Monte Carlo simulations of quantum systems with global updates

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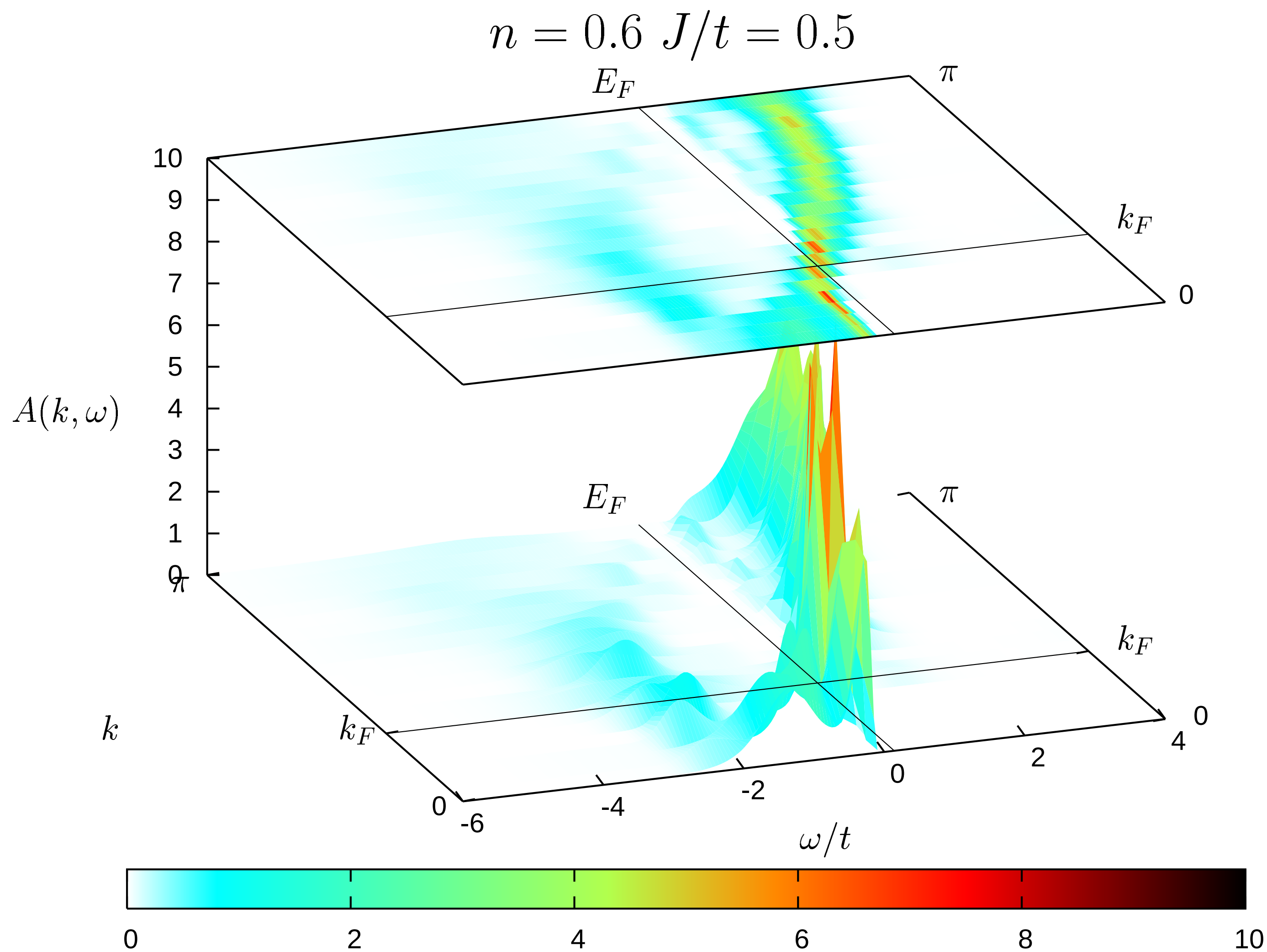
Institut für Theoretische Physik III
Universität Stuttgart

Spinons, holons, and antiholons in one dimension



5.1 The t-J model in one dimension

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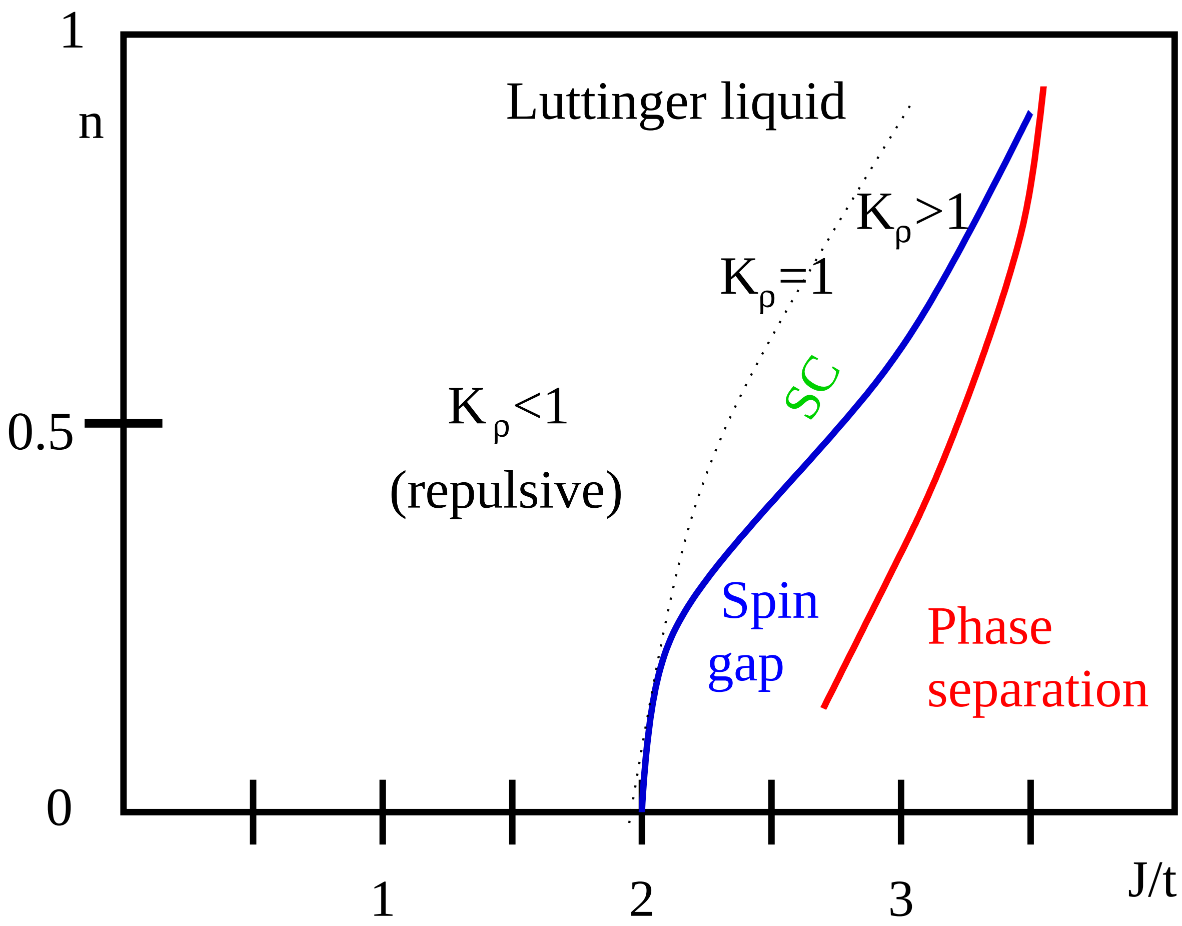
M. Ogata, M.U. Luchini, S. Sorella, and F.F. Assaad, Phys. Rev. Lett. **66**, 2388 (1991)



