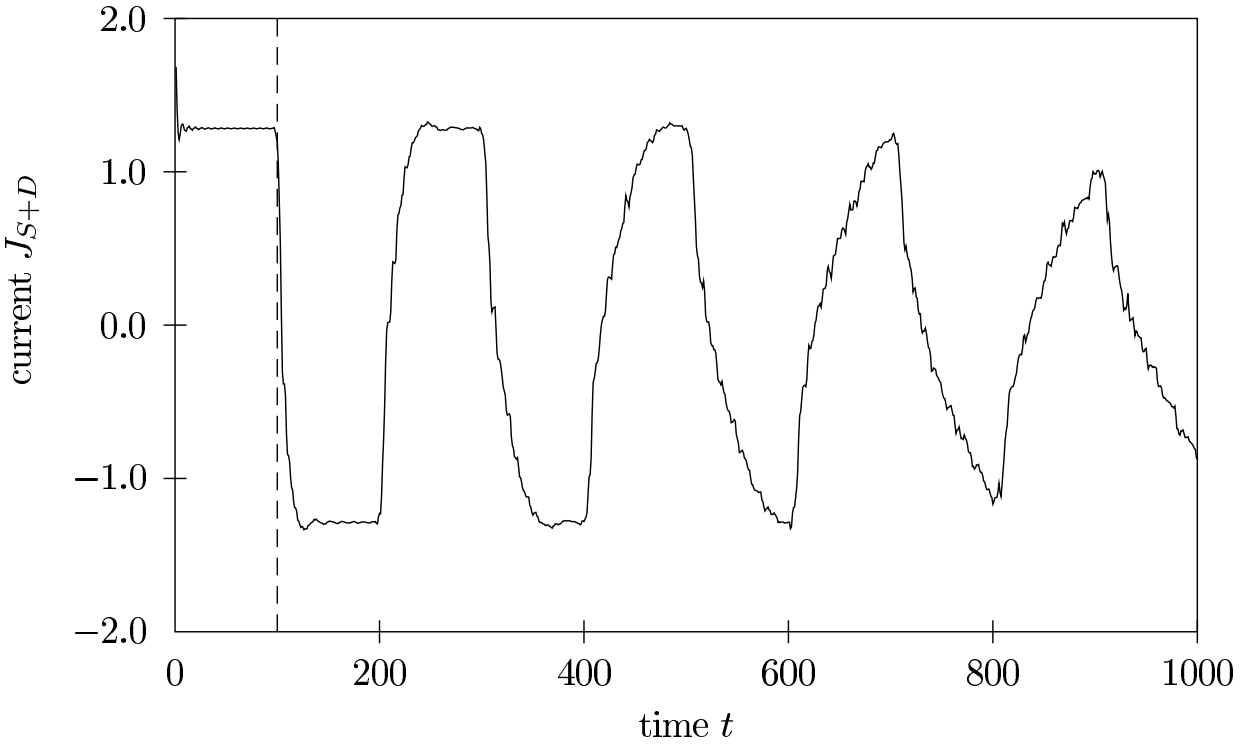
- Isolated systems $\Rightarrow$ no dissipation $\Rightarrow$ no resistor
- Only linear transport (no difference between setups I and II)

Classical finite-size effects



- Long time scale: Rectangle wave with period $T \propto N$
- Short time scale: Transient regime + finite-size fluctuations
- Intermediate time scale: Quasi-stationary current

