Ionic Hubbard chain at half filling

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1) Model
2) 3 Phases
3) Arguments for the intermediate phase
4) Fractional charge excitations
5) Methods of crossings of excited levels and jumps in Berry phases
6) Phase diagram
7) Charge correlations in the MI phase
8) Transport through a ring

The model:

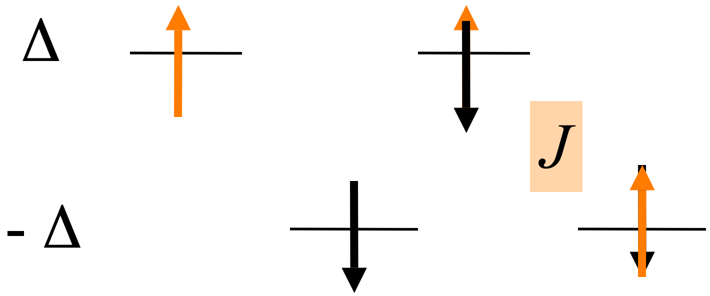
$$
\begin{aligned}
H &= -t\sum_{i\sigma}(c^\dagger_{i+1\sigma}c_{i\sigma} + \mathrm{H.c.}) + \Delta\sum_{i\sigma}(-1)^i n_{i\sigma} \\
&\quad + U\sum_i n_{i\uparrow}n_{i\downarrow}.
\end{aligned}
$$

Interest:

1) Neutral-ionic transition in mixed-stack donor-acceptor organic crystals ...DADADA… (Avignon, Balseiro, Proetto, Alascio, Phys. Rev. B 33, 205 (1986))

2) Ferroelectric perovskites (Egami et al., Science 261, 1307 (1993), R. Resta and S. Sorella, Phys. Rev. Lett. 74, 4738 (1995), Fabrizio, Gogolin, Nersesyan, ibid 83, 2014 (1999))

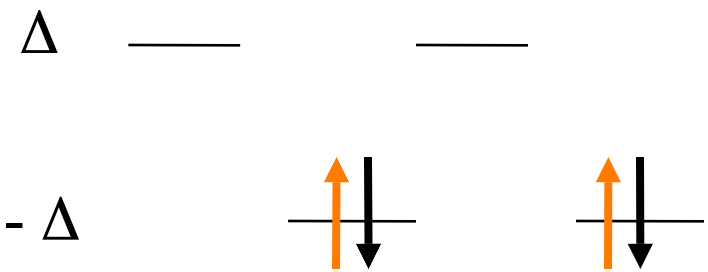
Phases of the model:



$t << U - 2\Delta$ **MI**

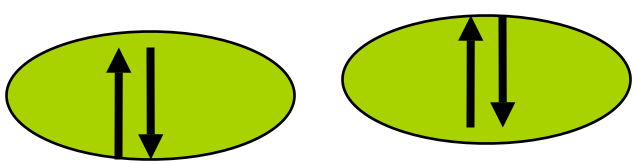
Mott insulator

$J = 2t^2/(U - 2\Delta) + 2t^2/(U + 2\Delta)$



$t << 2\Delta - U$ **BI**

Band insulator



$t > 2\Delta - U$

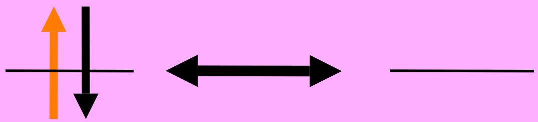
BOW or **SDI**

Arguments for the existence of the intermediate SDI phase

a) bosonization (Fabrizio et al.)

b) Mapping to an SU(3) AF Heisenberg (Batista-Aligia)

1) Electron-hole transformation at sites with energy - Δ



2) Elimination of doubly occupied sites

3) Mapping of the remaining three states into an SU(3) spin

Inclusion of nearest-neighbor repulsion V

SU(3)

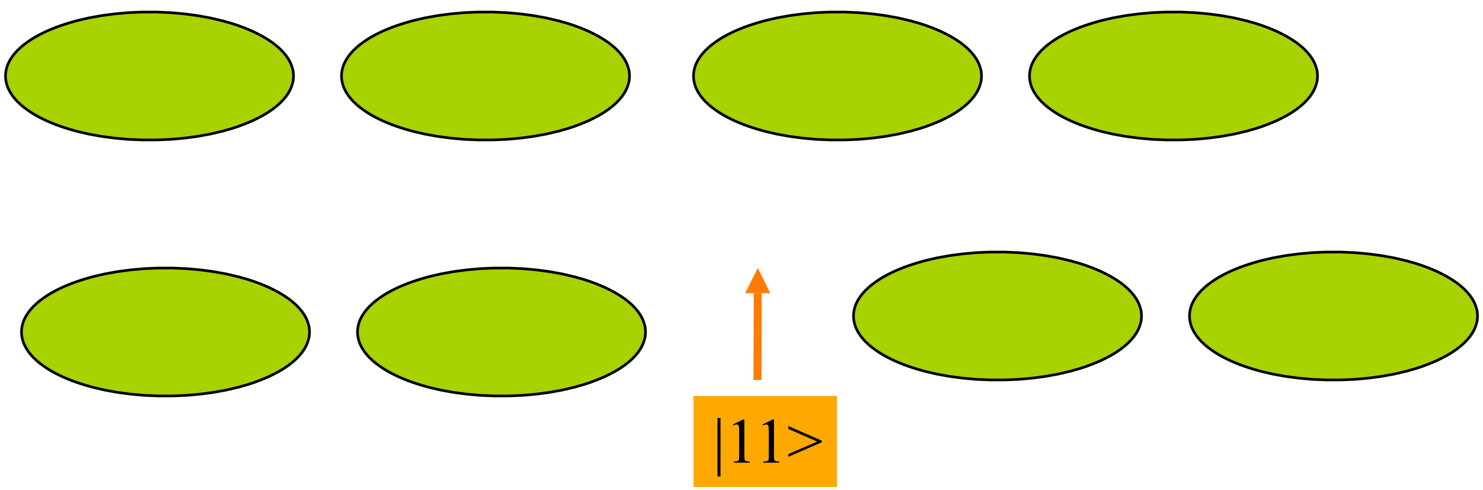
$$H_{eff} = \sum_{i\in A} J_{\mu\nu} S^{\mu\nu}(i)\bar{S}^{\nu\mu}(i+1) - B\sum_i S^{11}(i), \quad (1)$$

For $V = J/2 = t$ and $U = 2\Delta$, H_{eff} is an *isotropic* SU(3) *antiferromagnetic Heisenberg model*, $J_{\mu\nu} = -t$, $B = 0$. ITS GROUND STATE IS DIMERIZED. Also for $V = J/2 = t$

S=1

$$H_{eff} = -t\sum_i (\mathbf{S}_i \cdot \mathbf{S}_{i+1})^2 + (\Delta - U/2)\sum_i (S_i^z)^2. \quad (2)$$

Original charge $Q = \Sigma_i (-1)^i |S_i^z|$.



Method of crossings of excited levels **(weak coupling):**

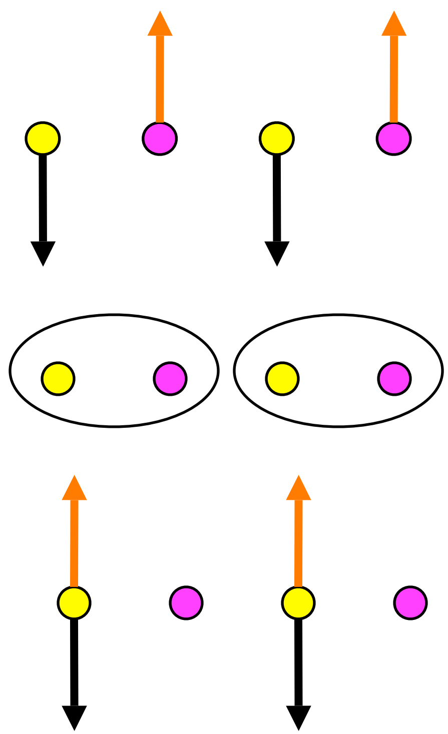
For critical systems: $\langle O_i O_{i+d} \rangle \propto \frac{1}{d^{\lambda}}, E_o - E_g = \frac{\pi v \lambda}{L}$

