Low-energy local density of states of the 1D Hubbard model

Imke Schneider,
Institut für Theoretische Physik, TU Dresden

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In collaboration with: Stefan Söffing, Michael Bortz, Alexander Struck, and Sebastian Eggert, TU Kaiserslautern

Low energy properties of fermionic systems in 1D

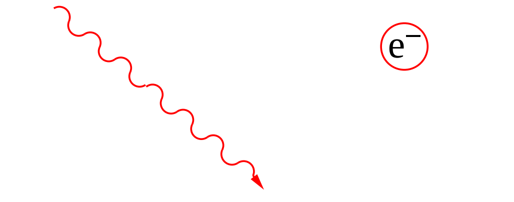
- Strong correlations, interactions dominant, universal behavior
- no single-particle picture possible, excitations collective bosonic modes

  Luttinger liquid

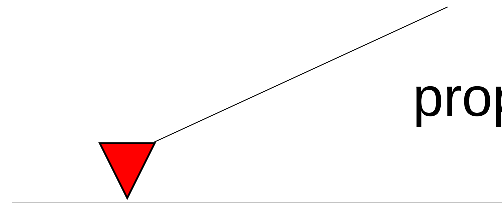
- Spin- and charge excitations decouple

Tunneling in quantum wires

Photo emission



Scanning tunneling spectroscopy



proportional to dI/dV

Density of states:

$$\rho(\omega) = -\frac{1}{\pi}\text{Im}\int_0^\infty e^{i\omega t} G^{\text{r}}(t)\,dt$$
$$= \sum_m |\langle \omega_m|\psi^\dagger|0\rangle|^2\,\delta(\omega - \omega_m)$$

Luttinger liquid: $\rho(\omega) \propto \omega^\alpha$

Momentum resolved tunneling experiments in 1D

Experimental signatures of spin-charge separation

- Semiconductor hetero-structures

  Auslaender, Steinberg, Yacoby, Tserkovnyak, Halperin, Baldwin, Pfeiffer, and West, Science 308, 88 (2005)

  Jompol, Ford, Griffiths, Farrer, Jones, Anderson, Ritchie, Silk, and Schofield, Science 325 (2009)

- Quasi one-dimensional crystals

  Kim, Koh, Rotenberg, Oh, Eisaki, Motoyama, Uchida, Tohyama, Maekawa, Shen, and Kim, Nature Phys. 2 (2006)

- Self-organized atomic chains

  (Segovia, Purdie, Hengsberger, and Baer, Nature 402 (1999))

Scanning tunneling spectroscopy in 1D

- Carbon nanotubes

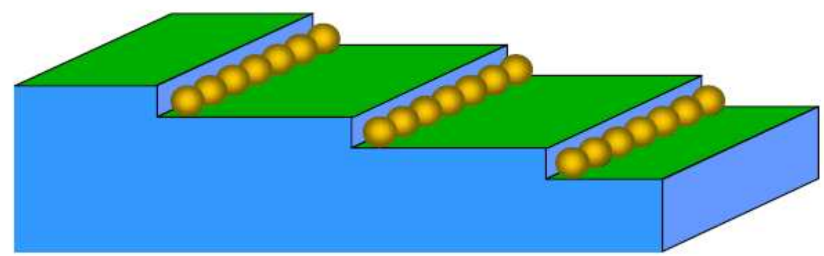
  Lee, Eggert, Kim, Kahng, Shinorara, and Kuk, Phys. Rev. Lett. 93 (2004)

  Venema, Wildöer, Janssen, Tans, Tuinstra, Kouwenhoven, and Dekker, Science 283 (1999)

  Lemay, Janssen, van den Hout, Mooij, Bronikowski, Willis, Smalley, Kouwenhoven, and Dekker, Nature 412 (2001)

- Self-organized atomic gold chains

  Blumenstein, Schäfer, Mietke, Meyer, Dollinger, Lochner, Cui, Patthey, Matzdorf, and Claessen, Nature Phys. 7 (2011)



Signatures of power law density of states $\rightarrow$ Luttinger liquid behavior

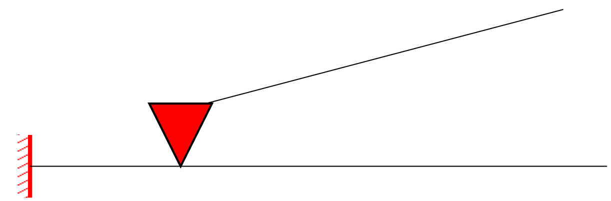
Outline

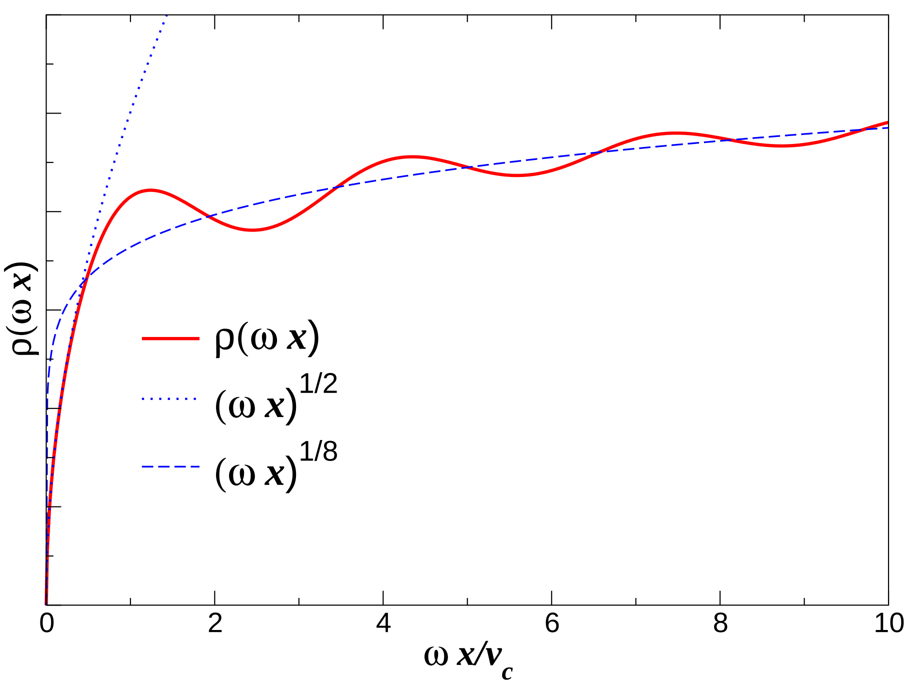
- Local density of states of interacting fermions in 1D
  - Luttinger liquid: power laws
    here: Effects of boundaries and finite system sizes
  - DMRG: lattice model of spinless fermions
    Spectral weight of individual excitations
  - Bosonization: Recursion formula
  - DMRG: Hubbard model

Luttinger liquid with impurity

Local density of states

$$\rho(\omega, x) = \sum_m |\langle \omega_m | \psi^\dagger(x) | 0 \rangle|^2 \, \delta(\omega - \omega_m)$$
$$= \frac{1}{2\pi} \int_{-\infty}^{\infty} e^{i\omega t} \langle \psi(x,t) \psi^\dagger(x,0) \rangle dt$$