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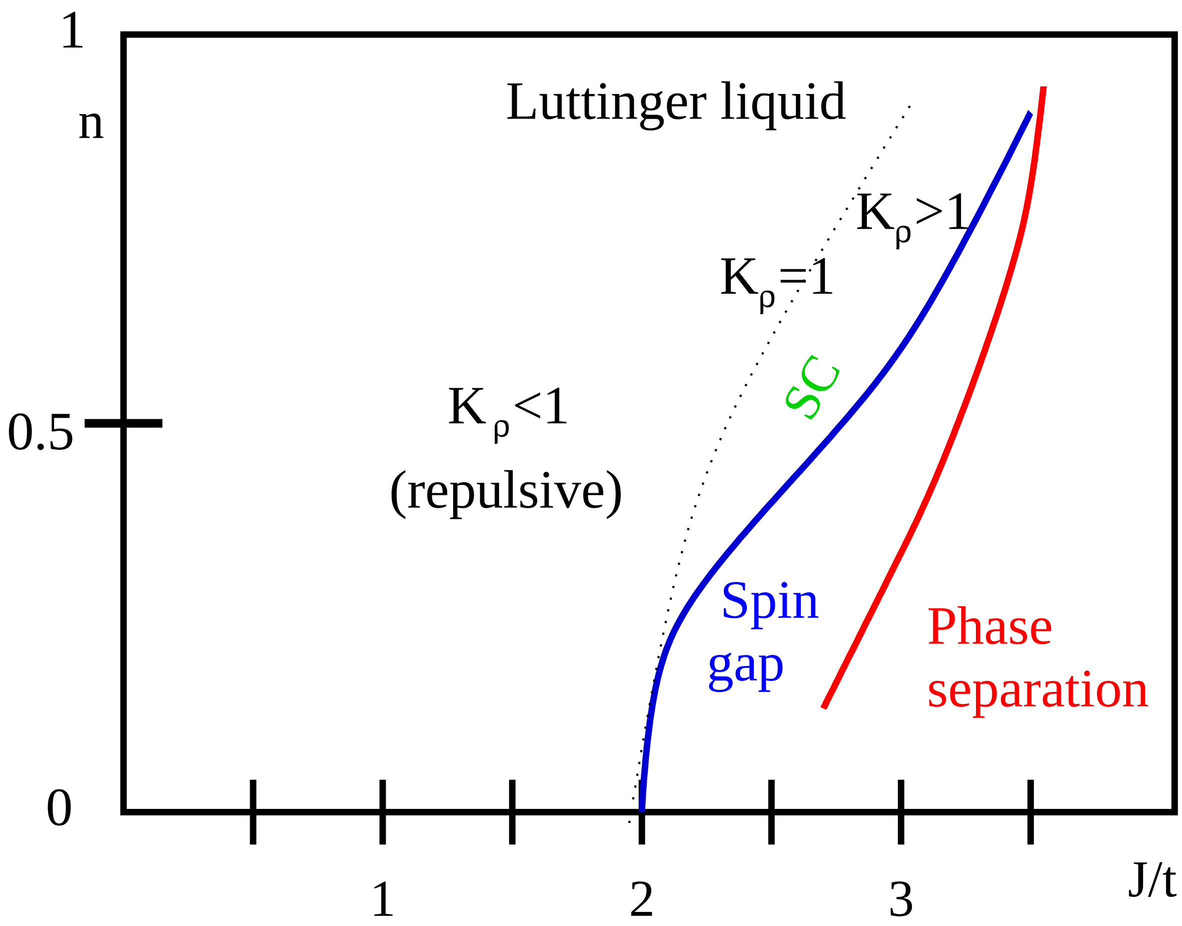

Phase diagram, with phases similar to those in high T_C superconductors

Exact results for the nearest neighbor t-J model

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- **At $J = 0$**
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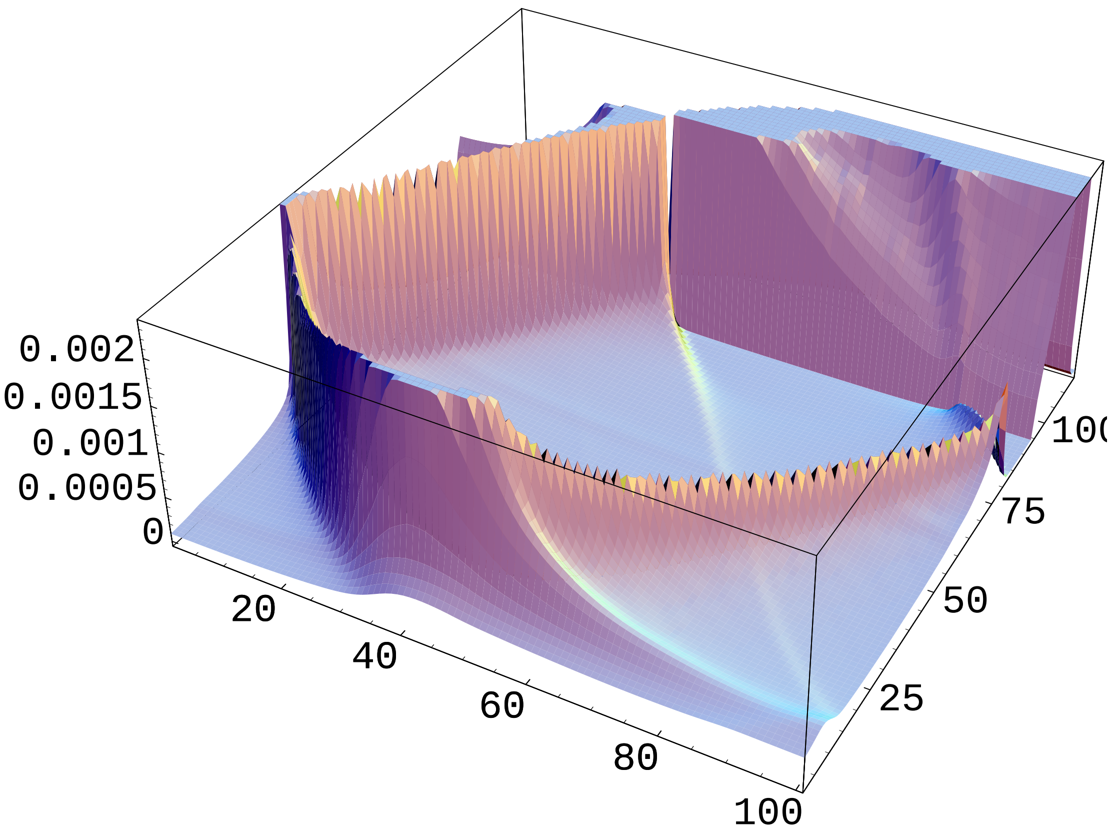

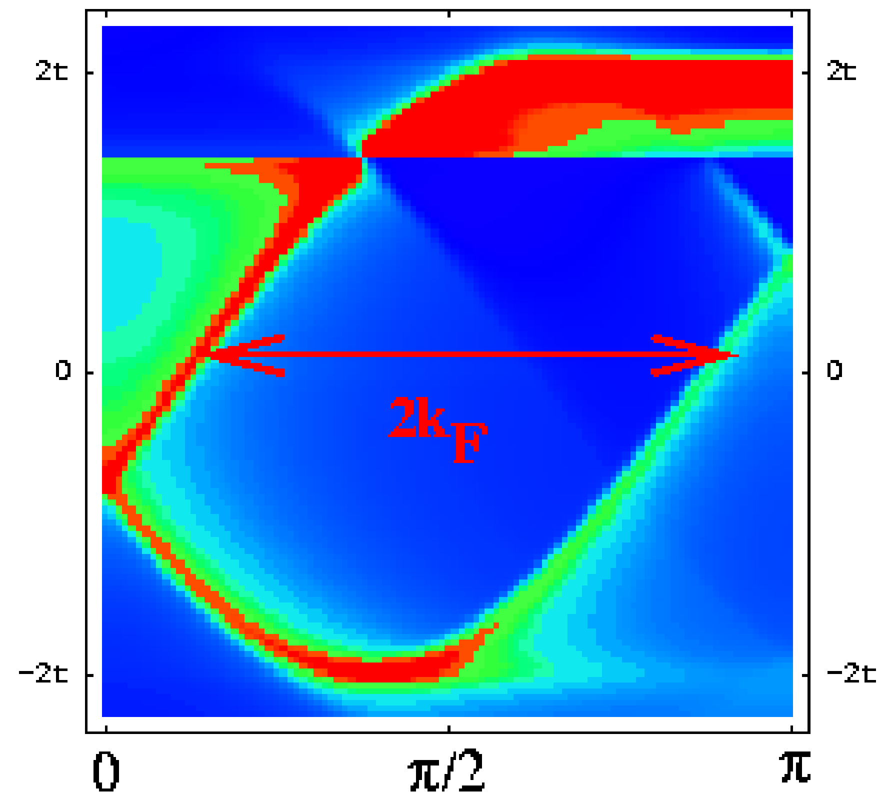

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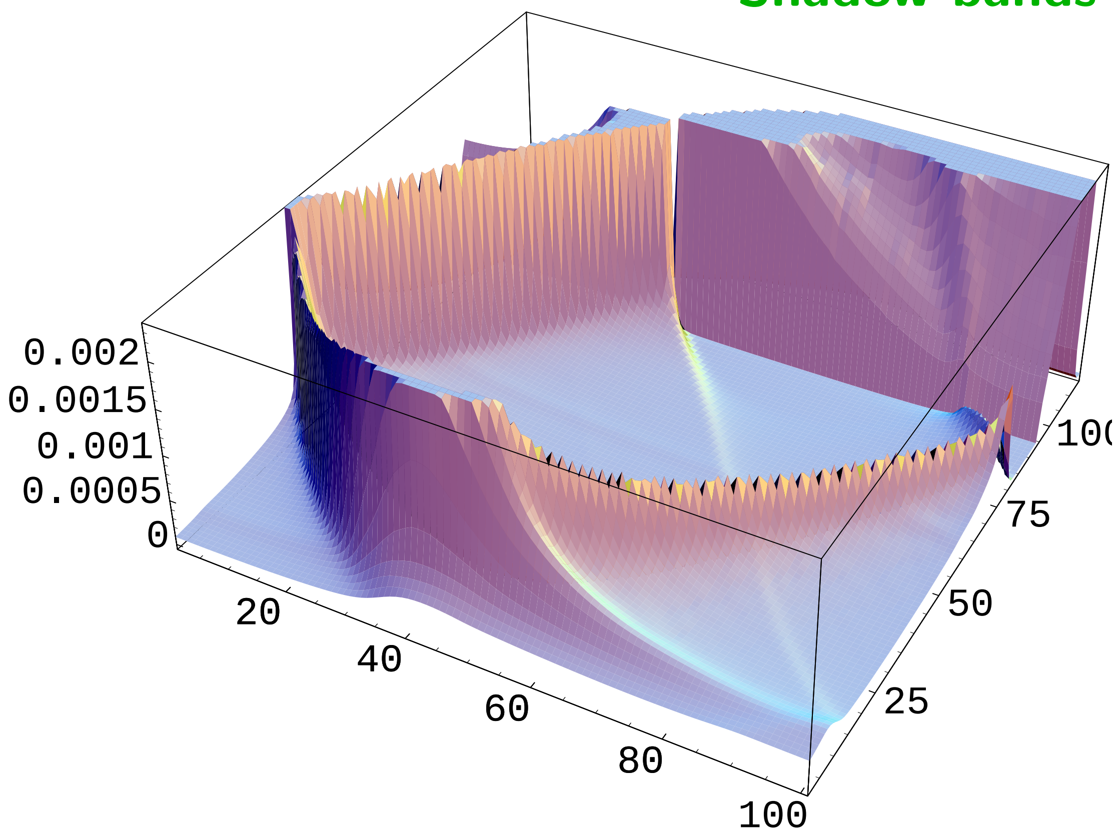

