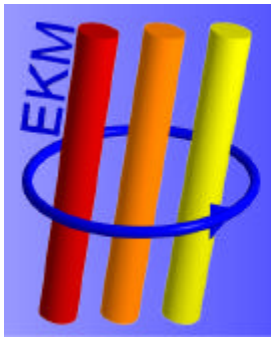

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Nature of Band- to Mott-insulator Transitions in 1D

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Outlook:

- *Insulator-insulator transitions*
- *Defining criteria for insulating phases*
- *Experimental realizations and theoretical model*
- *Simple limits for the ionic Hubbard model*
- *DMRG results*
- *Summary*

A. P. Kampf, M. Sekania, G. I. Japaridze, and Ph. Brune J. Phys.: Condens. Matter 15 5895-5907 (2003)

H. Fehske, A. P. Kampf, M. Sekania, G. Wellein Eur. Phys. J. B 31 , 11 (2003).

Insulator - Insulator Transitions

Origin: competition between charge density wave (CDW) formation and local Coulomb repulsion.

Sources for CDW formation:

- finite range Coulomb interactions
- electron-phonon coupling
- staggered potential
- alternated on-site Coulomb interaction

1D Model Hamiltonians:

U-V Hubbard Model:

$$H = -t\sum_{i,s}\left(c^{+}_{i,s}\,c_{i+1,s} + H.c.\right) + U\sum_{i} n_{i,\uparrow}n_{i,\downarrow} + V\sum_{i,s} n_{i,s}\,n_{i+1,s}$$

Pierls-Hubbard Model:

$$H = -t\sum_{i,s}\left(1+(-1)^{i}d\right)\left(c^{+}_{i,s}\,c_{i+1,s} + H.c.\right) + U\sum_{i} n_{i,\uparrow}n_{i,\downarrow}$$

Ionic Hubbard Model:

$$H = -t\sum_{i,s}\left(c^{+}_{i,s}\,c_{i+1,s} + H.c.\right) + U\sum_{i} n_{i,\uparrow}n_{i,\downarrow} + \frac{\Delta}{2}\sum_{i,s}(-1)^{i}\,n_{i,s}$$

Defining criteria for insulating phases:

- **Band insulator** **(BI)** $D_c = D_s$
- **Mott insulator** **(MI)** $D_c > D_s = 0$
- **Correlated insulator** **(CI)** $D_c > D_s > 0$

$$\Delta_c = E_0\left(N = L+1, S^z = 1/2\right) + E_0\left(N = L-1, S^z = 1/2\right) - 2E_0\left(N = L, S^z = 0\right)$$

$$\Delta_s = E_0\left(N = L, S^z = 1\right) - E_0\left(N = L, S^z = 0\right)$$

Δ_{opt} ° minimal excitation energy $(E_m\text{-}E_0)$ in the same particle number sector

<u>*Selection rule*</u> for optical transitions: $\langle 0|\hat{j}|m\rangle \neq 0$ only if $|m\rangle$ and $|0\rangle$ have different site-parities

Motivation

- Neutral-ionic transition in organic mixed-stack charge-transfer crystals with alternating donor (D) and acceptor (A) molecules

$$(\ldots D^{+r} A^{-r} D^{+r} A^{-r} \ldots)$$

J. Torrance (1981)
N. Nagaosa (1986)

- Ferroelectrics transition in perovskite materials such as

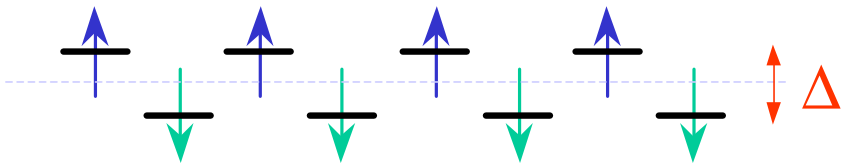
  $BaTiO_3$ *(T. Egami, S. Ishihara, M. Tachiki 1993)*

