Using defects to probe strongly-correlated many-body states

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RPMBT-15
OSU 2009

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Acknowledgements:
Discussions: S. Chandrasekharan, M. Metliski, O. Motrunich & S. Sachdev

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-1dimensional 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

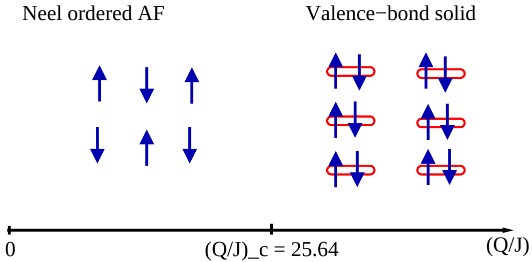
- Use impurity effects to probe character of correlated ground state.
- Need: Efficient numerical techniques allowing computation for systems with impurities

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 $P_{\langle ij \rangle} = (\frac{1}{4} - \vec{S}_i \cdot \vec{S}_j)$

(S=1/2 spins on a square lattice)

Sandvik 2007, Melko & Kaul 2007.

Why so unusual?

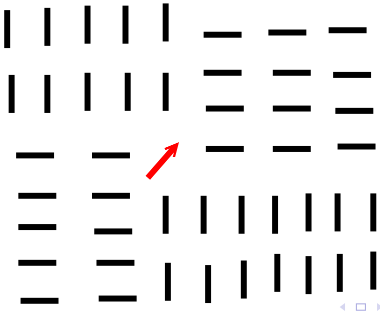
- J term favours Neel ordered state that spontaneously breaks spin rotation symmetry
- Q term favours valence bond solid that spontaneously breaks lattice translation symmetry
- Standard Landau theory argument $\rightarrow$ First order transition or intermediate phase with co-existing orders

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

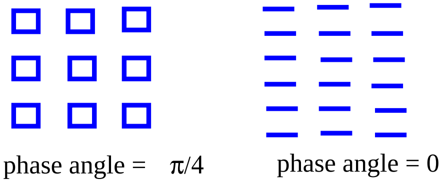
Theoretical framework

- 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



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): $\eta_n = \eta_{\mathrm{VBS}} \approx 0.26 \pm 0.03$)
- Kaul & Melko (07): Correlation length exponent $\nu \approx 0.68 \pm 0.04$
  (Sandvik (07): $\nu \approx 0.78 \pm 0.03$)

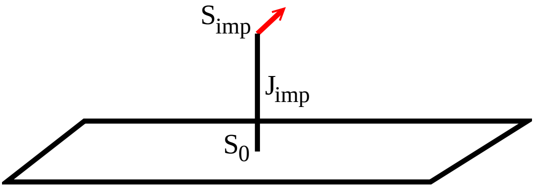
Sandvik 2009 (better data): η_n, ν agree with Kaul & Melko;
$\eta_{\mathrm{VBS}} \approx 0.20 \pm 0.02$ (unpublished)

Controversy:

- Jiang, Chandrasekharan, Nyeffler & Wiese 2008: Very similar numerical data
- But: Analysis by 'flowgram' method (Kuklov *et. al.* 2006) $\longrightarrow$ 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 $\rightarrow$ 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?

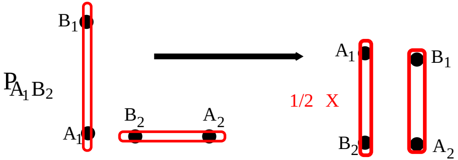
Singlet sector algorithm of Sandvik

- Singlet sector $\{|s\rangle\}$ of $2N$ spin $S = 1/2$ moments spanned by overcomplete basis.
  Decompose into N A-sublattice sites, and N B-sublattice sites
  $\{|s\rangle\}$ spanned by $\{|\mathcal{P}\rangle = \otimes_{\mathrm{A}} |\mathrm{A}\mathcal{P}(\mathrm{A})\rangle\}$
  $|\mathrm{A}\mathcal{P}(\mathrm{A})\rangle$ is singlet state of spin at A with spin at $\mathrm{B} = \mathcal{P}(\mathrm{A})$
  Basis is (very) overcomplete
- Start with arbitrary singlet state $|v_0\rangle$ and compute $\langle v_0|(-H)^m \hat{O}(-H)^m|v_0\rangle / \langle v_0|(-H)^{2m}|v_0\rangle$.
- Gives ground state expectation value of operator $\hat{O}$ for 'large enough' m (in practice $m \sim N \times \Delta_S^{-1}$).