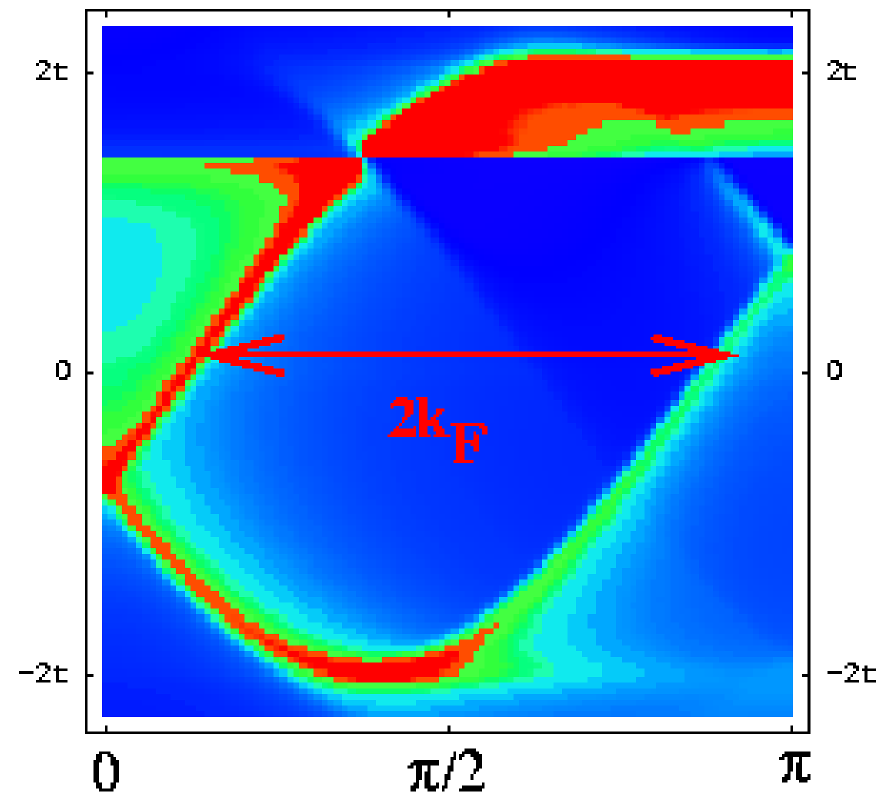

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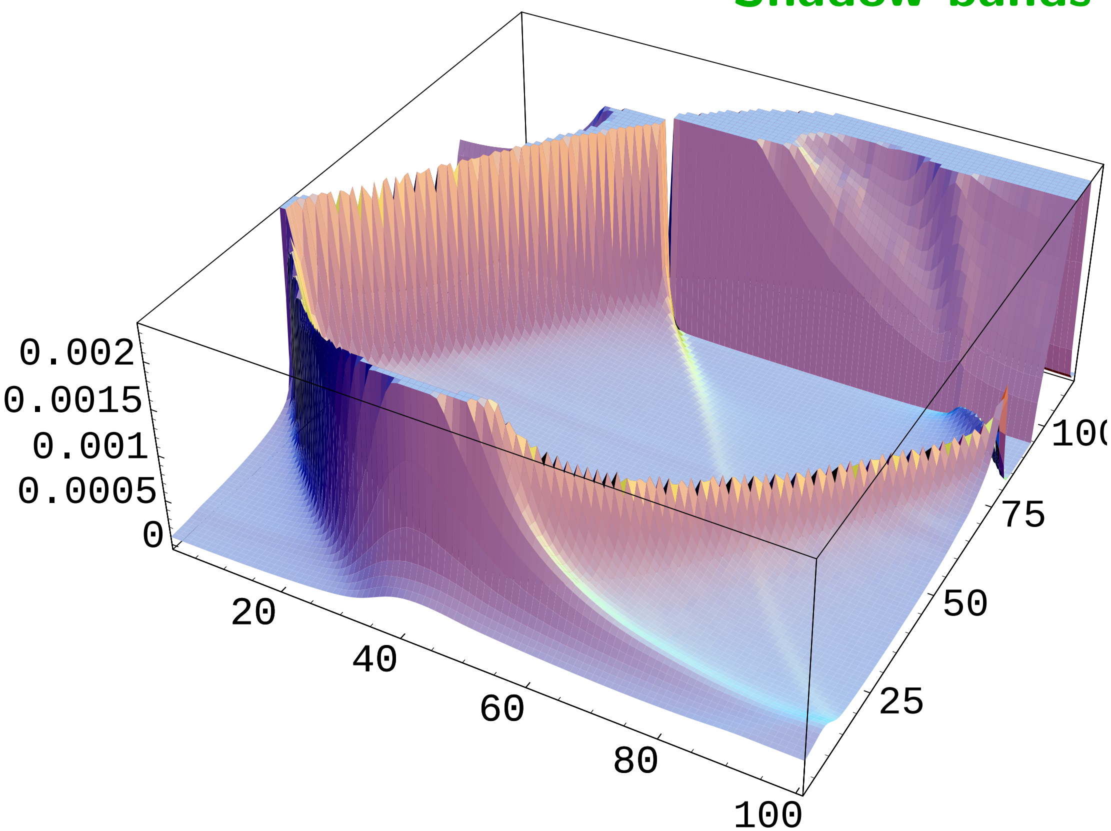

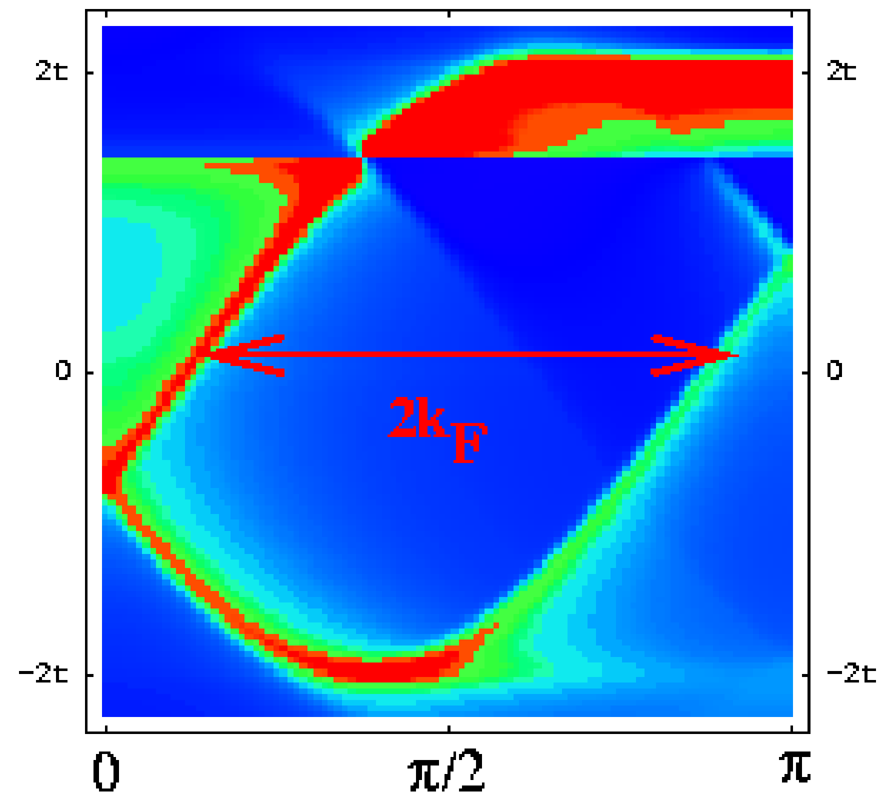

- **At J = 2t**
  Bethe-Ansatz solution
  P.A. Bares and G. Blatter, Phys. Rev. Lett. **64**, 2567 (1990)
  No correlations functions

5.2 The $1/r^2$ (inverse square) t-J model in one dimension

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$$H_{IS-t-J} \;=\; -\sum_{i<j,\sigma} t_{ij}(\tilde{c}^{\dagger}_{i,\sigma}\tilde{c}_{j,\sigma} + \mathrm{h.c.}) + \sum_{i<j} J_{ij}\left(\boldsymbol{S}_i \cdot \boldsymbol{S}_j - \frac{1}{4}\tilde{n}_i\tilde{n}_j\right) \;,$$

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Compact support and excitation content

Z.N.C. Ha and F.D.M. Haldane, Phys. Rev. Lett. **73**, 2887 (1994)

spinon	**Q=0,**	**S=1/2**	**semion**
holon	**Q=+e,**	**S=0**	**semion**
antiholon	**Q=–2e,**	**S=0**	**boson**

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Semion $\longrightarrow s_j s_\ell = i s_\ell s_j \longrightarrow$ **'half a fermion'**