  KNbO3 *(T. Neumann et al 1992)*

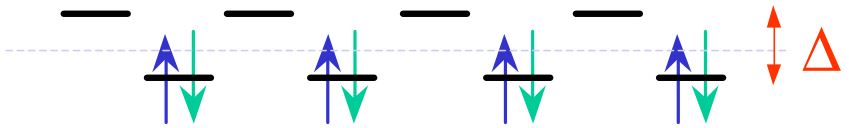
Simple Limits for the Ionic Hubbard Model

❖ *t = 0 (atomic limit)*

D < **U**



D > **U**



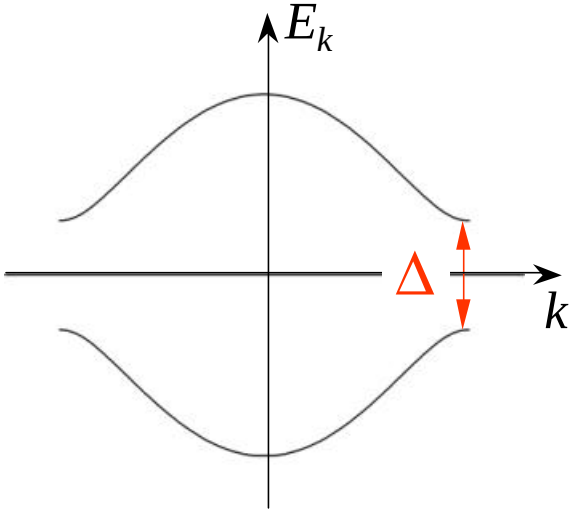
one electron per site, 2^N states

$D_c = U - D$, $D_s = 0$ Þ **"MI"**

$D_c = D_s = D - U$ Þ **BI**

❖ *U = 0*

$$E_k = \pm\sqrt{4t^2\cos^2 k + \frac{D^2}{4}}$$



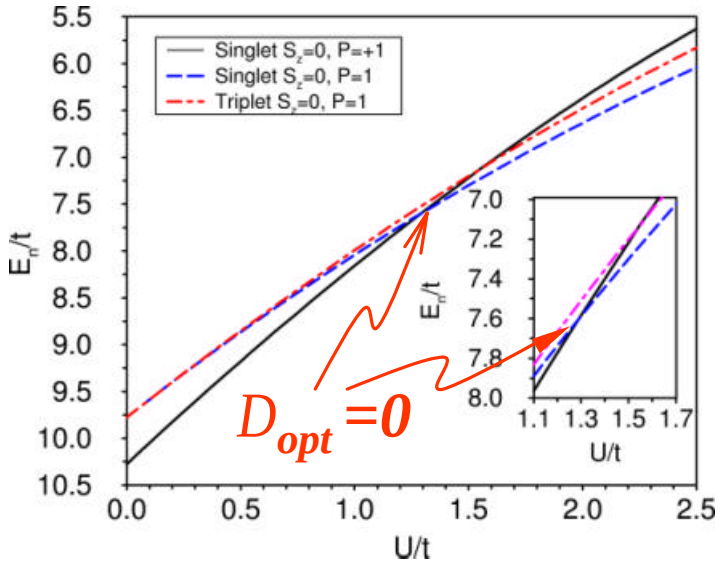
$D_c = D_s = D$ Þ **BI**

- site inversion operator: $\hat{P}$

$$\hat{P} c^{+}_{i,s} \hat{P} = c^{+}_{L-i,s}, \qquad for \qquad i = 0,\ldots, L-1$$

- translation by j sites: $\hat{T}_j$

$$[H,\hat{P}] = 0, \quad [H,\hat{T}_2] = 0, \quad [H,\hat{T}_1] \neq 0$$



Strong Coupling Limit ($U>>D$)

$$H^{eff} = J\sum_i S_i \cdot S_{i+1} + J'\sum_i S_i \cdot S_{i+2}$$

$$J = \frac{4t^2}{U}\left(\frac{1}{1-x^2} - \frac{4t^2}{U^2}\frac{\left(1+4x^2-x^4\right)}{\left(1-x^2\right)^3}\right), \qquad J' = \frac{4t^4}{U^3}\frac{\left(1+4x^2-x^4\right)}{\left(1-x^2\right)^3}, \qquad x = \frac{\Delta}{U}$$

