Investigations of Metal-Insulator and Insulator-Insulator Transitions using the DMRG

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- Gaps
- Electric susceptibility
- Discussion

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  - gaps
  - bond–order parameter
  - bond–order susceptibility
  - electric susceptibility
- Discussion

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References:

C. Aebischer, D. Baeriswyl and R.M. Noack, Phys. Rev. Lett. **86**, 468 (2001).

C. Aebischer, Ph.D. thesis, Fribourg, January 2002.

S. Manmana, Diploma thesis, Göttingen, May 2002.

S. Manmana, V. Meden, R.M. Noack, and K. Schönhammer, cond-mat/0307741, to appear in Phys. Rev. B.

Characterizing Metals and Insulators

ground-state DMRG, open BCs

- order parameters

  $\rightarrow$ ionicity $\langle n_A - n_B \rangle = \frac{1}{L} \sum_j (-1)^j \langle n_j \rangle$

  $\rightarrow$ polarization $\langle \mathcal{P} \rangle = \frac{1}{L} \sum_j x_j \langle n_j \rangle$

  $\rightarrow$ bond order $\langle B \rangle = \frac{1}{L} \sum_j (-1)^j \left\langle c^\dagger_{j+1} c_j + c^\dagger_j c_{j+1} \right\rangle$

- gaps

"single-particle gap" $\Delta_1 = \mu_+ - \mu_- = E_0(N+1) + E_0(N-1) - 2E_0(N)$

"spin gap" $\Delta_s = E_0(S=1,N) - E_0(S=0,N)$

"exciton gap" $\Delta_e = E_1(S=0,N) - E_0(S=0,N)$

- susceptibilities

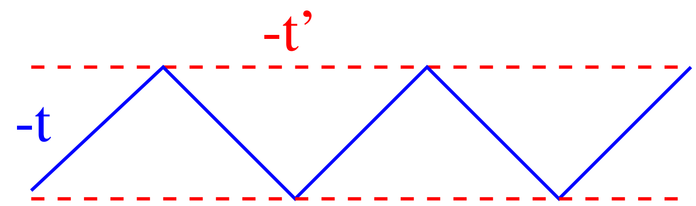
  $\rightarrow$ electric $\chi = \left. \frac{\partial \langle \mathcal{P} \rangle}{\partial E} \right|_{E=0} \approx \frac{1}{LE} \sum_i x_i \langle n_i \rangle$ (c.f. Drude weight)

  $\rightarrow$ bond $\chi = \left. \frac{\partial \langle B \rangle}{\partial \rho} \right|_{\rho=0}$

- correlation functions $C_d(r) = \langle n_i n_{i+r} \rangle - \langle n_i \rangle \langle n_{i+r} \rangle, \ldots$

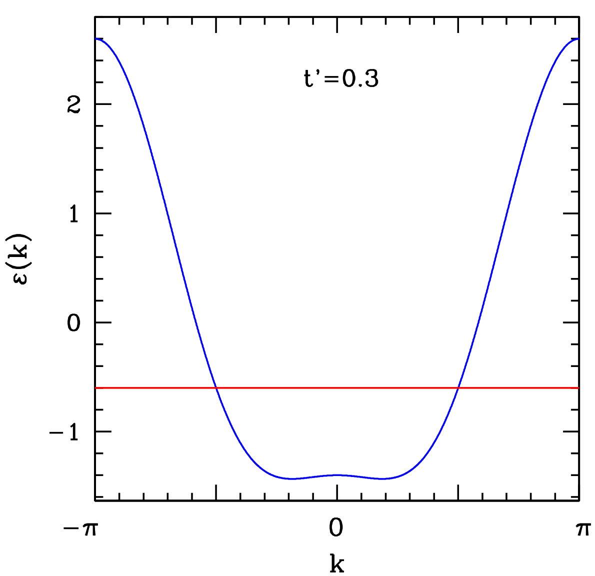
t–t′–U Chain at Half-Filling

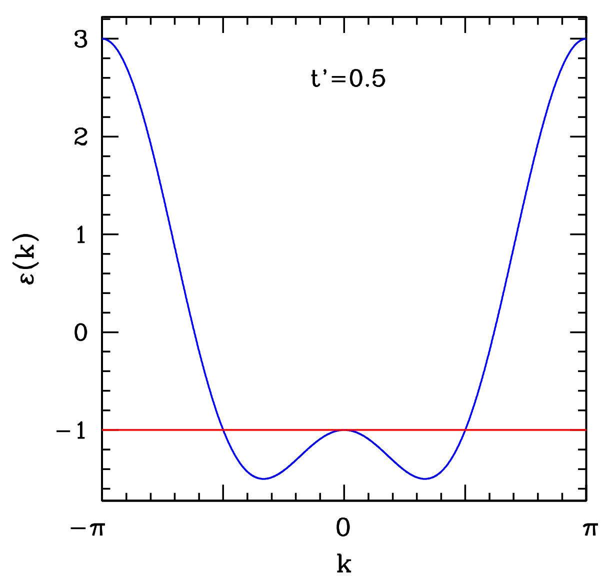
1D Hubbard model with next–nearest–neighbor hopping:



$$H = -\sum_{i,\sigma}(t\, c^\dagger_{i\sigma}c_{i+1\sigma} \; + \; t'\, c^\dagger_{i\sigma}c_{i+2\sigma} + \text{h.c.}) + \; U \; \sum_i n_{i\uparrow}n_{i\downarrow}$$

Dispersion: $\varepsilon(k) = -2t\cos k - 2t'\cos 2k$ $(t = 1)$





$n = 1:$ $t' < 0.5$: two Fermi points $t' > 0.5$: four Fermi points

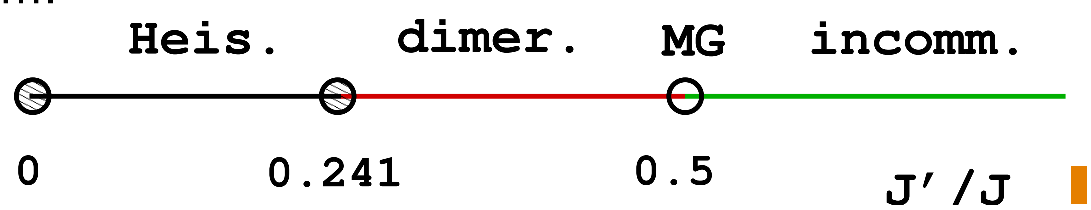
Limiting Cases

- Strong coupling ($U \gg t, t'$)

  Frustrated Heisenberg model

$$H = \sum_j \left[J \mathbf{S}_j \cdot \mathbf{S}_{j+1} + J' \mathbf{S}_j \cdot \mathbf{S}_{j+2} \right] \ , \qquad J = \frac{4t^2}{U} \ , \quad J' = \frac{4t'^2}{U}$$

  phase diagram:



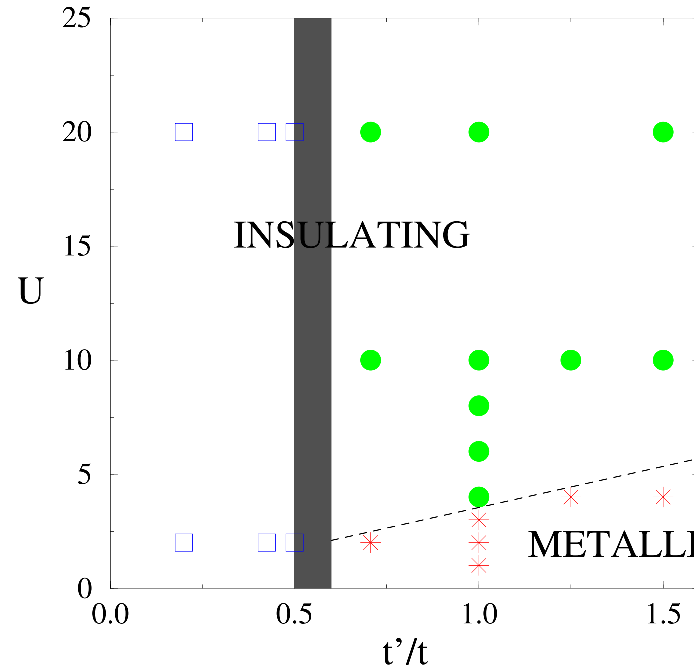
- Weak coupling

  Bosonization (Fabrizio, 1996)

  - two Fermi points: 1D Heisenberg
  - four Fermi points: no relevant nesting $\Rightarrow$ generic two-chain case
    $\Delta_s \neq 0$, $\Delta_c = 0$ (C1S0)

Phase Diagram

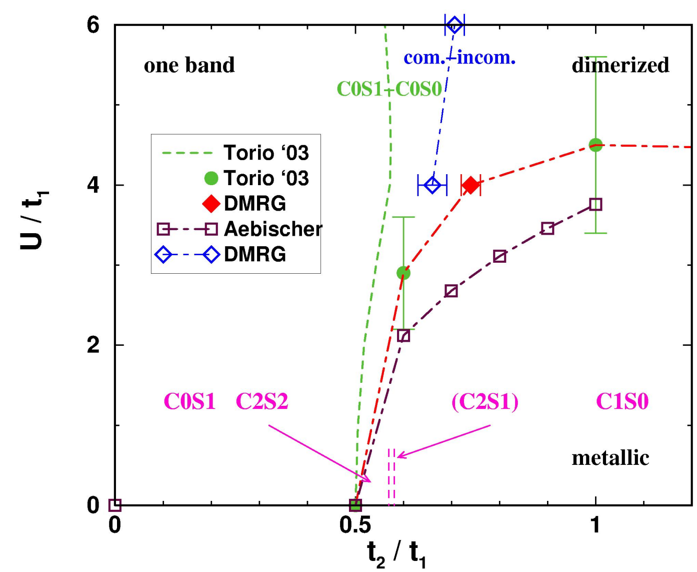
Ground–state phase diagram, $n = 1$:
(Daul & Noack, 1999)
From calculation of Δ_2, Δ_S



Behavior as a function of U:

- $t' < 0.5$: 1D Hubbard, $U_c = 0$
- $t' > 0.5$: Mott–Hubbard transition at finite U_c

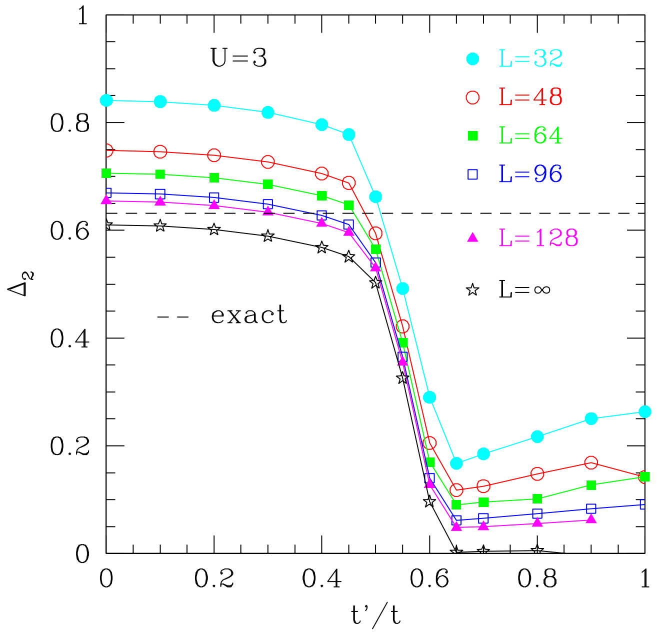
Recent work:
DMRG with n_k
(Gros, Hamacher, & Wenzel, 2004)
ED with Berry phase/level crossing
(Torio et al., 2003)
DMRG with χ
(Aebischer, Baeriswyl, & Noack, 2003)