Crucial: Efficient importance sampling algorithm for computing $\langle v_0'|(-H)^m|v_0\rangle$ exploiting overcompleteness of basis
Sandvik 2007; Sandvik & Beach 2007, Sandvik & Evertz 2008

Key ingredient of Sandvik's method

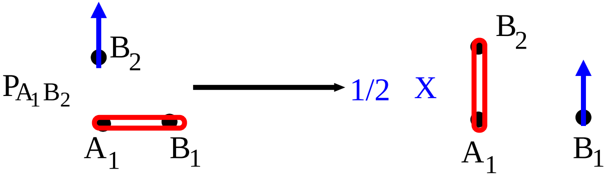
- Action of P_{AB} is either a rearrangement of valence bonds



- Or trivial

Generalizing to $S_{\rm tot} = 1/2$

- Simple but powerful generalization possible for $\{|S^z_{\rm tot} = +1/2; S_{\rm tot} = 1/2\rangle\}$ sector of $2N+1$ $S = 1/2$ moments ($N+1$) A-sublattice sites and N B-sublattice sites
- Basis: $\left\{|\mathrm{A_{free}}; \mathcal{P}\rangle = |S^z_{\mathrm{A_{free}}} = +\frac{1}{2}\rangle \otimes_{\mathrm{A}\neq\mathrm{A_{free}}} |\mathrm{A}\mathcal{P}(\mathrm{A})\rangle\right\}$
- What makes it work:

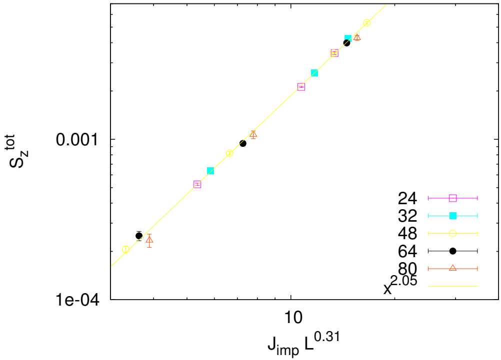


- $\langle v'_{1/2}|(-H)^{2m}|v_{1/2}\rangle$ can be efficiently computed by efficient generalization of singlet sector method of Sandvik & Evertz.

Banerjee & KD 2009

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

- For small J_{imp}, $\langle S^z_{\mathrm{tot}} \rangle_{\mathrm{bulk}}$ is quadratic in scaling variable $J_{\mathrm{imp}} L^{0.31}$ for $L \times L$ system.



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

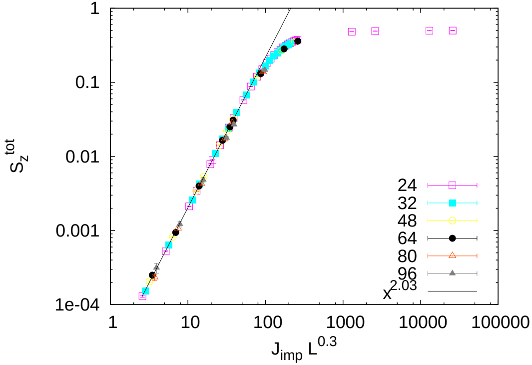
What is the interpretation of λ_{imp}?

Interpreting $\lambda_{\rm imp}$

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

Going with the flow...

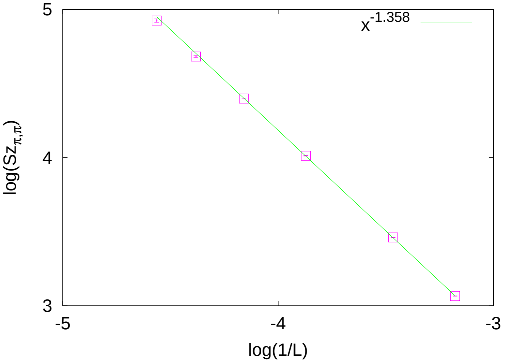
- $J_{\rm imp}$ relevant and flows to $J_{\rm imp} = \infty$ fixed point
  $S_{\rm imp}$ binds S_0 into a singlet $\rightarrow L \times L$ system with center site missing