Spectral function for electron addition

M. Arikawa, Y. Saiga, and Y. Kuramoto, Phys. Rev. Lett. **86**, 3096 (2001)

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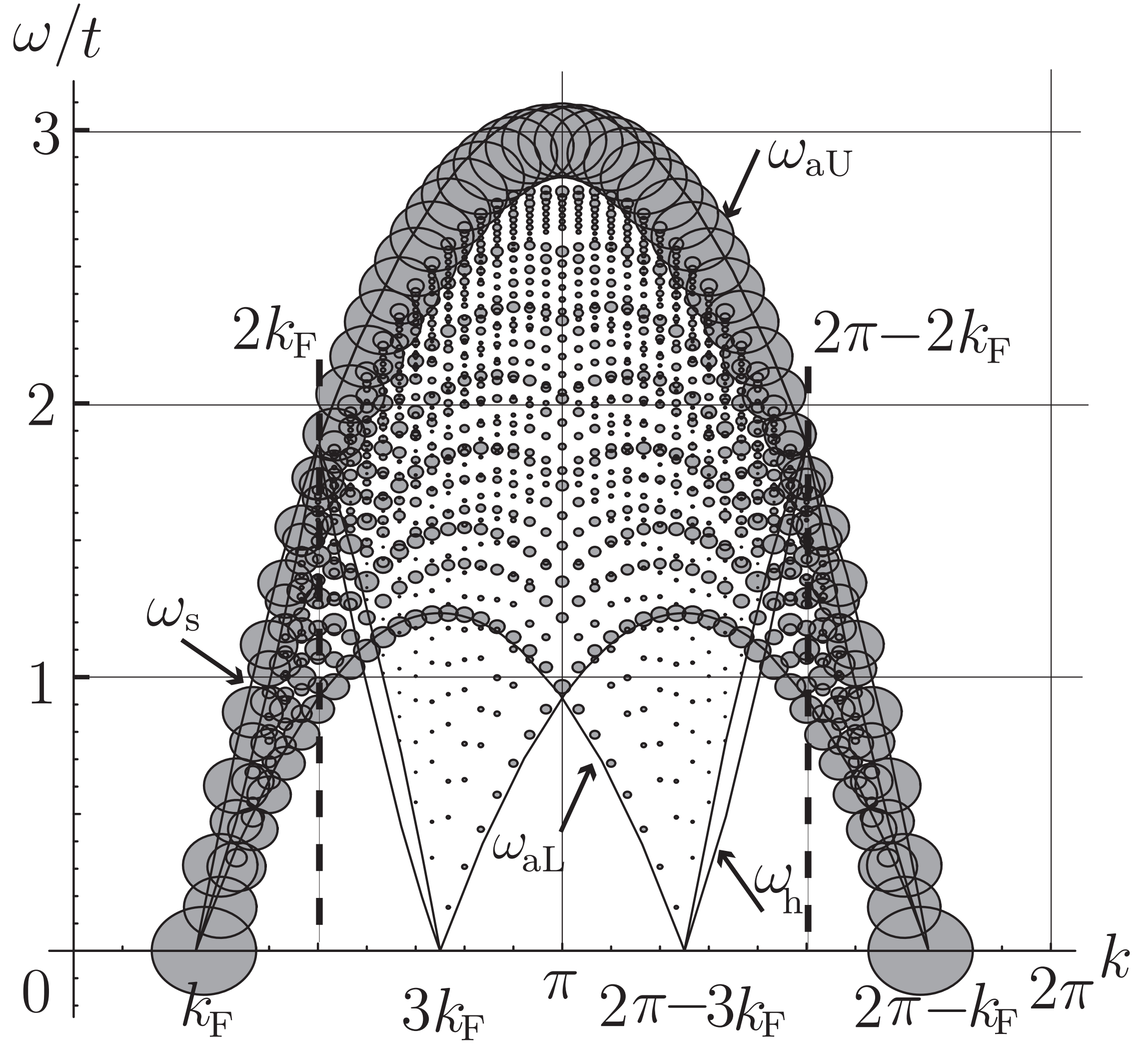

Analytic expressions

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Spectral function for electron addition $(0 \leq k < 2\pi)$

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$$A^+(k,\omega) = A_R(k,\omega) + A_L(k,\omega) + A_U(k,\omega)$$

where

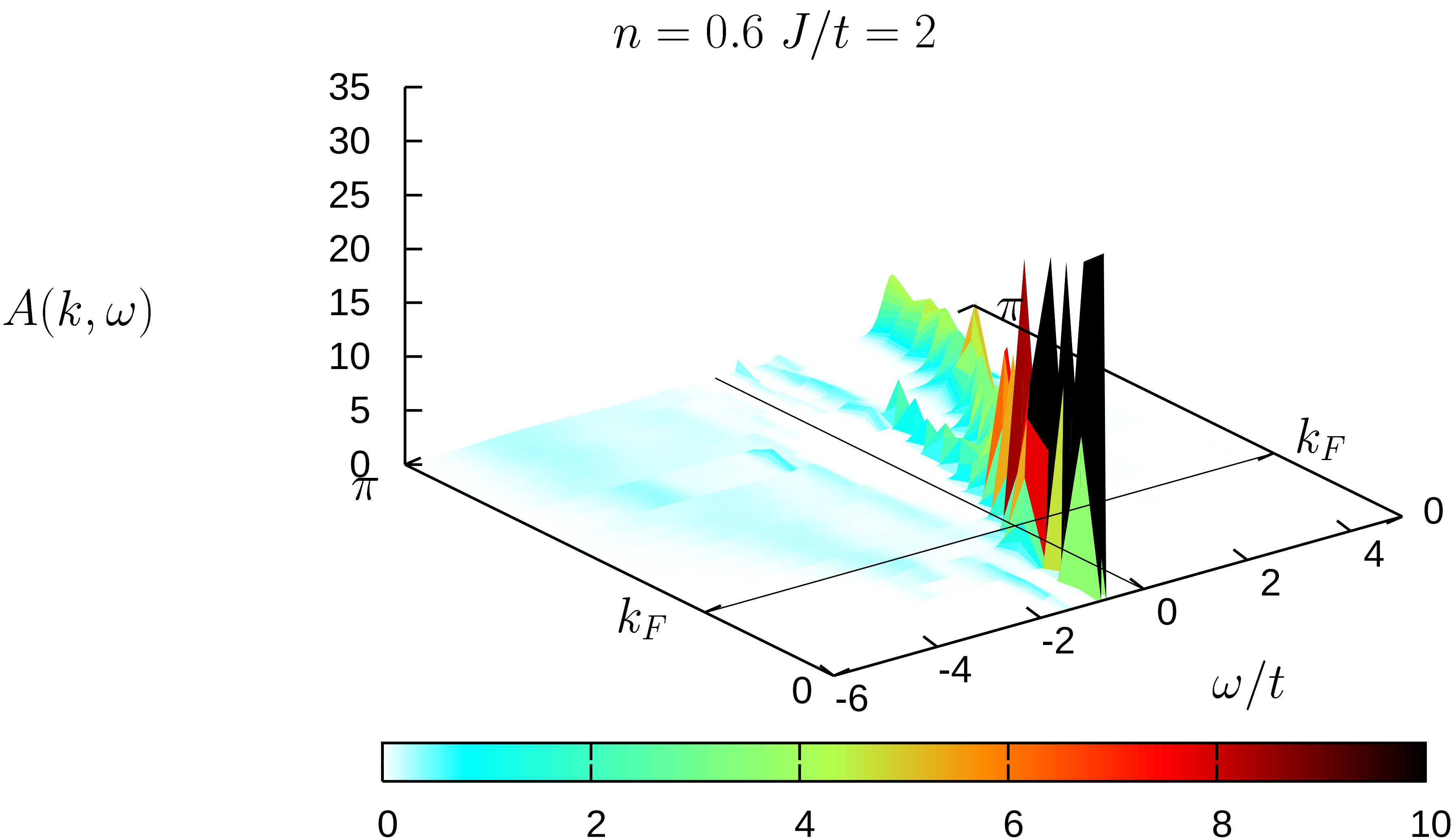
$$\begin{aligned} A_R(k,\omega) &= \frac{1}{4\pi}\int_0^{k_F} dq_h \int_0^{k_F-q_h} dq_s \int_0^{2\pi-4k_F} dq_a\, \delta\left(k-k_F-q_s-q_h-q_a\right) \\ &\times\delta\left[\omega-\epsilon_s(q_s)-\epsilon_h(q_h)-\epsilon_a(q_a)\right] \frac{\epsilon_s^{g_s-1}(q_s)\,\epsilon_h^{g_h-1}(q_h)\,\epsilon_a^{g_a-1}(q_a)}{\left(q_h+q_a/2\right)^2}\,, \end{aligned}$$

with $A_L(k,\omega) = A_R(2\pi-k,\omega)$
$g_s = 1/2$, $g_h = 1/2$, **and** $g_a = 2$, **statistical parameters, and**