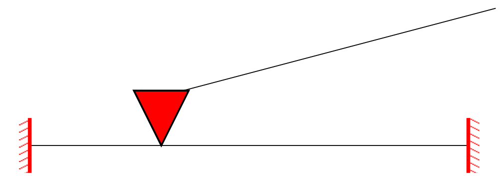
strong depletion for small energies and at the boundary

(here $K_s = 1, K_c = \frac{1}{2}$)

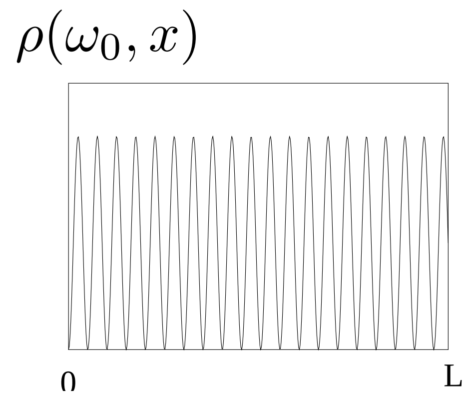
Eggert, Johannesson, Mattsson, Phys. Rev. Lett. 76, (1996)

Finite Luttinger liquid with boundaries

$$\rho(\omega,x) = \sum_m |\langle \omega_m|\psi^\dagger(x)|0\rangle|^2\,\delta(\omega-\omega_m)$$
$$= \frac{1}{2\pi}\int_{-\infty}^{\infty} e^{i\omega t}\,\langle\,\psi(x,t)\psi^\dagger(x,0)\rangle dt$$



Free fermions:

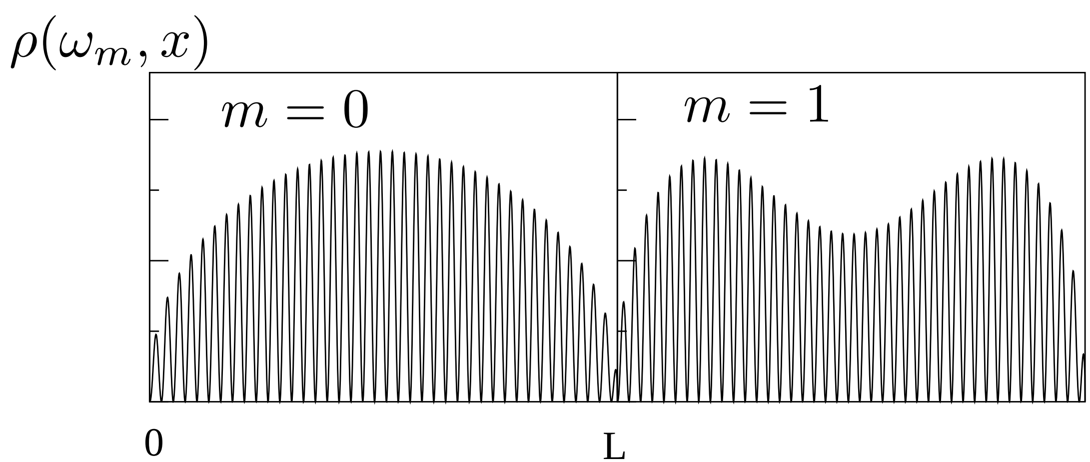


single particle wave function:

$\rho(\omega_m,x) = |\Psi_m(x)|^2$

Interacting:

Bosonization



Anfuso, Eggert, Phys. Rev. B 68 (2003)

Exact lattice model: local density of states in DMRG

$$H = -t \sum_{x=1}^{L-1} \left(\psi_x^\dagger \psi_{x+1} + \psi_{x+1}^\dagger \psi_x \right) + U \sum_{x=1}^{L-1} n_x n_{x+1}, \quad n_x = \psi_x^\dagger \psi_x - 1/2$$

- Approach 1: Dynamical DMRG and tDMRG
  + entire spectrum
  - energy levels not resolvable

  Jeckelmann, arXiv:1111.6545

- Approach 2: transition matrix elements in DMRG
  + energy levels resolvable
  - only for low energy excitations

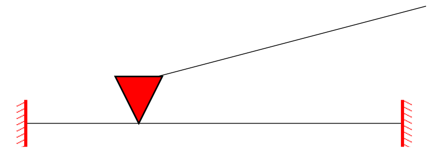
  Schneider, Struck, Bortz, and Eggert, Phys. Rev. Lett. 101, 206401 (2008)

  Söffing, Schneider, and Eggert, arXiv:1204.0003

$$\rho(\omega, x) = \sum_m |\langle \omega_m | \psi_x^\dagger | 0 \rangle|^2 \delta(\omega - \omega_m) = \quad -\tfrac{1}{\pi} \mathrm{Im} \int_0^\infty e^{i\omega t} G^{\mathrm{r}}(x,t)\, dt$$

Understanding of individual excitations

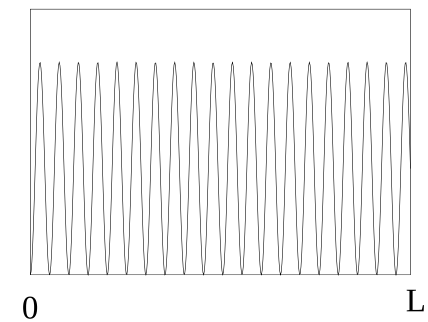
Free fermions

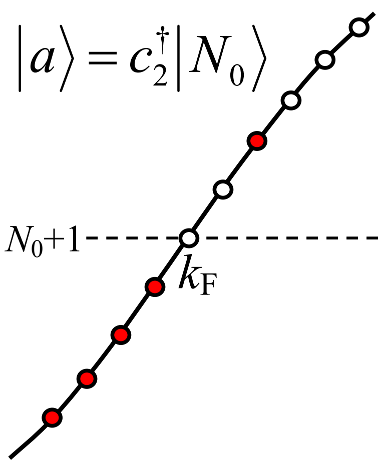


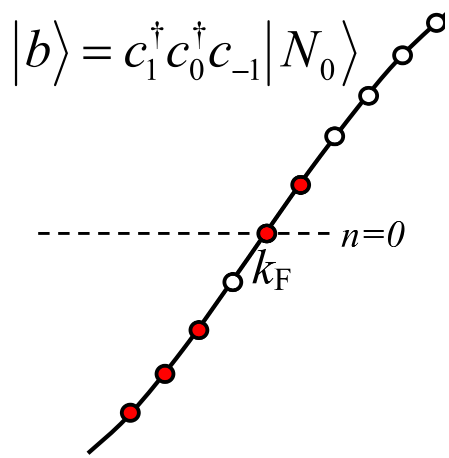
$$H = \sum_k \epsilon(k)\, c_k^\dagger c_k \qquad k = \frac{\pi}{L} n \qquad n = 0, 1, 2, \ldots$$