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

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

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

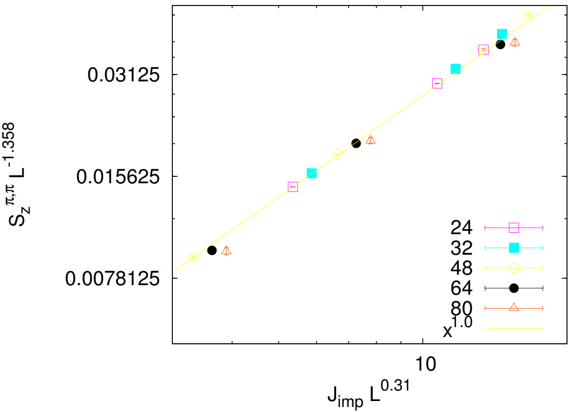


Gives $\eta_n = 0.28 \pm 0.05$

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

Back to weak-coupling: $\langle S^z_{\rm bulk}(\mathbf{Q} = (\pi/a, \pi/a))\rangle$

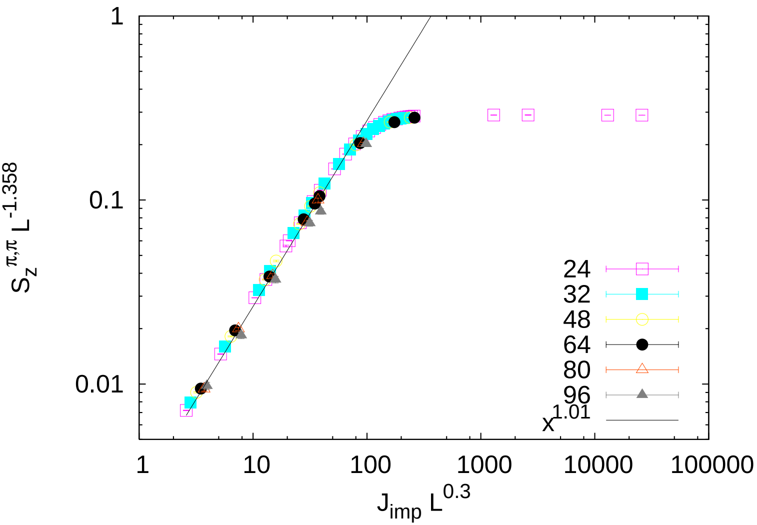
- Look at $\langle S^z_{\rm bulk}(\mathbf{Q})\rangle L^{(3-\eta_n)/2}$ for small $J_{\rm imp}$.
  Use the value of η_n obtained from $J_{\rm imp} = \infty$ results



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

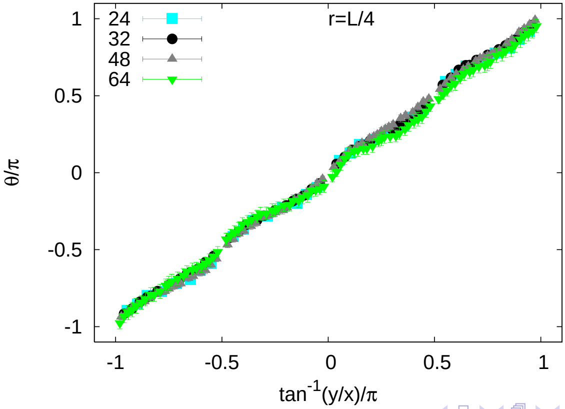
Going with the flow...