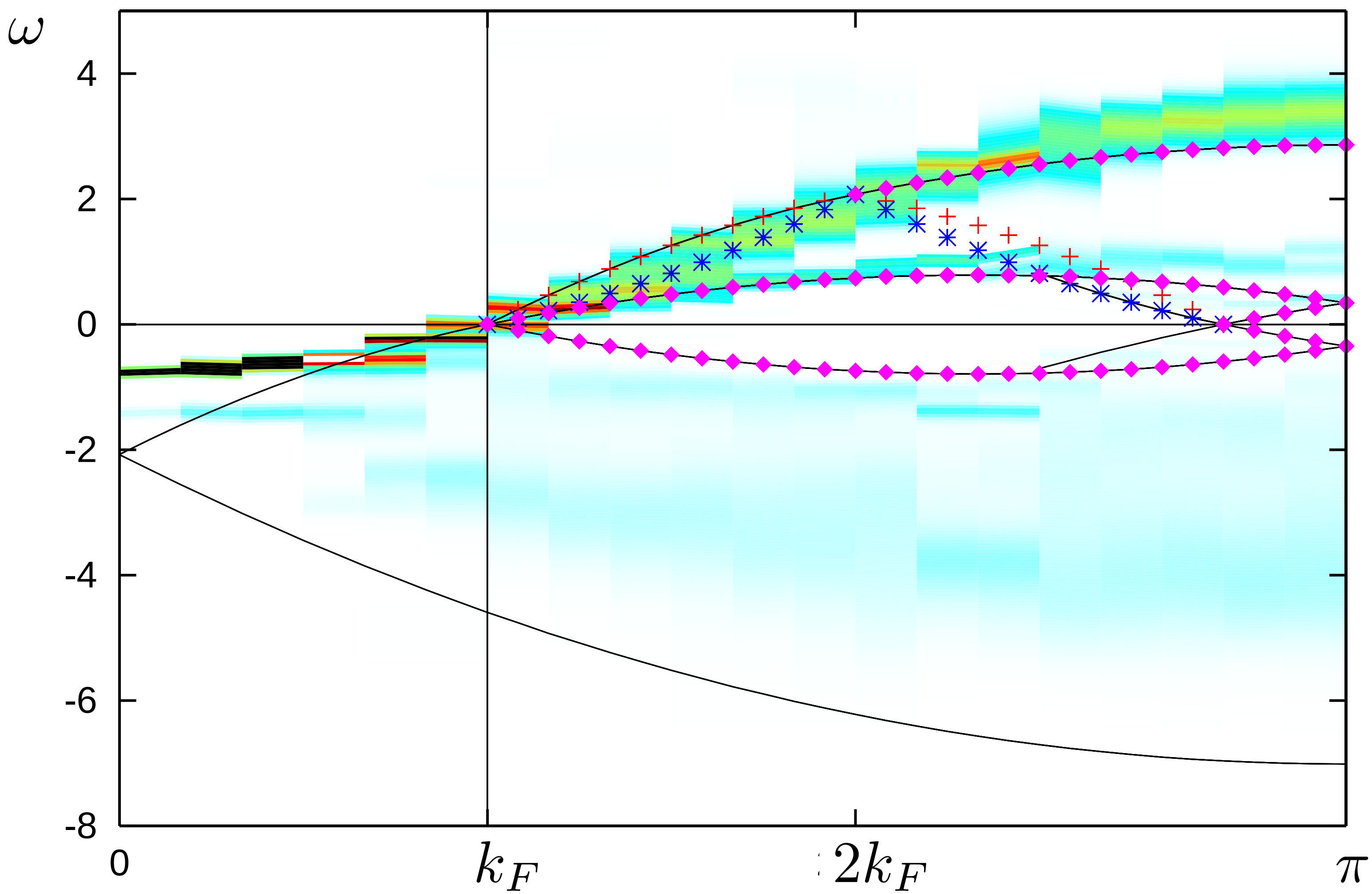
$$A_U(k,\omega) = \sqrt{\frac{\epsilon_a(k-2k_F)}{k(\pi-k/2)}}\,\delta\Big\{\omega-\left[\epsilon_s(k_F)+\epsilon_a(k-2k_F)\right]\Big\}\,, \quad (2k_F \leq k \leq 2\pi-2k_F)$$

5.3 Spectral functions for the n.n. t-J model from QMC

C. Lavalle, M. Arikawa, S. Capponi, F.F. Assaad, and A. Muramatsu, PRL **90**, 216401, (2003)



Spinon, holons, and antiholons in the n.n. t-J model at J=2t



$+$ **spinon:** $\epsilon_{sR(L)}(q_s) = tq_s\left(\pm v_s^0 - q_s\right) \quad 0 \leq q_s \leq k_F$

$*$ **holon:** $\epsilon_{hR(L)}(q_h) = tq_h\left(q_h \pm v_c^0\right) \quad 0 \leq q_h \leq k_F$

◆ **antiholon:** $\epsilon_{\bar{h}}(q_{\bar{h}}) = tq_{\bar{h}}(2v_c^0 - q_{\bar{h}})/2 \quad 0 \leq q_{\bar{h}} \leq 2\pi - 4k_F$

$v_s^0 = \pi$, $v_c^0 = \pi(1-n)$

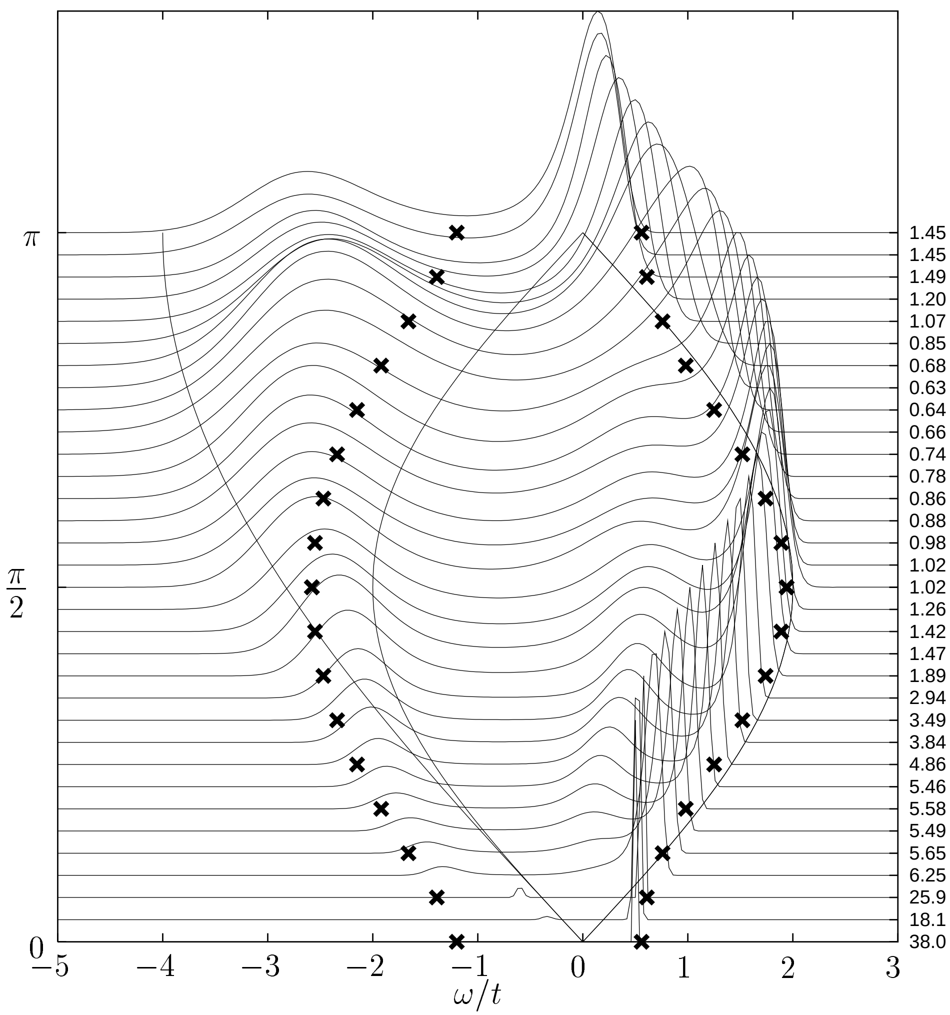
Excitation content of the hole spectrum at the supersymmetric point

M. Brunner, F.F. Assaad, and A. Muramatsu, Eur. Phys. J. B **16**, 209 (2000)

Supersymmetric point J/t = 2 ⟶ **exact holon and spinon dispersions from Bethe-Ansatz**

P.-A. Bares and G. Blatter, Phys. Rev. Lett. **64**, 2567 (1990)

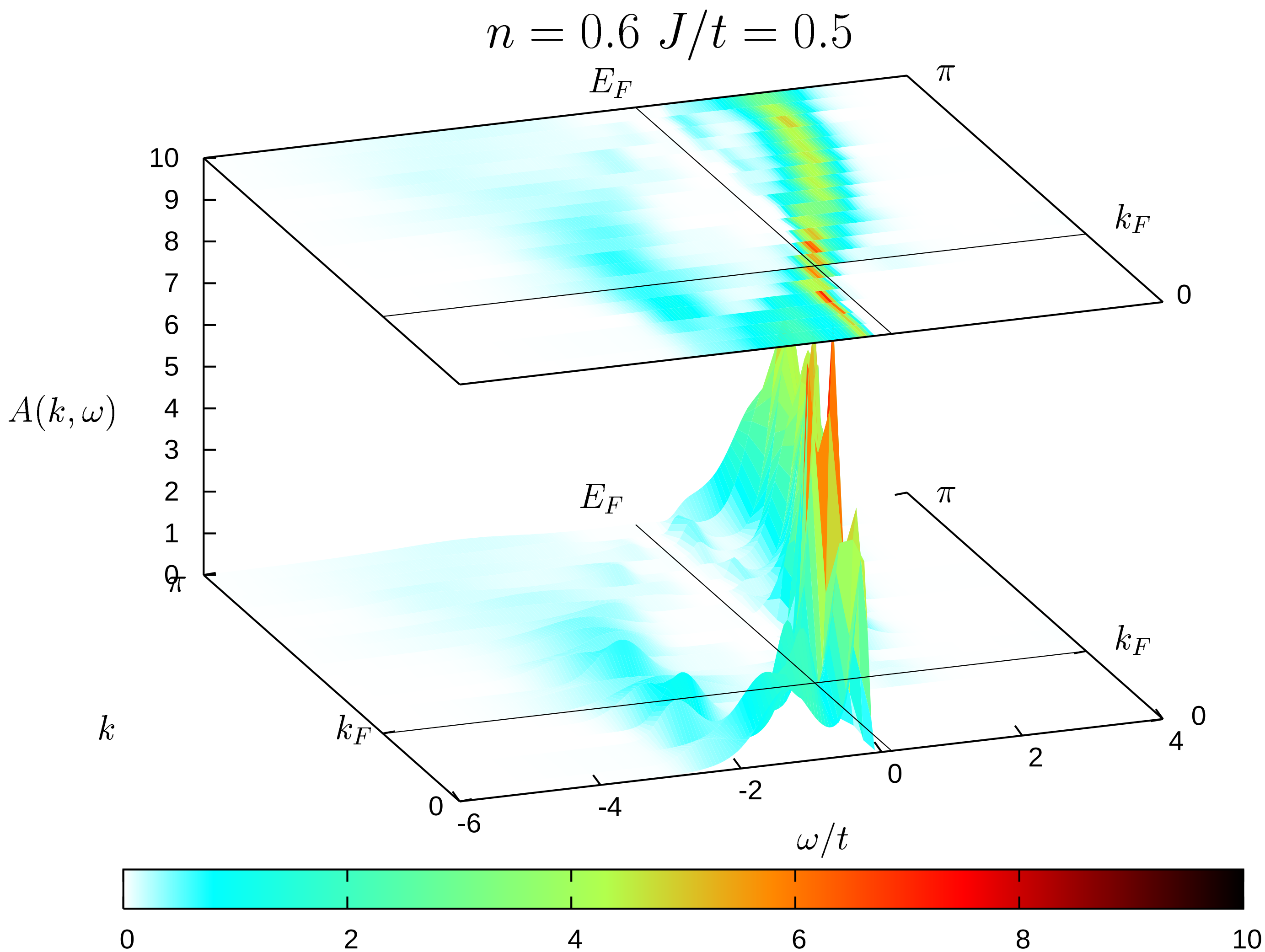
P.-A. Bares, G. Blatter, and M. Ogata, Phys. Rev. B **44**, 130 (1991)