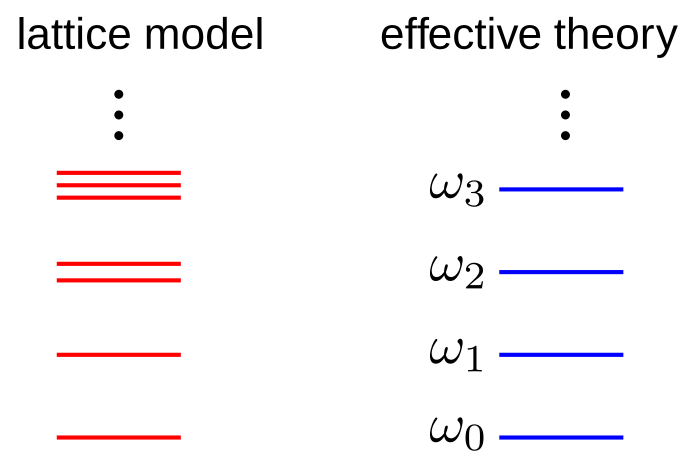
$$|\langle N_0 | c_n \psi_x^\dagger | N_0 \rangle|^2 = \frac{2}{L} |\sin(k_F + k_n) x|^2$$

$|\langle a | \psi_x^\dagger | N_0 \rangle|^2$



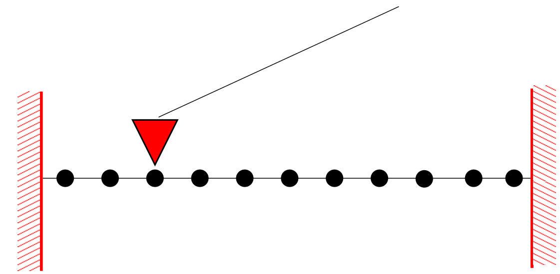


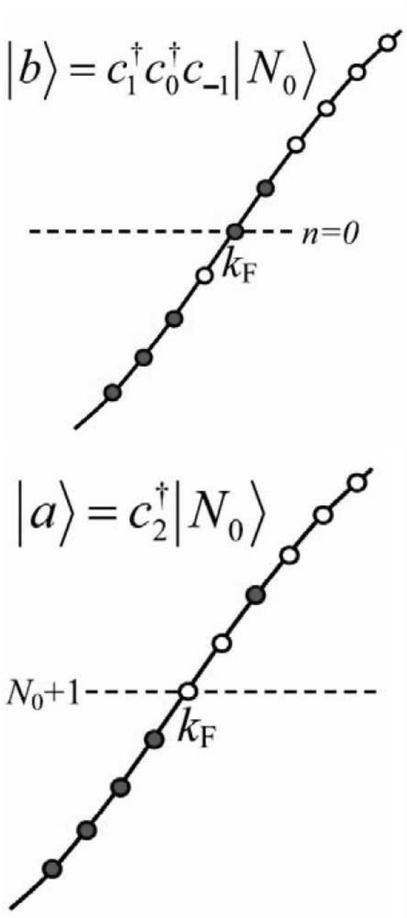


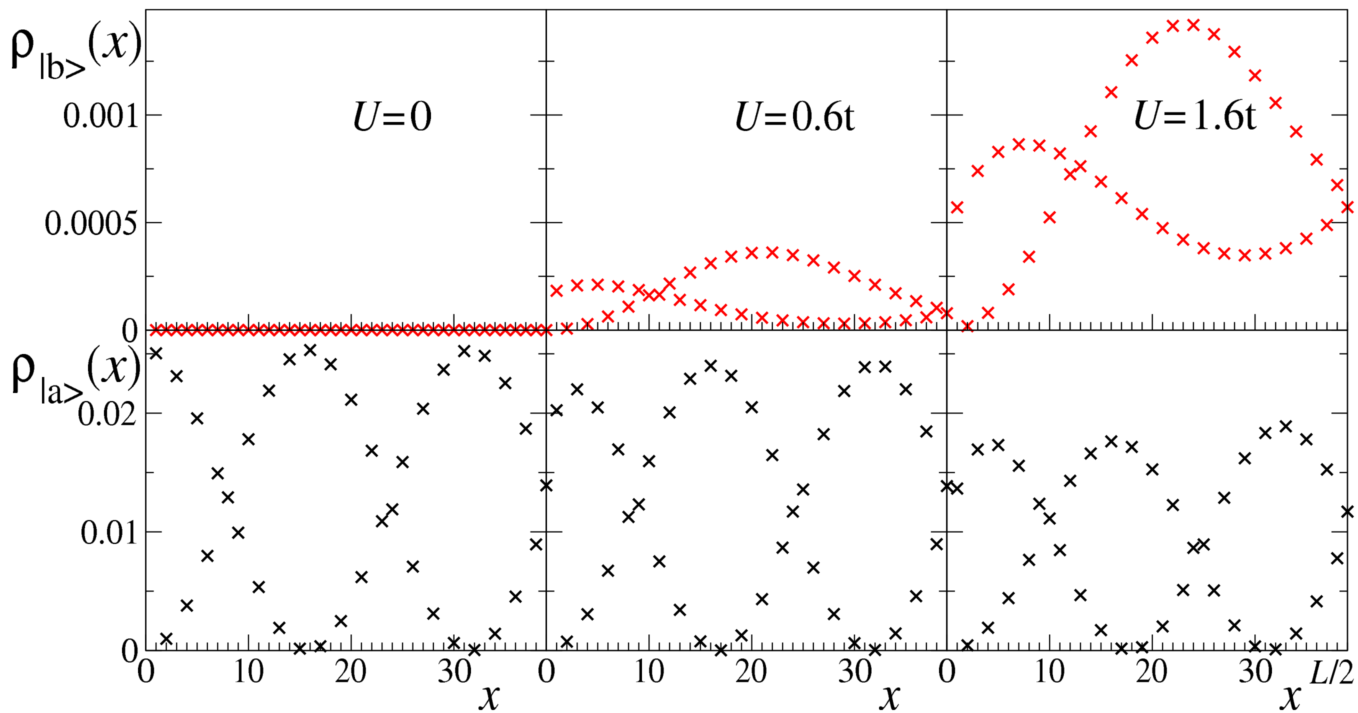


Local density of states: DMRG results

$$H = -t\sum_{x=1}^{L-1}\left(\psi_x^\dagger\psi_{x+1} + \psi_{x+1}^\dagger\psi_x\right) + U\sum_{x=1}^{L-1} n_x n_{x+1}$$