Then, crossing of two excited levels denotes a change of phase

MI or SDW

BOW or SDI

BI or CDW



S_{ix}

B_i

n_i

$S = 1, k = 0, P = -1$

Spin transition

$S = 0, k = 0, P = 1$

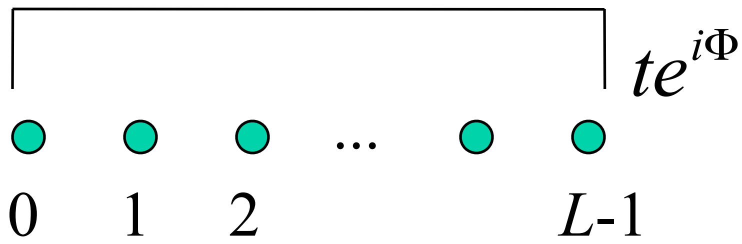
$S = 0, k = \pi, P = -1$

Charge transition

$S = 0, k = \pi, P = 1$

OPEN SHELL BC

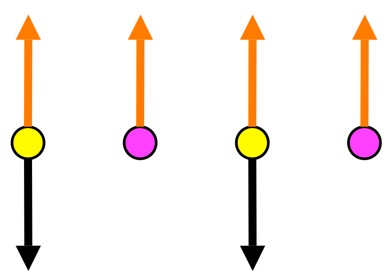
Method of jumps of Berry phases **(strong coupling):**



$$c^{+}_{L\sigma} = e^{i\Phi} c^{+}_{0\sigma}$$

Charge Berry phase g: phase captured by the ground state in the cycle $0 < \Phi < 2\pi$

a) In systems with inversion symmetry g = 0 or π (mod. 2π)
b) Changes in polarization $\Delta P = \Delta\, \mathrm{g}(e/2\pi)$



BI or CDW g = 0

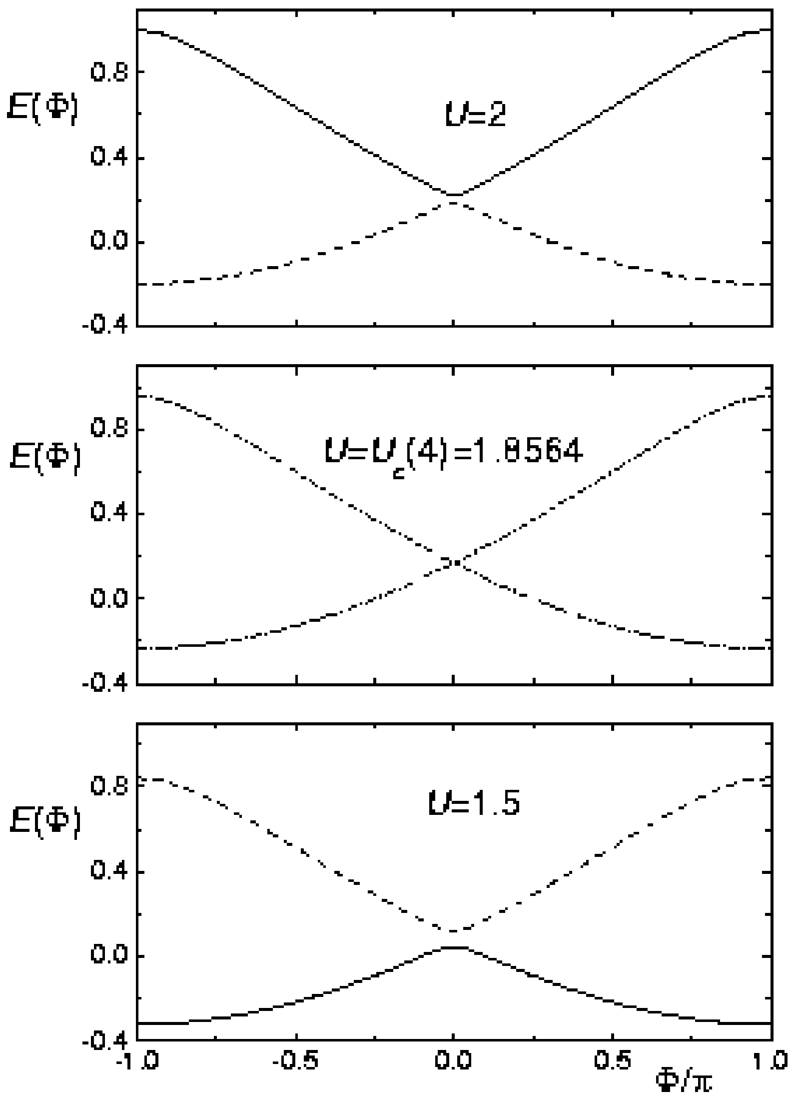
MI or SDW g = π

Spin Berry phase g_s

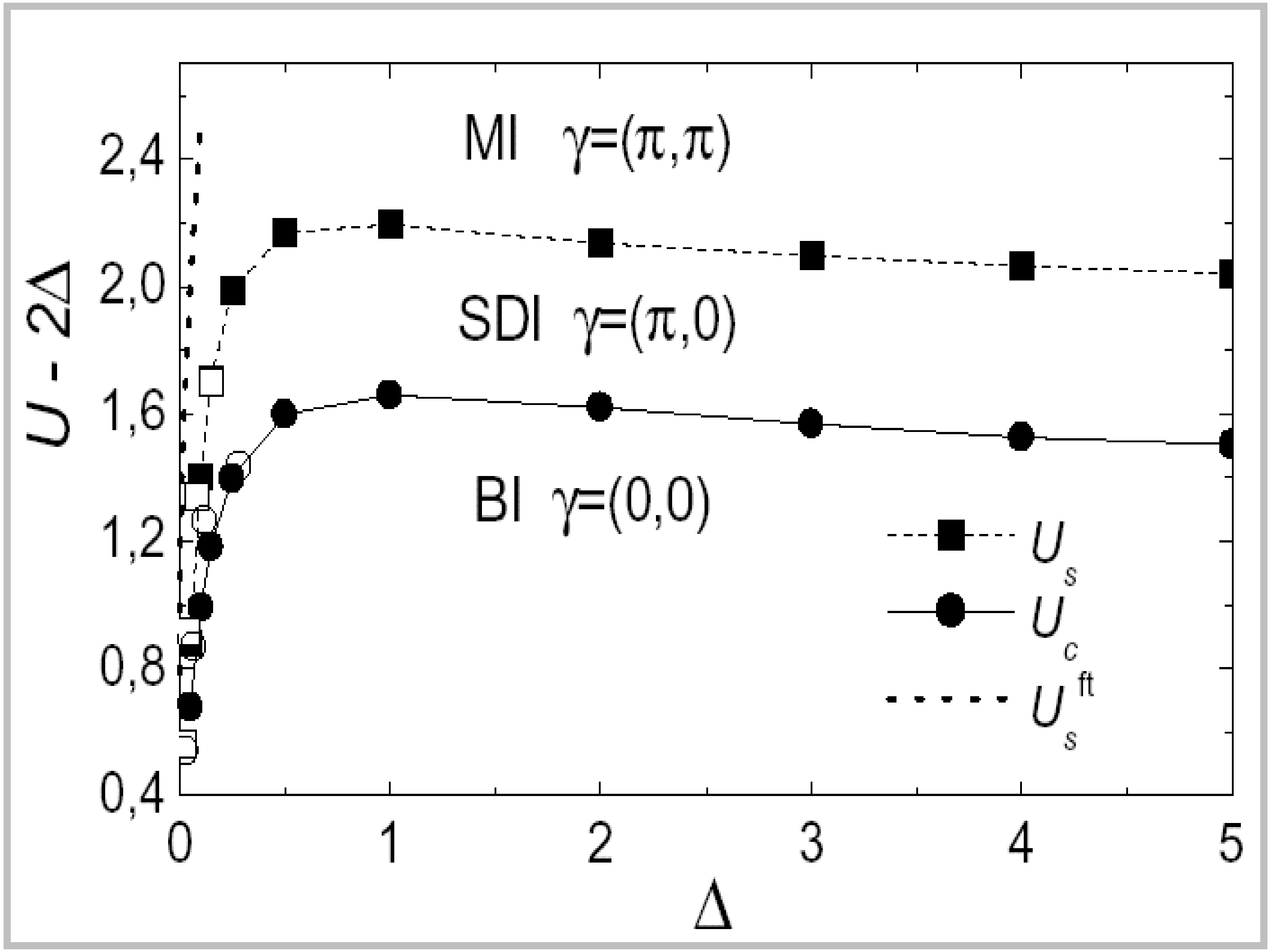
$$c_{L\sigma}^{+} = e^{i\sigma\Phi} c_{0\sigma}^{+}$$

$\Delta = 0$, $V = 1$

Both methods coincide!!