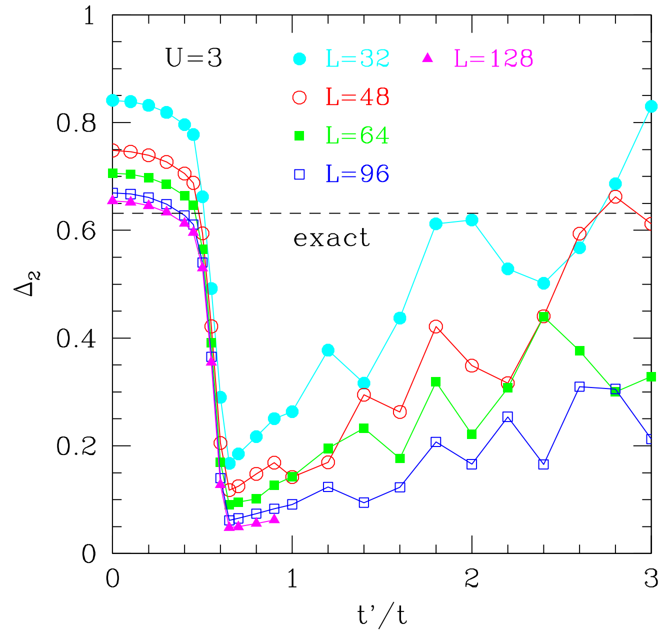


Gaps Reexamined

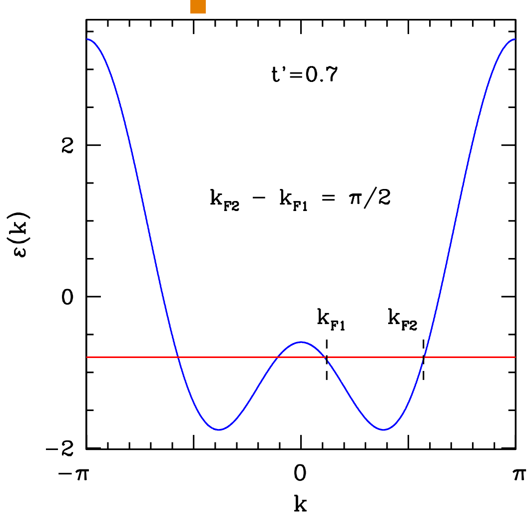
Two-particle gap $\Delta_2 = [E_0(N+2) + E_0(N-2) - 2E_0(N)]/2$

but for larger $t' \ldots$



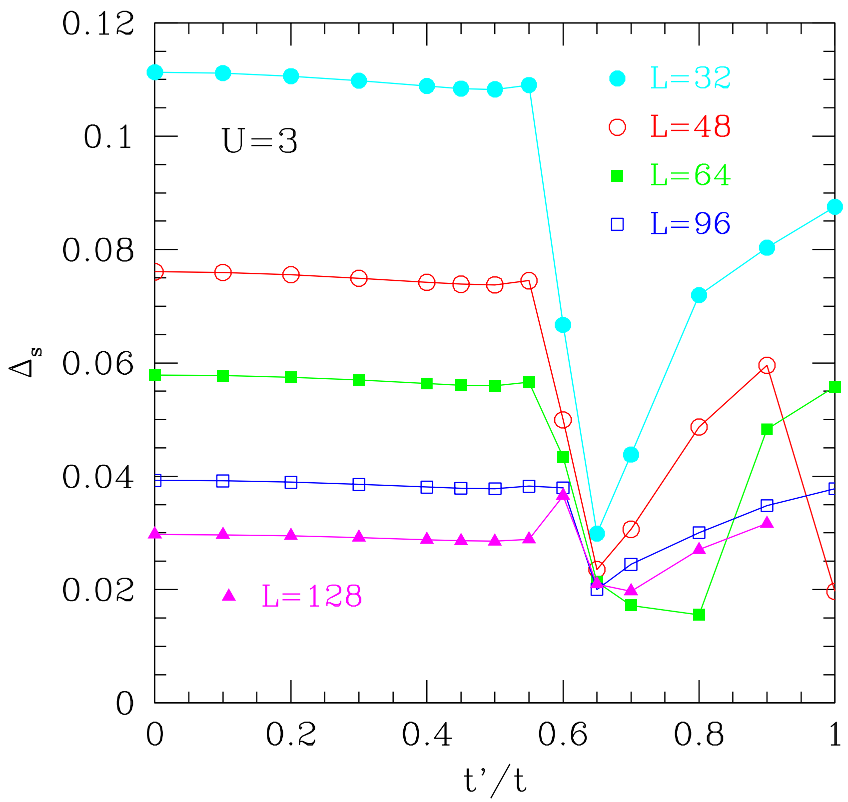


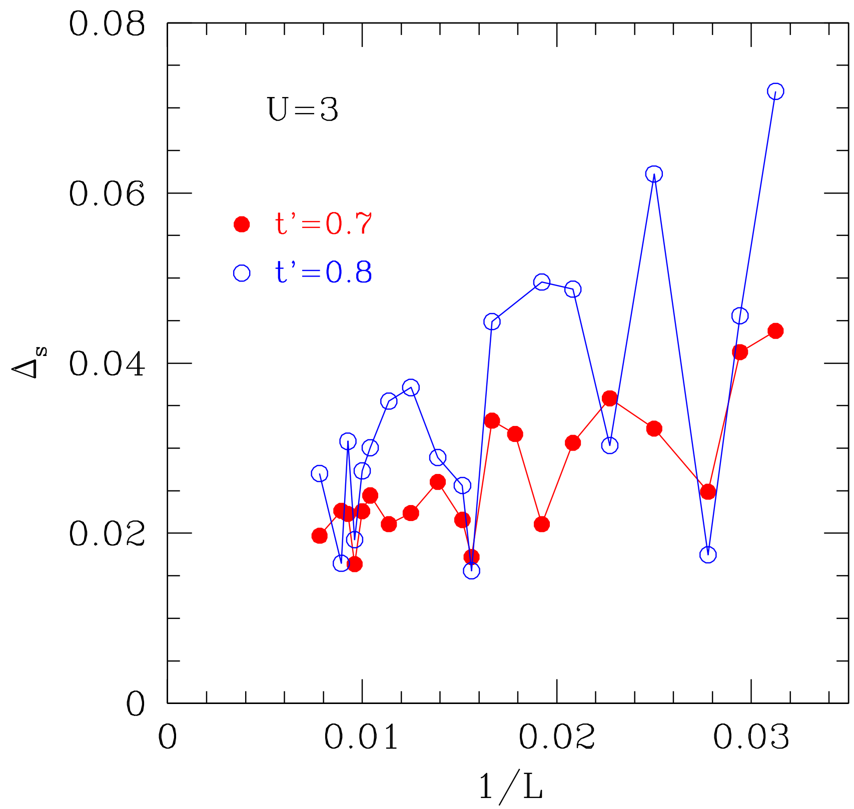
Cause:



incommensurate k_{F1}, k_{F2}

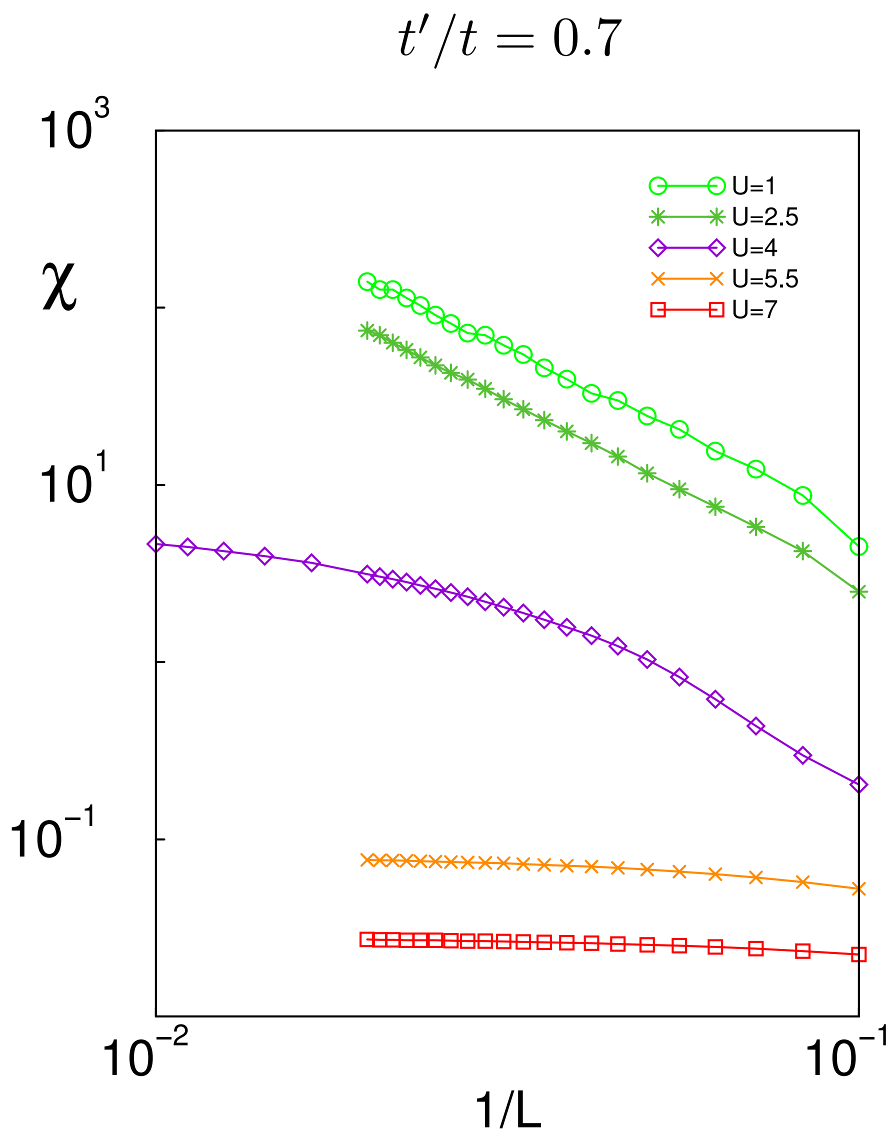
Spin Gap





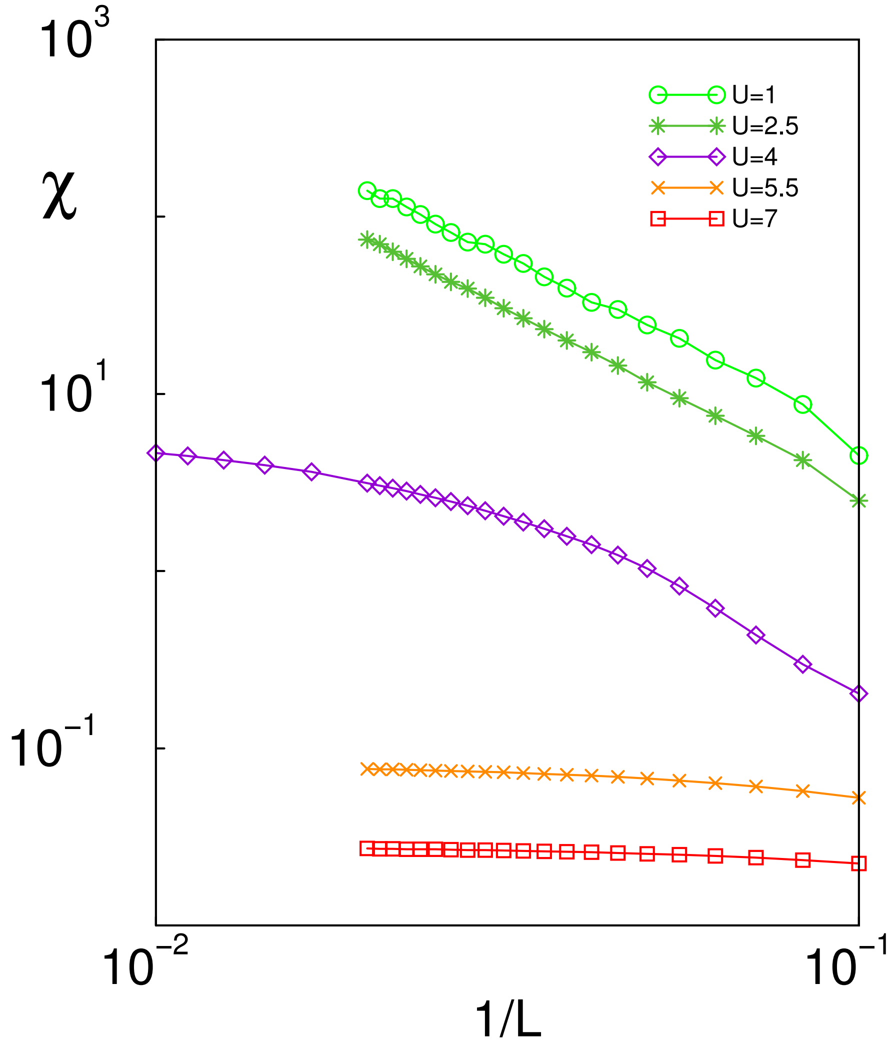
$\Rightarrow$ finite-size scaling erratic for $t' > t'_c$