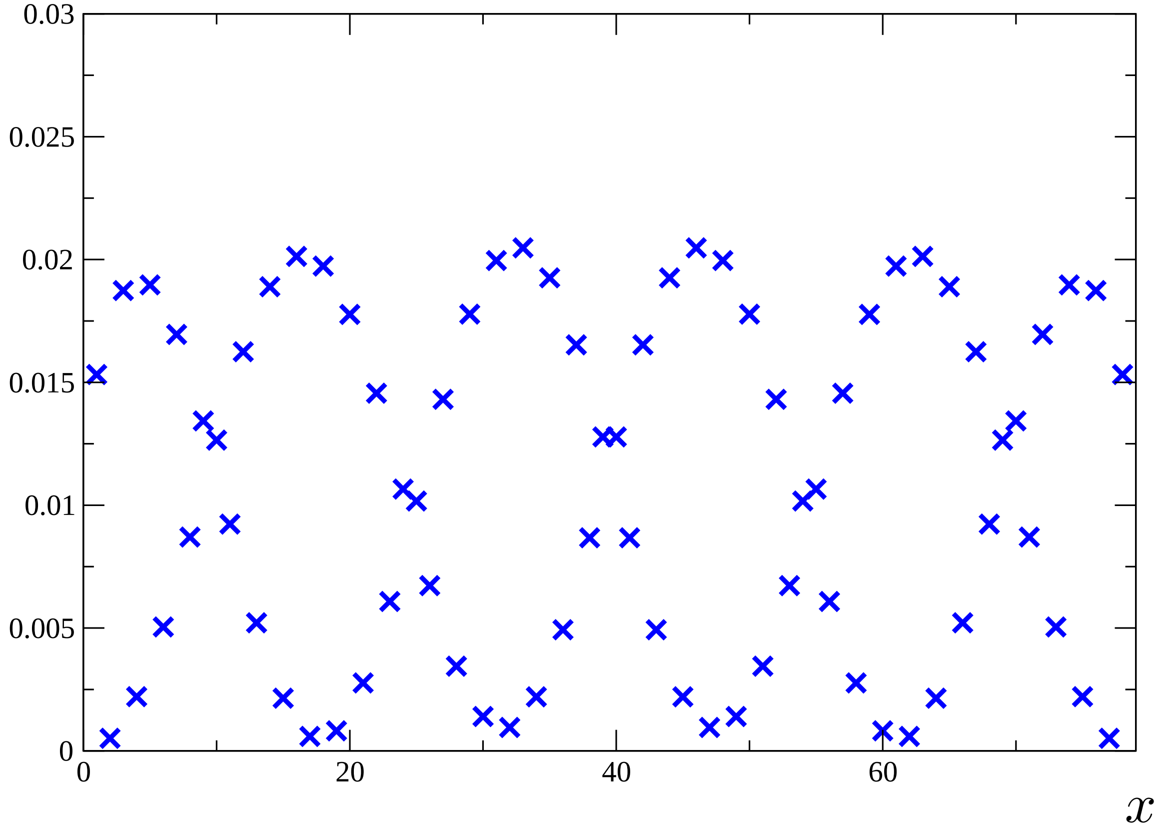






Local density of states: DMRG results

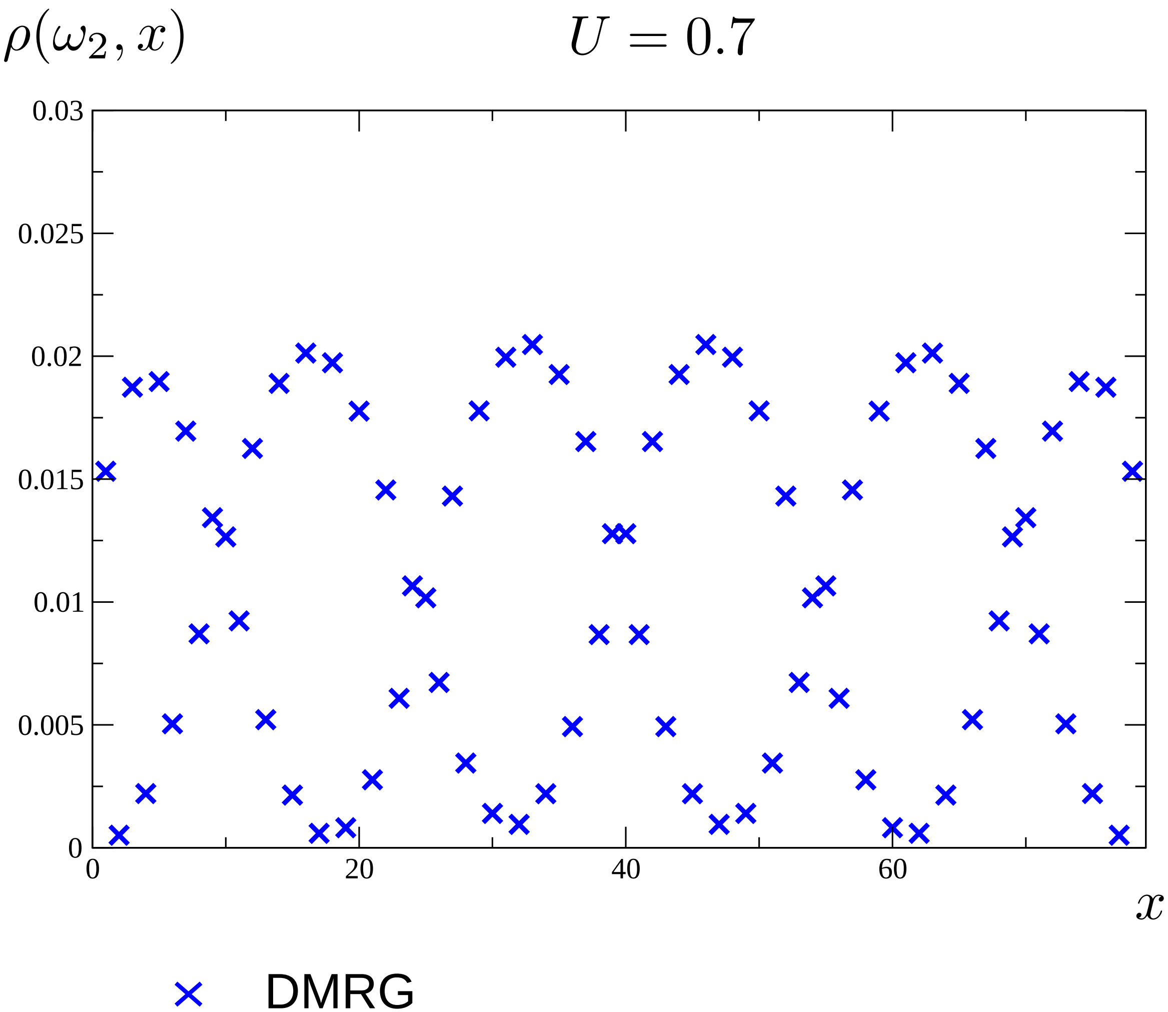
$\rho(\omega_2, x)$ $\quad U = 0.7$

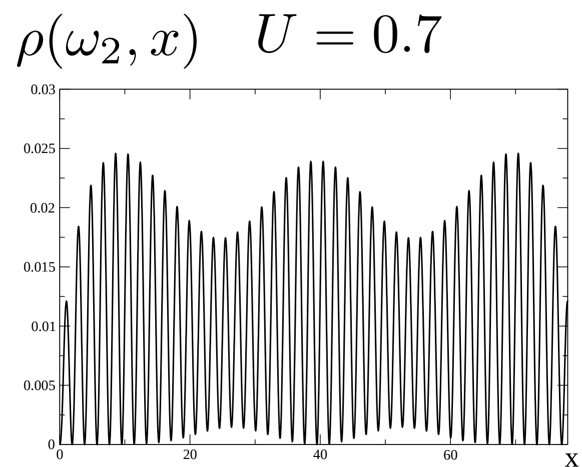


× DMRG

$$\rho(\omega_2, x) = |\langle a|\psi^\dagger(x)|0\rangle|^2 + |\langle b|\psi^\dagger(x)|0\rangle|^2$$