$D_s = 0$ for $J' < 0.24J$, ($U > 3.6t$ for $D < t$) ($U > 3.6D$ for $D > t$)

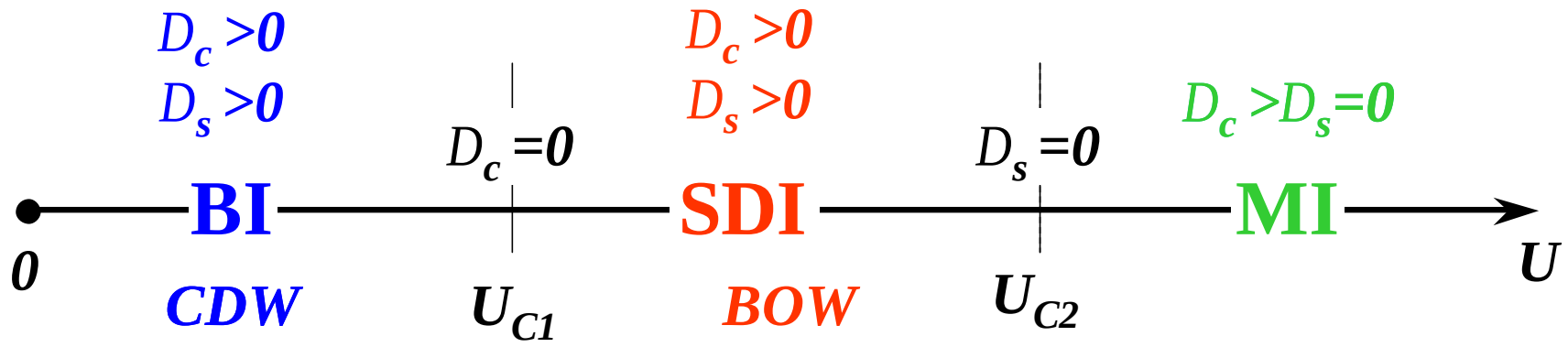
Effective Hamiltonian has higher symmetry than the original one !

$$[H,\hat{T}_1] \neq 0, \quad [n_i,\hat{T}_1] = 0 \quad \Rightarrow \quad [H^{eff},\hat{T}_1] = 0, \quad [n_i^{eff},\hat{T}_1] \neq 0$$

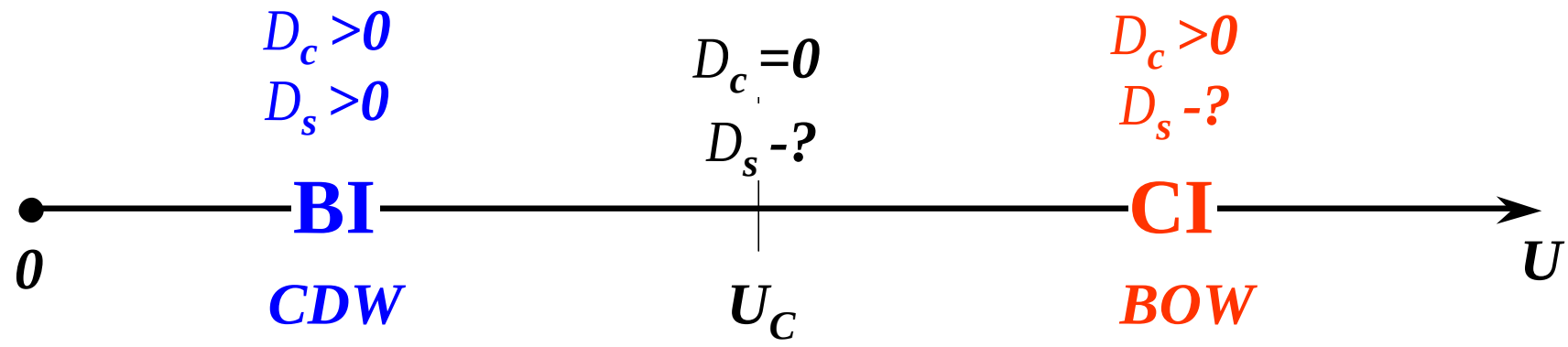
$$n_i^{eff} = 1 - (-1)^i \frac{2U\Delta}{\left(U^2-\Delta^2\right)}\sum_j \left(1 - 4\vec{S}_i\vec{S}_{i+j}\right)$$