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

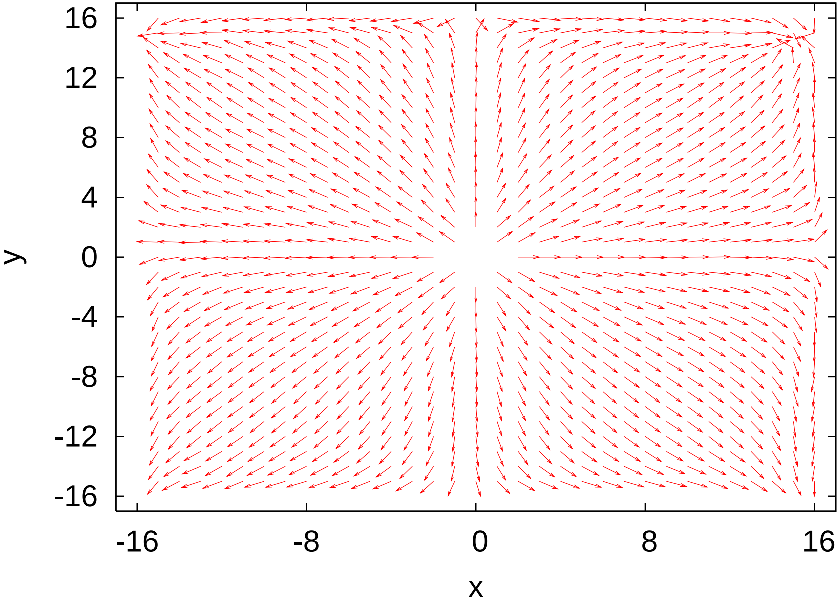


A twist at ∞: Induced VBS order has phase winding

- 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

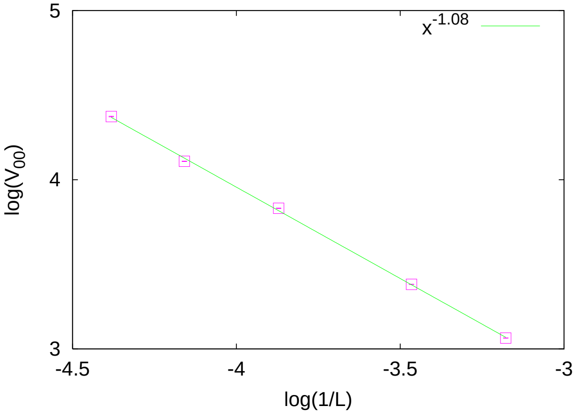


Snapshot of the spinon vortex



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}.
  $(\langle V(r=0,\tau)V(r=0,0)\rangle_C \sim 1/\tau^{\eta'_{\mathrm{VBS}}}$
- Case 1: $\eta''_{\mathrm{VBS}} < 2$
  $p = 2 - \left(\frac{\eta_{\mathrm{VBS}}}{2} + \frac{1}{2}\right)$
- Case 2: $\eta''_{\mathrm{VBS}} > 2$
  $p = 2 - \left(\frac{\eta'_{\mathrm{VBS}}}{2} + \frac{\eta_{\mathrm{VBS}}}{2} - \frac{1}{2}\right)$
- Our interpretation: Case 1 unlikely
  (Gives η_{VBS} very diferent from Sandvik (09): $\eta_{\mathrm{VBS}} \approx 0.20 \pm 0.02$)
- Case 2: implies $\eta'_{\mathrm{VBS}} = 2.64 \pm 0.06$

(for what it is worth...)

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

At second order critical point:

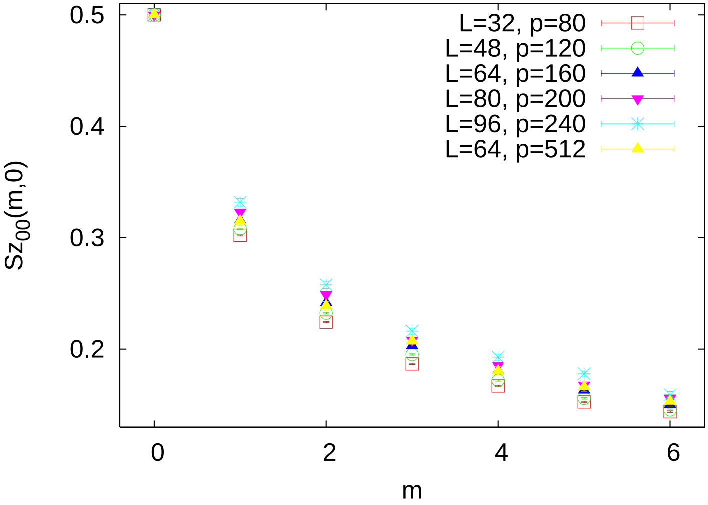
- $\langle S^z_{\mathbf{Q}}(\mathbf{r})\rangle = \frac{1}{L^{(1+\eta_\mathrm{n})/2}} f_{\mathbf{Q}}\left(\frac{\mathbf{r}}{L}\right)$ for $r >> 1$
- $\langle S^z_{\mathbf{0}}(\mathbf{r})\rangle = \frac{1}{L^2} f_0\left(\frac{\mathbf{r}}{L}\right)$ for $r >> 1$