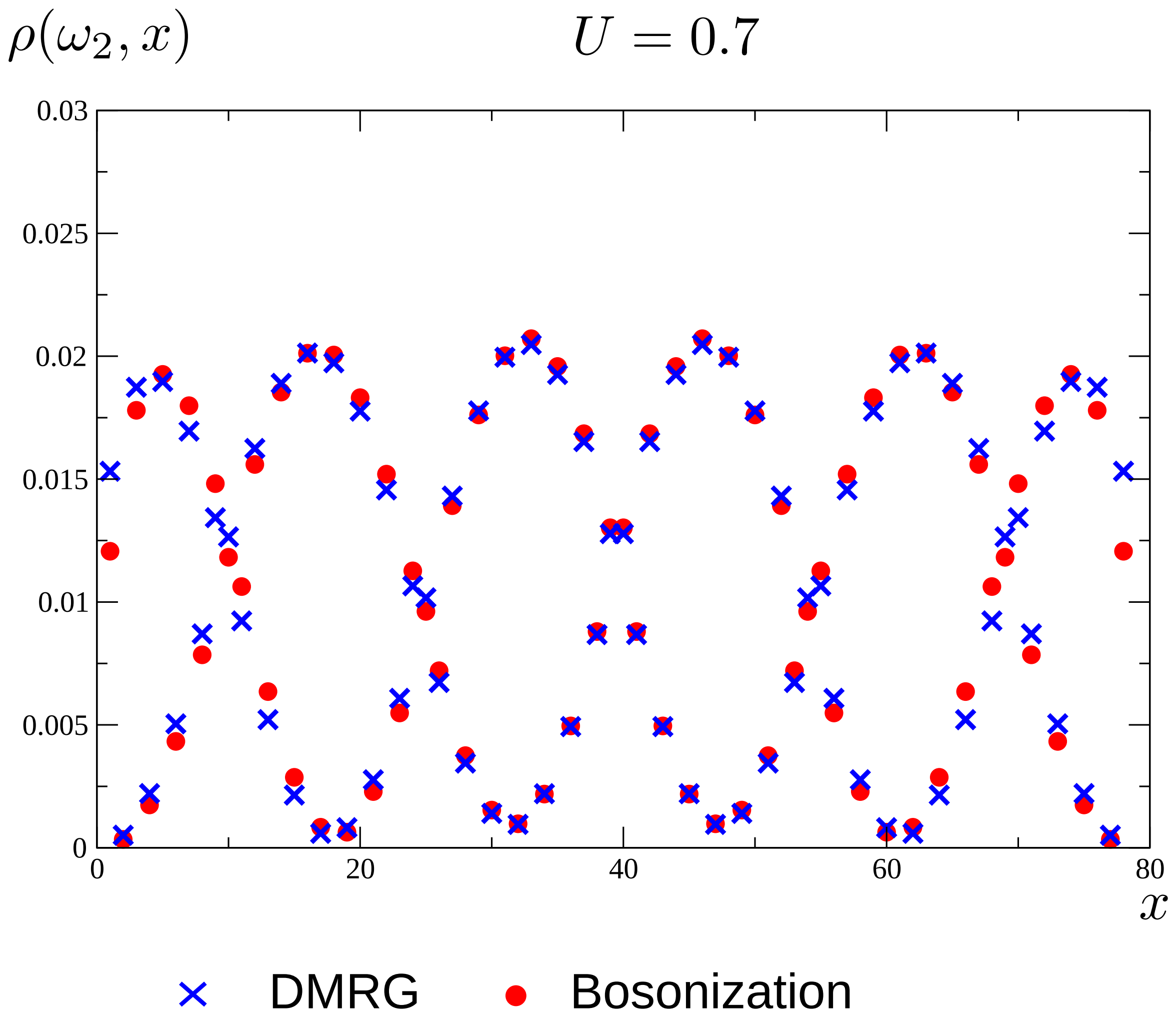
Local density of states: DMRG results

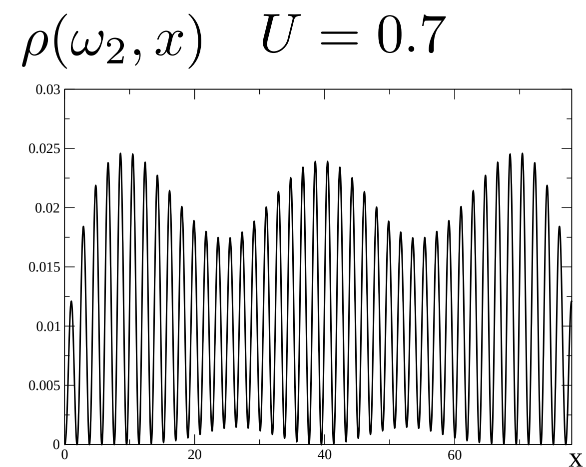




$$\rho(\omega_2, x) = |\langle a|\psi^\dagger(x)|0\rangle|^2 + |\langle b|\psi^\dagger(x)|0\rangle|^2$$