A.A. Aligia (2003)

Proposed Scenarios

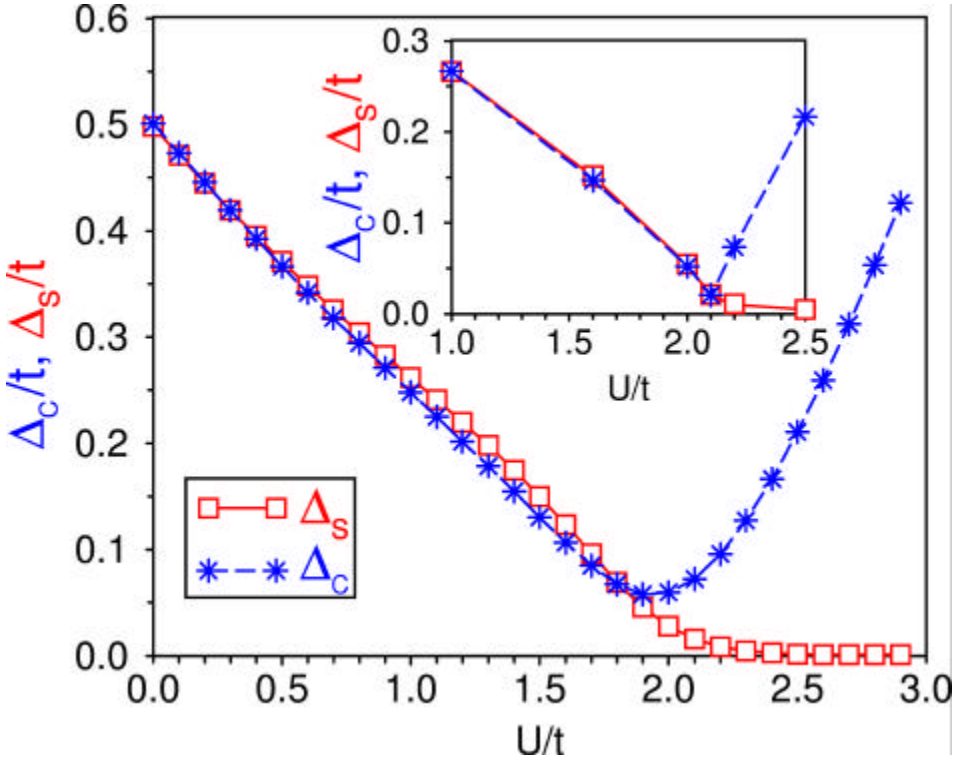


M. Fabrizio, A. O. Gogolin, and A.A. Nersesyan, (1999) weak coupling



T. Wilkens and R.M Martin (2001) QMC

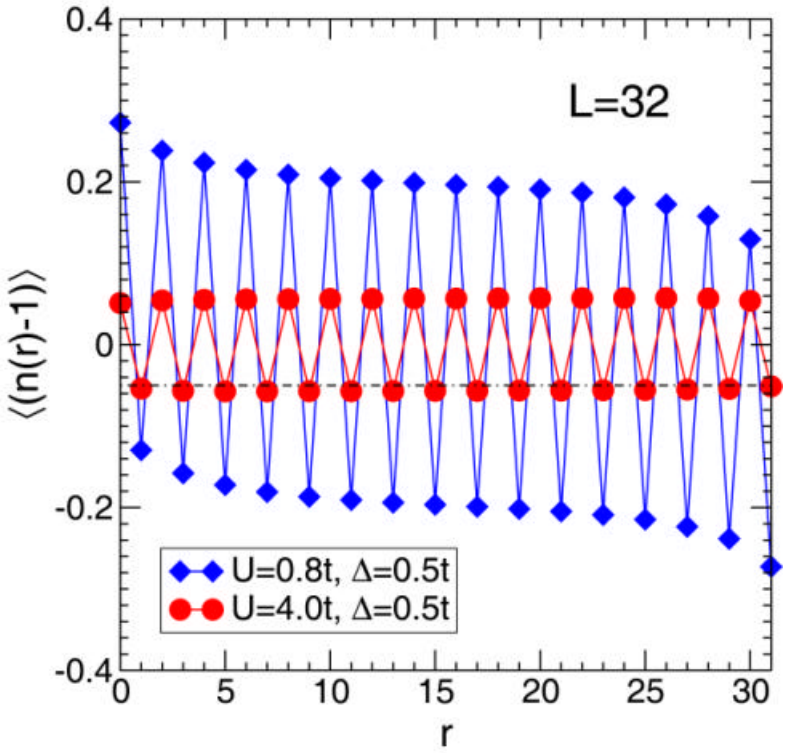