Numerical tests: To avoid relying on arbitrariness in definition of $\langle S^z_{\mathbf{Q}}(r)\rangle$ and $\langle S^z_0(r)\rangle$, 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?

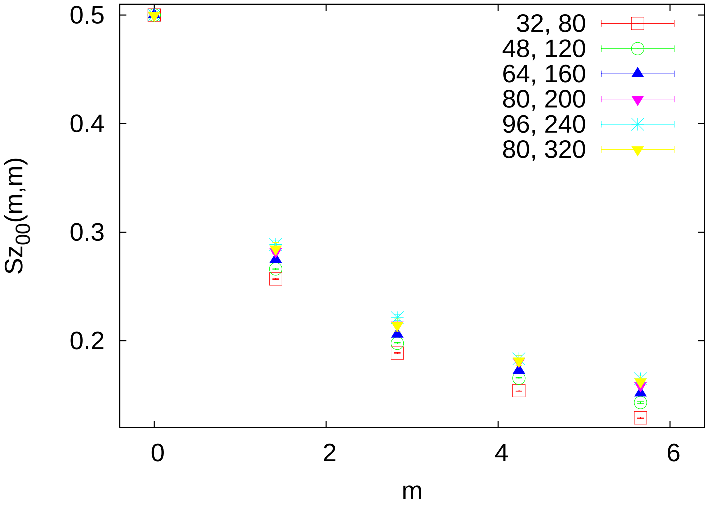
Test near zero wavevector



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

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

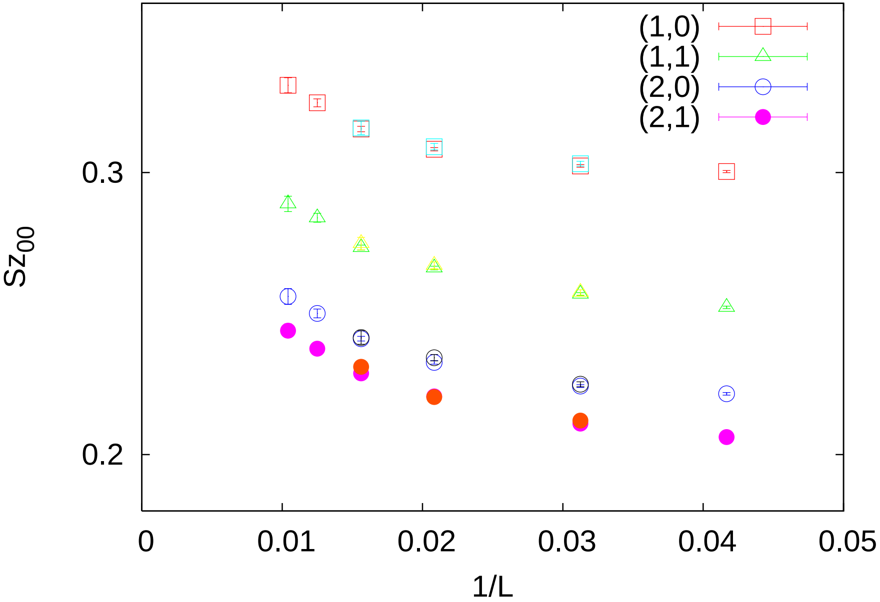
Test near zero wavevector



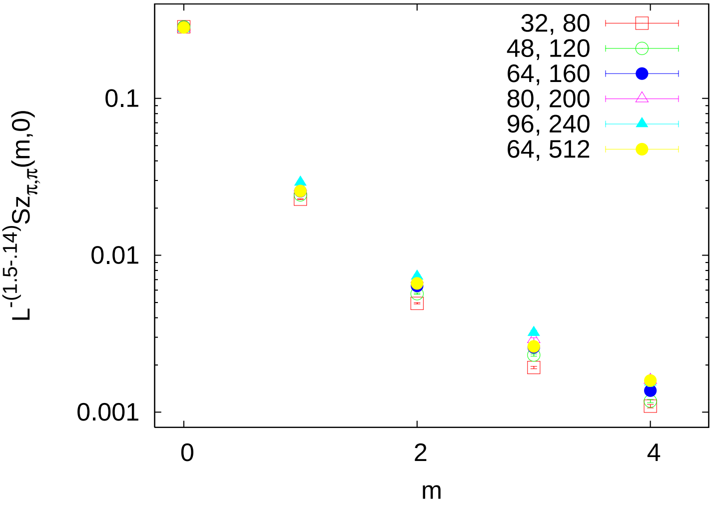
$m_x = m_y = m = qL/2\pi$—Scaling not very good

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

Zoom in on deviations from scaling



Test near wavevector **Q**



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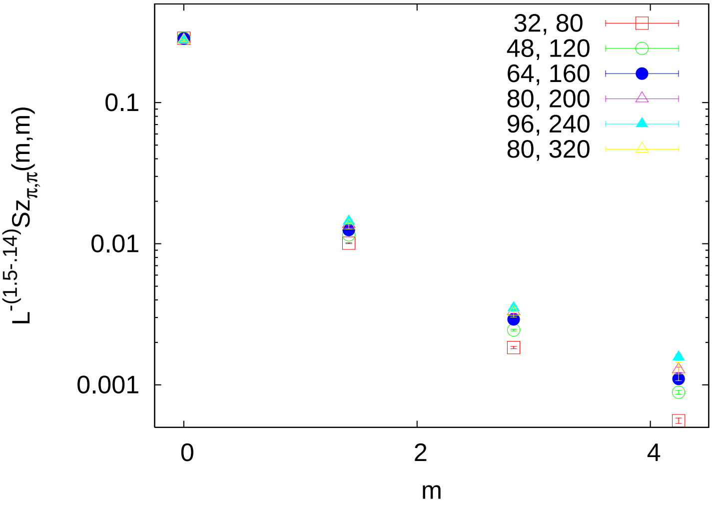