Finite-size effects in quantum systems



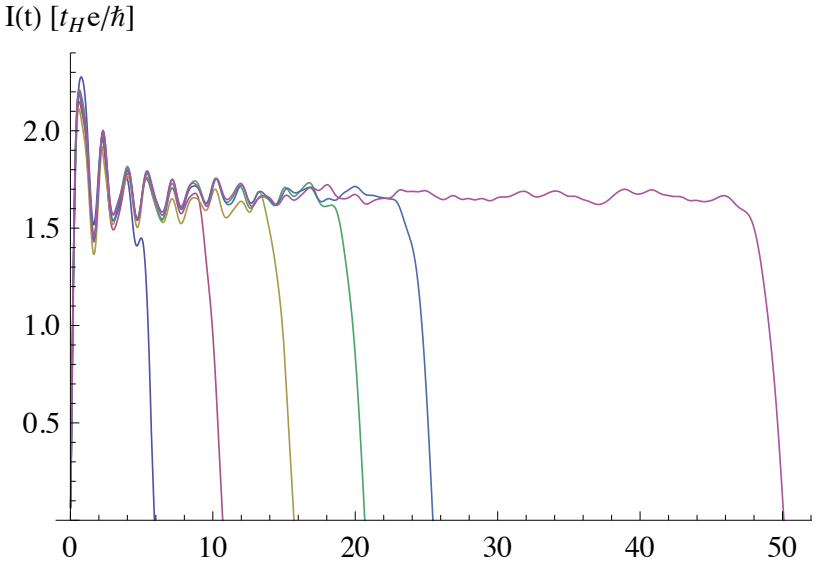
- Long time scale: Wave with *approximate period* $T \propto N$
- Intermediate time scale: Quasi-stationary current for $t < T/2$
- All time scales: Finite-size and initial-condition fluctuations

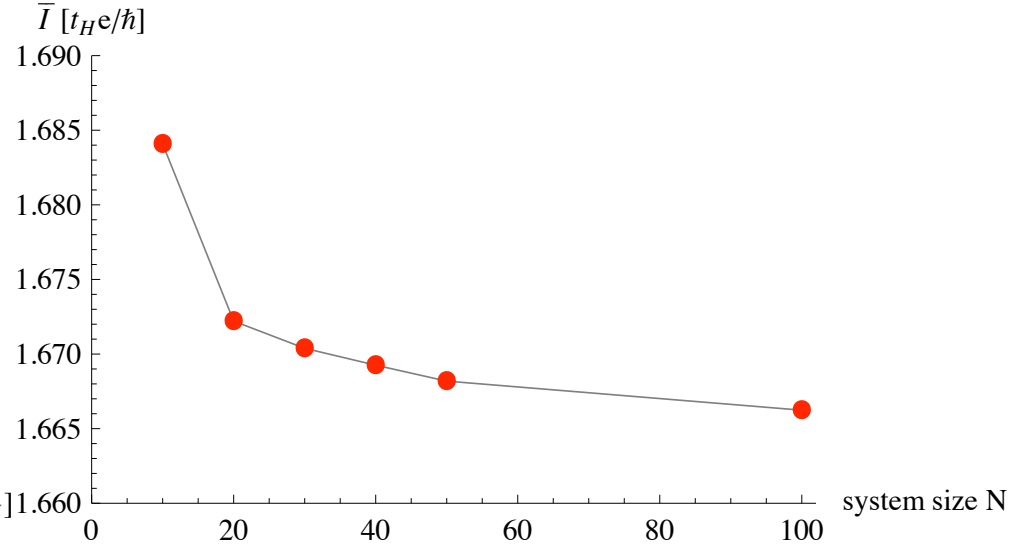
Steady-state current extrapolation

Method

- Assuming an *approximate* rectangle wave of period T
- Fourier transform $\tilde{I}(\omega = \frac{2\pi}{T})$ of signal $I(t)$ using $0 < t < T/4$
- Extrapolation $I_S = \lim_{N\to\infty} \frac{4}{\pi}\tilde{I}(\omega = \frac{2\pi}{T})$

