

Using defects to probe strongly-correlated many-body states

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Acknowledgements:

Discussions: S. Chandrasekharan, M. Metliski, O. Motrunich &
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Impurities yield information about host materials

- ▶ Impurities can be useful probes of interesting low temperature states of matter
Alloul et. al. Rev. Mod. Phys. 81, 45 (2009).
e.g Zn and Ni doping in CuO_2 planes of high- T_c superconductors
non-magnetic impurities that cut spin-chains in quasi-1 dimensional systems.
- ▶ Impurities change the state of system in immediate vicinity
Changes can be picked up by local probes such as NMR
- ▶ Particularly interesting if system has 'nearby' competing ground-states
Impurities can locally 'seed' a competing ground state with different ordering and symmetry properties

Borrowing from experiments

From experiments to numerical computations

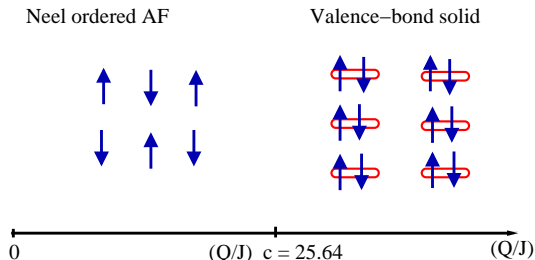
- ▶ Use impurity effects to probe character of correlated ground state.
- ▶ Need: Efficient numerical techniques allowing computation for systems with impurities

In this talk:

- ▶ Impurity spin effects in an antiferromagnet on the verge of transition to a valence-bond solid (quantum paramagnet)

An unusual phase transition

- ▶ Antiferromagnet on verge of transition to a quantum paramagnet



$$H_{JQ} = -J \sum_{\langle ij \rangle} P_{\langle ij \rangle} - Q \sum_{\langle ij \rangle || \langle kl \rangle} P_{\langle ij \rangle} P_{\langle kl \rangle}$$

where $P_{\langle ij \rangle} = \left(\frac{1}{4} - \vec{S}_i \cdot \vec{S}_j \right)$
($S=1/2$ spins on a square lattice)

Sandvik 2007, Melko & Kaul 2007.

Why so unusual?

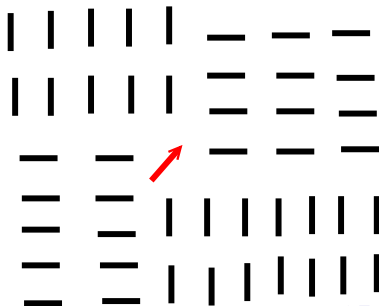
- ▶ J term favours Neel ordered state that spontaneously breaks spin rotation symmetry
- ▶ Q term favours valence bond solid that spontaneously breaks lattice translation symmetry
- ▶ Standard Landau theory argument \rightarrow First order transition or intermediate phase with co-existing orders

Apparently second order direct transition between two phases

- ▶ Sandvik 2007, using a new singlet-sector ground-state projection algorithm in valence bond basis ($T = 0$ results directly)
- ▶ Melko & Kaul 2007, using Quantum Monte Carlo at inverse temperature $\beta Q \approx L$ for $L \times L$ square lattice

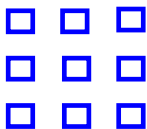
Theoretical framework

- ▶ Senthil *et. al.* 2004: Landau theory does not work due to Berry phases in the action
- ▶ Critical region not well-described using standard action written in terms of order-parameter fields
- ▶ Instead: 'Natural' variables are $S = 1/2 Z_4$ vortices in the four-fold symmetry breaking VBS order. Coupled at critical point to emergent $U(1)$ gauge field ('sound-mode' in order parameter phase)

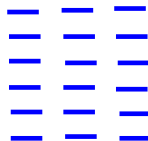


Consequences

- ▶ Direct second order quantum critical point between Neel and VBS phases
- ▶ Critical Neel order parameter correlations:
 $\langle \vec{n}(r)\vec{n}(0) \rangle_{\text{crit}} \sim r^{-(1+\eta_n)}$ with **large η_n unlike usual critical points**
- ▶ Pinning potential for phase ϕ of the VBS order parameter is irrelevant at transition \rightarrow System cannot immediately choose between columnar VBS order and plaquette VBS order upon entering VBS phase



phase angle = $\pi/4$



phase angle = 0

Deconfined critical point scenario:

- ▶ Claim of Melko and Kaul, and Sandvik:
 H_{JQ} provides an example of this physics
- ▶ Reasonably sharp, apparently second-order transition
Reasonably good scaling behaviour at low temperatures above
 $T = 0$ quantum critical point
- ▶ Melko & Kaul (07): Large $\eta_n \approx 0.35 \pm 0.03$ in agreement with expectations
(Sandvik (07): $\eta_n = \eta_{\text{VBS}} \approx 0.26 \pm 0.03$)
- ▶ Kaul & Melko (07): Correlation length exponent $\nu \approx 0.68 \pm 0.04$
(Sandvik (07): $\nu \approx 0.78 \pm 0.03$)

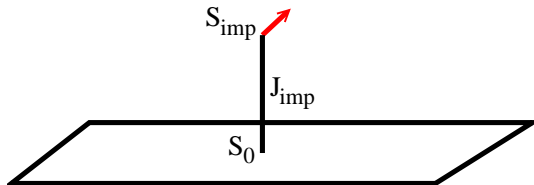
Sandvik 2009 (better data): η_n, ν agree with Kaul & Melko;
 $\eta_{\text{VBS}} \approx 0.20 \pm 0.02$ (unpublished)

Controversy:

- ▶ Jiang, Chandrasekharan, Nyeffler & Wiese 2008: Very similar numerical data
- ▶ But: Analysis by 'flowgram' method (Kuklov *et. al.* 2006) → apparent indication of (weakly) first order direct transition
If Q_c determined by some 'crossing criterion' (ρ_S vs Q/J for various sizes L), crossing point drifts as size gets large
'Universal' value of ρ_S at putative critical point increases with L beyond some system size L
Finite chance to be superfluid even at 'critical' point → first order transition
- ▶ Results inconsistent with deconfined critical point scenario favoured by Melko and Kaul, and by Sandvik

Our goal: Look at impurity physics at putative critical point

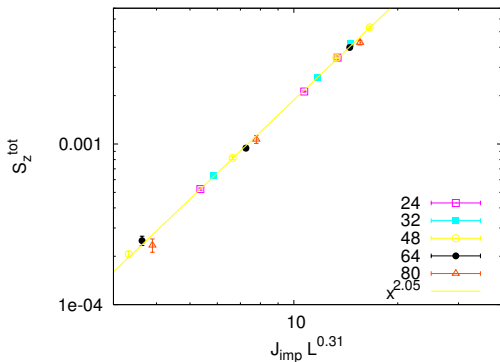
Adding an impurity



- ▶ $H_{JQ} + J_{\text{imp}} \vec{S}_{\text{imp}} \cdot \vec{S}_0$
- ▶ Is J_{imp} a 'relevant perturbation' at bulk transition?
- ▶ What effect does it have on the bulk?

Is small J_{imp} relevant at $Q_c \approx 25.64$?

- ▶ For small J_{imp} , $\langle S_{\text{tot}}^Z \rangle_{\text{bulk}}$ is quadratic in scaling variable $J_{\text{imp}} L^{0.31}$ for $L \times L$ system.



J_{imp} is relevant perturbation with eigenvalue $\lambda_{\text{imp}} = 0.31 \pm 0.03$

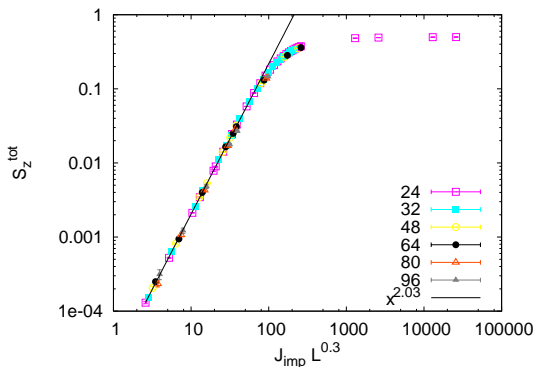
What is the interpretation of λ_{imp} ?