Results for D_c and D_s



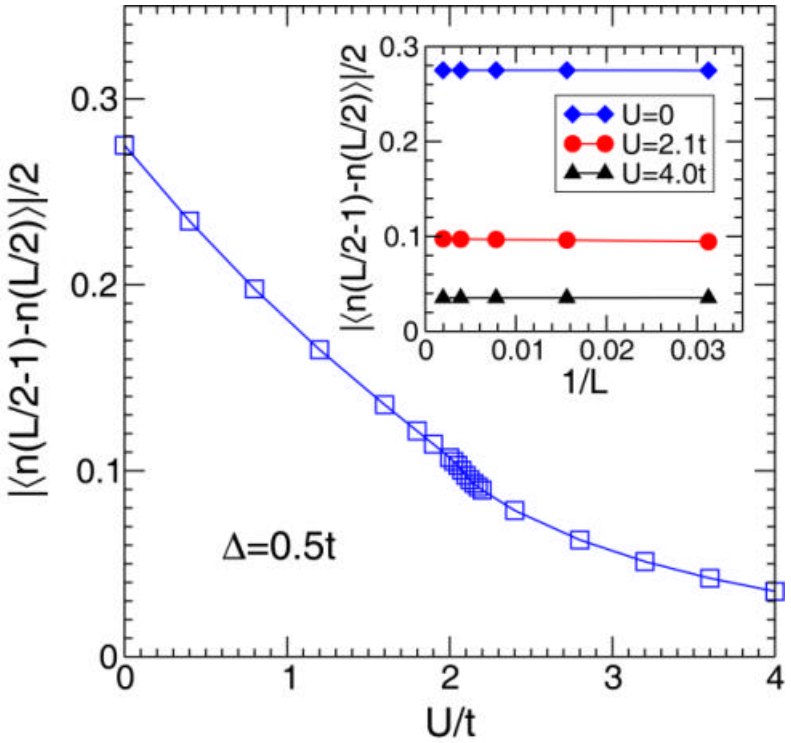
DMRG calculations were performed for $\Delta=0.5$, on open chains with $L=\{30,40,50,60\}$ (main plot) and up to $L=512$ (inset), and extrapolated to the limit of infinite chain length