Electric Susceptibility



Electric Susceptibility

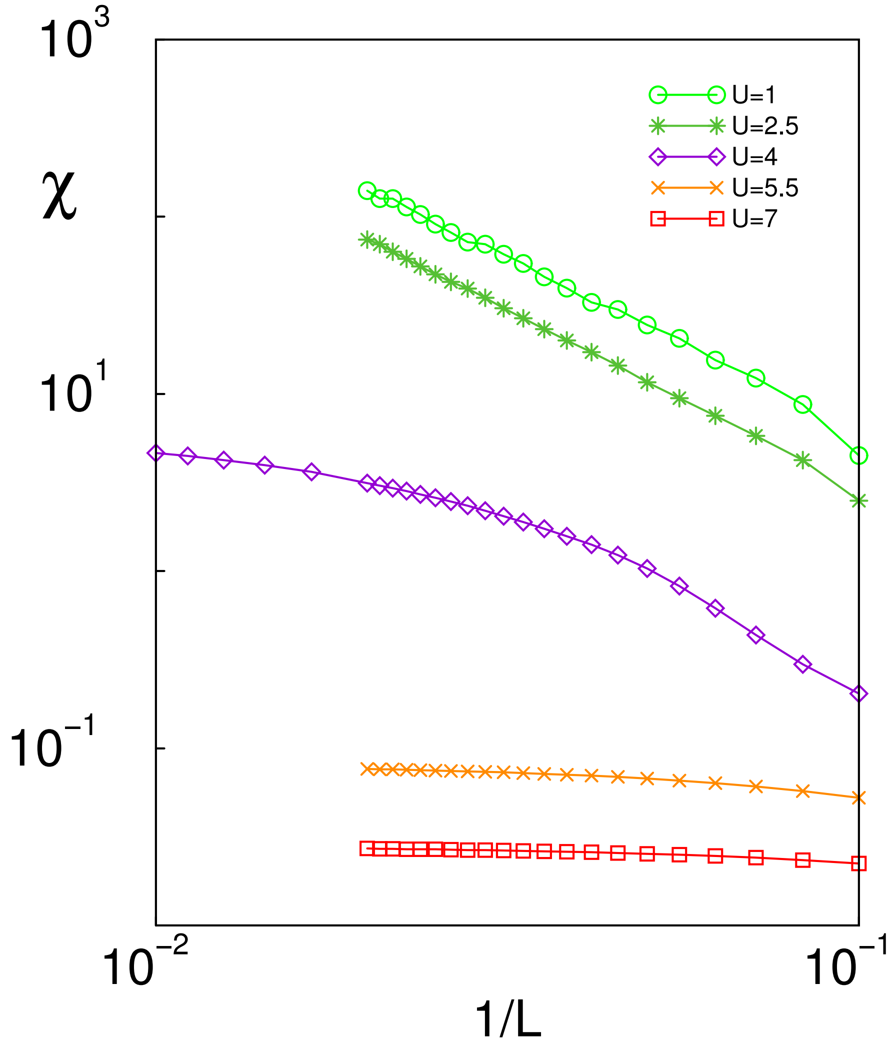
$t'/t = 0.7$



metal: $\chi \sim L^2$

Electric Susceptibility

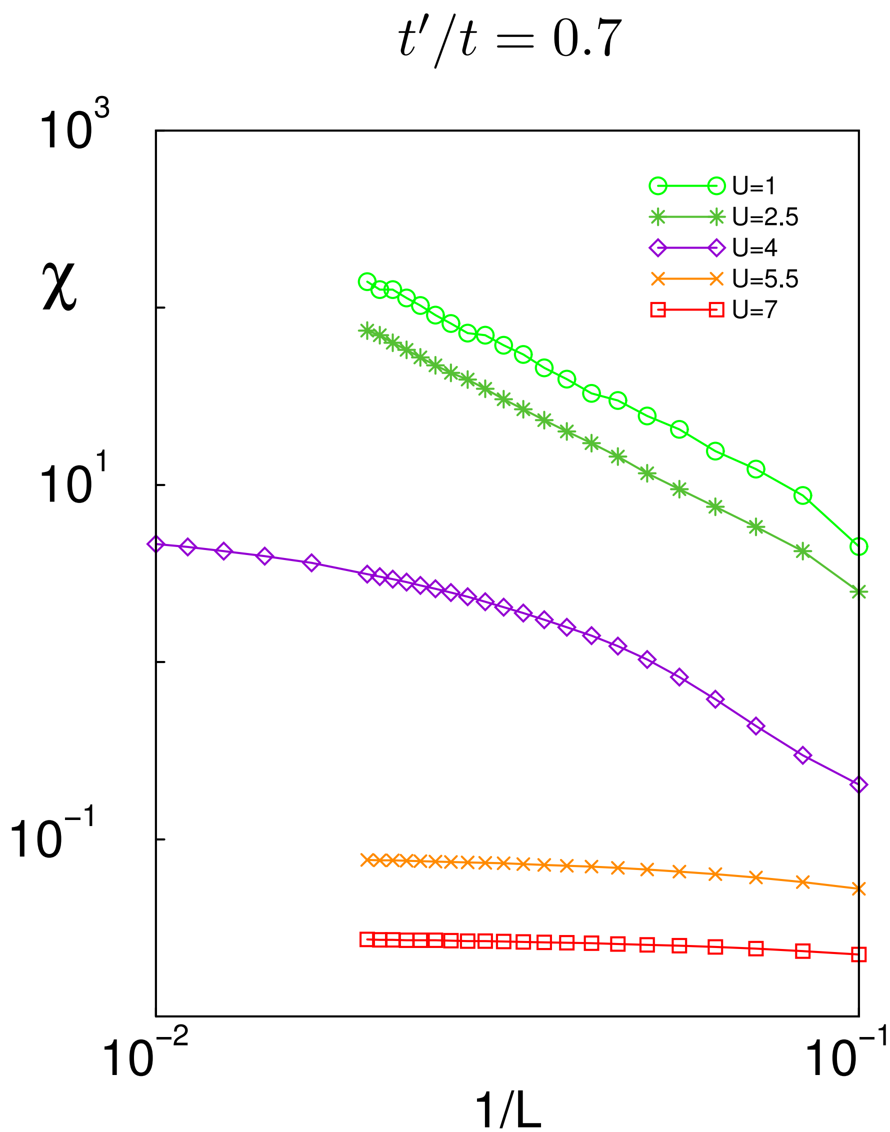
$t'/t = 0.7$



metal: $\chi \sim L^2$

critical

Electric Susceptibility



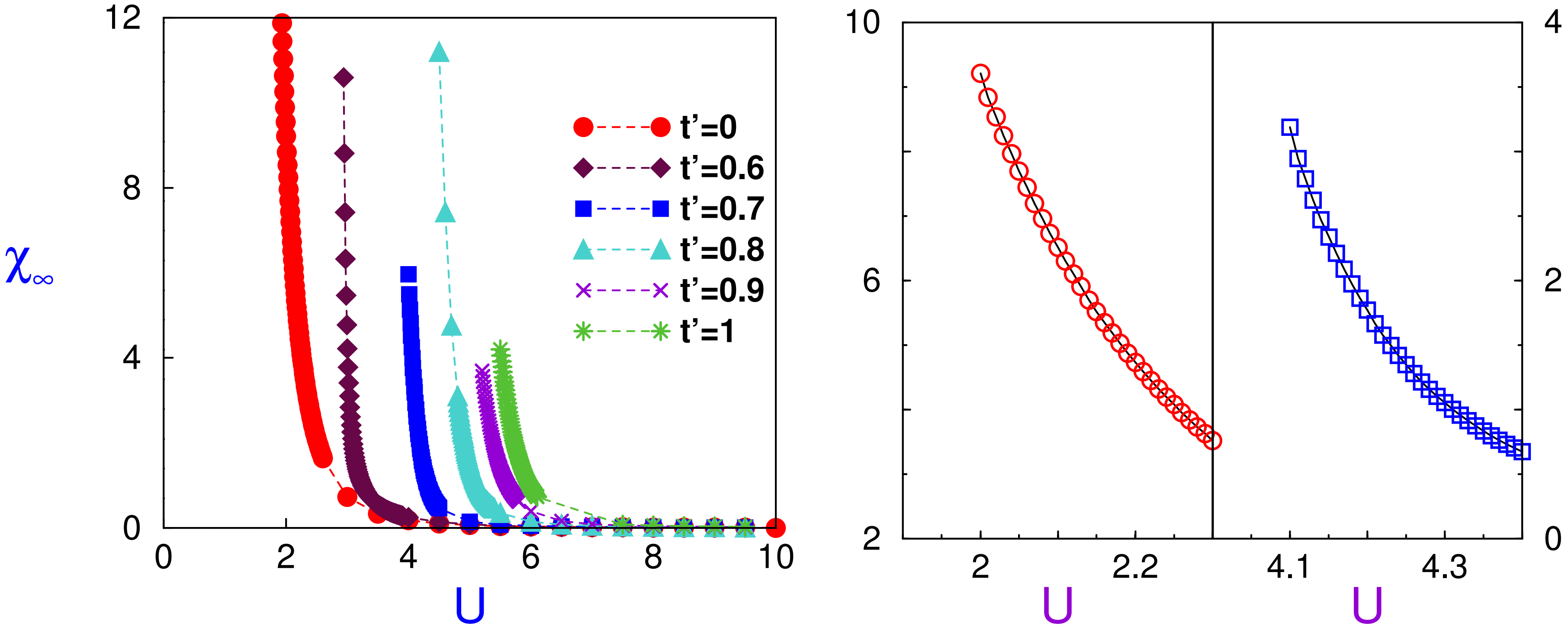
metal: $\chi \sim L^2$

critical

insulator: $\chi \longrightarrow$ const.

transition at $U_c/t \approx 4$

$L \to \infty$ extrapolation: $\chi_\infty(U)$

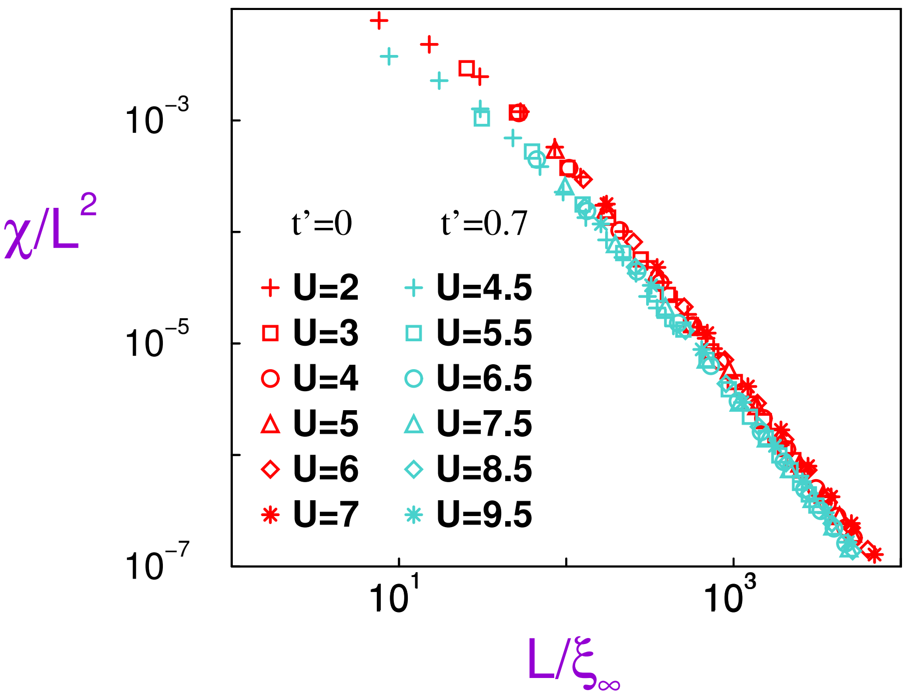


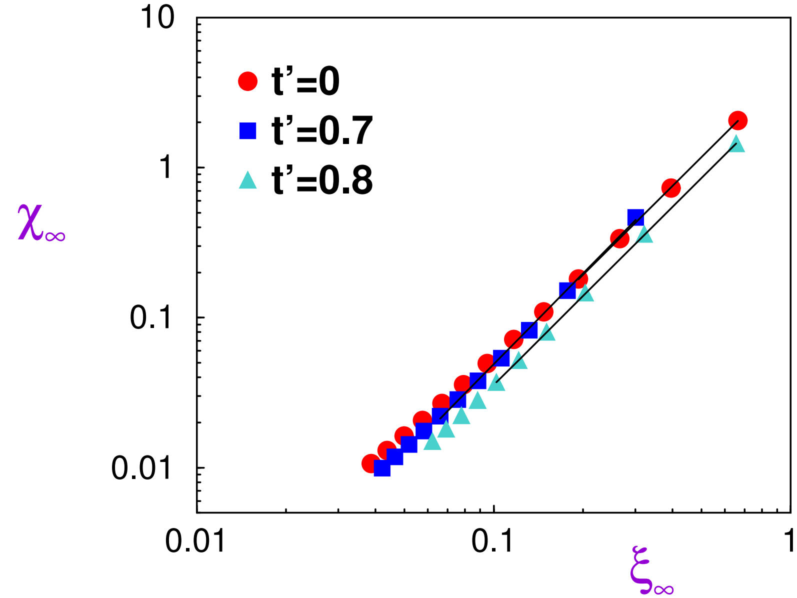
$$\chi \propto \exp\left(\frac{4\pi}{U - U_c}\right)$$

