Using impurity physics to probe a quantum critical point

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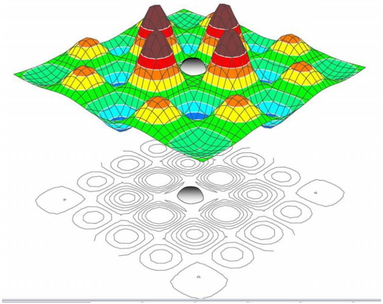
References:

A. Banerjee, KD, & F. Alet, Phys. Rev. B **82**, 155139 (2010).
A. Banerjee, KD, & F. Alet, Phys. Rev. B **83**, 235111 (2011).
S. Sanyal, A. Banerjee, & KD, arXiv:1107.1493.

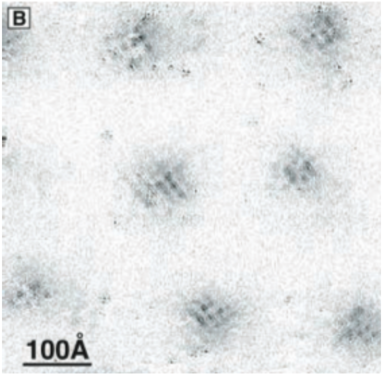
Impurities as probes



Alloul et. al. (Rev. Mod. Phys. 2009).

- Impurities can be useful probes of interesting low temperature states of matter—Zn doping in cuprates

Impurities as probes



Checkerboard around vortex—from Seamus Davis group-page

- Impurities change the state of system in immediate vicinity—Changes can be picked up by local probes such as STM
- Particularly interesting if system has 'nearby' competing ground-states Impurities can locally 'seed' a competing ground state with different ordering and symmetry properties

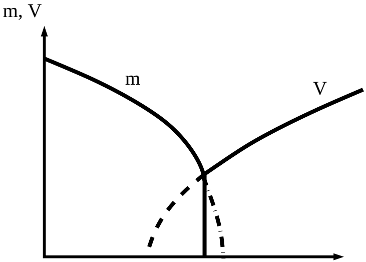
Numerical 'experiments' with impurities

- Impurity at the quantum phase transition from Néel state to lattice-symmetry breaking valence-bond solid (VBS) on square lattice.

  $\rightarrow$ Probe nature of quantum phase transition
- Compare with:
  1. Impurity at quantum phase transition from Néel state to quantum paramagnet on square lattice.
  2. Impurity at Néel-VBS transition in SU(3) magnets on square lattice.
  3. Impurity in gapless power-law ordered "Néel" phase in the $S = 1/2$ Heisenberg spin chain

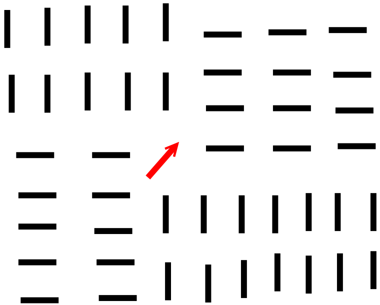
Néel-VBS transitions: Landau Theory

- 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



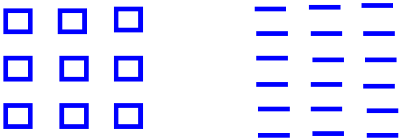
Néel-VBS transitions: Deconfined criticality

- Senthil *et. al.* (Science, PRB 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 NCCP[1] theory.
- Levin and Senthil (PRB 2004): '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

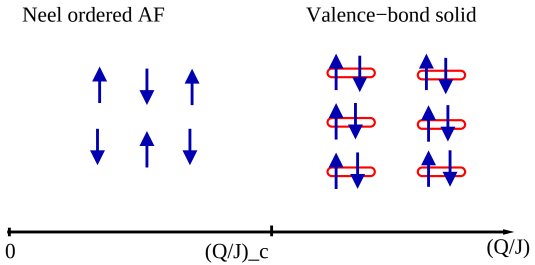
- Direct second order quantum critical point between Neel and VBS phases
- Critical Neel order parameter correlations: $\langle \vec{n}(r)\vec{n}(0)\rangle_{\mathrm{crit}} \sim r^{-(1+\eta_n)}$ with large η_n unlike usual critical points
- Pinning potential for phase ϕ of the VBS order parameter is irrelevant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