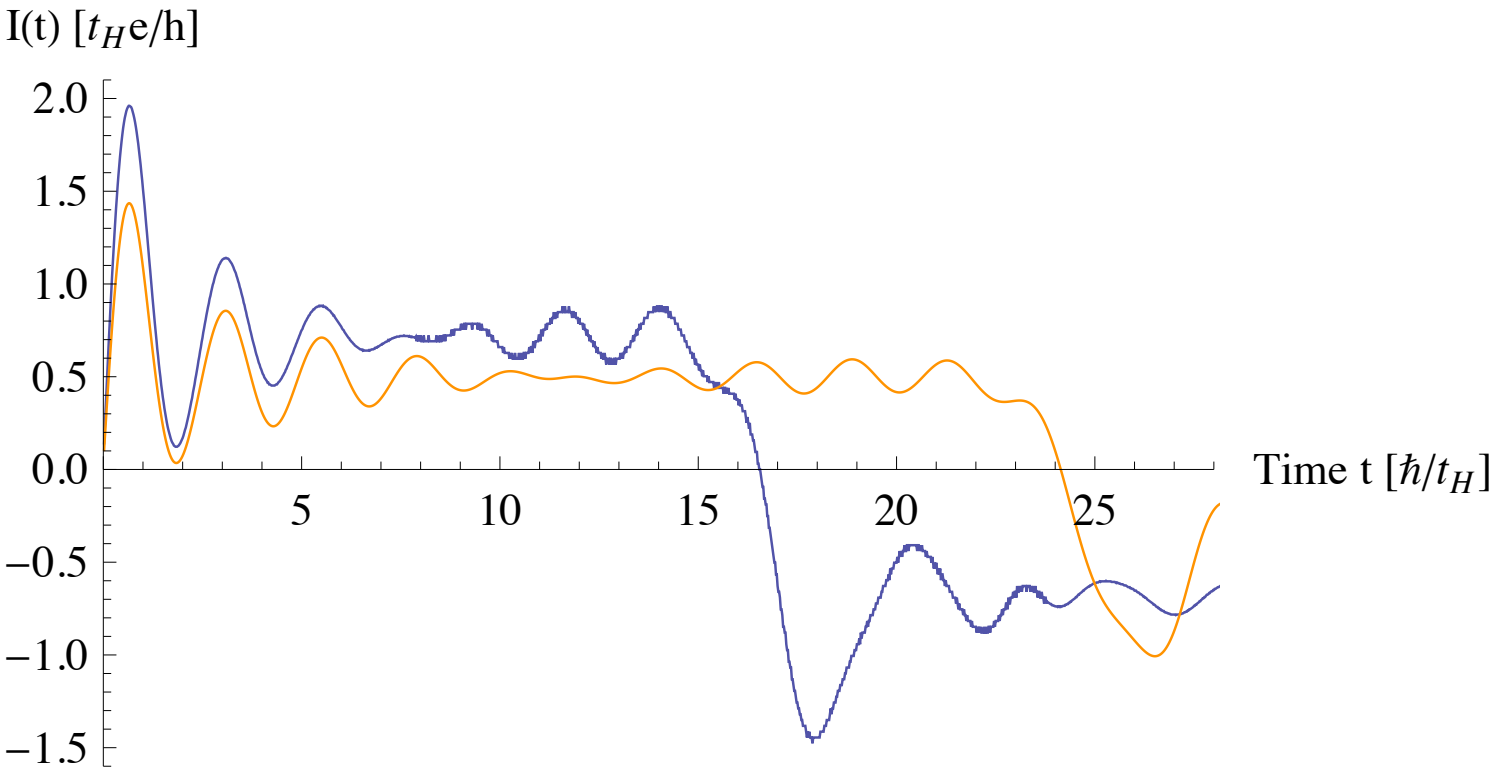
Example: Hubbard chain, $U = 1$, $n = \frac{2}{3}$, $\Delta\mu(t < 0) = 1.2$, $N = 10-100$