Interpreting λ_{imp}

- ▶ $\vec{S}(r=0, \tau) = c_n \vec{n}(r=0, \tau) + c_L \vec{L}(r=0, \tau)$
- ▶ Assuming \vec{n} is dominant piece:
$$H_{\text{imp}} = J_{\text{imp}} \int d\tau \vec{S}_{\text{imp}} \cdot \vec{n}(r=0, \tau)$$
- ▶ $[J_{\text{imp}}] = 1 - [\vec{n}]$
assuming time scales like space ($z = 1$)
- ▶ $[\vec{n}] = (1 + \eta_n)/2$
- ▶ $\lambda_{\text{imp}} = (1 - \eta_n)/2$
- ▶ Implies $\eta_n \approx 0.38 \pm 0.06$

Going with the flow...

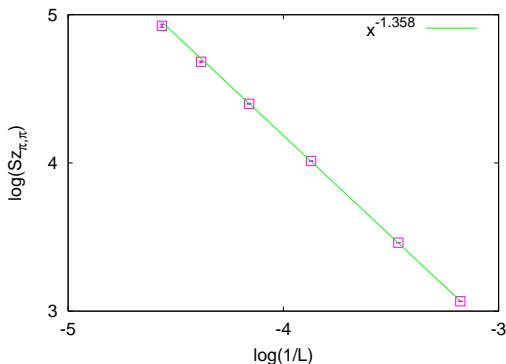
- ▶ J_{imp} relevant and flows to $J_{\text{imp}} = \infty$ fixed point
 S_{imp} binds S_0 into a singlet $\rightarrow L \times L$ system with center site missing



Scaling at $J_{\text{imp}} = \infty$

- ▶ Standard scaling (Hoglund, Sandvik & Sachdev 2007, Metliski & Sachdev 2008):

Vacancy-induced Neel order at critical point $\sim L^{2-(1+\eta_n)/2}$:



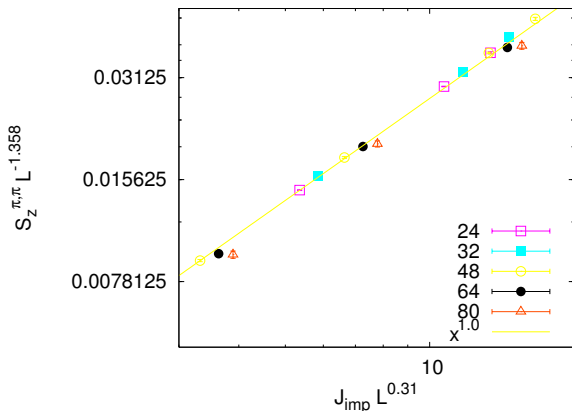
Gives $\eta_n = 0.28 \pm 0.05$

Caveat emptor: slightly outside of error bars of $(1 - 2\lambda_{\text{imp}})$

Back to weak-coupling: $\langle S_{\text{bulk}}^z(\mathbf{Q} = (\pi/a, \pi/a)) \rangle$

- ▶ Look at $\langle S_{\text{bulk}}^z(\mathbf{Q}) \rangle L^{(3-\eta_n)/2}$ for small J_{imp} .

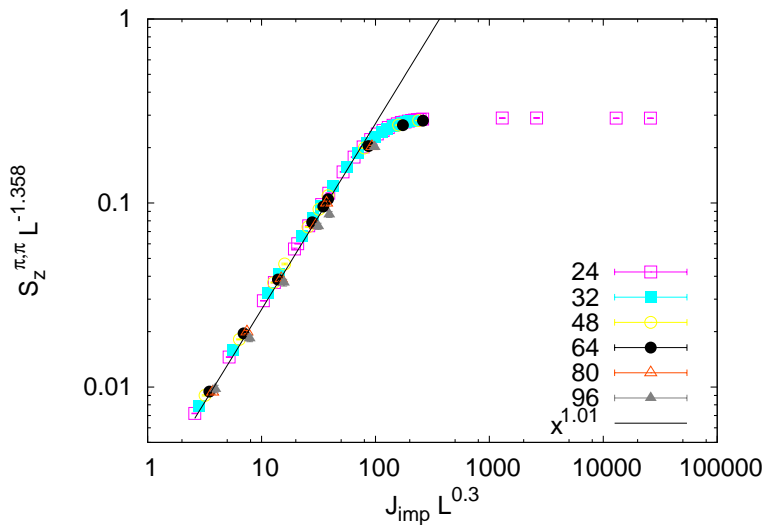
Use the value of η_n obtained from $J_{\text{imp}} = \infty$ results



Scaling collapse as *linear* function of $J_{\text{imp}}(L) = J_{\text{imp}} L^{0.31}$

Going with the flow...