phase angle = π/4 phase angle = 0

Accessing the Néel-VBS transition: Models

- Néel-VBS transitions in *unfrustrated* spin models



$$H_{JQ_2} = -J \sum_{\langle ij \rangle} P_{\langle ij \rangle} - Q \sum_{\langle ij \rangle || \langle kl \rangle} P_{\langle ij \rangle} P_{\langle kl \rangle}$$

$$H_{JQ_3} = -J \sum_{\langle ij \rangle} P_{\langle ij \rangle} - Q \sum_{\langle ij \rangle || \langle kl \rangle || \langle rs \rangle} P_{\langle ij \rangle} P_{\langle kl \rangle} P_{\langle rs \rangle}$$

$$\text{where } P_{\langle ij \rangle} = \left(\tfrac{1}{4} - \vec{S}_i \cdot \vec{S}_j\right)$$

Sandvik (PRL 2007), Lou, Sandvik & Kawashima (PRB 2009), Melko & Kaul (PRL 2008).

Initial results

Apparently second order direct transition between two phases

- Sandvik (PRL 2007): JQ_2 model using singlet-sector ground-state projection algorithm in valence bond basis ($T = 0$ results directly)
- Melko & Kaul (PRL 2008): JQ_2 using Quantum Monte Carlo at inverse temperature $\beta Q \approx L$ for $L \times L$ square lattice

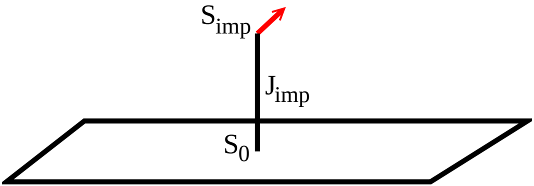
Conflicting claim of first order behaviour

- Jiang *et. al.* (J.Stat.Mech. 2008)

Evidence for deconfined criticality

- Lou, Sandvik, & Kawashima (PRB 2009).
  No sign of first order behavour.
- Both H_{JQ_2} and H_{JQ_3} yield *same* exponents.
- $\eta_s \approx 0.34$.
- $\eta_d \approx 0.20$.
- $\nu \approx 0.68$.
  Such universal behaviour unlikely if first order transition.

Adding an impurity



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

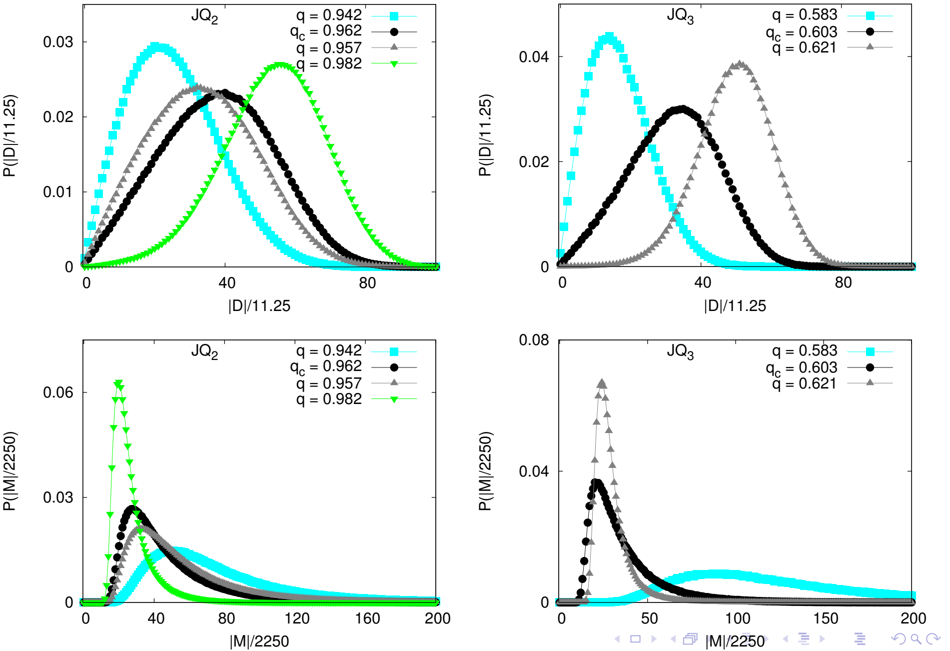
$J_{\mathrm{imp}} = \infty$: Doping by non-magnetic ion to create missing-spin defect