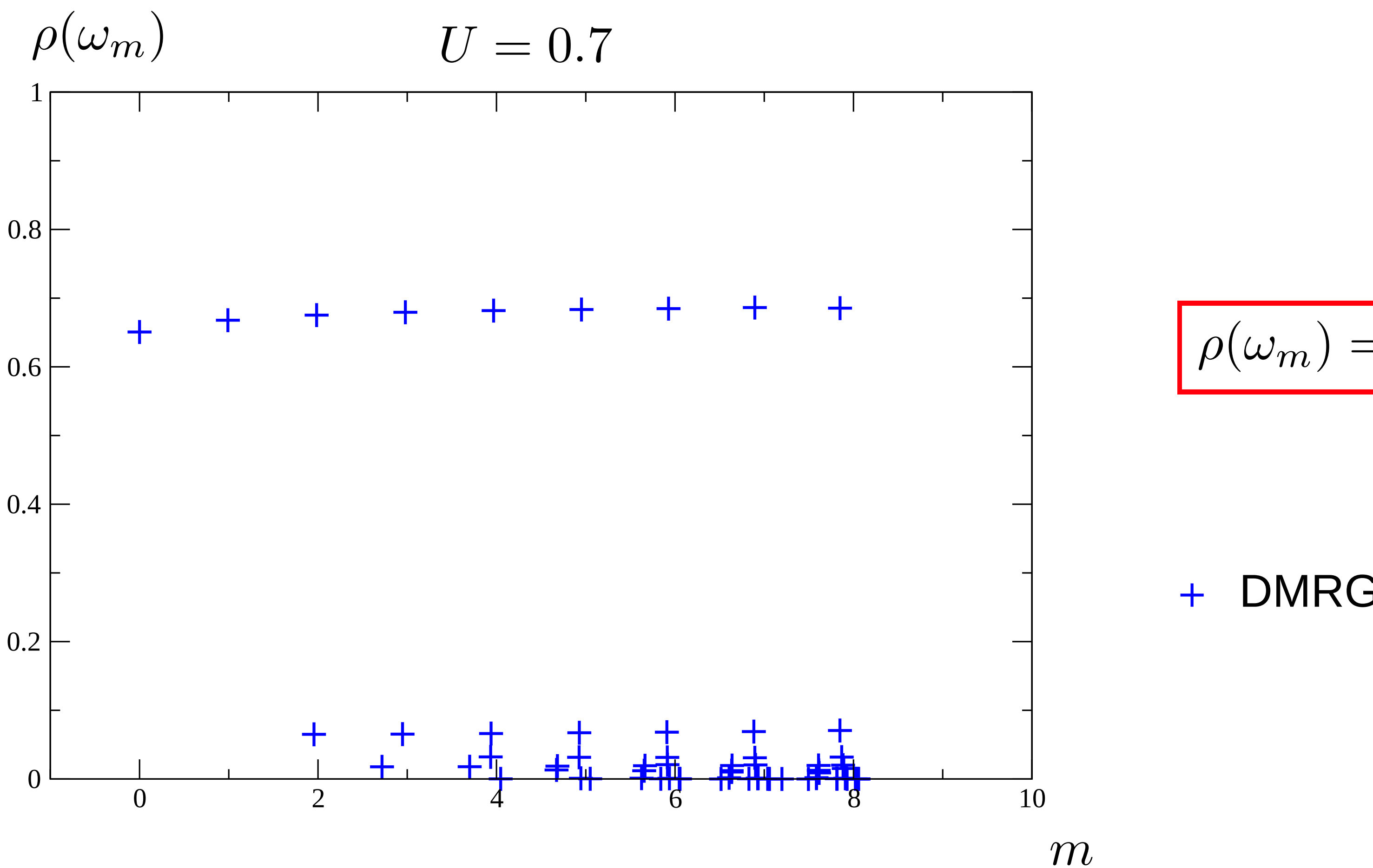
Local density of states: DMRG results





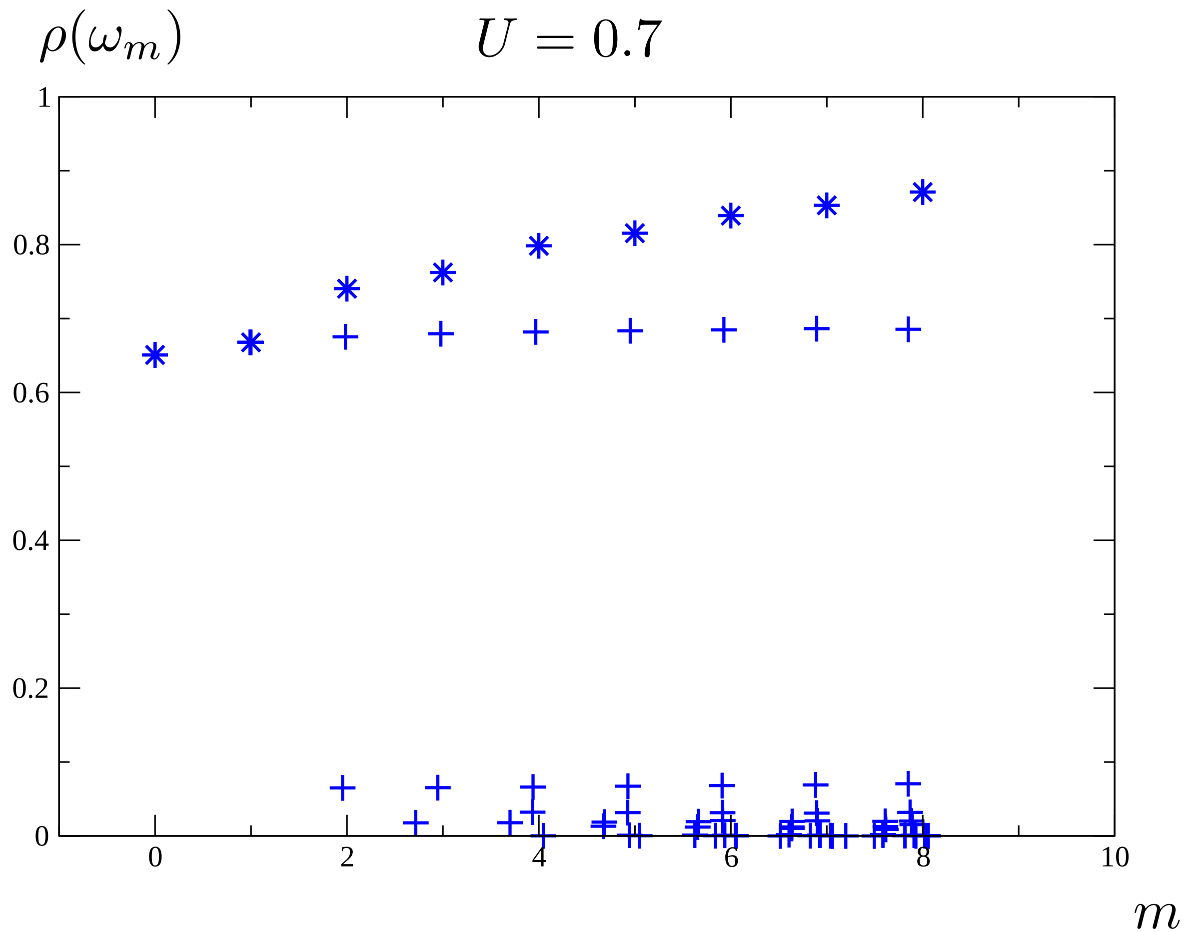
$$\rho(\omega_2, x) = |\langle a|\psi^\dagger(x)|0\rangle|^2 + |\langle b|\psi^\dagger(x)|0\rangle|^2$$