Understand flow with $J_{\text{imp}}(L)$ quite well

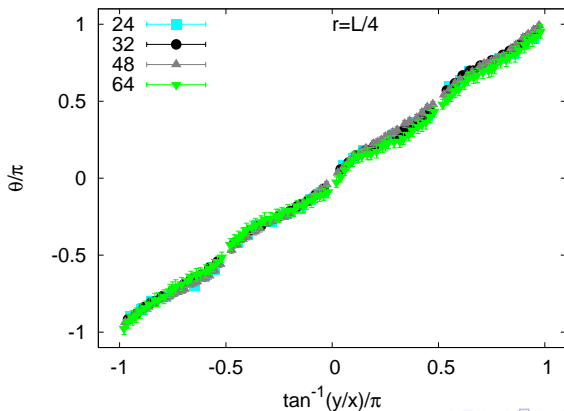


A twist at ∞ : Induced VBS order has phase winding

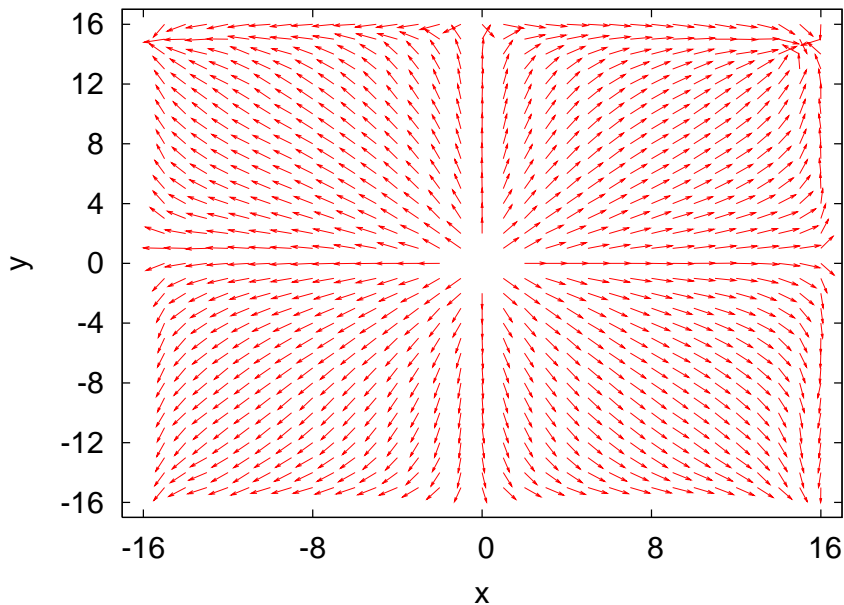
- ▶ Look at $\langle V_x(\vec{r}) \rangle = \langle (-1)^x \vec{S}_{\vec{r}} \cdot (\vec{S}_{\vec{r}+\hat{x}} - \vec{S}_{\vec{r}-\hat{x}}) \rangle$
and $\langle V_y(\vec{r}) \rangle = \langle (-1)^y \vec{S}_{\vec{r}} \cdot (\vec{S}_{\vec{r}+\hat{y}} - \vec{S}_{\vec{r}-\hat{y}}) \rangle$

Local site-centered complex VBS order parameter $V = V_x + iV_y$

- ▶ Phase $\phi_V = \arctan(V_y/V_x)$ is linear function of angular coordinate θ

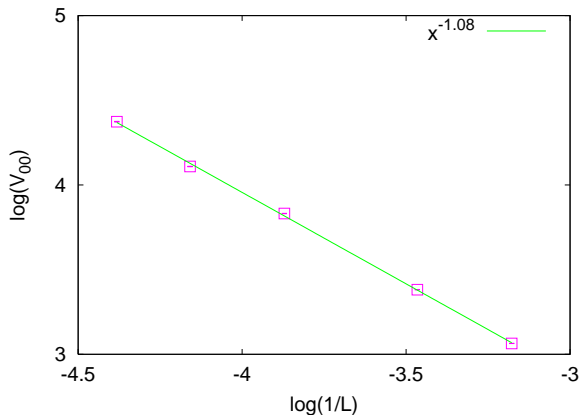


Snapshot of the spinon vortex



Scaling with size of induced VBS order

- ▶ How does $V_{00} = \sum_r V_r \exp(-i\theta_r)$ scale with L ?