Charge Density Distribution

CDW on a L=32 open chain

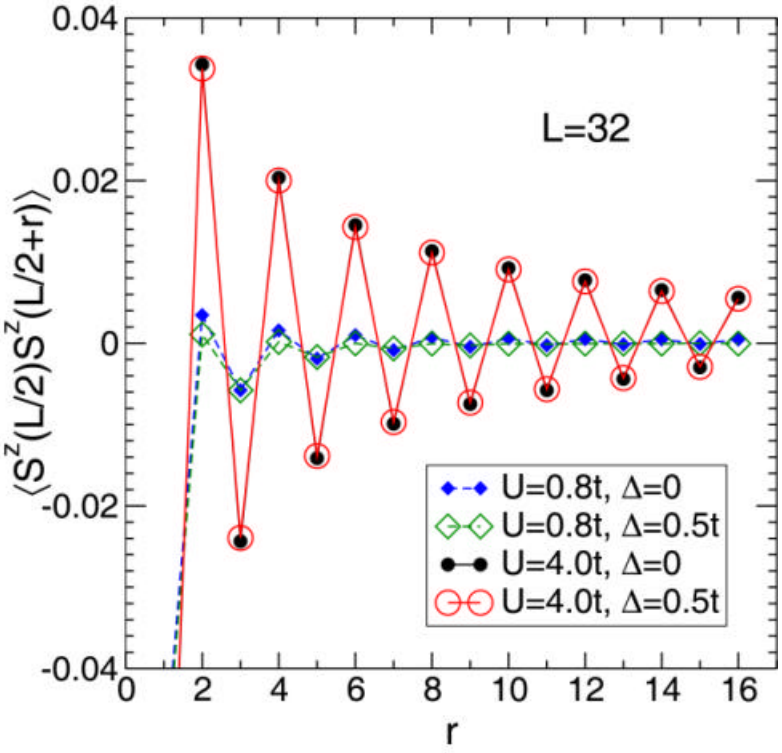


Staggered charge density component for L=512

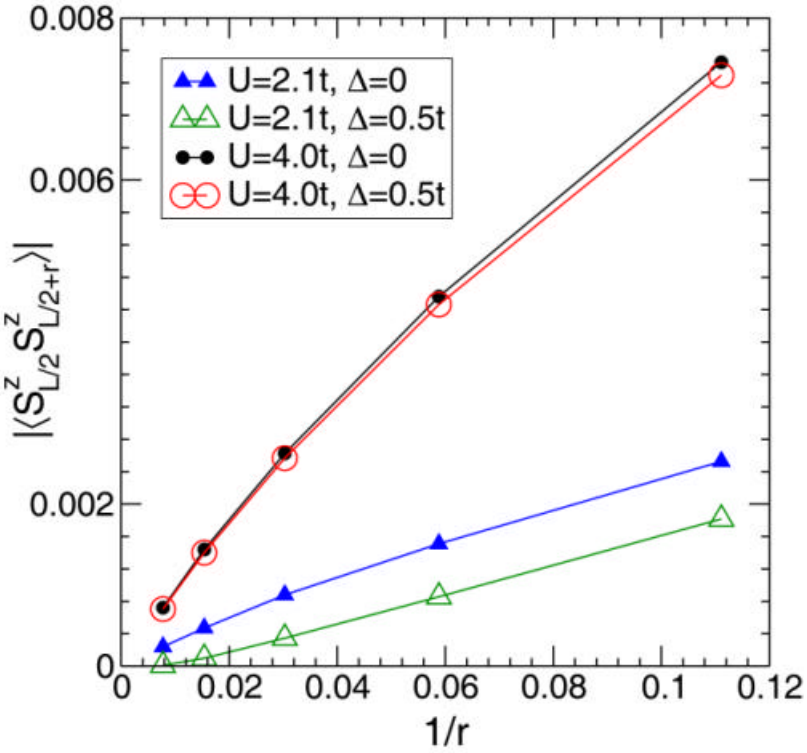


➥ **For finite D the CDW persists for *arbitrary* $U<¥$**

Spin-Spin Correlation Function