Density of states: position integrated



$$\rho(\omega_m) = \sum_x \rho(\omega_m, x)$$

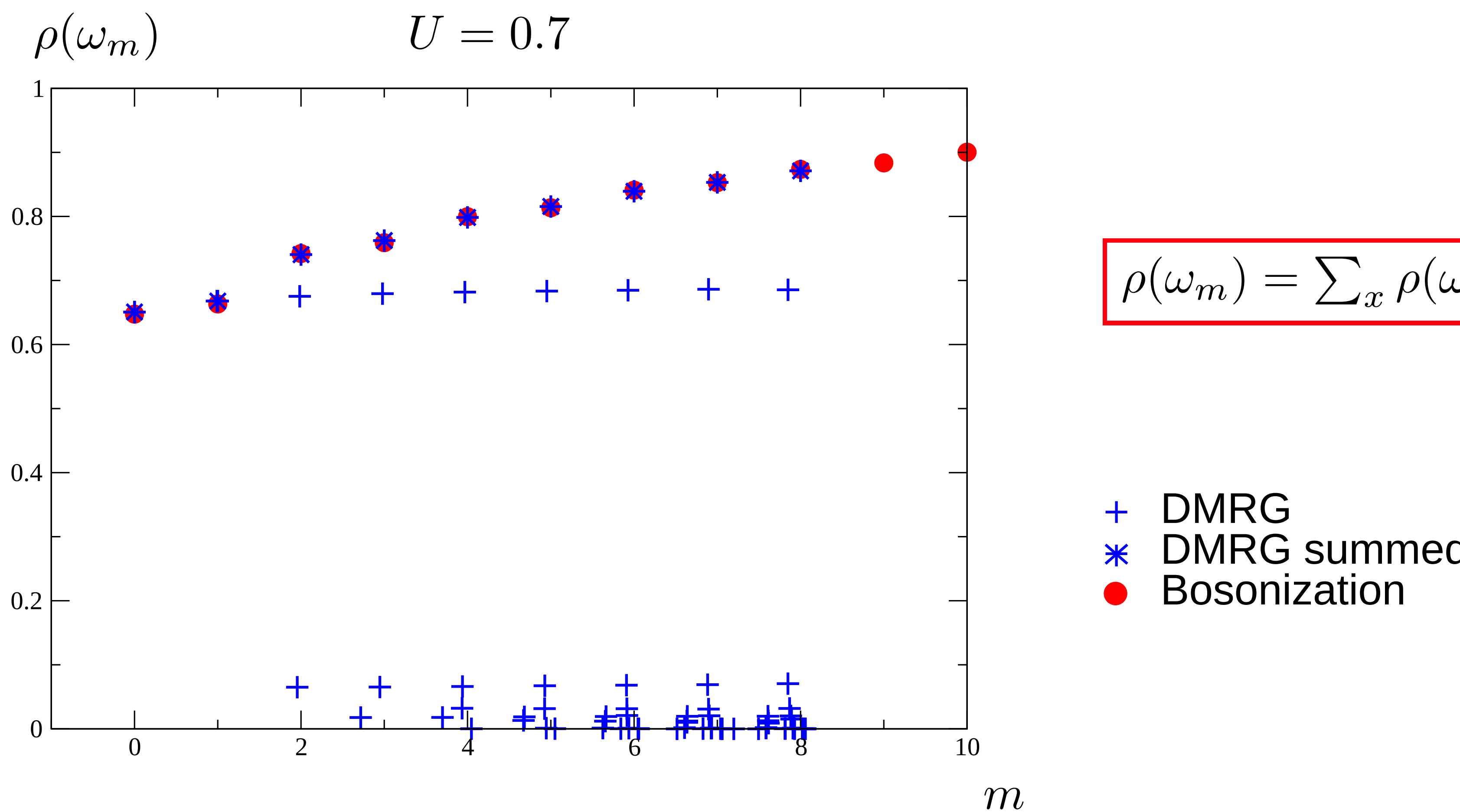
Density of states: position integrated



$$\rho(\omega_m) = \sum_x \rho(\omega_m, x)$$

+ DMRG
∗ DMRG summiert

Density of states: position integrated



$$\rho(\omega_m) = \sum_x \rho(\omega_m, x)$$

Recursive method for the density of states

- $\rho(\omega, x) = \frac{1}{2\pi} \int_{-\infty}^{\infty} e^{i\omega t} \langle \psi(x,t)\psi^\dagger(x,0)\rangle dt$
- Correlation functions in standard bosonization

$$\langle \psi_R(x,t)\psi_R^\dagger(x,0)\rangle = |c|^2 \exp\left(\sum_{\ell=1}^{\infty} \frac{1}{\ell} e^{-i\ell\Delta\omega t}\gamma_\ell(x)\right)$$

$$\psi_R^\dagger(x,t) := c(x) \exp\left[i\sum_{\ell=1}^{\infty} \frac{1}{\sqrt{\ell}} e^{i\ell\Delta\omega t} A_\ell^\dagger(x)\right] \exp\left[i\sum_{\ell=1}^{\infty} \frac{1}{\sqrt{\ell}} e^{-i\ell\Delta\omega t} A_\ell(x)\right]$$

$$\gamma_\ell(x) = [A_\ell(x), A_\ell^\dagger(x)], \; A_\ell(x) = \alpha(K)e^{ik_\ell x} b_\ell^R - \beta(K)e^{-ik_\ell x} b_\ell^L$$

- Finite systems

$$\frac{1}{2\pi}\int_{-\infty}^{\infty} dt\, e^{i\omega t} \langle \psi_R(x,t)\psi_R^\dagger(x,0)\rangle = \sum_m \rho_m\, \delta(w - m\Delta\omega)$$

$$\rho_m = \frac{1}{m}\left(\rho_{m-1}\gamma_1 + \rho_{m-2}\gamma_2 + \cdots + \rho_1\gamma_{m-1} + \rho_0\gamma_m\right) \quad \text{mit} \quad \rho_0 = |c|^2$$

Schneider and Eggert, Phys. Rev. Lett. 104 (2010)

earlier recursive approach: **Schönhammer and Meden, Phys. Rev. B 47 (1993)**

Spinless fermions with periodic b. c.

Density of states: $\rho_m = \frac{1}{m}(\rho_{m-1}\gamma_1 + \rho_{m-2}\gamma_2 + \cdots + \rho_1\gamma_{m-1} + \rho_0\gamma_m)$

- Commutator mode independent

$$\gamma = \frac{1}{2}\left(\frac{1}{K} + K\right)$$ Luttinger-parameter K

- Recursion formula exacty solvable

$$\rho_m = |c|^2 \frac{\Gamma(m+\gamma)}{\Gamma(\gamma)\Gamma(m+1)} \approx |c|^2 \frac{1}{\Gamma(\gamma)} m^{\gamma-1}$$ well known power law

- in general $\gamma_\ell(x)$ mode and x dependent

Spinful fermions with open b. c.