$V_{00} \sim L^p$ with $p = 1.08 \pm 0.03$ (imaginary part of V_{00} negligible)
What exponent(s) is p related to?

Interpreting p

- ▶ Power p not straightforward to interpret

Metliski & Sachdev 2008

- ▶ Depends on numerical values of bulk and boundary exponents η_{VBS} and η'_{VBS} .

$$\langle \langle V(r=0, \tau) V(r=0, 0) \rangle \rangle_{\text{C}} \sim 1/\tau^{\eta'_{\text{VBS}}}$$

- ▶ Case 1: $\eta'_{\text{VBS}} < 2$

$$p = 2 - \left(\frac{\eta_{\text{VBS}}}{2} + \frac{1}{2} \right)$$

- ▶ Case 2: $\eta'_{\text{VBS}} > 2$

$$p = 2 - \left(\frac{\eta'_{\text{VBS}}}{2} + \frac{\eta_{\text{VBS}}}{2} - \frac{1}{2} \right)$$

- ▶ Our interpretation: Case 1 unlikely

(Gives η_{VBS} very different from Sandvik (09): $\eta_{\text{VBS}} \approx 0.20 \pm 0.02$)

- ▶ Case 2: implies $\eta'_{\text{VBS}} = 2.64 \pm 0.06$

(for what it is worth...)

Scaling of $\langle S^Z(r) \rangle$ at $J_{\text{imp}} = \infty$

At second order critical point:

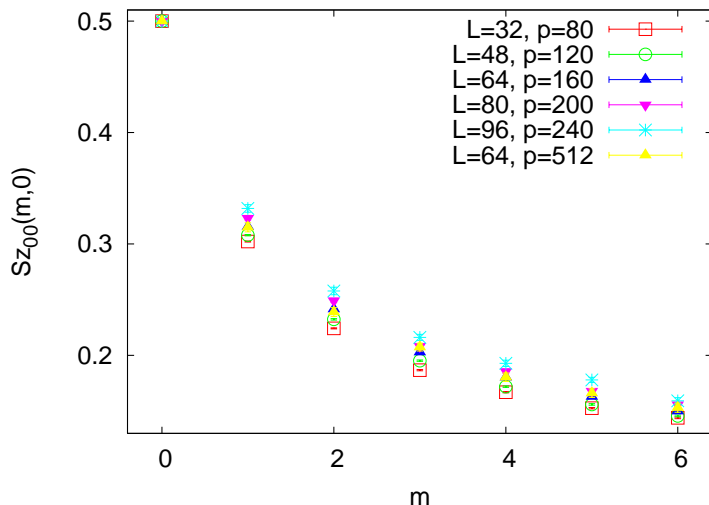
- ▶ $\langle S_{\mathbf{Q}}^Z(\mathbf{r}) \rangle = \frac{1}{L^{(1+\eta_n)/2}} f_{\mathbf{Q}}\left(\frac{\mathbf{r}}{L}\right)$ for $r \gg 1$
- ▶ $\langle S_{\mathbf{0}}^Z(\mathbf{r}) \rangle = \frac{1}{L^2} f_0\left(\frac{\mathbf{r}}{L}\right)$ for $r \gg 1$

Numerical tests: To avoid relying on arbitrariness in definition of $\langle S_{\mathbf{Q}}^Z(r) \rangle$ and $\langle S_{\mathbf{0}}^Z(r) \rangle$, Fourier transform $\langle S^Z(r) \rangle$ and translate predictions to q space

- ▶ $\langle S^Z(\mathbf{q}) \rangle = g_0(\mathbf{q}L)$ for $|\mathbf{q}| \ll \pi$
- ▶ $\langle S^Z(\mathbf{Q} + \mathbf{q}) \rangle = L^{2-(1+\eta_n)/2} g_{\mathbf{Q}}(\mathbf{q}L)$ for $|\mathbf{q}| \ll \pi$

How well does this work?