Phase diagram

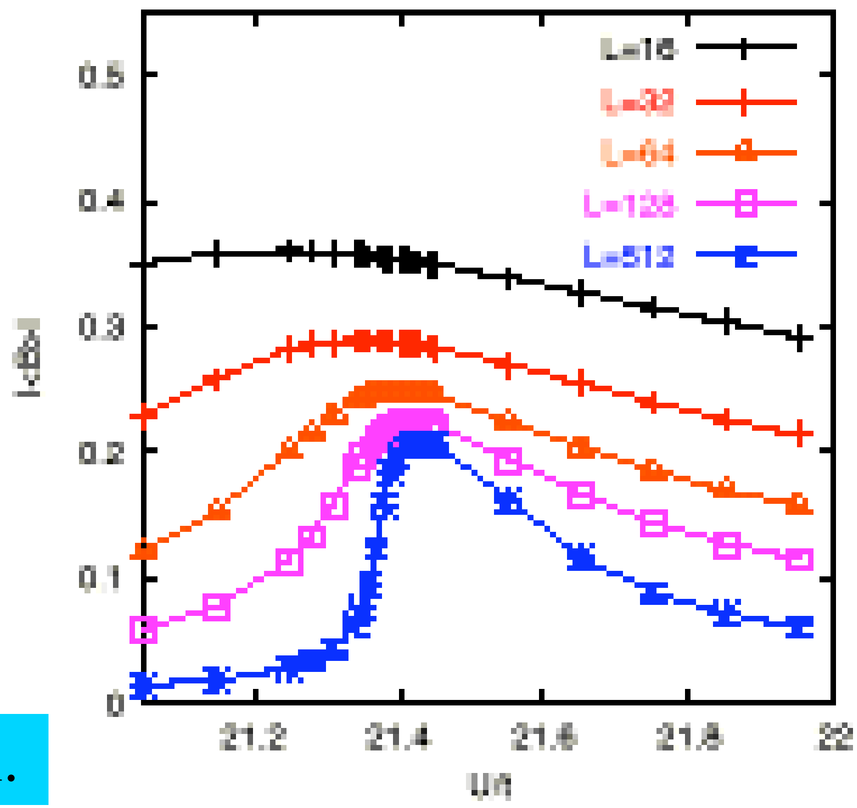


Bond Order Parameter

$$B \equiv \frac{1}{L-1} \sum_{j,\sigma} (-1)^j \left[c^\dagger_{j\sigma} c_{j+1\sigma} + \text{h.c.} \right]$$