$\Rightarrow$ infinite-order transition

U_c finite for $t'/t \gtrsim 0.5$

Scaling Behavior





$\Rightarrow \chi_\infty \propto \xi_\infty^2$

finite-size scaling: $\dfrac{\chi}{L^2} = C(t')\Phi(L/\xi_\infty)$

(Privman & M.E. Fisher, 1984)

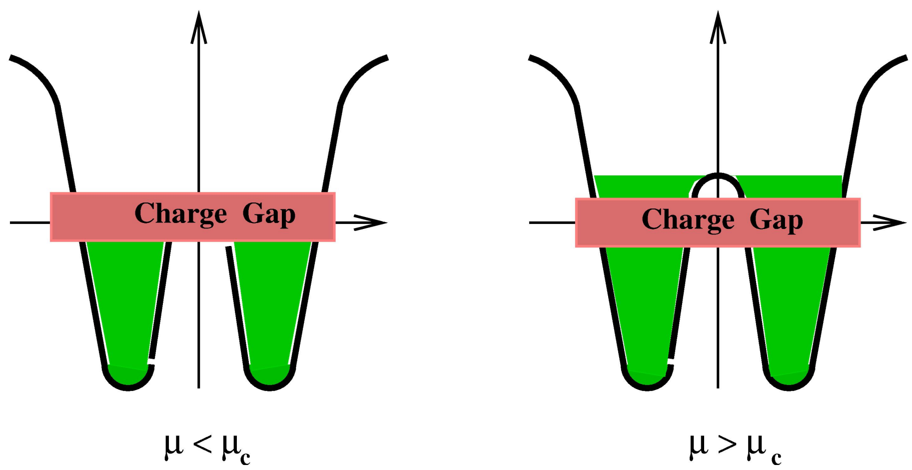
hyperscaling: $\chi_\infty \sim \xi_\infty^{2+z-d}$

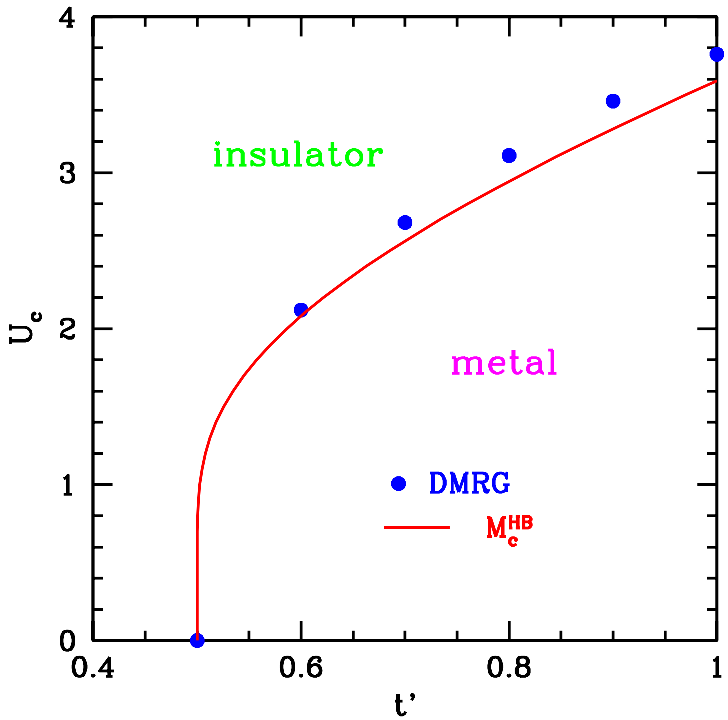
(Kim & Weichman, 1991)

Estimate for MI Phase Boundary

Band minimum must overcome Hubbard gap

$\mu_{\text{eff}} = 2t'_c - t^2/t'_c = M_c^{HB}(U)$

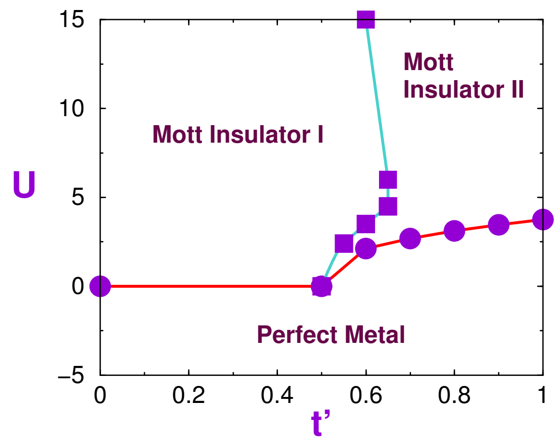




$\Rightarrow$ agreement surprisingly good

Remaining Issues: t-t'-U Model

- Opening of spin gap/dimerization



$L \to \infty$ behavior of $\langle B \rangle$
(C. Aebischer, Ph.D. thesis)

Better: bond-order or magnetic susceptibility

- Do intermediate CnSm phases exist?
  $\Rightarrow$ How to calculate gaps/gapless modes?
- Dynamics: single-particle, charge, spin
- Doping into dimerized phase – Pairing?

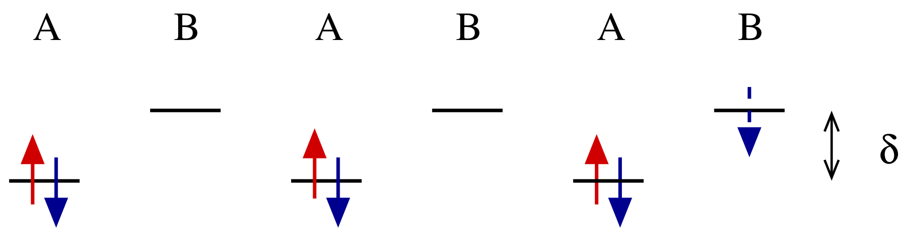
Ionic Hubbard Model

Hubbard chain with alternating potential (half-filled, n=1)

$$H = -t \sum_{j,\sigma} (c^\dagger_{j\sigma} c_{j+1\sigma} + c^\dagger_{j+1\sigma} c_{j\sigma}) + U \sum_j n_{j\uparrow} n_{j\downarrow} + \delta/2 \sum_{j\sigma} (-1)^j \, n_{j\sigma}$$

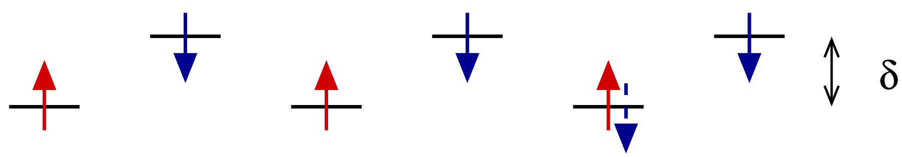
Atomic limit ($t = 0$):

$U < \delta$:



ionic
$\Delta_c = \delta - U$

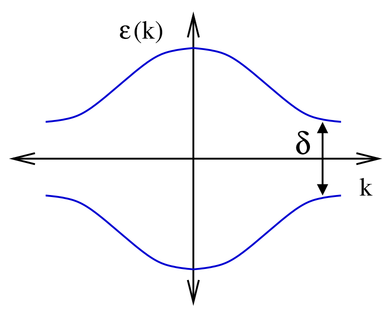
$U > \delta$:



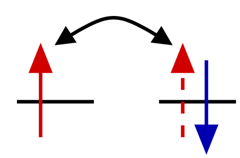
Mott
$\Delta_c = U - \delta$

Effect of hopping term

$U = 0$:
band insulator



$\delta = 0$:
antiferromagnetic

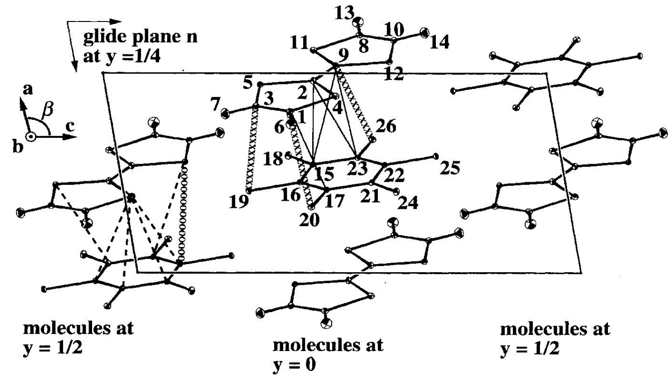


Motivation

- neutral-ionic transition in organic charge-transfer salts
  (Torrance et al., 1981)

  stack of donor-acceptor atoms,
  e.g. TTF-CA (Le Cointe et al., 1995)

  sharp change in $\langle n_A - n_B \rangle$ at transition



- ferroelectric transition in $BaTiO_3$ and $KNbO_3$
  (Egami, Ishihara, & Tachiki, 1993)

- theoretical
  - transition from a "renormalized" band insulator to a Mott insulator

    $$\Delta_s = \Delta_c = \delta_{\text{renorm}} \longrightarrow \Delta_s = 0, \Delta_c \sim U - \delta, \text{ AF}$$

  - Contrast: dimerized band insulator

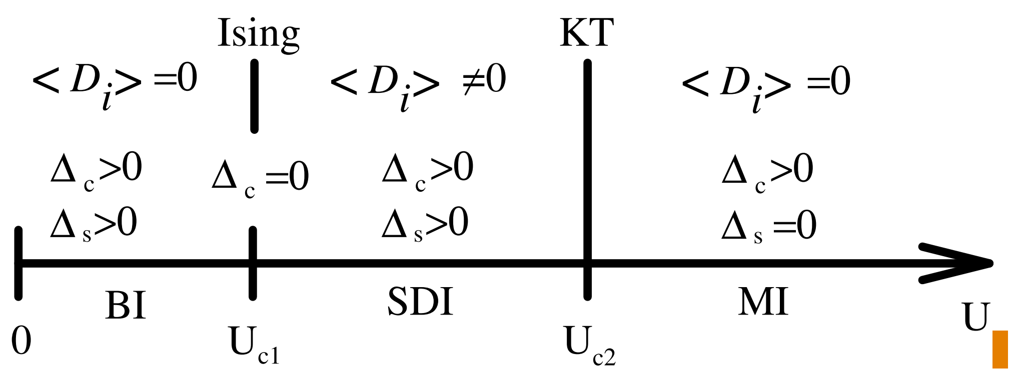
    $$H_{\text{kin}} = -t \sum_{j,\sigma} \left[1 + (-1)^j \gamma\right] \left(c_{j\sigma}^\dagger c_{j+1\sigma} + c_{j+1\sigma}^\dagger c_{j\sigma} \right)$$

    strong coupling limit: dimerized spin chain: $\Delta_c > \Delta_s > 0$

$\Rightarrow$ no transition, just crossover behavior

Scenarios for the Transition

Weak coupling: bosonization (Fabrizio, Gogolin, & Nersesyan, 1999)



Numerical:

- Gidoupolos, Sorella, & Tosatti, 2000: (ED, Berry phase) 2 transitions, metallic intermediate phase
- Wilkens & Martin, 2001: (var. QMC) 1 transition, dimerized for $U > U_c$
- Torio, Aligia, & Ceccatto, 2001: (ED, Berry phase) 2 transitions
- Takada & Kido, 2001: (DMRG) 2 transitions
- Qin et al., 2003 (DMRG) 2 transitions, $\Delta_1 \rightarrow 0$ at U_{c2}
- Brune et al., cond-mat/0106007; Kampf et al., 2003: (ED &DMRG) 1 transition - first order (?), dimerized for $U > U_c$ (?)
- Y.Z. Zhang et al., 2003: (DMRG) two transitions

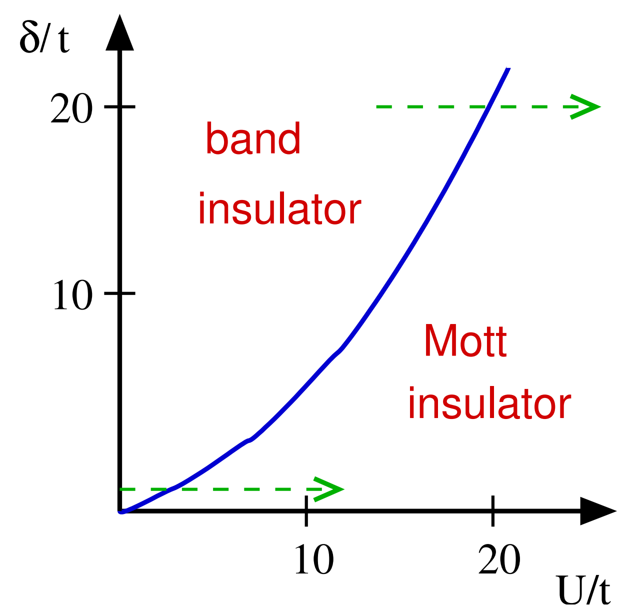
Unclear Questions

- How many phase transitions?
- Is there an intermediate dimerized phase?
- Order of the phase transition(s)?
- Behavior in the large-U limit?
- Behavior of the various gaps?
- Metallic point?

DMRG calculations

parameter values: $\delta/t = 1$, $\delta/t = 20$

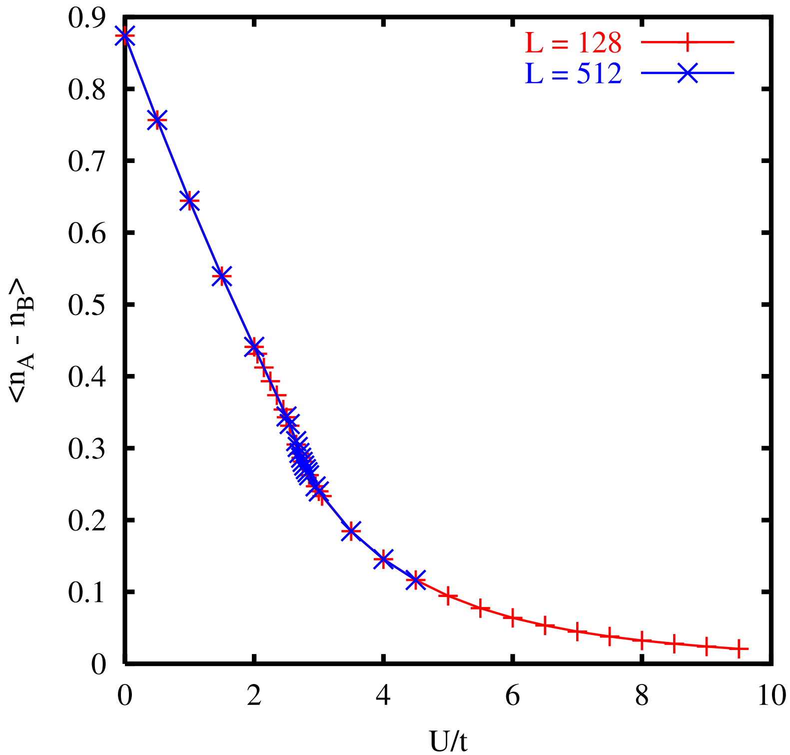
$\Rightarrow$ behavior as a function of U/t
at $T = 0$, open BCs

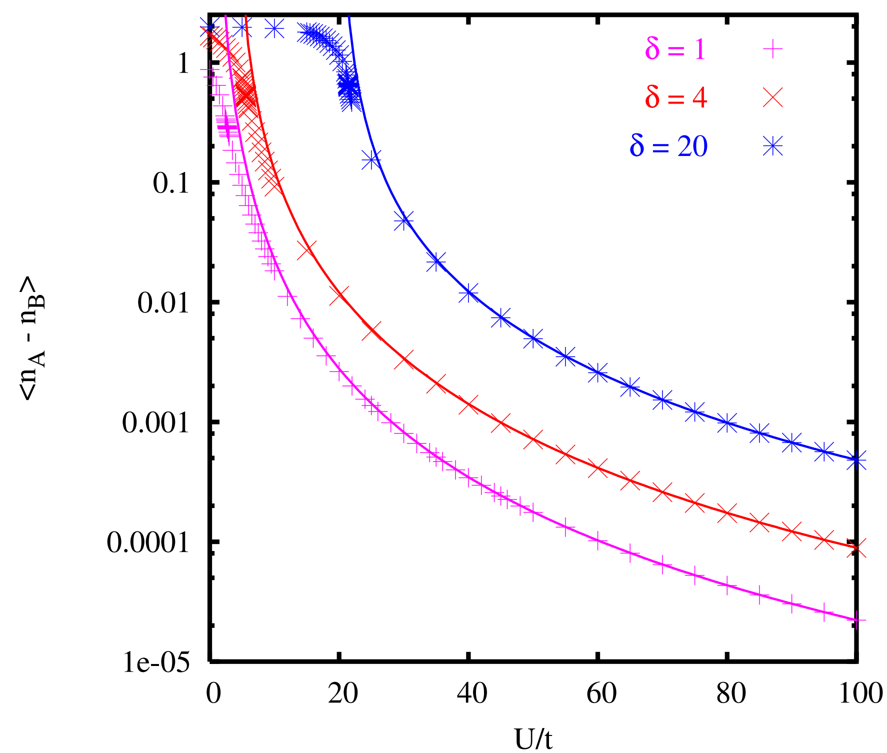


Ionicity

$$\langle n_A - n_B \rangle = \frac{1}{L} \sum_j (-1)^j \langle n_j \rangle$$

$$\delta/t = 1$$





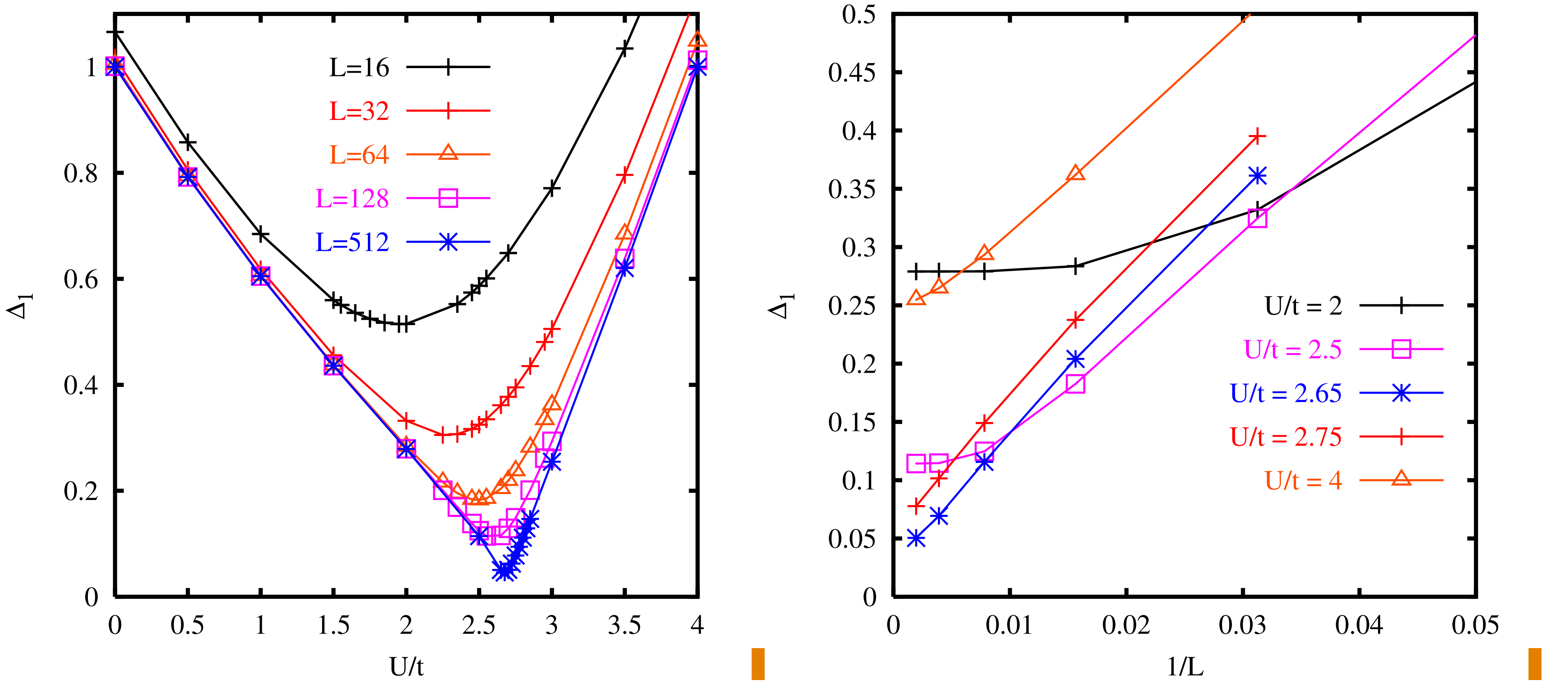
Continuous - no jump
inflection point at U_{c1} (??)

$\sim \frac{1}{U^3}$ for $U \gg t$
effective Heisenberg model:
$\langle n_A - n_B \rangle = 32 \ln 2 \frac{t^2 U \delta}{(U^2 - \delta^2)^2}$

Gaps

single-particle gap: $(\delta/t = 1)$

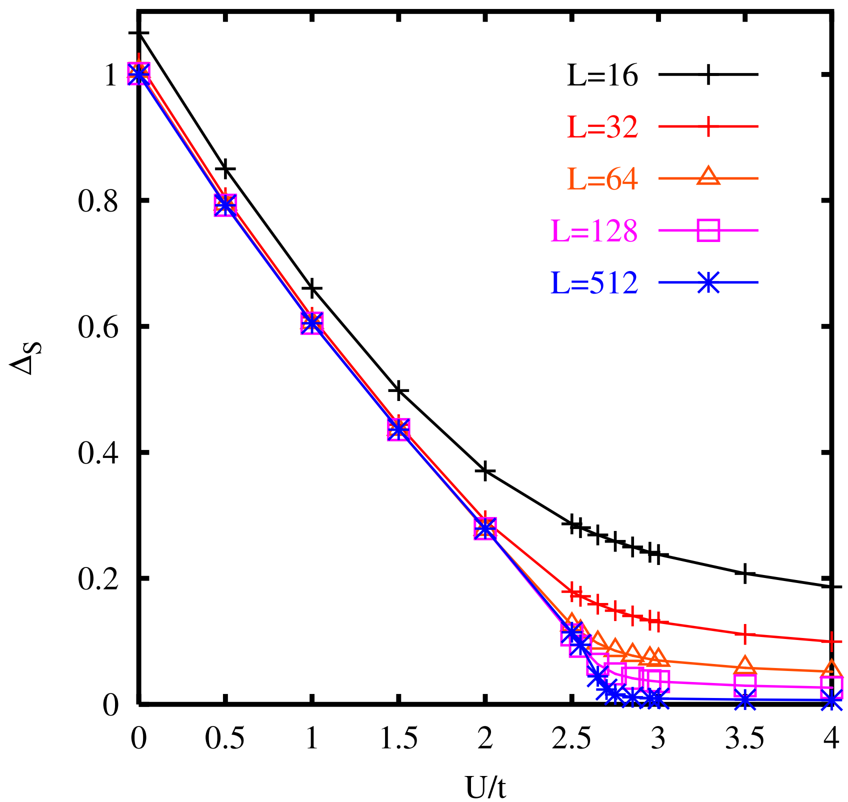
$$\Delta_1 = \mu_+ - \mu_- = E_0(N_{\rm el} = L+1) + E_0(N_{\rm el} = L-1) - 2E_0(N_{\rm el} = L)$$