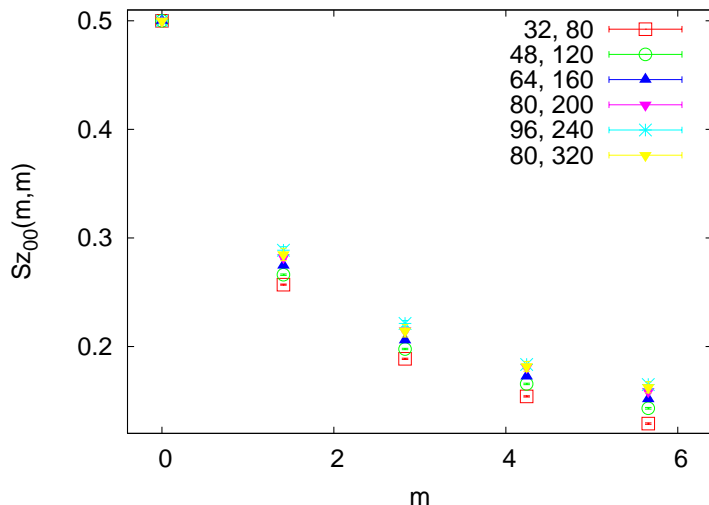
Test near zero wavevector



$m = q_x L / 2\pi$ — **Scaling not very good**

Check on systematic error: $L = 64$ calculation done with two projection powers

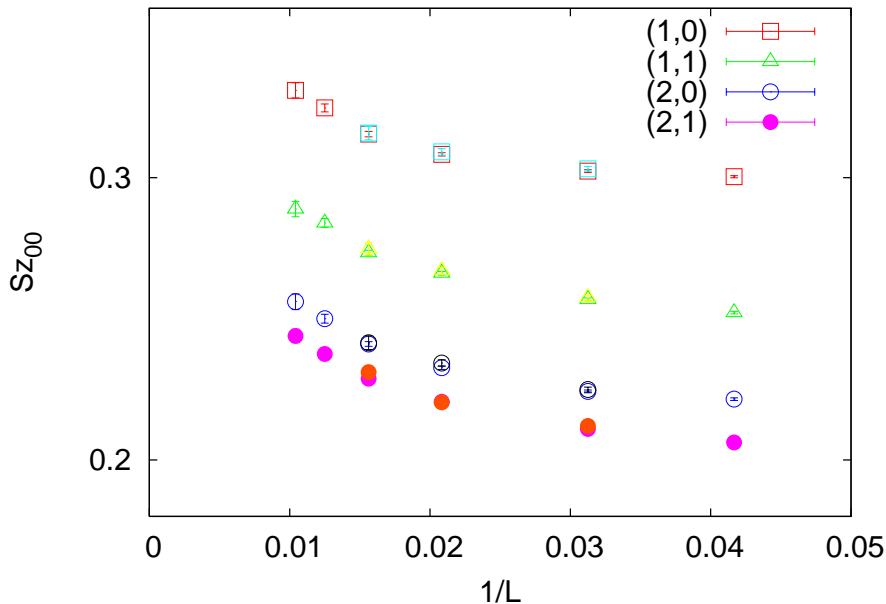
Test near zero wavevector



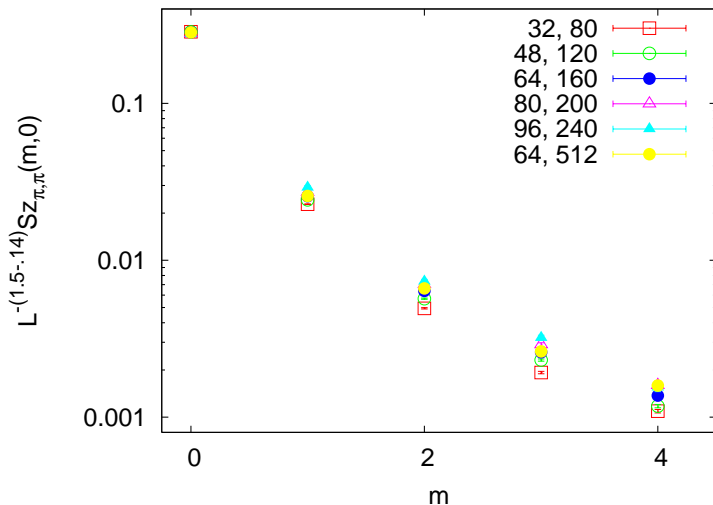
$m_x = m_y = m = qL/2\pi$ — Scaling not very good