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

d=2
Δ

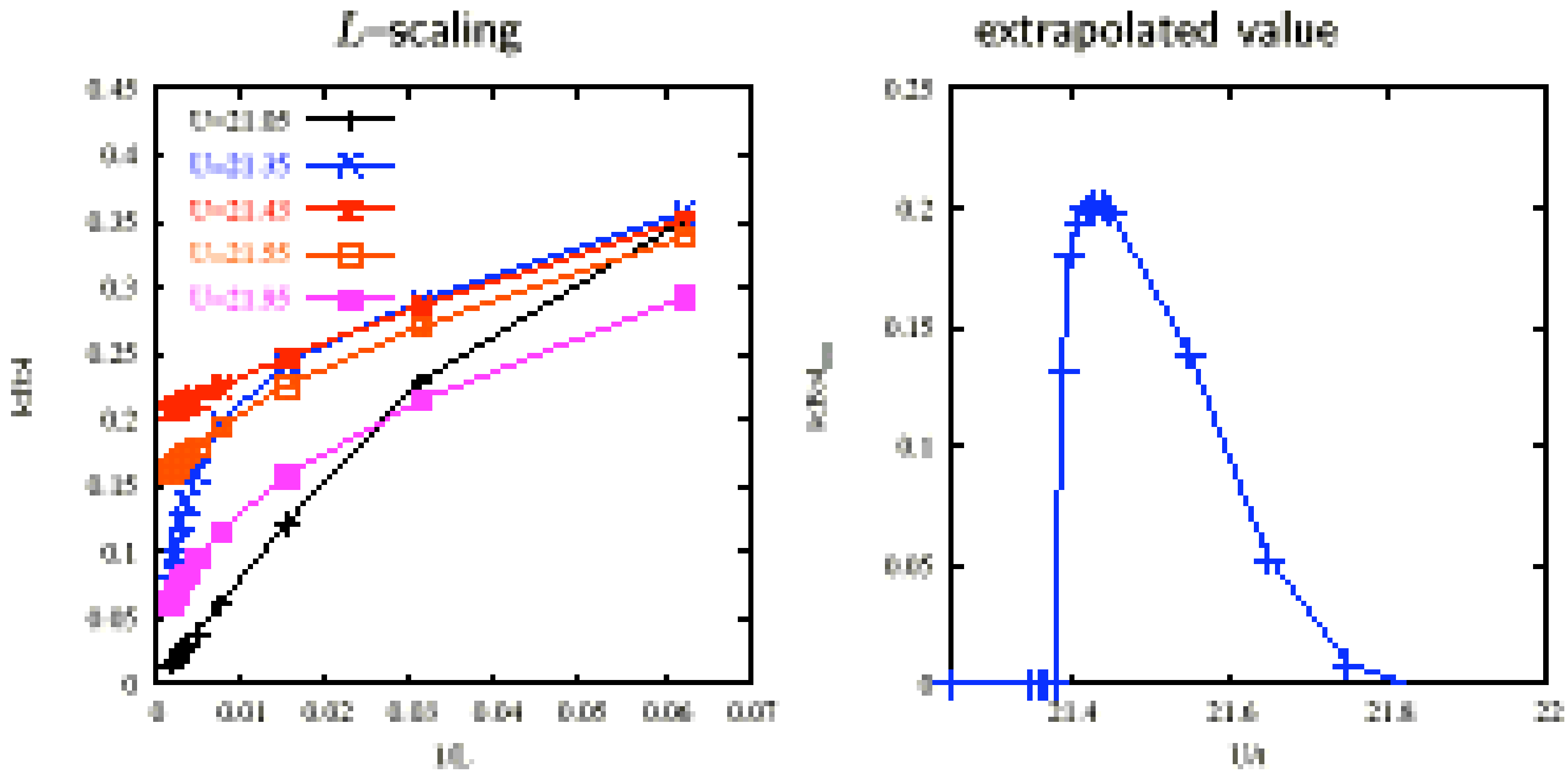


$\delta/t = 20$

S. Manmana et al.

Bond order parameter: $L \to \infty$ extrapolation

$\delta/t = 20$

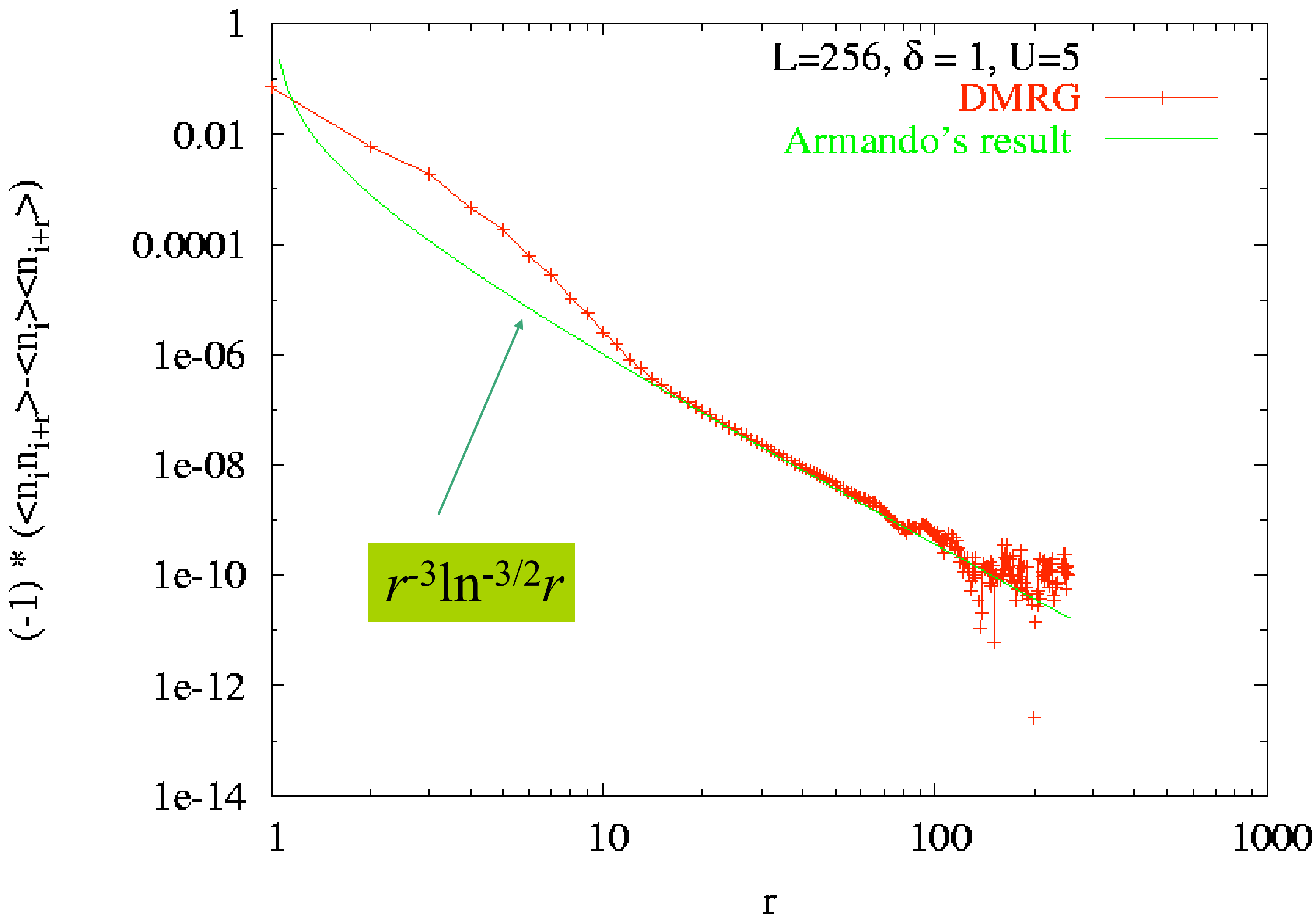


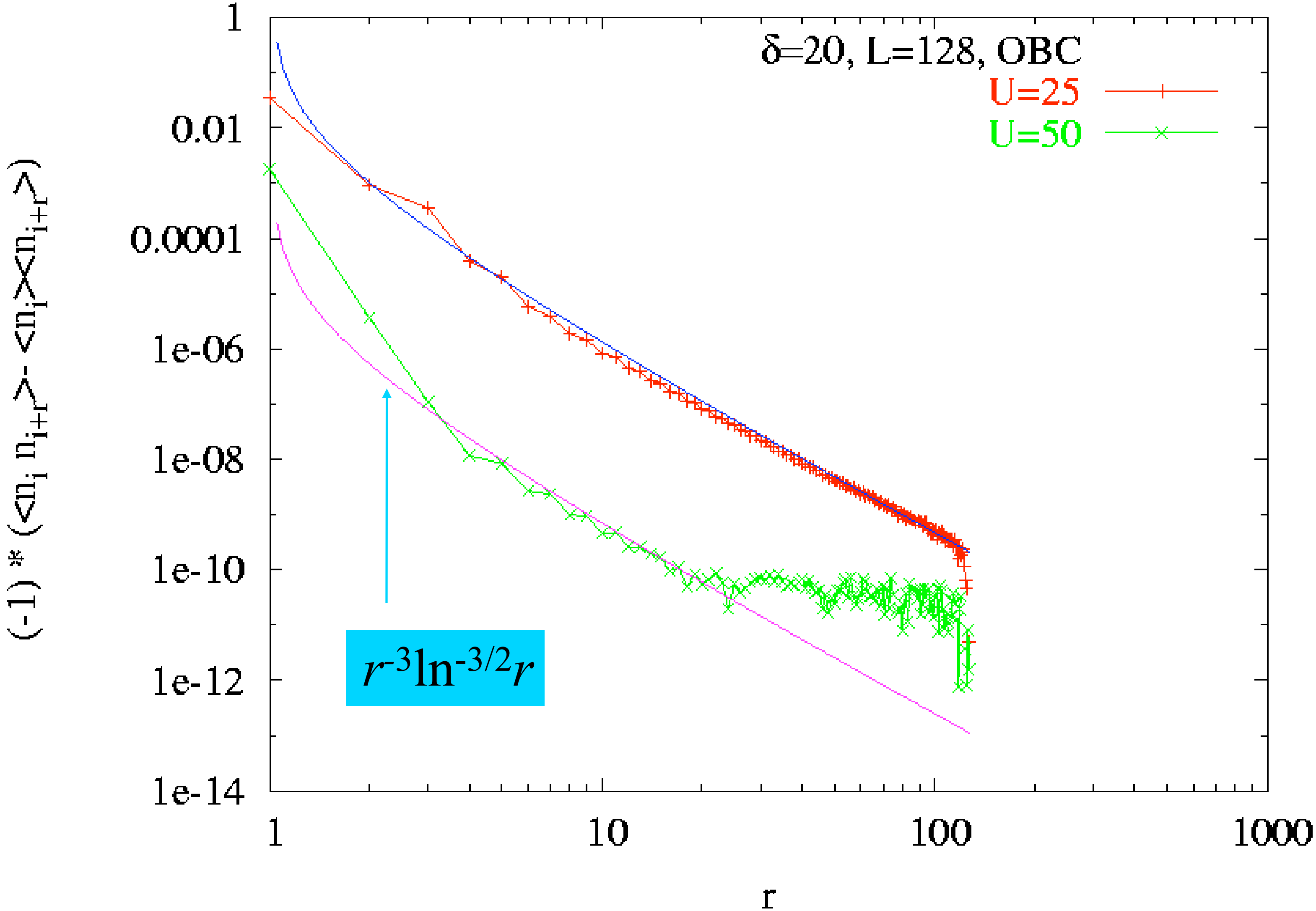
In the band insulator $\langle B \rangle \sim \frac{1}{L}$, in the Mott phase $\langle B \rangle \sim \frac{1}{\sqrt{L}}$

very small region with dimerization

S. Manmana et al.

Charge-charge correlation functions in the MI phase





δ=20, L=128, OBC
U=25
U=50
$r^{-3}\ln^{-3/2}r$
(-1) * (<n_i n_{i+r}>- <n_i><n_{i+r}>)
r
1
0.01
0.0001
1e-06
1e-08
1e-10
1e-12
1e-14
1
10
100
1000

Under a canonical transformation for $t \ll U - 2\Delta$

$$\tilde{H} = Pe^{-S} H e^{S} P = \frac{4t^2 U}{(U^2 - 4\Delta^2)} \sum_{\langle ij \rangle} (\mathbf{S}_i \cdot \mathbf{S}_j - \frac{1}{4}). \tag{1}$$

Doing the same with the charge operator:

$$\tilde{n}_i = 1 - (-1)^i \frac{4U\Delta t^2}{(U^2 - 4\Delta^2)^2} \sum_{\delta = \pm 1} (1 - 4\mathbf{S}_i \cdot \mathbf{S}_{i+\delta}). \tag{2}$$

After a Jordan Wigner trans. and bosonization:

$$\sum_{\delta} (S_j^+ S_{j+\delta}^- + \text{H.c.}) \to \sum_{\delta} ((a_j^\dagger a_{j+\delta} + \text{H.c.}) \to c(-1)^j \frac{\partial}{\partial x} \cos(\sqrt{2}\varphi) + \ldots \tag{3}$$