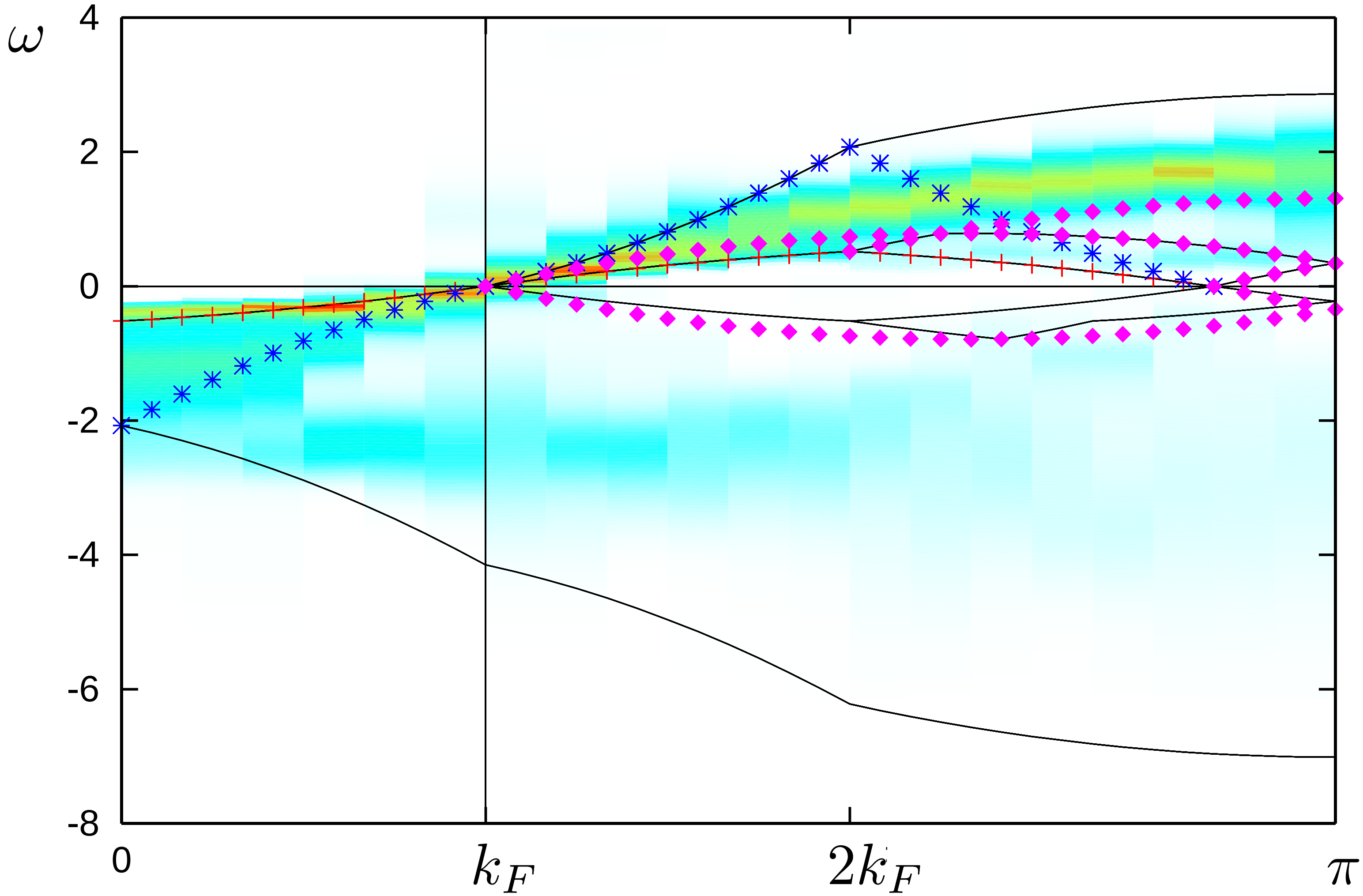
Full line: One holon + one spinon with dispersions given by charge-spin separation Ansatz.

Crosses: One holon + one spinon with. dispersions given by Bethe-Ansatz

Spectral function at J = 0.5 t



Spinon, holons, and antiholons at J = 0.5 t and n = 0.6



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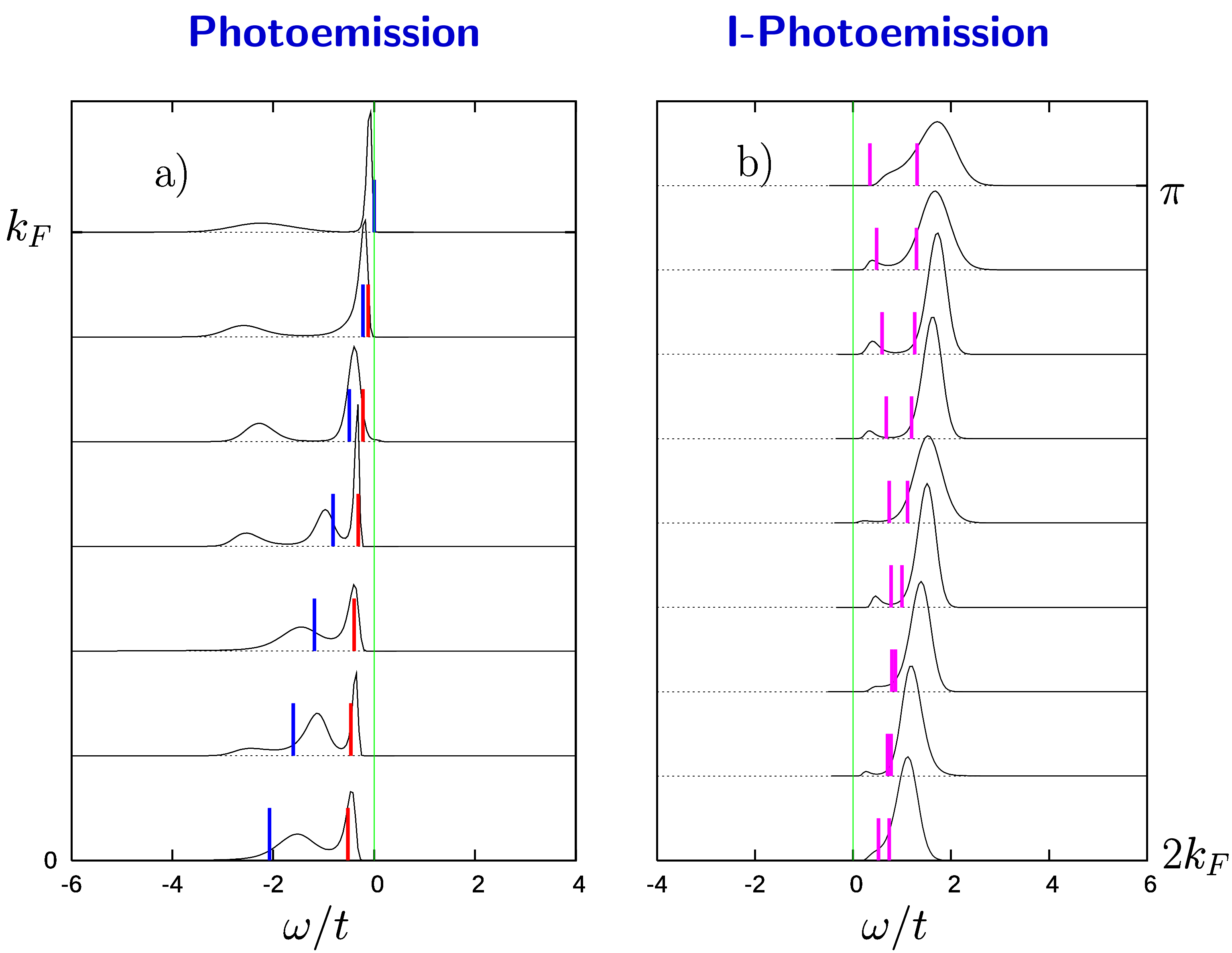
$v_s^0 = \pi$, $v_c^0 = \pi(1-n)$