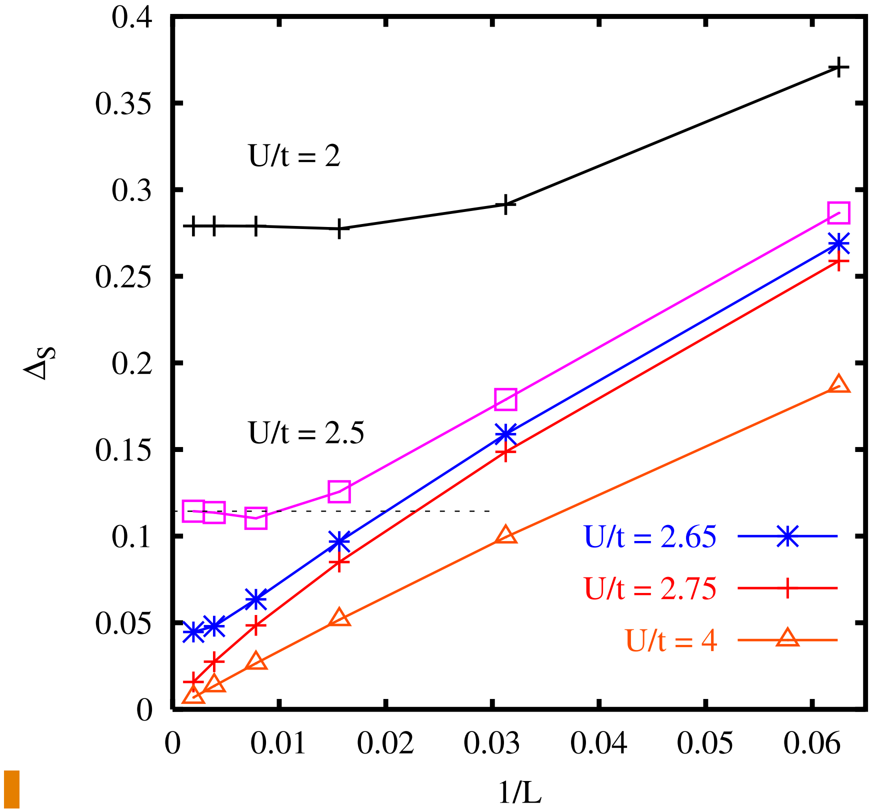


$\Rightarrow$ transition instead of crossover?

Spin Gap

$$\Delta_s = E_0(S=1, N_{\rm el}=L) - E_0(S=0, N_{\rm el}=L) \qquad (\delta/t = 1)$$



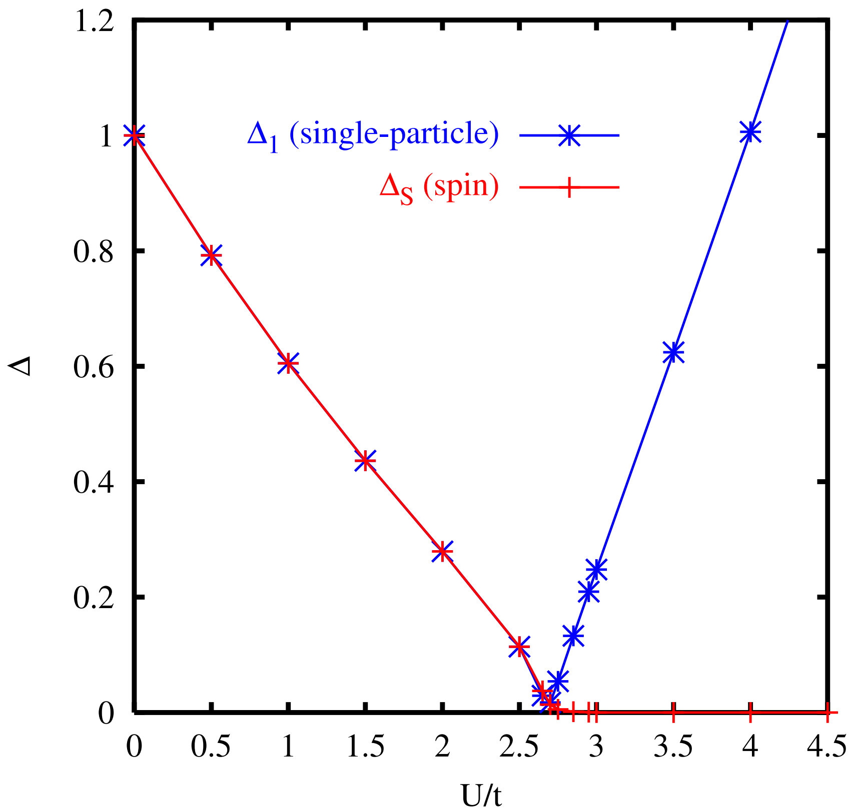


⇒ vanishes above the transition, as expected

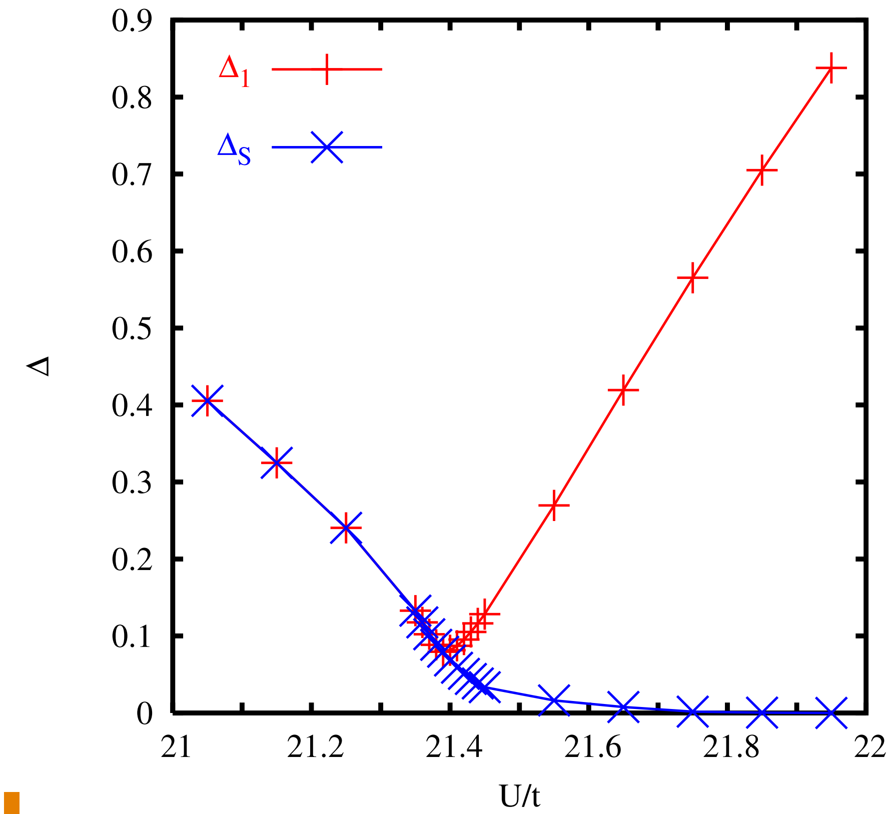
Relationship between spin and single-particle gaps

gaps at $L \to \infty$:

$\delta/t = 1$



$\delta/t = 20$



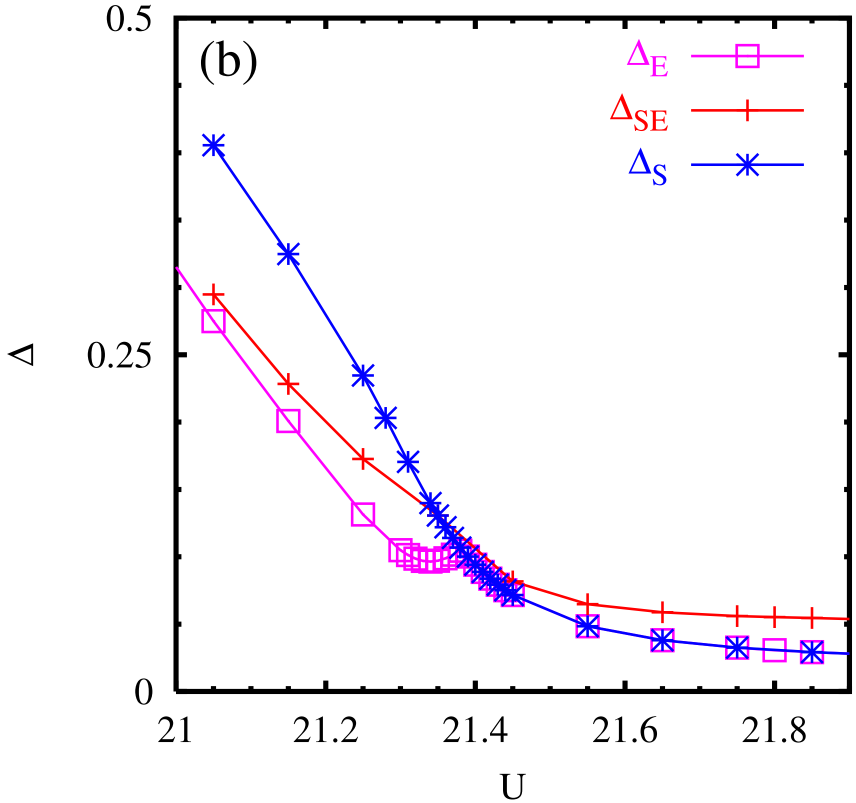
$\Rightarrow$ one transition point!

or maybe more?