Method

- Singlet sector $\{|s\rangle\}$ of $2N$ spin $S = 1/2$ moments spanned by overcomplete valence bond basis.
- Start with arbitrary singlet state $|v_0\rangle$ and compute $\langle v_0|(-H)^m \hat{O}(-H)^m|v_0\rangle / \langle v_0|(-H)^{2m}|v_0\rangle$ stochastically.
  Sandvik (PRL 2005)
- Gives ground state expectation value of operator $\hat{O}$ for 'large enough' m (in practice $m \sim Volume \times \Delta_S^{-1}$).
- Crucial: Efficient importance sampling algorithm for computing $\langle v_0'|(-H)^m|v_0\rangle$ exploiting overcompleteness of basis
  Sandvik & Evertz (PRB 2010)

- Our approach: Modify this to work for $S_{\text{tot}} = 1/2$ doublet ground state of system with one impurity.
  Banerjee & KD (J.Stat.Mech. 2010)

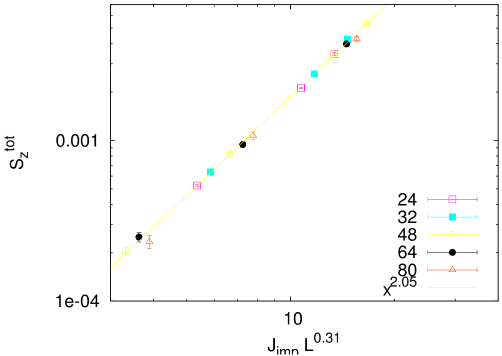
First things first: Any bulk first order signatures?



Thinking (un)critically (a first pass):

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

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



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

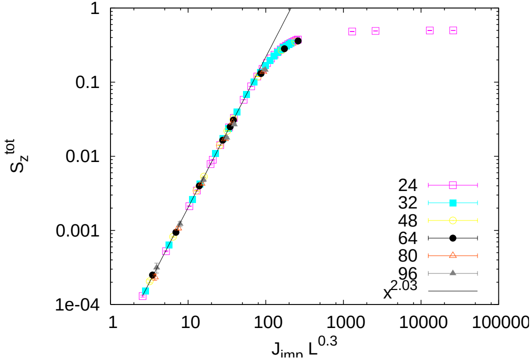
What is the interpretation of $\lambda_{\rm imp}$?

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:
  $H_{\rm imp} = J_{\rm imp} \int d\tau \vec{S}_{\rm imp} \cdot \vec{n}(r=0,\tau)$
- $[J_{\rm imp}] = 1 - [\vec{n}]$
  assuming time scales like space ($z = 1$)
- $[\vec{n}] = (1+\eta_n)/2$
- $\lambda_{\rm imp} = (1-\eta_n)/2$
- Implies $\eta_n \approx 0.35 \pm 0.06$
  consistent with $\eta_n \approx 0.34$ (Lou,Sandvik,Kawashima PRB2009)

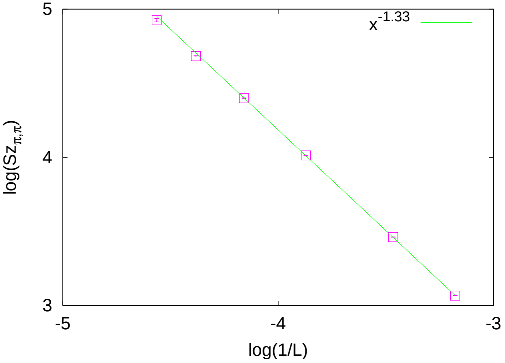
Going with the flow...