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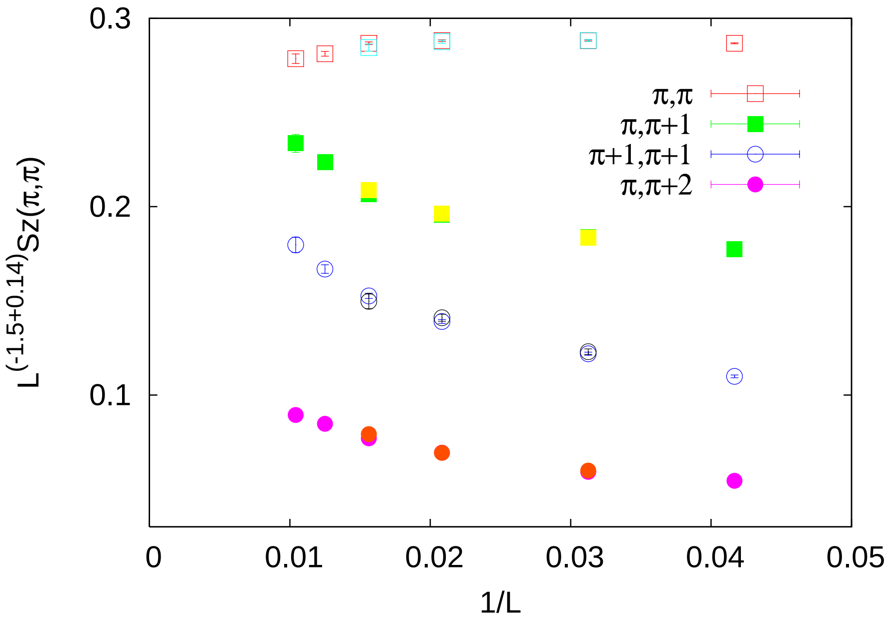
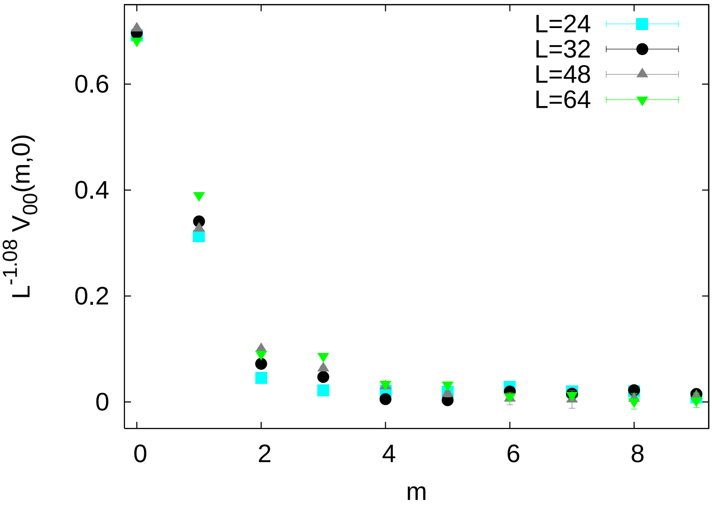
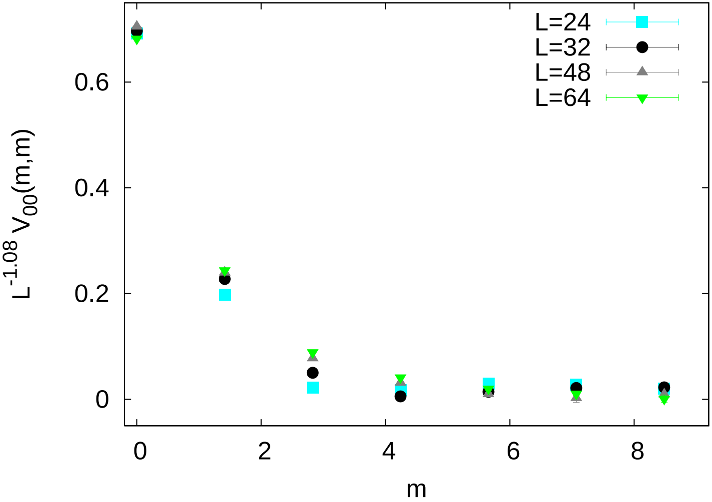


Similar results of $V_r \exp(-i\theta_r)$