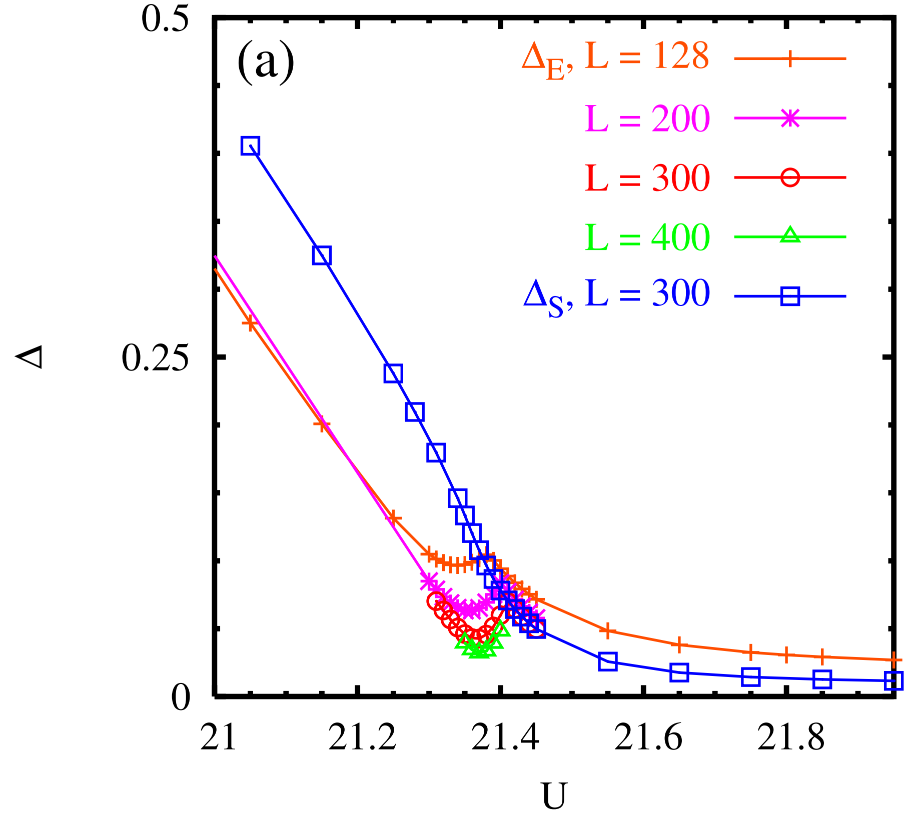
Excited States

Gap to the $S = 0$ and $S = 1$ excited states $(\delta/t = 20)$

$L = 128$



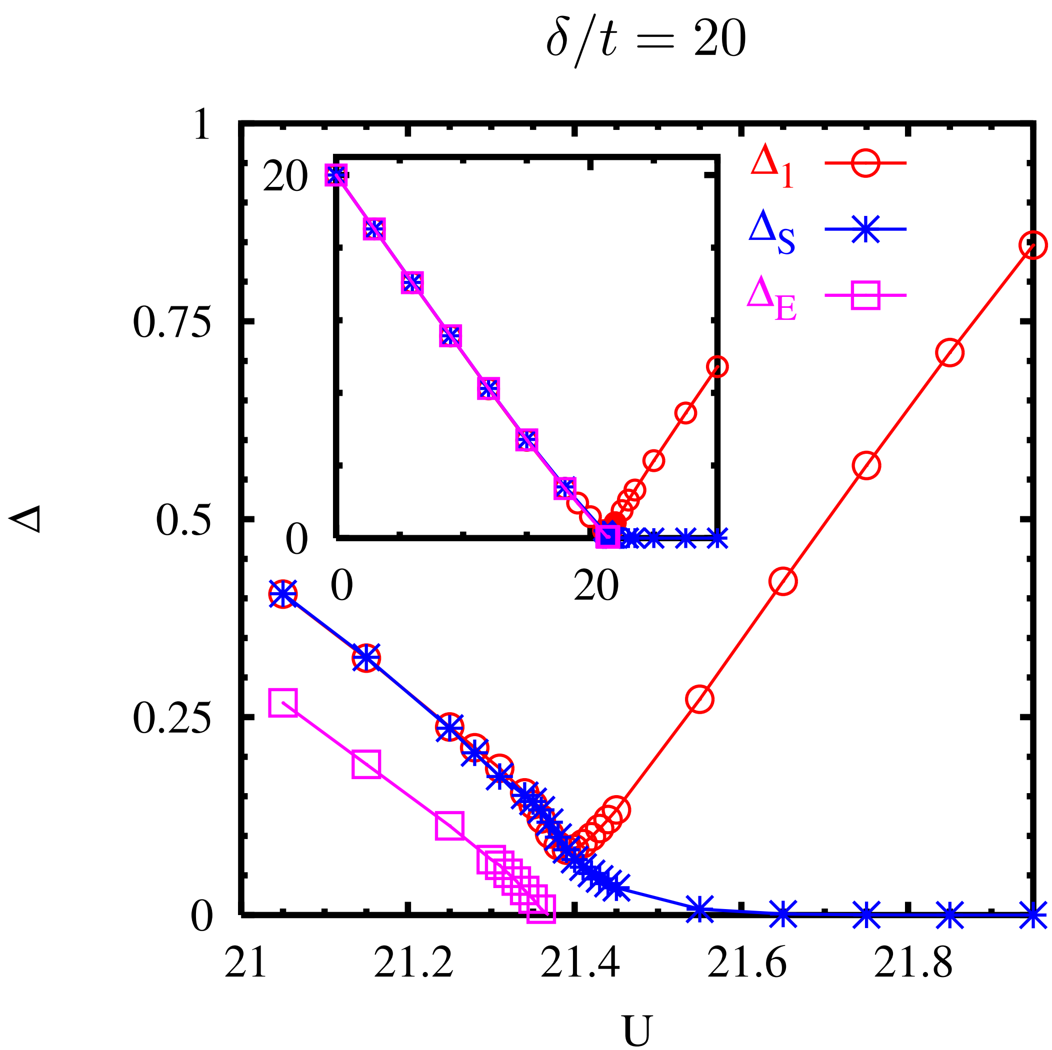
finite-size scaling



⇒ continuum of $S = 0$ excitations below the spin gap

⇒ separate minimum in the charge excitations

Extrapolation and Comparison



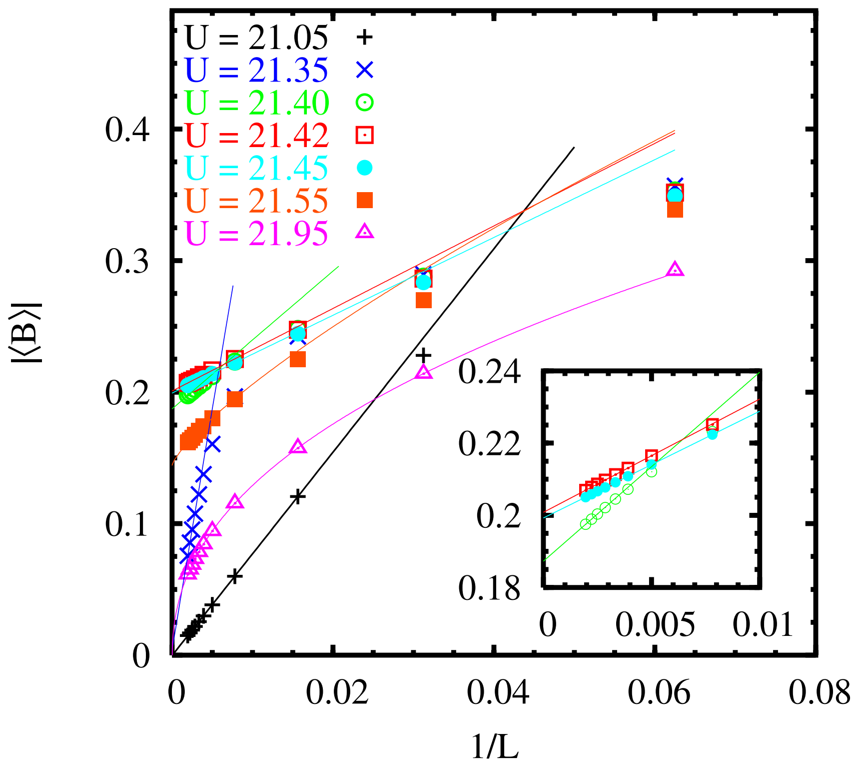
- Δ_e vanishes linearly at $U \equiv U_{c1}$
- Δ_s, Δ_1 nonzero at U_{c1}
- Δ_s vanishes at $U_{c2} > U_{c1}$

Bond Order Parameter

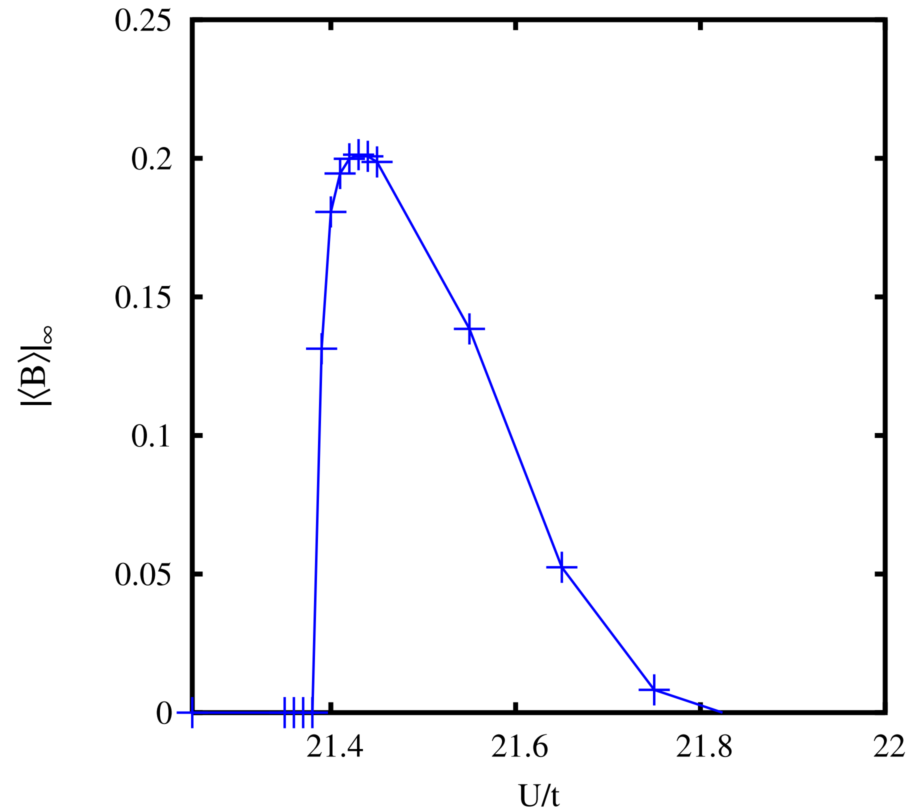
$\langle B \rangle$ can be nonzero for open BCs

$$\delta/t = 20$$

L–scaling



extrapolated value



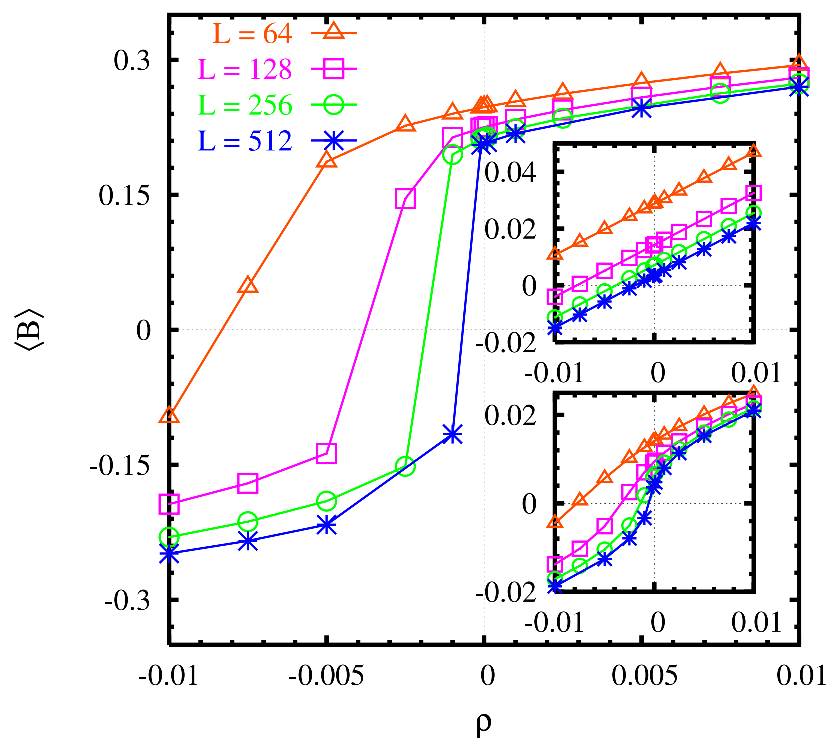
In the band insulator $\langle B \rangle \sim \frac{1}{L}$, in the Mott phase $\langle B \rangle \sim \frac{1}{\sqrt{L}}$

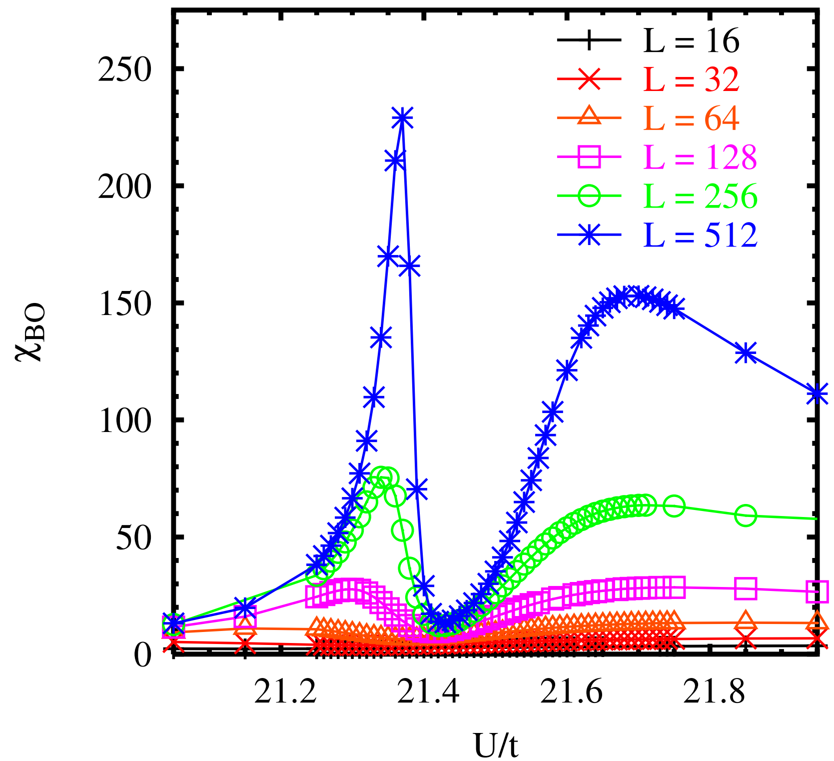
very small region with dimerization

Characterizing the Dimerization Transition(s)