Check on systematic error: $L = 80$ calculation done with two projection powers

Zoom in on deviations from scaling



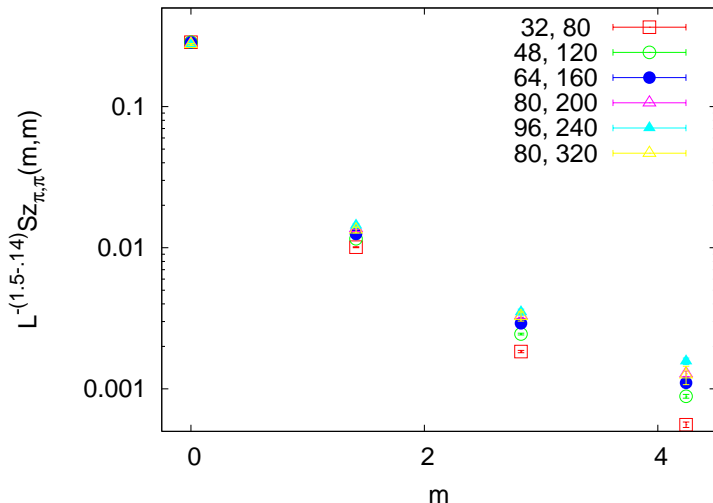
Test near wavevector Q



$m = q_x L / 2\pi$ — **Scaling not very good**

Check on systematic error: $L = 64$ calculation done with two projection powers

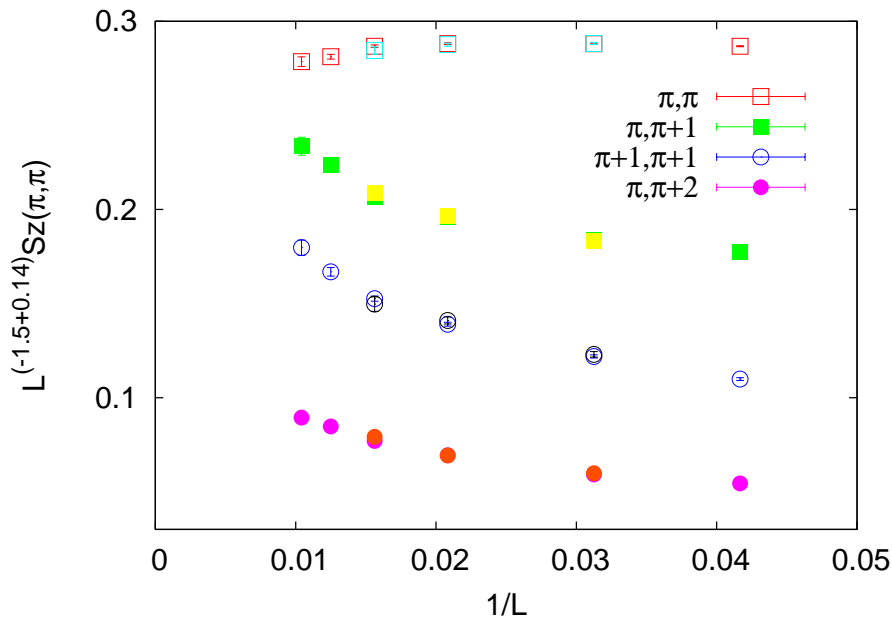
Test near wavevector Q



$m_x = m_y = m = qL/2\pi$ — **Scaling not very good**

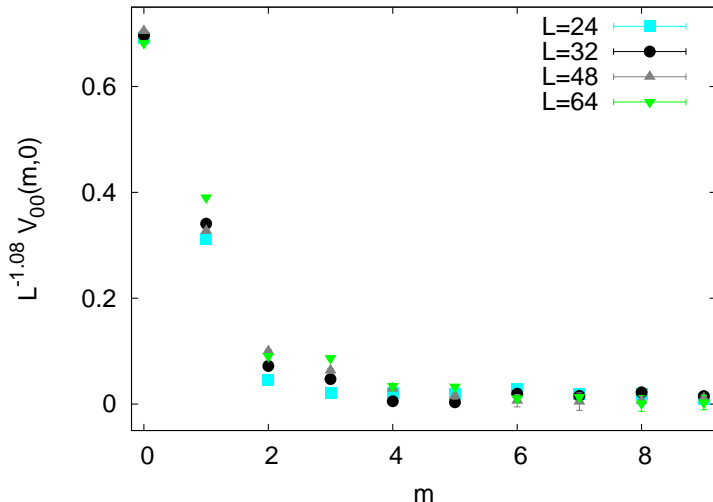
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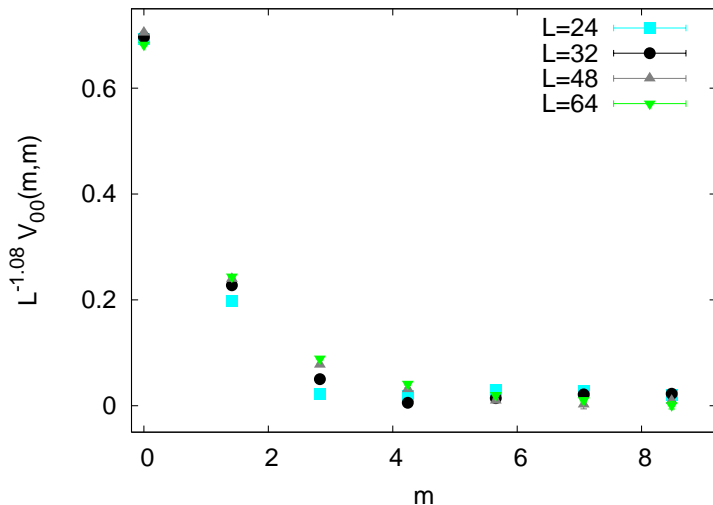


Similar results of $V_r \exp(-i\theta_r)$

Fourier transform of $V_r \exp(-i\theta_r)$ should scale like $L^p g_V(\mathbf{q}L)$ for $|\mathbf{q}| \ll \pi$



Similar results of $V_r \exp(-i\theta_r)$