Charge-spin separation at J = 0.5 t



Antiholons at $J = 0.5\ t$ vs. doping

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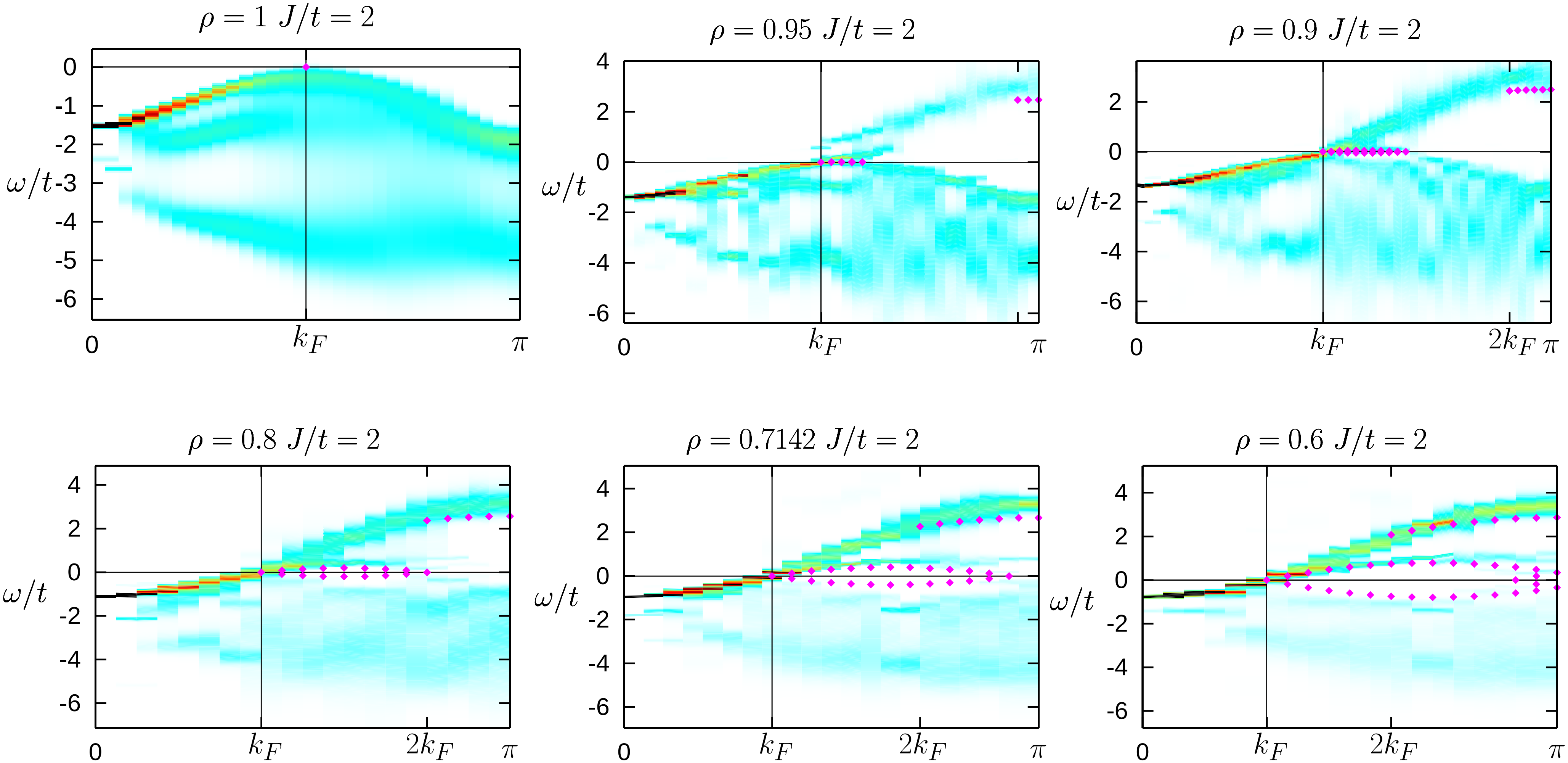

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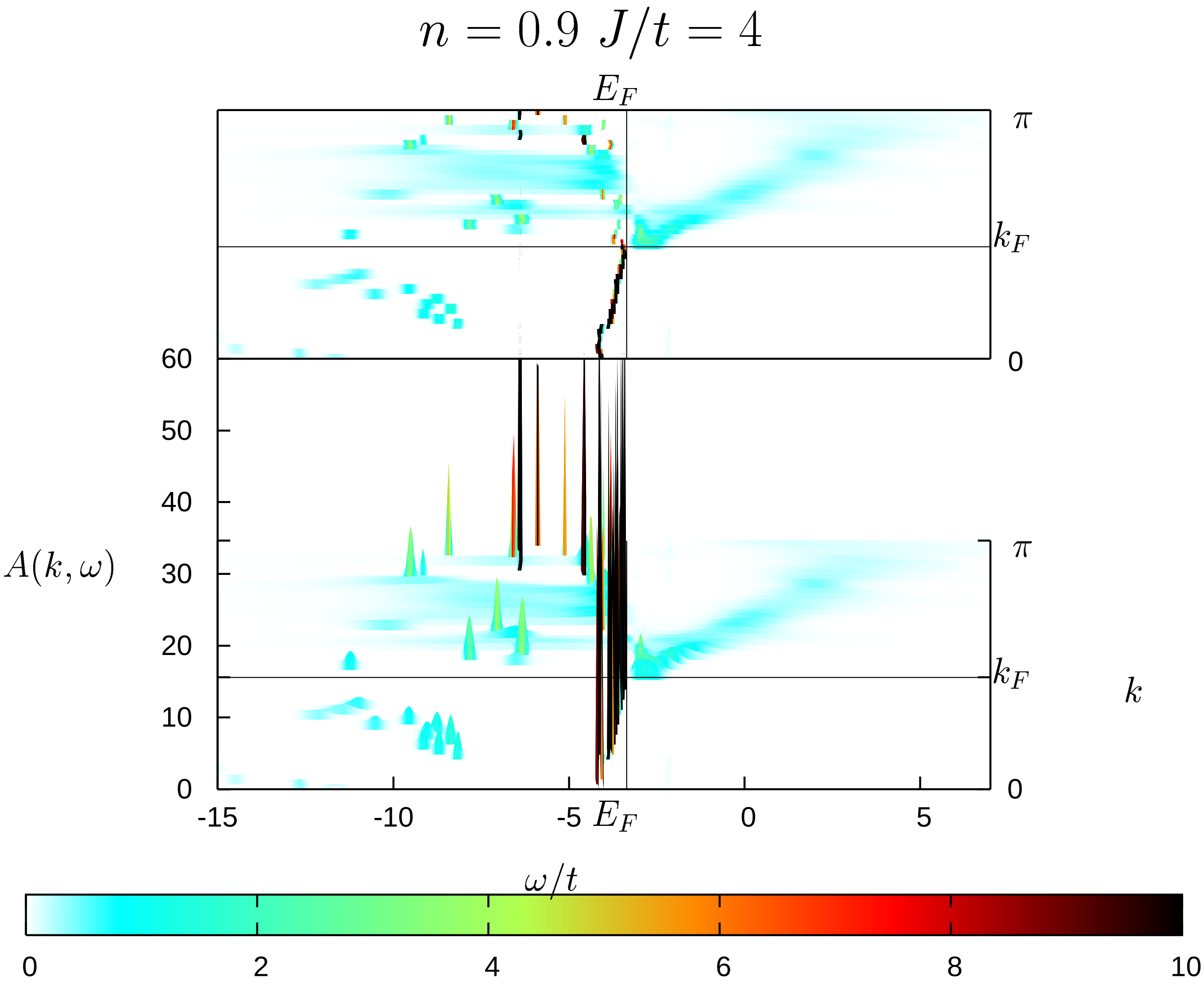
- **Can they help to understand D = 2?**

Photoemission and inverse photoemission with phase separation



Discontinuous spectrum on the photoemission side

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  $\longrightarrow$ **spin-gap and phase separation**

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- Extension to finite temperature