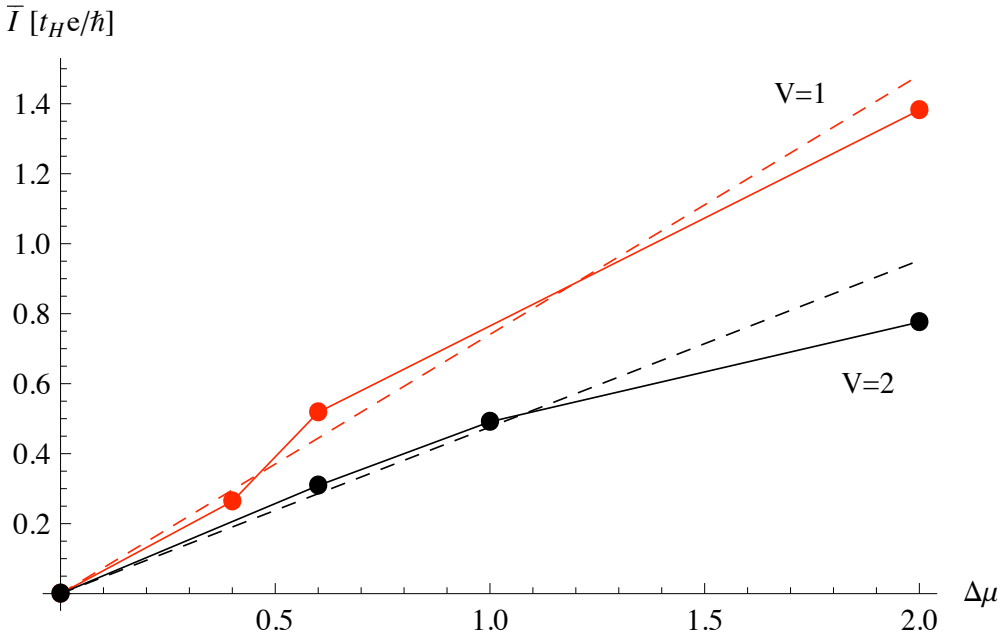
Results for the spinless fermion model

$V = 1,\ N = 40, 60,$ Setup I: $\Delta\mu(t < 0) = 0.6$

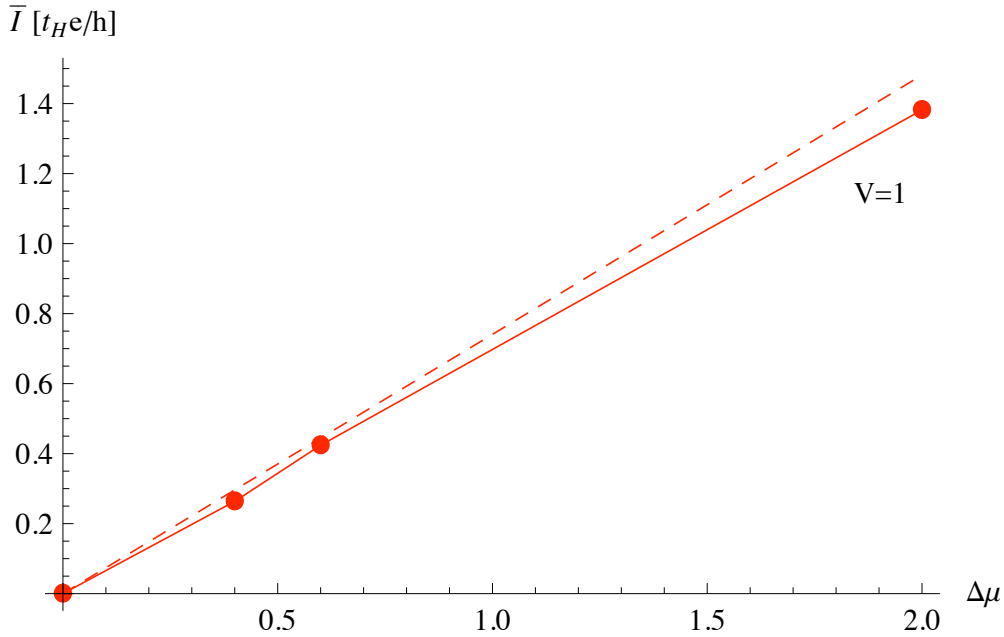


Results for the spinless fermion model

Finite system ($N = 60$)