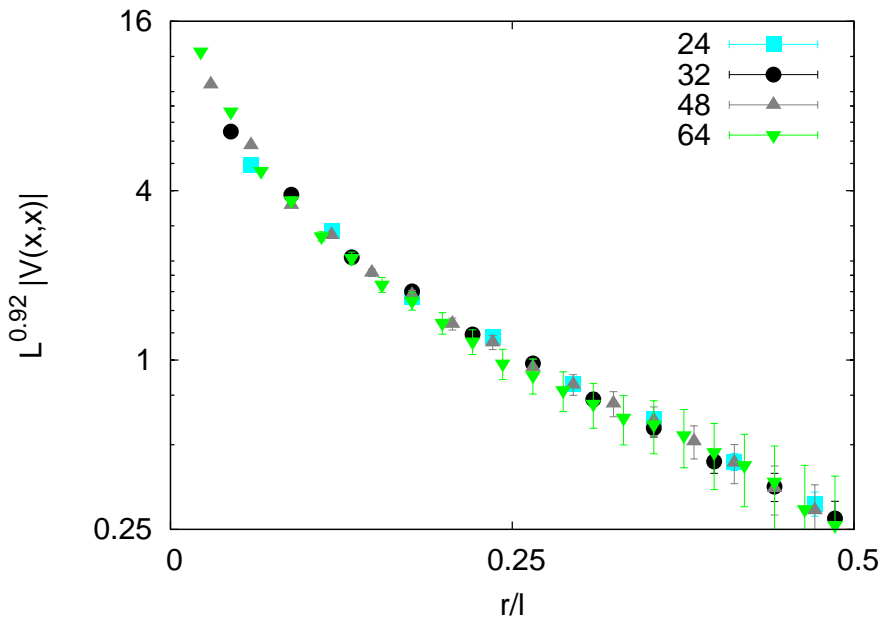


Again: scaling has corrections that go away very slowly with size

What have we learnt?

- ▶ Bulk properties at transition seem to agree with expectations at the deconfined critical point of Senthil *et al.* (up to sizes $L \sim 100$).
no direct evidence of first-order transition
- ▶ Impurity scaling predictions not as successful:
Slow transients that seem to violate scaling at least up to size $L \sim 100$
- ▶ Real question: What is this very slow crossover?
Is this again a signature of a weakly-first order transition at asymptotically large sizes?
Or is there some irrelevant impurity operator (at $r = 0$) causing this slow crossover?

$V_r \exp(-i\theta_r)$ along diagonal



$V_r \exp(-i\theta_r)$ along y axis