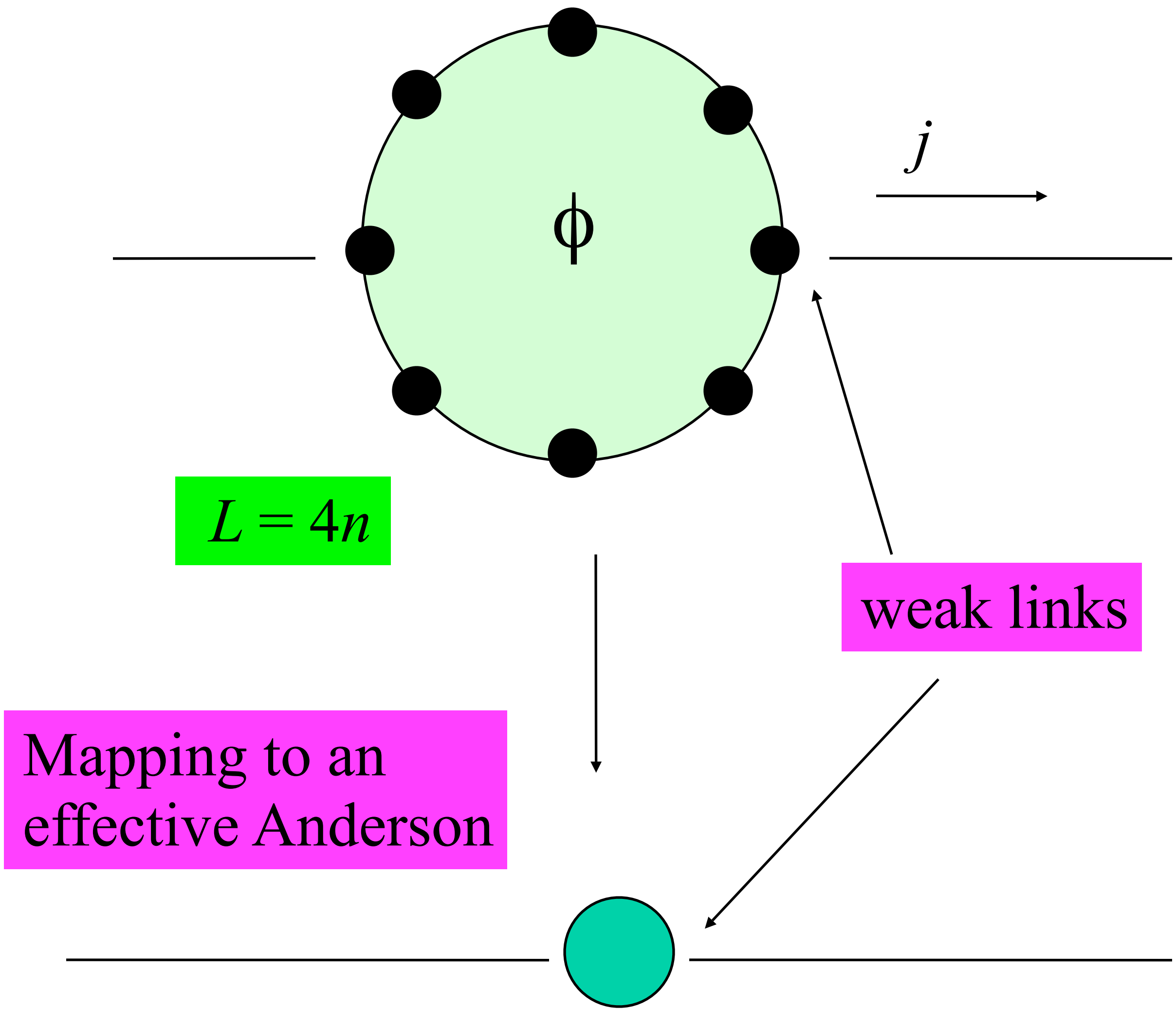
Using:

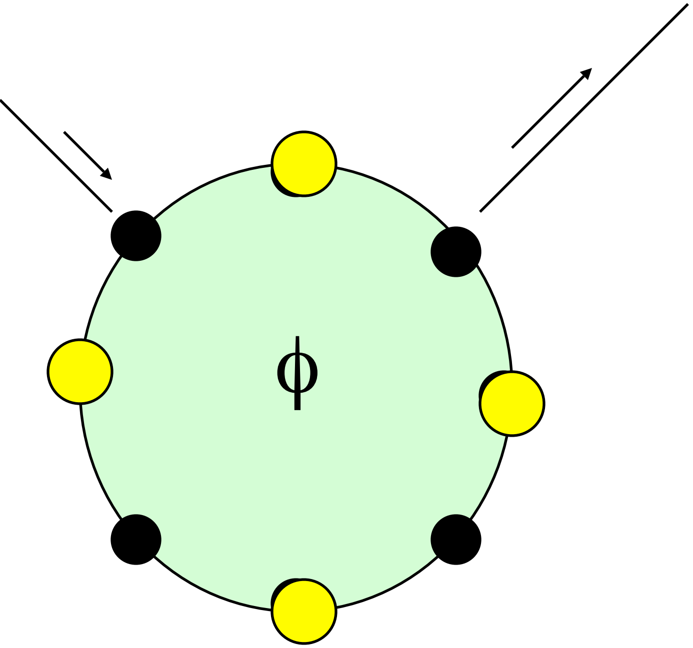
$$\langle : \cos(\sqrt{2}\varphi(x)) :: \cos(\sqrt{2}\varphi(y)) : \rangle \sim \frac{1}{|x - y| \ln^{3/2} |x - y|}, \tag{4}$$

one obtains:

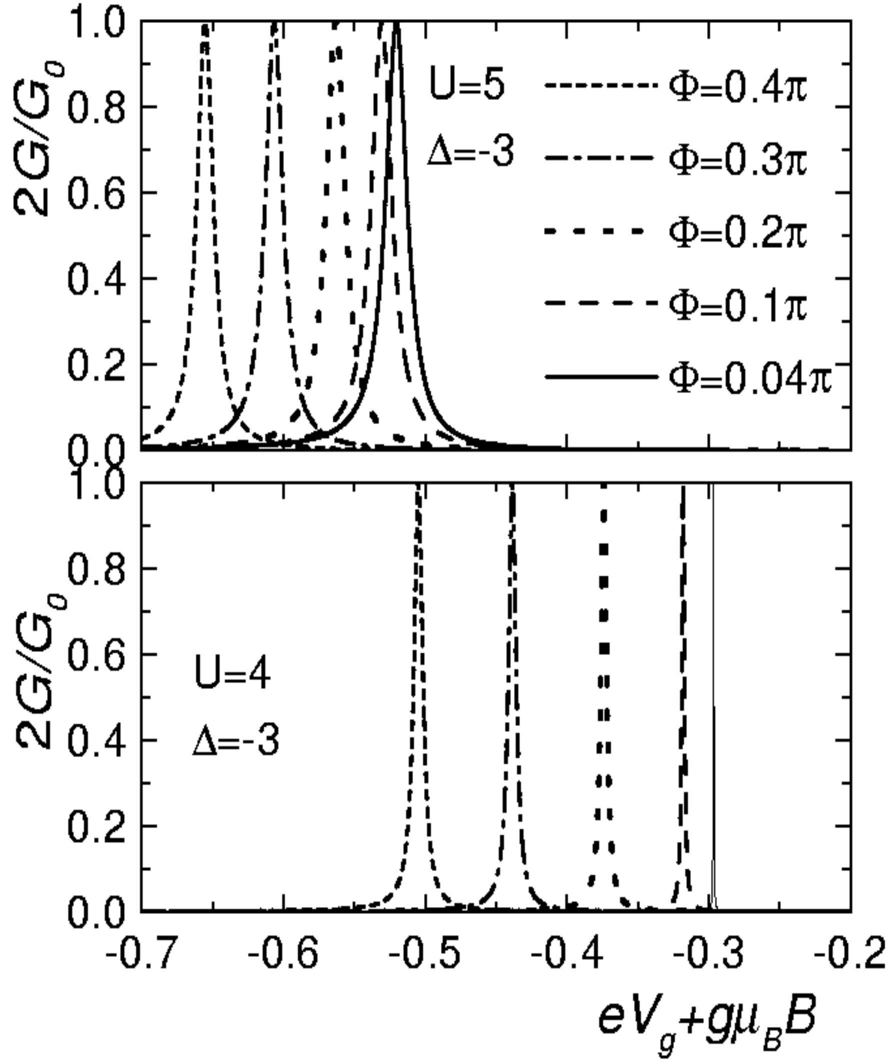
$$\langle n_i n_{i+d} \rangle - \langle n_i \rangle_H \langle n_{i+d} \rangle \approx d^{-3} \ln^{-3/2} d. \tag{5}$$