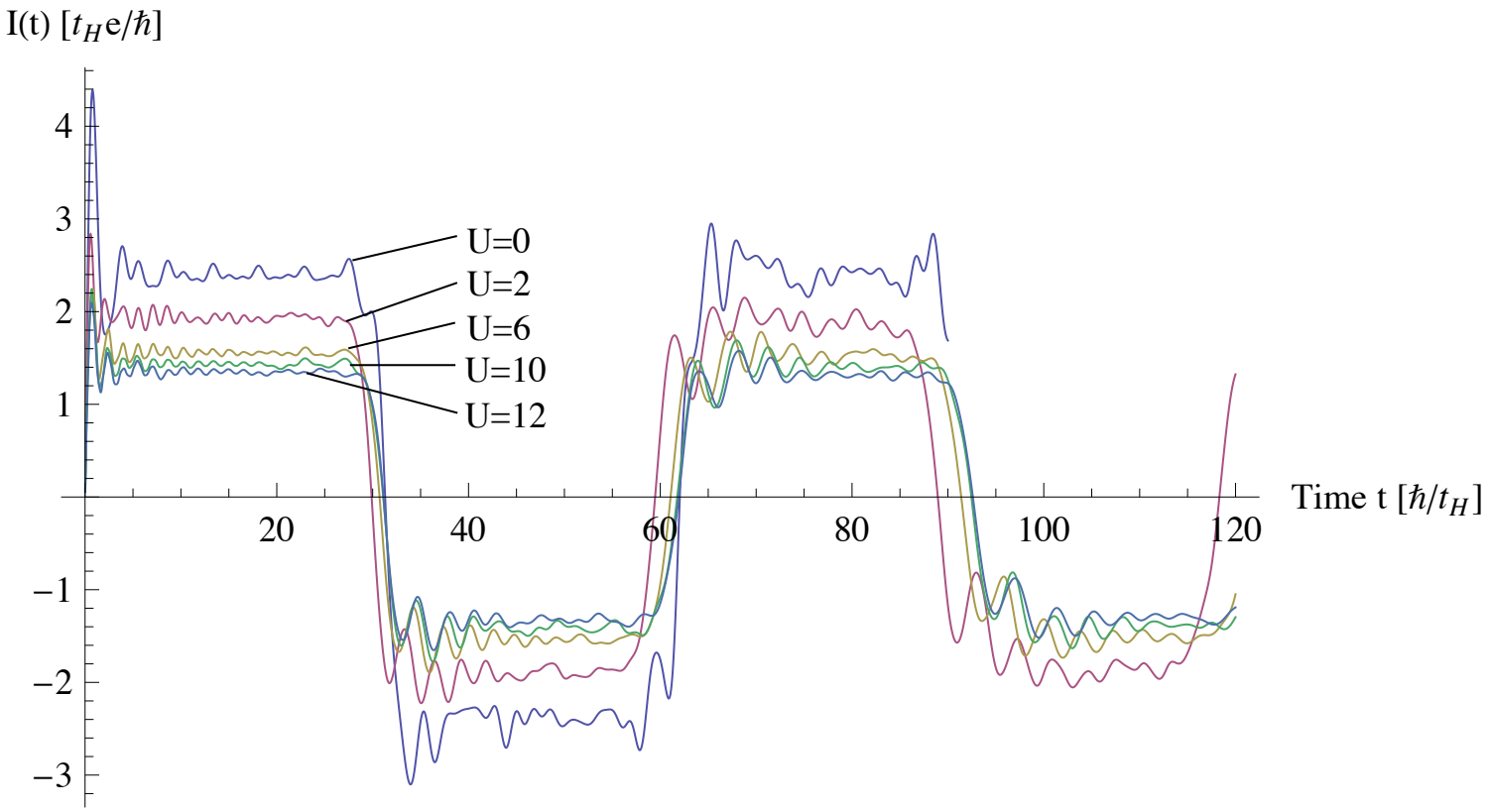
Infinite system ($N \to \infty$)



- Setup I $[\Delta\mu(t < 0) \neq 0] \Rightarrow$ linear response at $V = 0$
- Luttinger liquid $\Rightarrow$ linear response $I = \frac{e^2}{h} K \Delta\mu$
- Bethe Ansatz $\Rightarrow K = \frac{\pi}{2} \frac{1}{\pi - \arccos(V/2)}$

Results for the Hubbard model

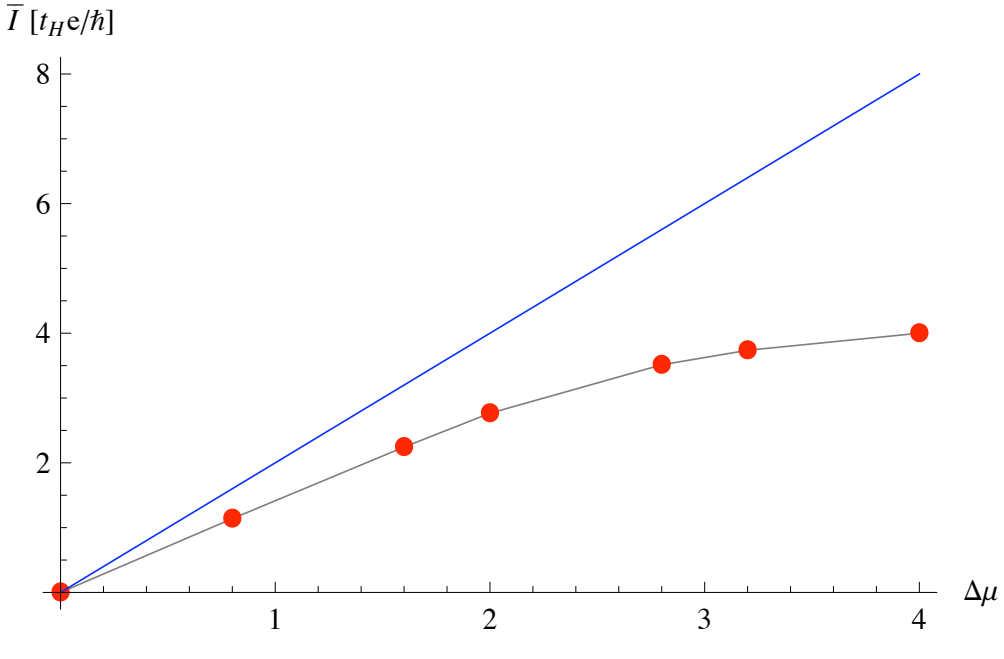
$N = 60,\ n = 2/3$, Setup I: $\Delta\mu(t < 0) = 1.2$