Luttinger liquid picture:

States described by integer spin and charge quantum numbers $\{m_s, m_c\}$

Energies: $\omega_{m_s,m_c} = (m_s v_s + m_c v_c)\frac{\pi}{L+1}$ with $v_s \leq v_c$

Density of states:

$$\rho_{m_s,m_c}(x) \quad = \quad |c_x|^2 \left[\rho^{uni}_{s,m_s}(x)\rho^{uni}_{c,m_c}(x) - \cos(2k_F x)\rho^{osc}_{s,m_s}(x)\rho^{osc}_{c,m_c}(x)\right]$$

Calculate recursively, e.g. :

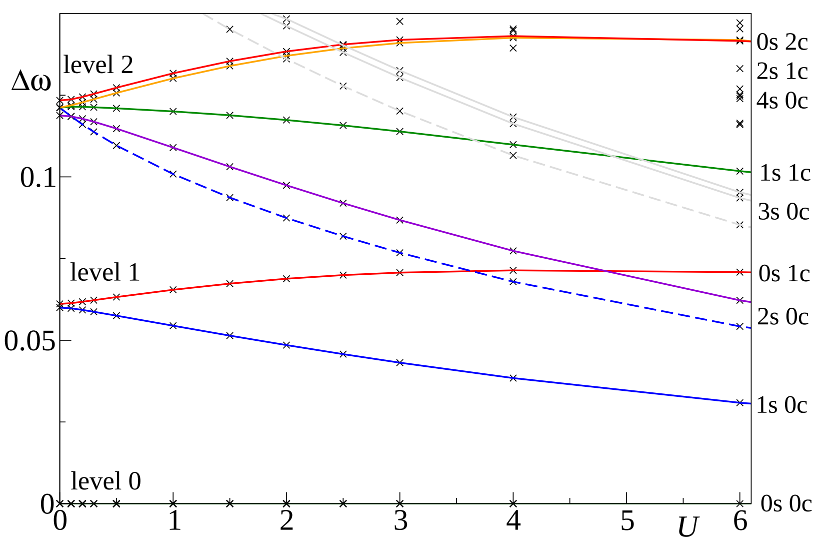
$$\rho^{uni}_{c,m_c}(x) = \frac{1}{m_c}\sum_{\ell=1}^{m_c}\rho^{uni}_{c,m_c-\ell}(x)\gamma^{uni}_{c,\ell}(x)$$

$$\gamma^{uni}_{c,\ell}(x) = (1/K_c + K_c)/4 + (1/K_c - K_c)\,\cos(2k_\ell x)$$

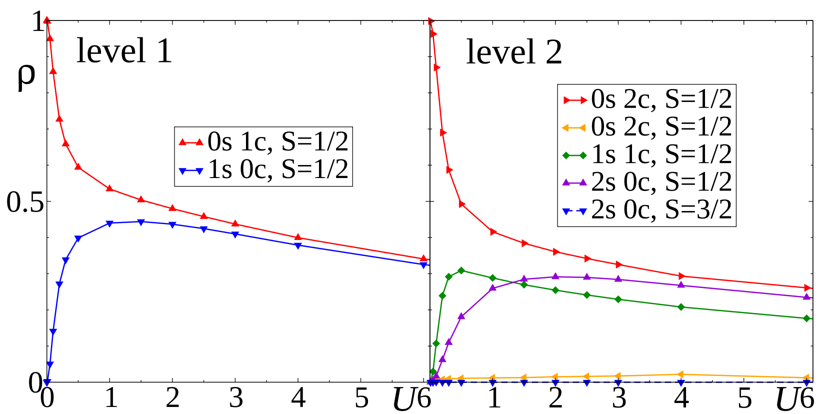
Comparison to DMRG results (1/3)

Hubbard model: $H = -t \sum_{\sigma,\, x=1}^{L-1} \left(\psi^\dagger_{\sigma,x}\psi_{\sigma,x+1} + \text{h.c.}\right) + U \sum_{x=1}^{L} n_{\uparrow,x} n_{\downarrow,x}$

Energies $\Delta\omega$



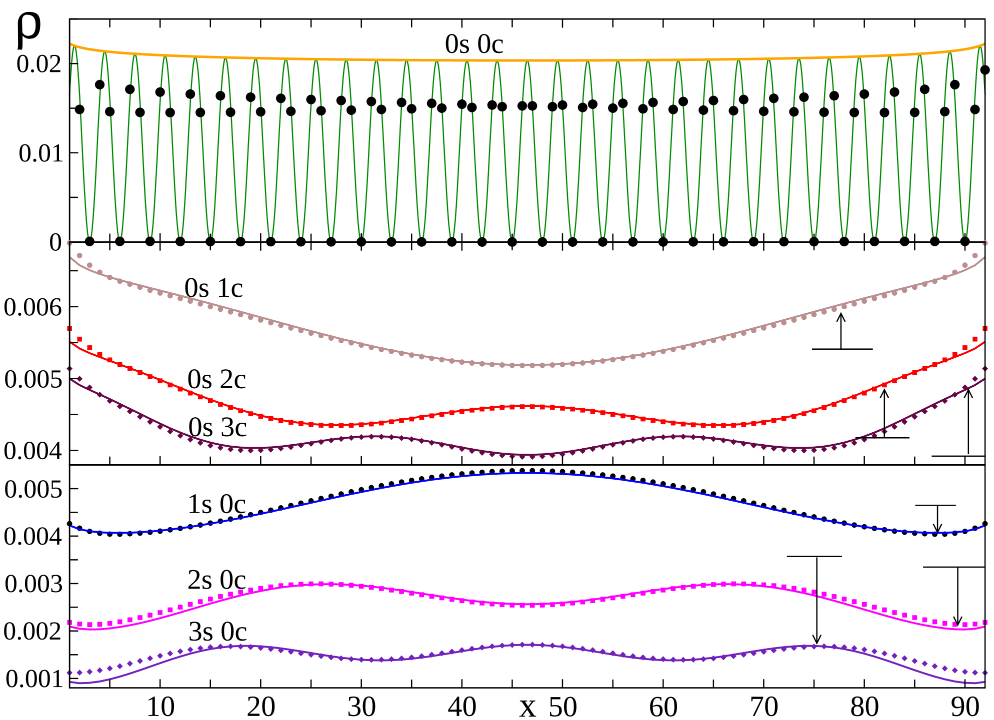
Total density of states



Parameter: $N_\uparrow = N_\downarrow + 1 = 31$ and $L = 90$

Comparison to DMRG results (2/3)

Local density of states:



$$N_\uparrow = N_\downarrow + 1 = 31$$
$$L = 92$$
$$U = 1$$

Lines: predictions for $K_c = 0.9081$ and $K_s = 1.16$ adjusted by shifts

Local density of states *increases* near boundary

Comparison to DMRG results (3/3)

Local density of states does *not* fit predictions by theory:

- Theory curves must be shifted down for charge and up for spin modes (competition of energy scales: band curvature vs interaction
- Luttinger parameter K_s must be chosen considerably larger than unity $\rightarrow$ attractive behavior in the spin

  Boundary exponent $\alpha_B = (1/K_s + 1/K_c)/2 - 1$ may become negative

  Similar observations: **Schuricht, Andergassen, and Meden preprint arXiv:1111.7174,**

  Andergassen, Enss, Meden, Metzner, Schollwöck, and Schönhammer, Phys. Rev. B 73 (2006),

  Meden, Metzner, Schollwöck, Schneider, Stauber, and Schönhammer, Eur. Phys. J. B 16 (2000),

  Schönhammer, Meden, Metzner, Schollwöck, and Gunnarsson, Phys. Rev. B 61, (2000)

- Multiplicative corrections to $G^r(x,t)$ due to marginal irrelevant operator?

Summary

- Local density of states for individual energy levels by DMRG
- Recursive formula: simple calculation of the density of states
- Numerical results in agreement with bosonization for spinless fermions
- Large deviations for the Hubbard model
  $\rightarrow$ effective negative boundary exponent