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 $V_r \exp(-i\theta_r)$

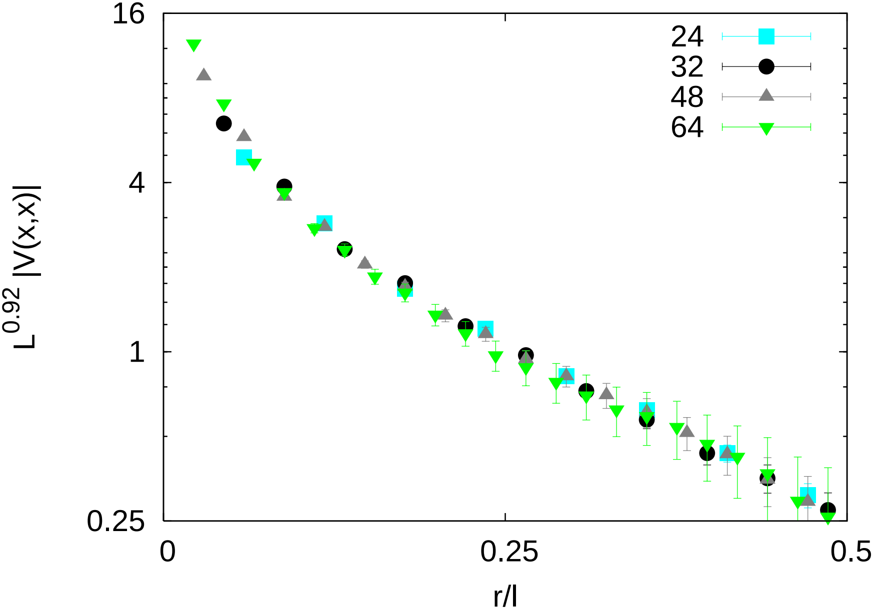


Again: scaling has corrections that go away very slowly with size

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