Results for the Hubbard model

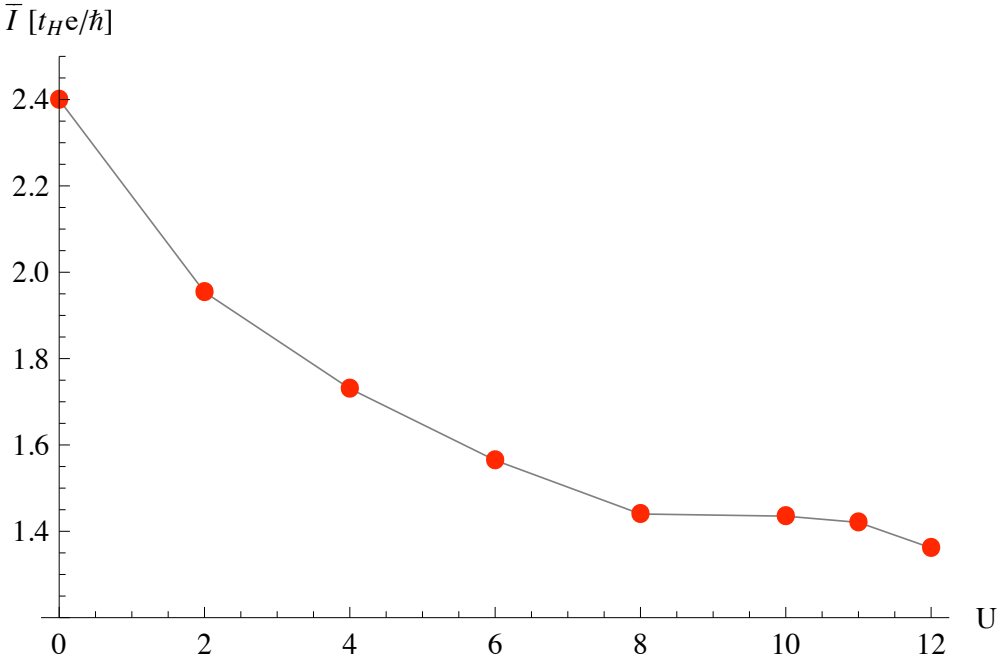
$$N = 60,\ n = \frac{2}{3}$$

$U = 1$, Setup I $[\Delta\mu(t < 0) \neq 0]$



- Problem in the linear regime

Setup I $[\Delta\mu(t < 0) = 1.2]$



- Significant interaction effects in the non-linear regime

Results: Interpretation

- $\frac{I_S}{\Delta\mu} = \frac{e^2}{h}K = \mathit{conductance} < \infty$
- Isolated system $\Rightarrow$ energy conservation, no dissipation
- $\Delta\mu$ is an externally applied potential
- What is the actual voltage bias ?

Summary

- Steady-state current from the nonequilibrium dynamics of finite systems

- Highly scalable TEBD method
- Accuracy seems good enough

- Wave function accuracy / “large“discarded weight
- Setup dependence of the non-linear response
- Influence of initial conditions
- Analysis of finite-size effects
- Definition and computation of actual voltage bias

- Work in progress