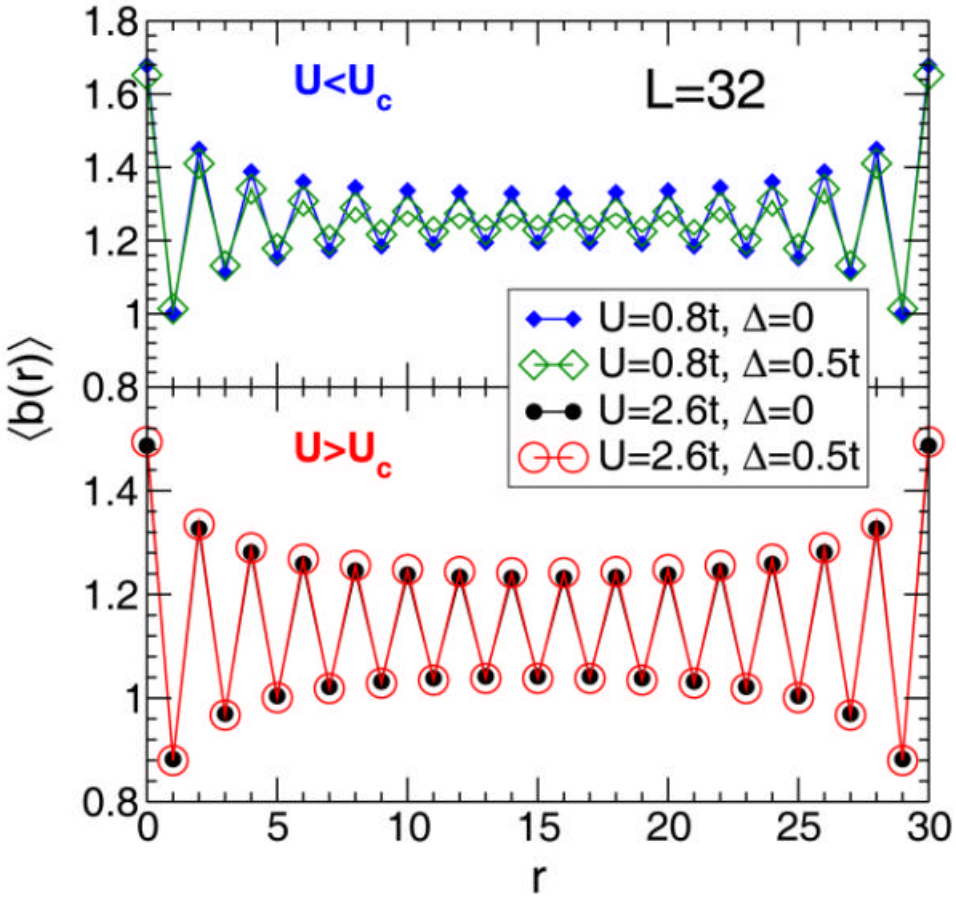
Scaling of the spin-spin correlation function at r=L/4+1



- ***U=4t:*** long distance behavior of the spin correlations of the IHM and Hubbard model are quite similar

- ***U=2.1t:*** spin-spin correlation function manifestly supports the finiteness of the spin gap