- $J_{\rm imp}$ 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 impurity scaling (Hoglund, Sandvik & Sachdev (PRL 2007), Metliski & Sachdev (PRB 2007,2008): $Sz(\pi,\pi) \sim L^{2-(1+\eta_n)/2}$

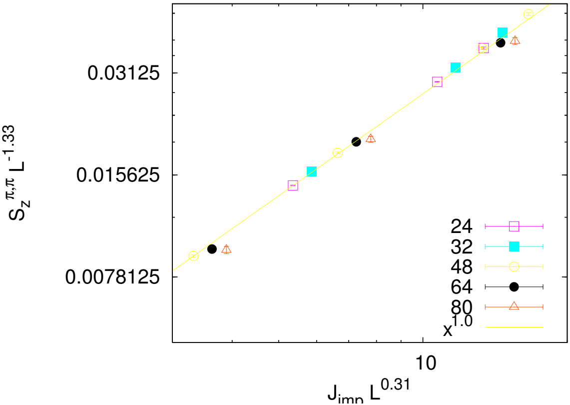


Gives $\eta_n \approx 0.34$

Consistent with earlier estimate via $\eta_n = (1 - 2\lambda_{\mathrm{imp}})$ and with $\eta_n \approx 0.34$ (Lou, Sandvik, Kawashima PRB 2009)

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

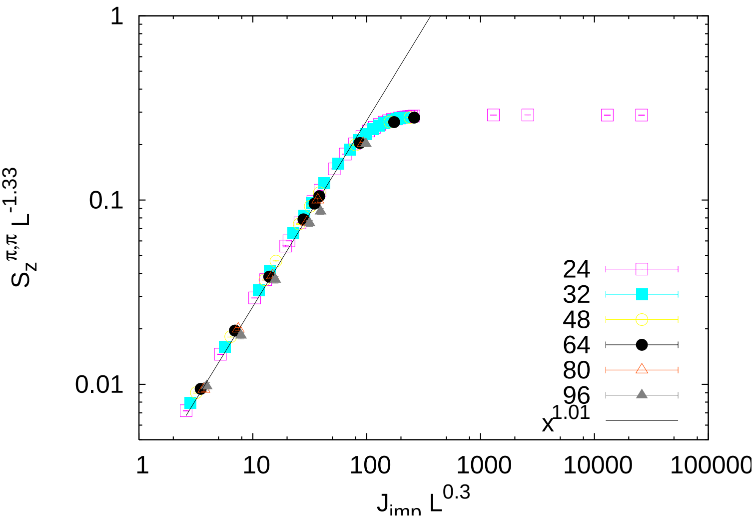
- Look at $\langle S^z_{\rm bulk}(\mathbf{Q})\rangle L^{(3-\eta_n)/2}$ for small $J_{\rm imp}$.
  Use the value of η_n obtained from $J_{\rm imp} = \infty$ results



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

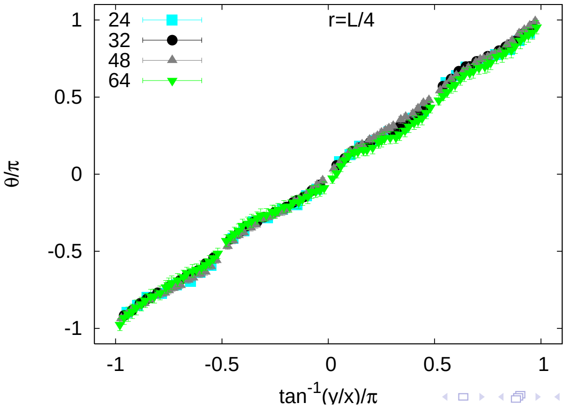
Going with the flow...