New representation and the minus-sign problem

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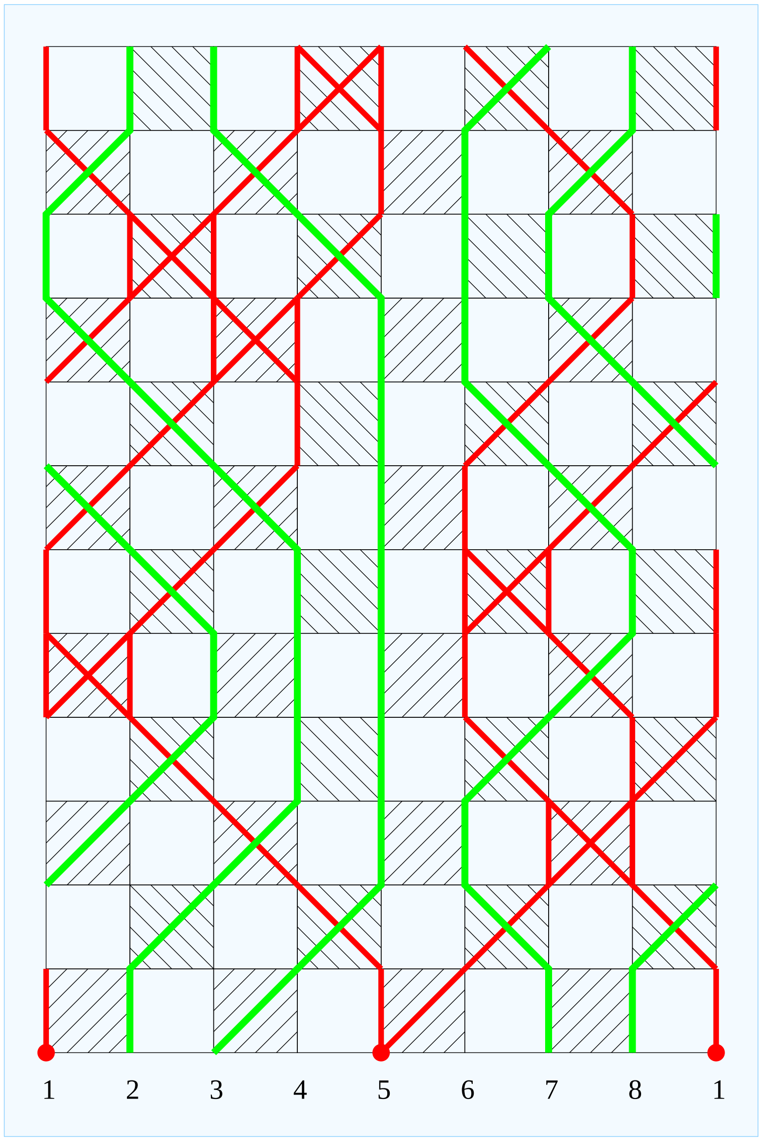

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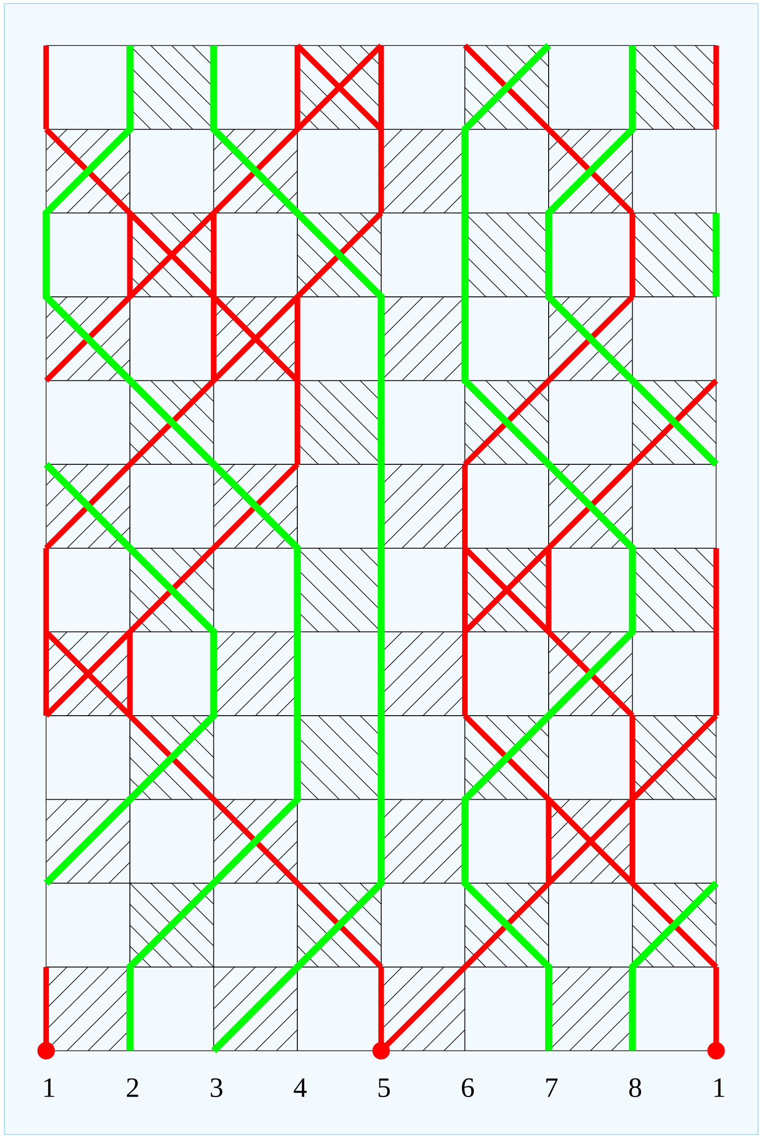

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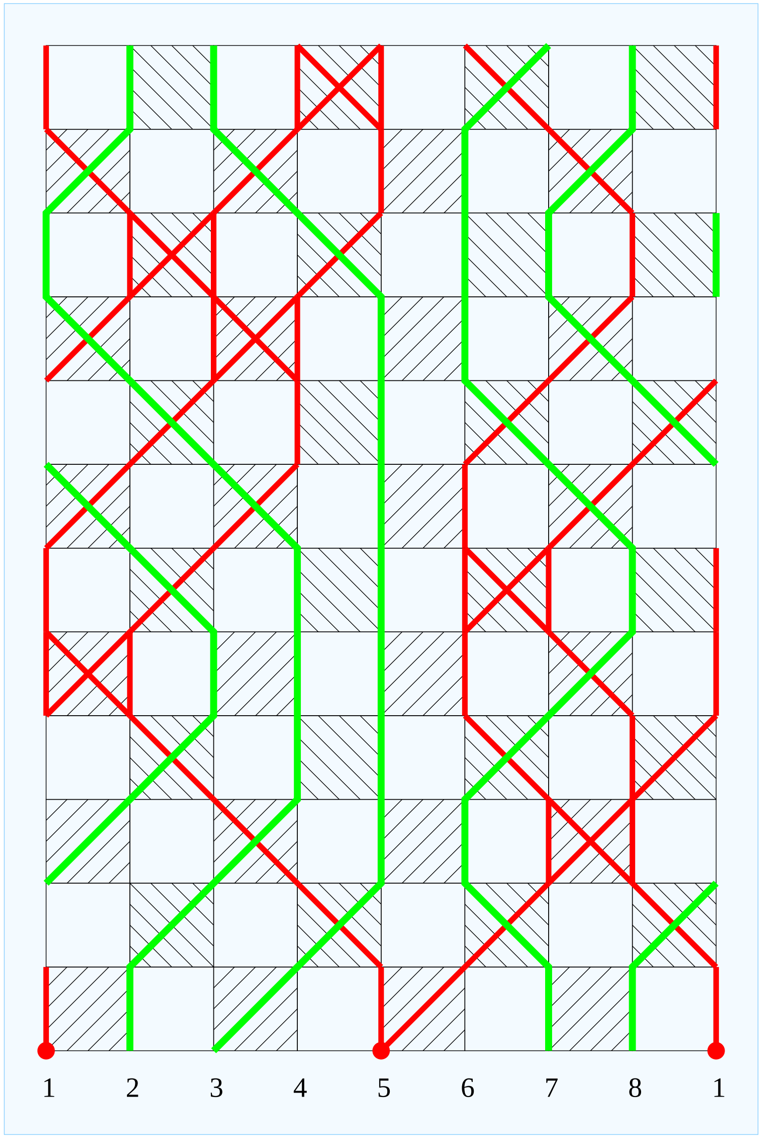

$|{\downarrow}>$ **is a barrier for holes**

expect also less severe minus sign problem for J small, low doping, and large systems in two dimensions

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- **Fast Fourier transformation** ⟶ **alternative to checkerboard decomposition.**
- **Jordan-Wigner transformation** ⟶ **from bosons to fermions in 1-D**
  For 2-D see

  E. Frradkin, Phys. Rev. Lett. bf 63, 322 (1989)

  Y.R. Wang, Phys. Rev. B **43**, 3786 (1991)

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- **Loop-algorithm** $\longrightarrow$ **particular form of cluster algorithms. Statistical mechanics of graphs**

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- **Minus-sign problem** $\longrightarrow$ **eliminated in special cases with the Meron method**

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- Canonical transformation $\longrightarrow$ pseudospins + spinless holes
- Single hole dynamics and loop-algorithm $\longrightarrow$ exact treatment of single hole dynamics
- Single hole in a 2-D quantum antiferromagnet
  $\longrightarrow$ coherent quasiparticle with internal dynamics
  holons and spinons confined by string potential
  Self-consistent Born approximation agrees very well with QMC

Summary of Lecture 4

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- **Hybrid-loop algorithm** $\longrightarrow$ **new algorithm for doped antiferromagnets**

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- Static and dynamical correlation functions $\longrightarrow$ spectral functions

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- **One-particle spectral functions** $\longrightarrow$ **QMC for the nearest neighbor t-J model vs. analytical results for the** $1/r^2$ **t-J model**

Summary of Lecture 5

- t-J model in 1-D $\longrightarrow$ rich phase diagram reminiscent of high T_C superconductors
- $1/r^2$ t-J model $\longrightarrow$ free excitations with fractional statistics
- One-particle spectral functions $\longrightarrow$ QMC for the nearest neighbor t-J model vs. analytical results for the $1/r^2$ t-J model
- Antiholon $\longrightarrow$ new generic excitation of the nearest neighbor t-J model

Collaborators

- Dr. Michael Brunner (HypoVereinsbank-München)
- Dr. Catia Lavalle (University of Stuttgart)
- Dr. Sylvain Capponi (Université Paul Sabatier, Toulouse)
- Dr. Mitsuhiro Arikawa (University of Stuttgart)
- Prof. Dr. Fakher F. Assaad (University of Würzburg)