Measuring the charge transition

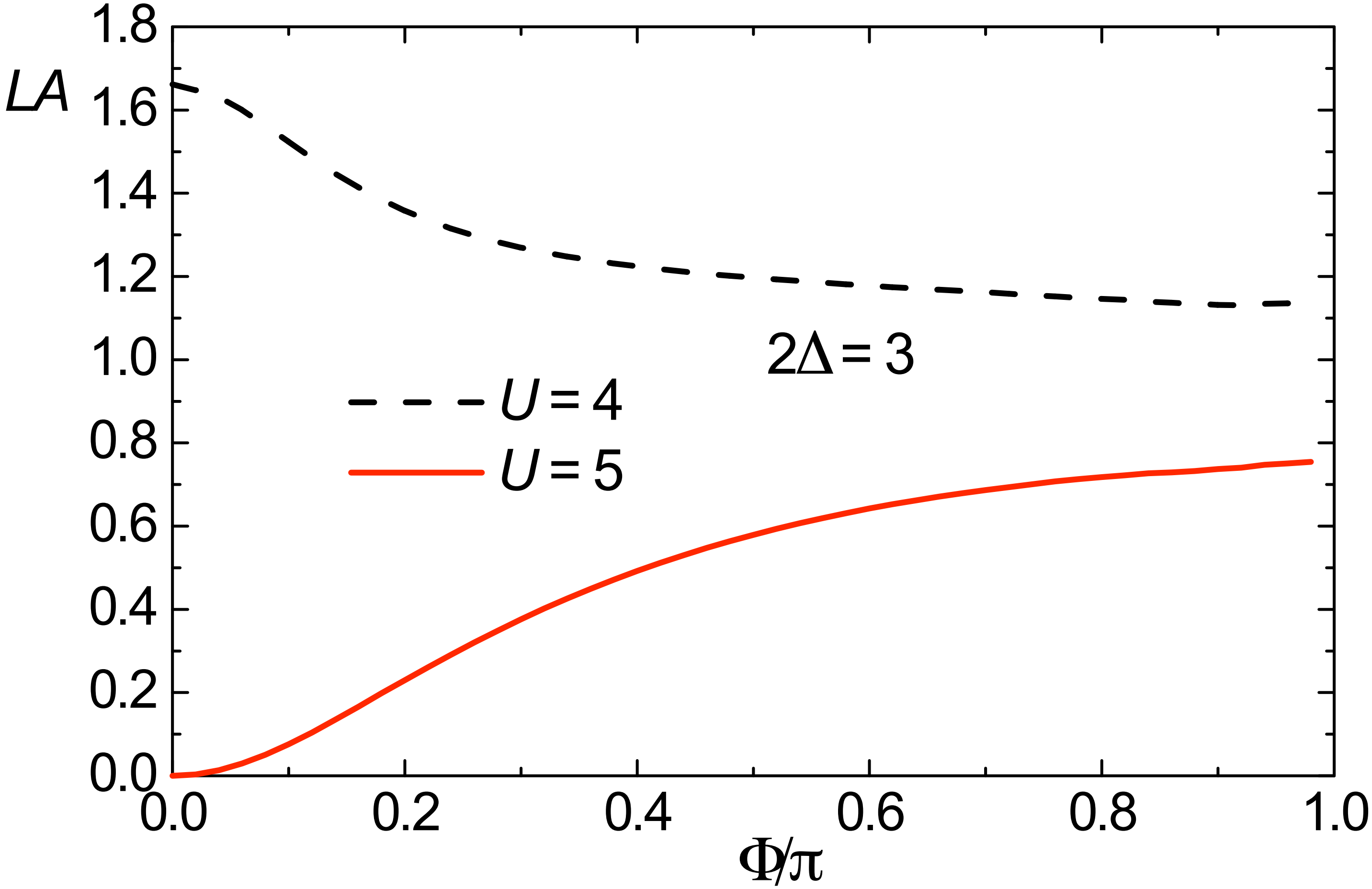




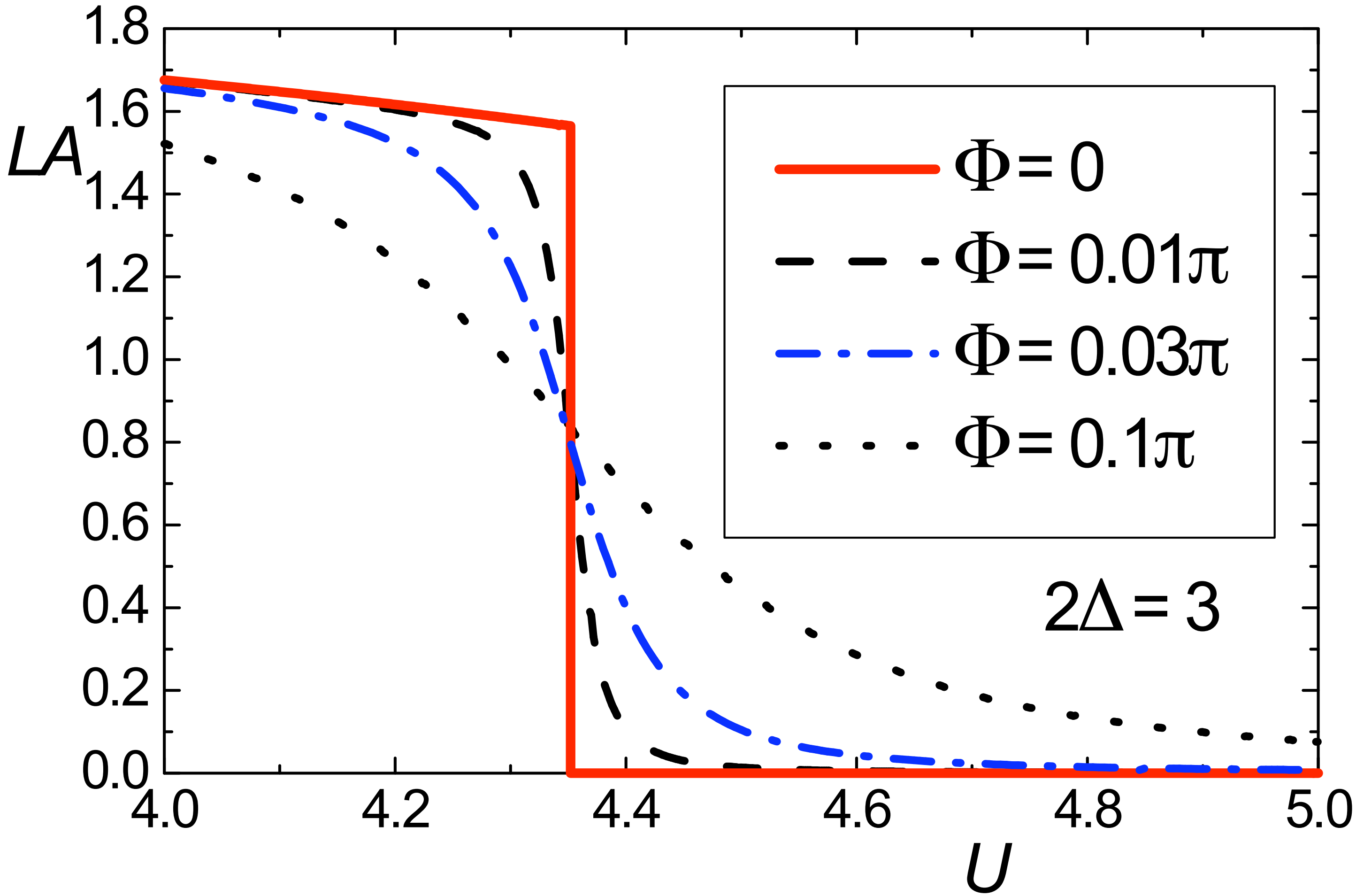
$B>>T_K$



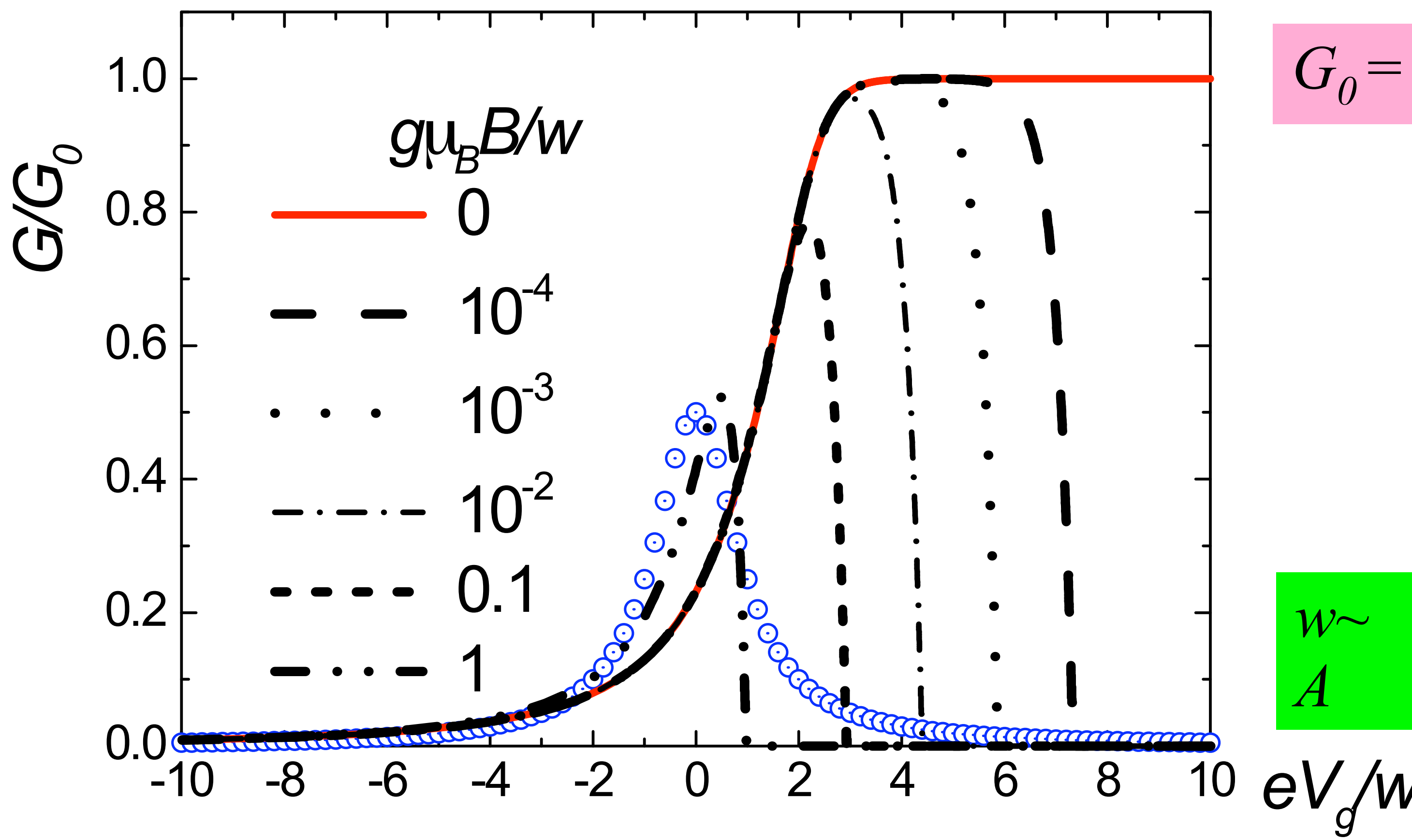
Intensity of the first peak in the transmittance



Intensity of the first peak in the transmittance



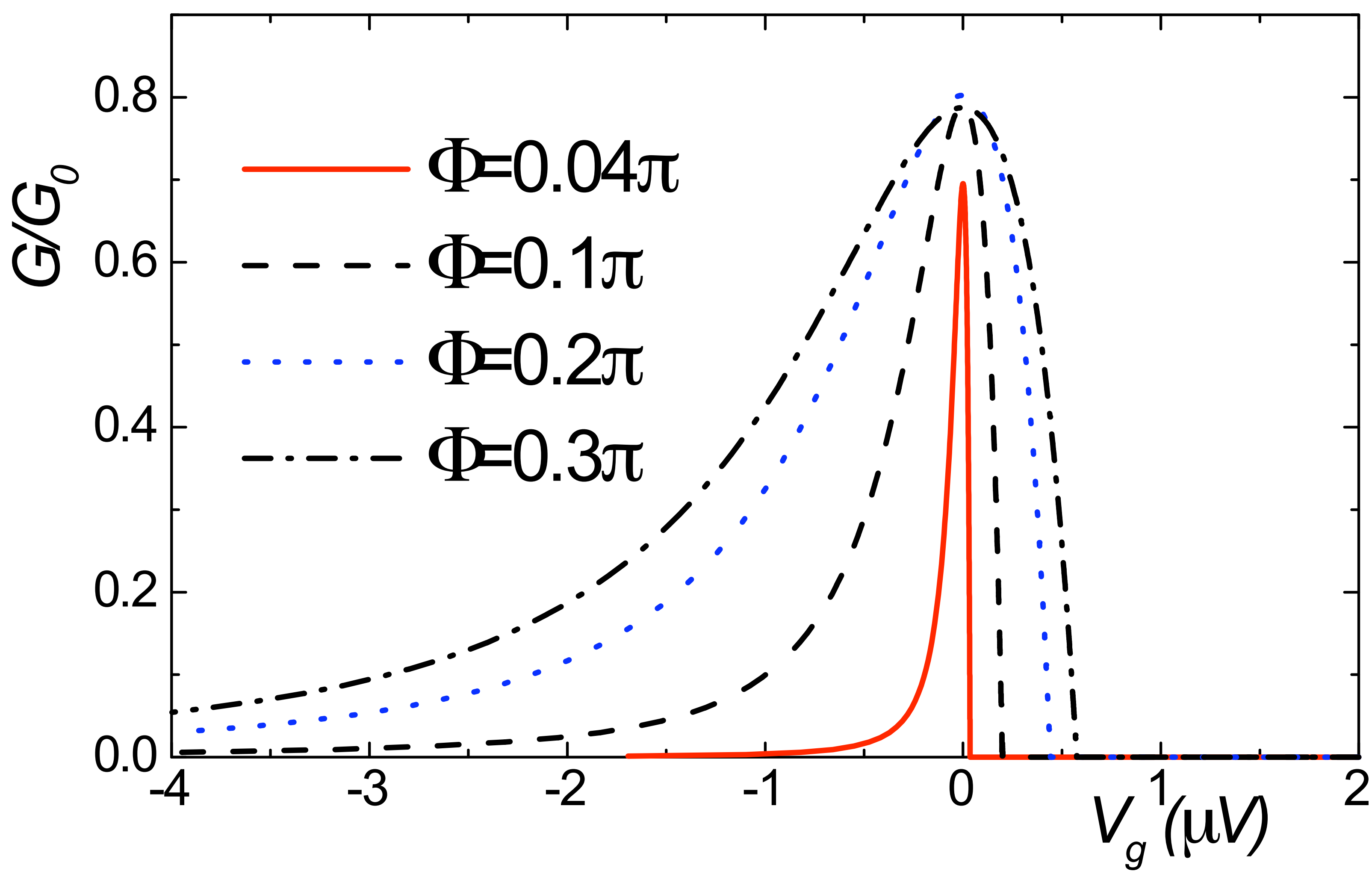
Conductance effective Anderson



$G_0 = 2e^2/h$

$w \sim A$

R.L.Width *w* proportional to quasiparticle weigth *A*



G/G$_0$
0.8
0.6
0.4
0.2
0.0
-4
-3
-2
-1
0
1
2
V_g (μV)
Φ=0.04π
Φ=0.1π
Φ=0.2π
Φ=0.3π

Conclusions

The transition from the BI tothe MI takes place through an intermediate dimerized **ferroelectric** phase

The topological jumps allow to determine **accurately** the transitions

Charge correlations in the MI phase have **power law** decay due to **relevant** coupling between charge and spin

The topological transition can be measured in nanodevices or molecules

References:

Phase diagram: M.E. Torio, A.A. Aligia, and H.A. Ceccatto, Phys. Rev. B 64, 121105 (2001) (Rapid Comm)

Dimerized phase: C.B. Batista and A.A. Aligia, Phys. Rev. Lett. 92, 246405 (2004) ; Phys. Rev. B 71, 125110 (2005).

Charge dynamics in the MI phase: A.A. Aligia, Phys. Rev. B 69, 041101(R) (2004) (Rapid Comm.)