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

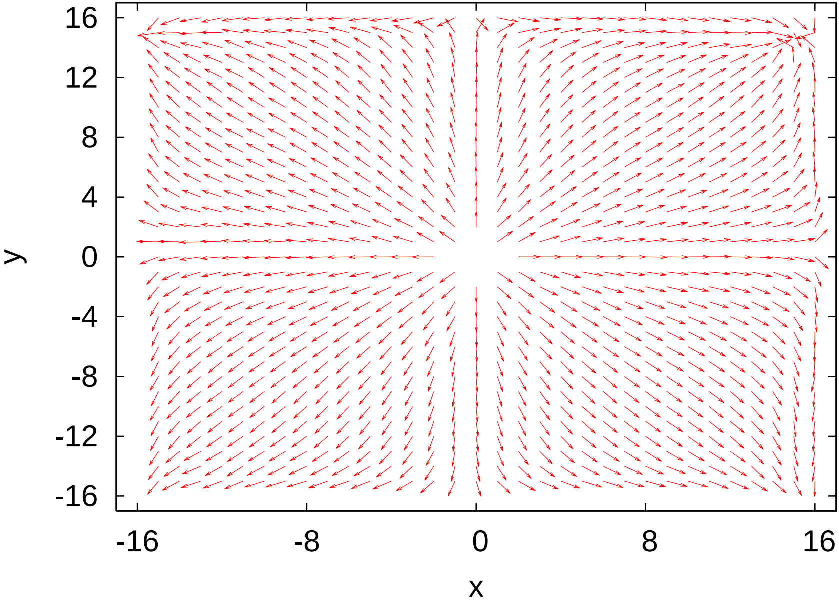


A twist at ∞: Induced local VBS order has phase winding

- 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 of impurity spin texture: A more careful look

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 $r >> 1$
  Hoglund, Sandvik, Sachdev (PRL 2007), Metlitski & Sachdev (PRB 2007,2008)

Numerics: How to define uniform and staggered parts *unambiguously*?

- Our approach: Finesse the question in q space
  $\langle S^z(\mathbf{q})\rangle = g_0(\mathbf{q}L)$ for $|\mathbf{q}| \ll \pi/2$
  $\langle S^z(\mathbf{Q}+\mathbf{q})\rangle = L^{2-(1+\eta_n)/2} g_{\mathbf{Q}}(\mathbf{q}L)$ for $|\mathbf{q}| \ll \pi/2$

How well does this work?

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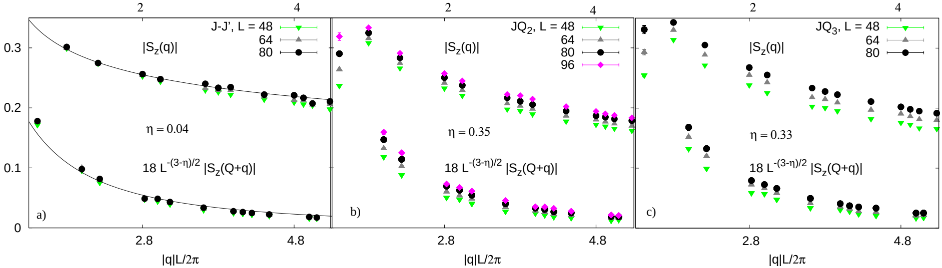


Impurity scaling does not work at Neel-VBS transitions

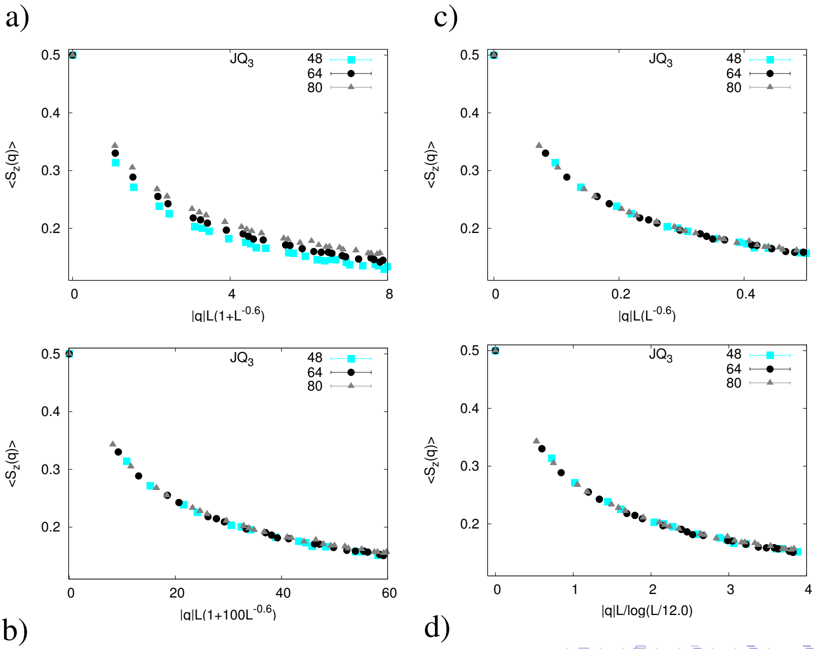
Ordinary but strong finite size corrections?