Bond-Charge Density



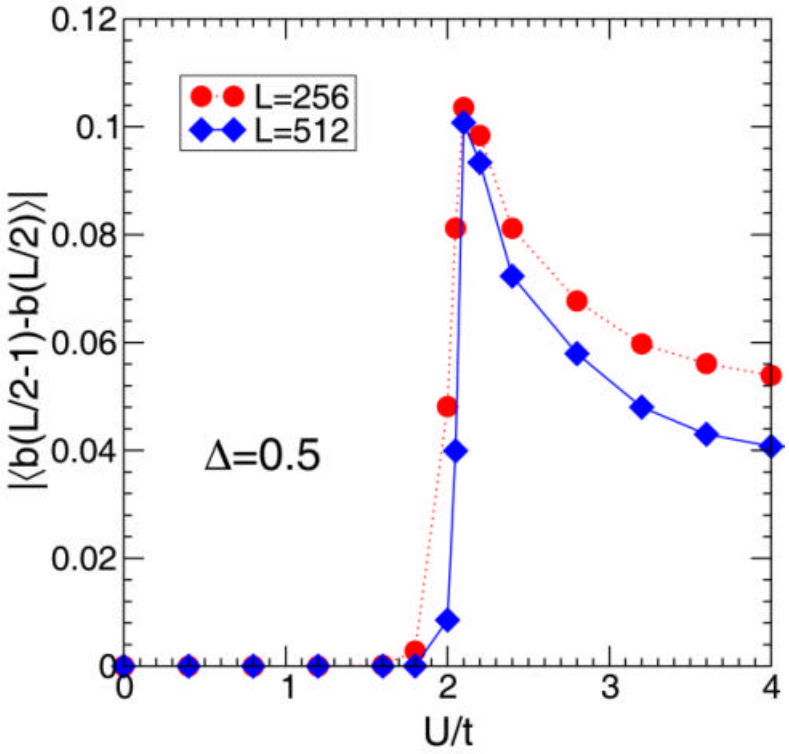
Modulation of the bond density due to strong open boundary effect in the pure Hubbard model.

- $U<U_C$: reduction of bond density oscillation in IHM comparing to Hubbard

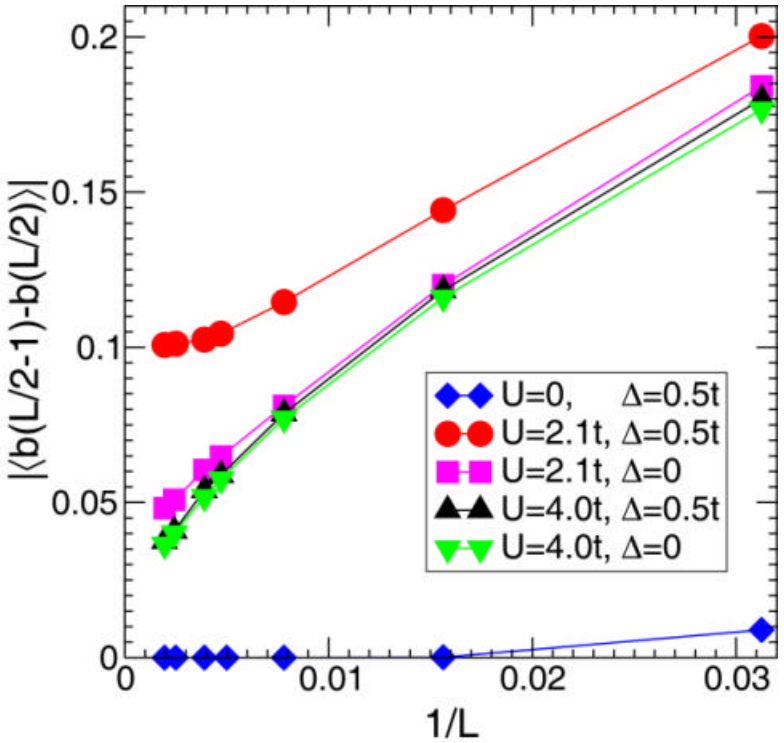
- $U>U_C$: enhancement of bond density oscillation in IHM comparing to Hubbard

$$b(i) = \sum_s \left(c^+_{i,s} c_{i+1,s} + H.c. \right)$$

Staggered bond-density component



Scaling behavior of the staggered bond-density component



- $U<U_C$: (BI) absence of bond-density oscillation
- $U=2.1t$: (CI) upward curvature of the staggered bond density versus $1/L$ points to a finite value in the infinite chain length limit, i.e long range BOW
- $U=4t$: starts to resemble the results for the pure Hubbard model

Summary

- The ionic potential leads to long range CDW order for all interaction strength
- DMRG resolves one transition point from the BI to the CI phase.
- At the transition point $D_c = D_s > 0$
- Close above transition we identify signal for long range BOW order
- With increasing U above U_C the finite size scaling behavior of the staggered bond and spin-spin correlation function changes qualitatively and approaches the scaling behavior of the Hubbard model