Transport through a ring: A.A. Aligia, K. Hallberg, A.P. Kampf, B. Normand, Phys. Rev. Lett. 93, 076801 (2004)

Fractional charge excitations from phenomenological G-L energy:

$F = g_8 a_c^2 + g_1 a_s^2 + \Delta a_c a_s,$

$a_\nu = \cos(\sqrt{2}\phi_\nu)$. with $g_1 < 0$, $g_8 > 2\Delta$.

Minimum for either $a_c = \Delta/(2g_8)$, $a_s = -1$ or $a_c = -\Delta/(2g_8)$, $a_s = 1$.

$\Delta\phi_c = \pm C_{1/2}(\pi/\sqrt{2})$, $C_{1/2} = 1 - 2\arccos[\Delta/(2g_8)]/\pi$.

$C_0 = 1 - C_{1/2}$.

Polarization

$P - P_0 = \frac{e}{2\pi}\gamma_c = \lim_{L\to\infty} \frac{e}{2\pi} \mathrm{Im}\ln z_L^c$

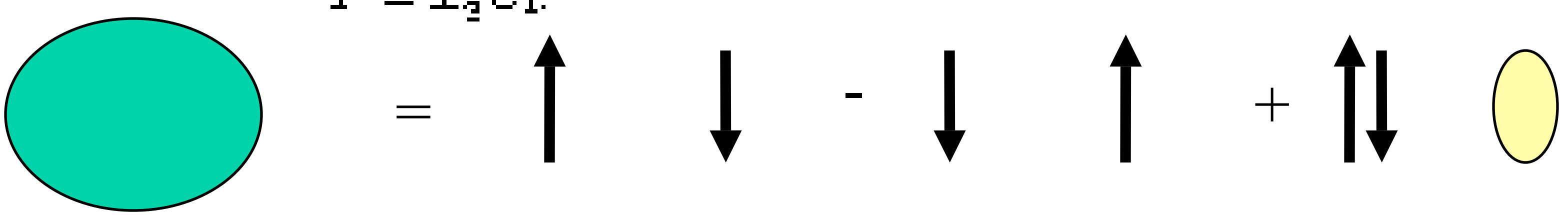
$z_L^c = \langle g|U_L^c|g\rangle$, $U_L^c = \exp[i\frac{2\pi}{La}X]$, $X = \sum_j ja(n_{j\uparrow} + n_{j\downarrow})$.

From bosonization:

$U_L^c = \exp(i\sqrt{8}\phi_c^0)$, $\phi_c^0 = \frac{1}{La}\int dx\phi_c(x)$.

$P = 0$ for the MI $\Longrightarrow P_0 = \pm e/2$. Then :

$P = \pm\frac{e}{2}C_1$.



Mapping to SU(3) AF Heisenberg

$$
\begin{aligned}
c^\dagger_{i\uparrow} &= -f_{i\downarrow}, \quad c^\dagger_{i\downarrow} = f_{i\uparrow}, \quad \text{for odd } i \\
c^\dagger_{i\sigma} &= f^\dagger_{i\sigma}, \qquad\quad \text{for even } i
\end{aligned} \tag{1}
$$

For $t \ll \Delta$ and $t \ll U$, but arbitrary $2\Delta - U$, we can eliminate the states with double occupancy on any site.

$$
\begin{aligned}
H_{eff} = -t\sum_i (c^\dagger_{i\uparrow} c^\dagger_{i-1\downarrow} - c^\dagger_{i\downarrow} c^\dagger_{i-1\uparrow} + \text{H.c.}) + \frac{2\Delta - U}{2}\sum_i n_i \\
+ \quad \sum_i \frac{2t^2}{U + 2\Delta}(\mathbf{s}_i \cdot \mathbf{s}_{i-1} - \frac{1}{4} n_i n_{i-1}) \\
+ \sum_{\delta = -1} \frac{t^2}{2\Delta} c^\dagger_{i-\delta\sigma} c_{i-\delta\sigma}(\frac{n_i}{2} + 2\mathbf{s}_i \cdot \mathbf{s}_{i-\delta}),
\end{aligned} \tag{2}
$$

Approximately:

$$
\begin{aligned}
H_{eff} = t\sum_{i,\sigma} (c^\dagger_{i,\sigma} c^\dagger_{i-1,\sigma} + \text{H.c.}) + \frac{2\Delta - U}{2}\sum_i n_i \\
+ J\sum_i (\sigma^z_i \sigma^z_{i-1} - \sigma^x_i \sigma^x_{i-1} - \sigma^y_i \sigma^y_{i-1} - \frac{1}{4} n_i n_{i-1}) \\
- V\sum_i (1 - n_i)(1 - n_{i-1}),
\end{aligned} \tag{3}
$$

At each site j of the A sublattice the mapping of the three states to the spin components is the following: $|j0\rangle \to |j1\rangle$ (the vacuum at site j is mapped to the first spin component), $c^\dagger_{j\uparrow} K_j |0\rangle \to |j2\rangle$, and $c^\dagger_{j\downarrow} K_j |0\rangle \to |j3\rangle$. Instead, for sublattice B the last two assignments are changed to $c^\dagger_{j\uparrow} K_j |0\rangle \to -|j2\rangle$, and $c^\dagger_{j\downarrow} K_j |0\rangle \to -|j3\rangle$.

Opening of a spin gap as U decreases: MI $\longrightarrow$ SDI transition

$$Z = \int D\varphi_c \varphi_s e^{-S}, S = S_c + S_s + S_{cs}$$

$$S_c = \frac{1}{2}\int d\tau\, dx [\frac{1}{v_c}(\partial\tau\varphi_c)^2 + v_c(\partial_x\varphi_c)^2 + \frac{g_{3\perp}}{(\pi a)^2}\cos(\sqrt{8\pi K_c}\varphi_c)]$$

$$S_c = \frac{1}{2}\int d\tau\, dx [\frac{1}{v_c}(\partial\tau\varphi_c)^2 + v_c(\partial_x\varphi_c)^2 + \frac{m}{v_c}\varphi_c^2]$$

$$S_s = \frac{1}{2}\int d\tau\, dx [\frac{1}{v_s}(\partial\tau\varphi_s)^2 + v_s(\partial_x\varphi_s)^2 + \frac{g_{1\perp}}{(\pi a)^2}\cos(\sqrt{8\pi K_s}\varphi_s)]$$

$$S_{cs} = \int d\tau\, dx \frac{2\Delta}{\pi a}\cos(\sqrt{2\pi K_c}\varphi_c)\cos(\sqrt{2\pi K_s}\varphi_s)$$

$$S_{cs} \cong \int d\tau\, dx \frac{2\Delta}{\pi a}\sqrt{2\pi K_c}\varphi'_c \cos(\sqrt{2\pi K_s}\varphi_s) = \int d\tau\, dx A\varphi'_c$$

$$Z = \int D\varphi_s e^{-S_{eff}} Z_c, Z_c = \int D\varphi_c e^{-S_c}, S_{eff} = S_s + S'$$

$$S' = -\ln[\int D\varphi_c e^{-S_c - S_{cs}}] + \ln Z_c = -\ln\left\langle e^{-S_{cs}} \right\rangle_c$$

$$S' = -\frac{1}{2}\left\langle \int d\tau_1 dx_1 d\tau_2 dx_2 A(\tau_1, x_1)\varphi_c(\tau_1, x_1) A(\tau_2, x_2)\varphi_c(\tau_2, x_2) \right\rangle_c$$

$$S' \cong -\frac{1}{2}\int d\tau_a dx_a A^2(\tau_a, x_a)\left\langle \int d\tau_d dx_d \varphi_c(0,0)\varphi_c(\tau_d, x_d) \right\rangle_c =$$

$$S' \cong -\frac{1}{2}\int d\tau_a dx_a \frac{4\Delta^2 K_c}{\pi a^2}(1 + \cos[\sqrt{8\pi K_s}\varphi_s(\tau_a, x_a)])\frac{v_c}{m^2}$$

$$S_s = \frac{1}{2}\int d\tau dx[\frac{1}{v_s}(\partial_\tau \varphi_s)^2 + v_s(\partial_x \varphi_s)^2 + \frac{g_{1\perp}}{(\pi a)^2}\cos(\sqrt{8\pi K_s}\varphi_s)]$$

$$g'_{1\perp} = g_{1\perp} - \frac{4\pi\Delta^2 v_c K_c}{m^2} = Ua - \pi v_c K_c \left(\frac{2\Delta}{m}\right)^2$$