Bond-Order susceptibility $\chi_{\rm BO} = \left.\frac{\partial\langle B\rangle}{\partial\rho}\right|_{\rho=0^+}$ $(\delta/t = 20)$

$U/t = 21.42, [19, 50]$





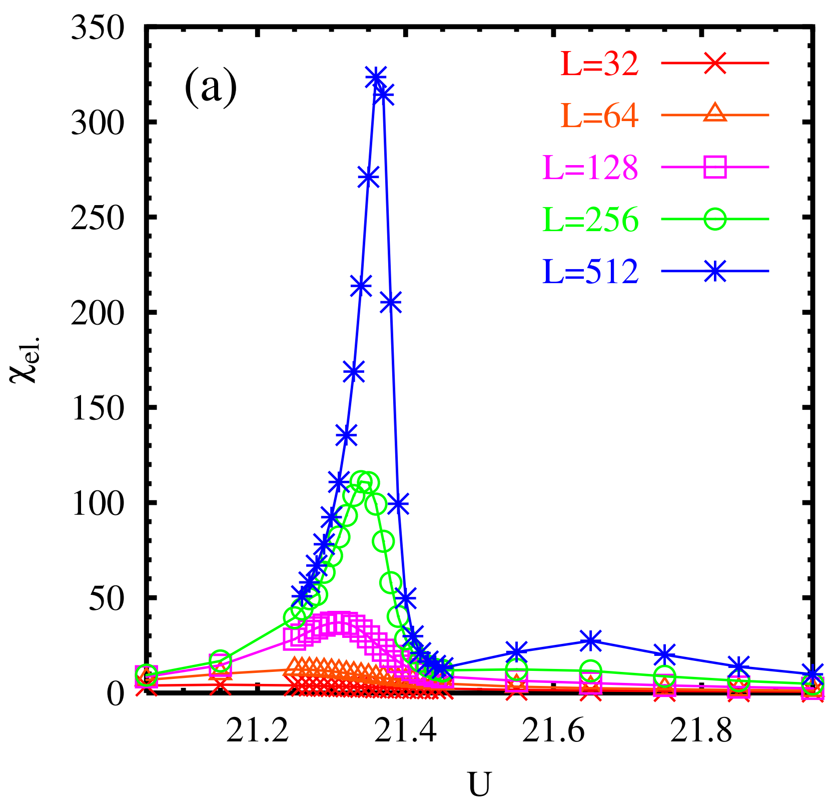
⇒ Two peaks, two divergences – two transitions

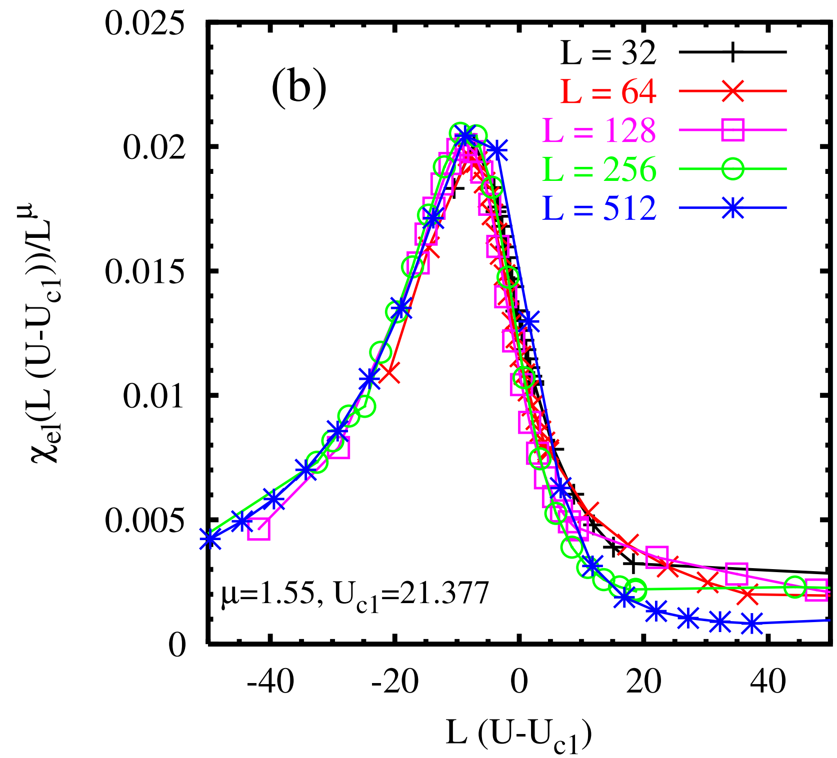
Complication: $\chi_{\rm BO}$ diverges in entire Mott insulator

Electric Susceptibility

Response to an applied electric field $\boldsymbol{E} = E\hat{\boldsymbol{x}}$ (along chain) $(\delta/t = 20)$

$$\chi = \frac{\partial \langle \mathcal{P} \rangle}{\partial E}\bigg|_{E=0} = -\frac{1}{L}\frac{\partial^2 E_0(E)}{\partial E^2}\bigg|_{E=0} \approx \frac{1}{LE}\sum_i x_i \langle n_i \rangle$$

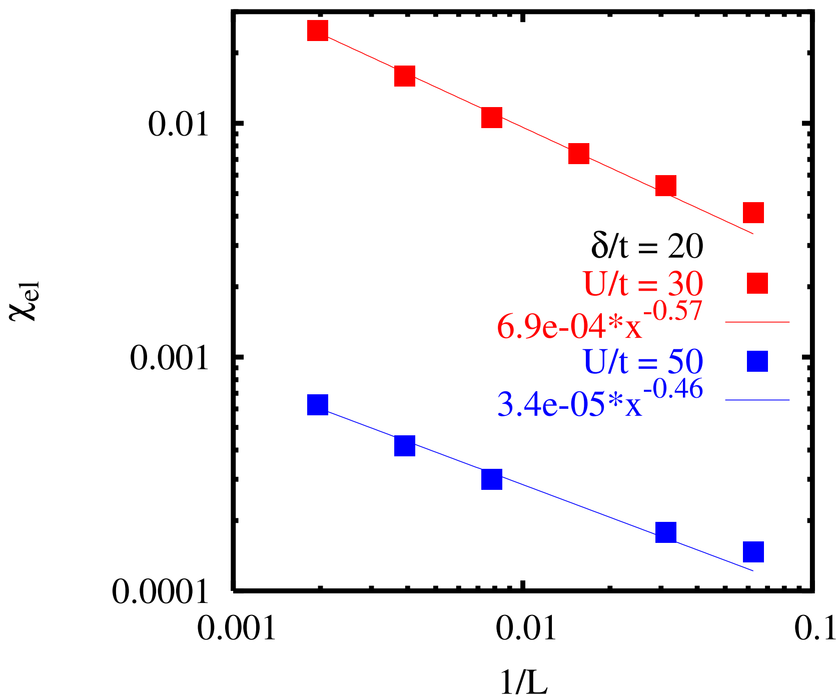


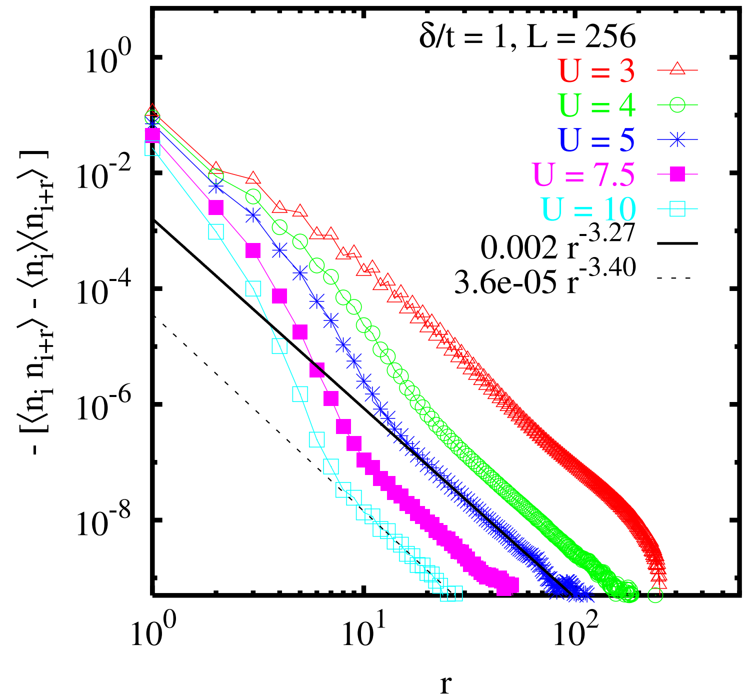


- diverges at the "metallic" point - U_{c1}
- finite-size scaling $\Rightarrow$ collapse, $\chi(U_{c1}) \sim L^{2-\eta}, \eta = 0.46$??

Strong Coupling Phase ($U \gg \delta$)

$$C_d(r) = \langle n_i n_{i+r} \rangle - \langle n_i \rangle \langle n_{i+r} \rangle$$





- Weak, but clear divergence in $\chi_{\rm el}$ in the strong coupling phase
  $\Rightarrow$ metal? strange Mott insulator?
- Power–law decay of density-density correlation function $\Rightarrow C_d(r) \sim r^{-3}$

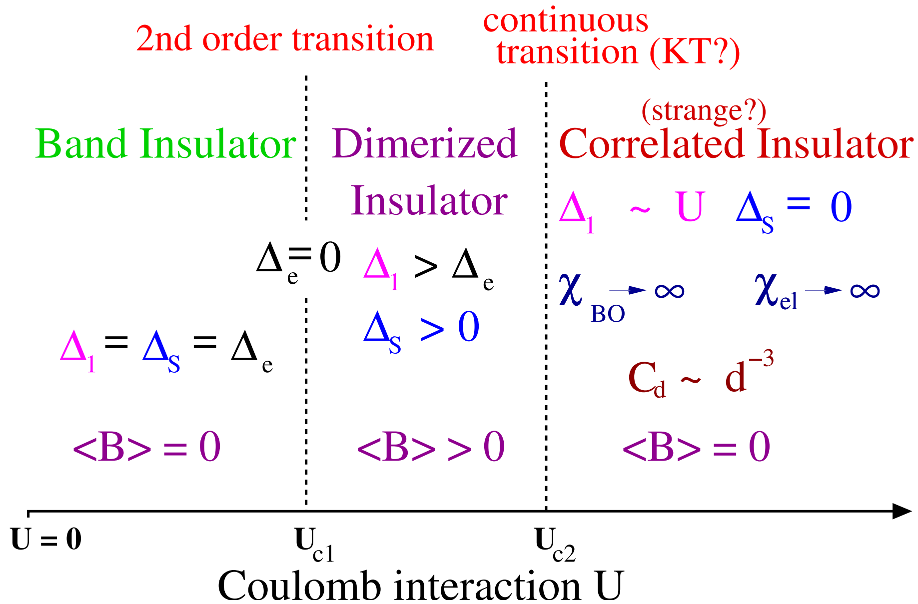
Explanation: strong coupling expansion for

$$C_d(r) \approx A\,(-1)^r\left[\langle(\mathbf{S}_i\cdot\mathbf{S}_{i+1})\,(\mathbf{S}_{i+r}\cdot\mathbf{S}_{i+r+1})\rangle - \langle\mathbf{S}_i\cdot\mathbf{S}_{i+1}\rangle\langle(\mathbf{S}_{i+r}\cdot\mathbf{S}_{i+r+1}\rangle\right]$$
$$\sim r^{-3}\ln^{-3/2} r$$

(A. Aligia, 2004)

Discussion

Our generic phase diagram:



$\Rightarrow$ Two transitions, spontaneously dimerized intermediate phase, in agreement with the scenario of Fabrizio, Gogolin, & Nersesyan, 1999.

Remaining Issues

- Is the system metallic at U_{c1}?
- Dynamical correlation functions: charge, spin, single-particle.
- Nature of "strange" Mott insulator.
- Why is dimerized phase of width $\sim t$?
  $\Rightarrow$ Effective $S = 1$ model for $U \approx \delta$