Dimensionless scaling argument $\mathbf{m} = \mathbf{q}L$.
$\rightarrow$ Standard finite-size corrections to scaling argument should look to replace $\mathbf{m}$ with

$$\mathbf{m} \times \left[1 + \left(\frac{l_{0/Q}}{L}\right)^p\right]$$

where power p controls approach to scaling regime for length scales $L \gg l_{0/Q}$.

Does this work?



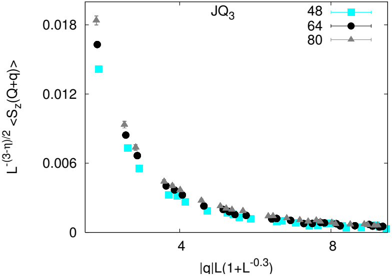
Forced to use $\mathbf{m}/L^{0.2}$ or $\mathbf{m}/\log(L/l_{0/Q})$

Unconventional scaling argument $\mathbf{m}/L^p$ with $p \approx 0.2$ hard to interpret

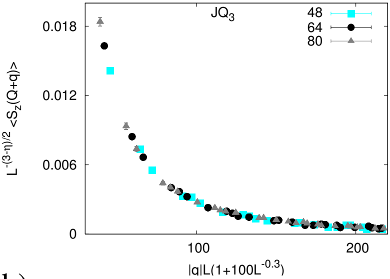
- $L^{0.2} \to \log(L/l_{0/Q})$.
- Scaling argument $\mathbf{m}/\log(L/l_{0/Q})$ can presumably arise from marginal operators at fixed point.
- Parallel work of Sandvik sees some log drifts in other things. (PRL 2010).

Interpret data in terms of “log” violations?

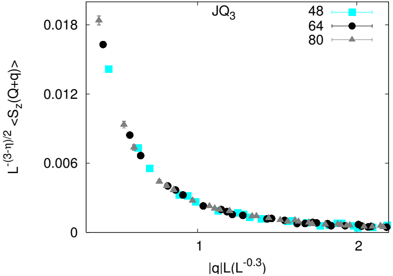
a)



b)



c)



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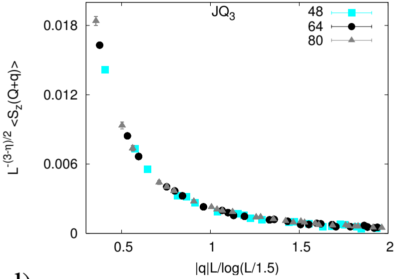
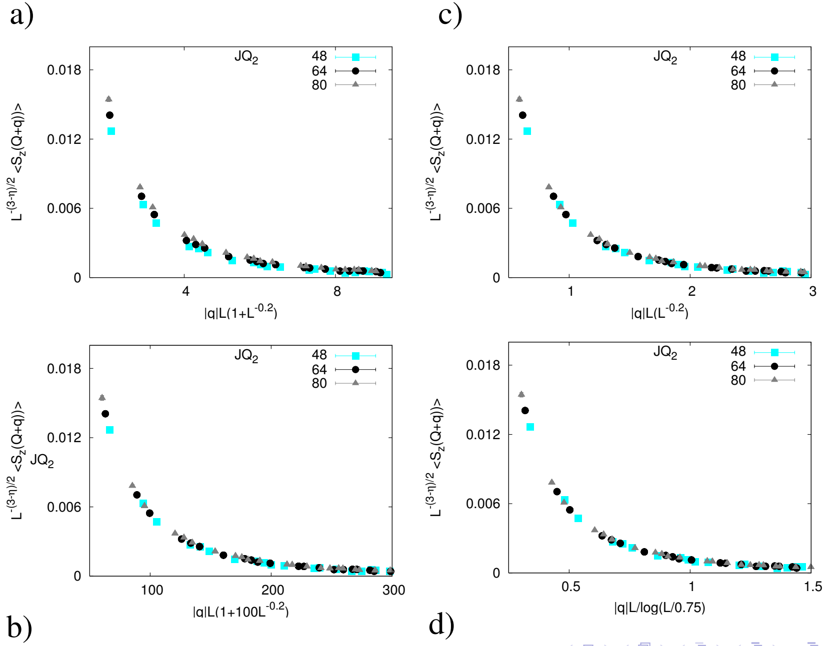


Ansatz: Logarithmic violations of scaling

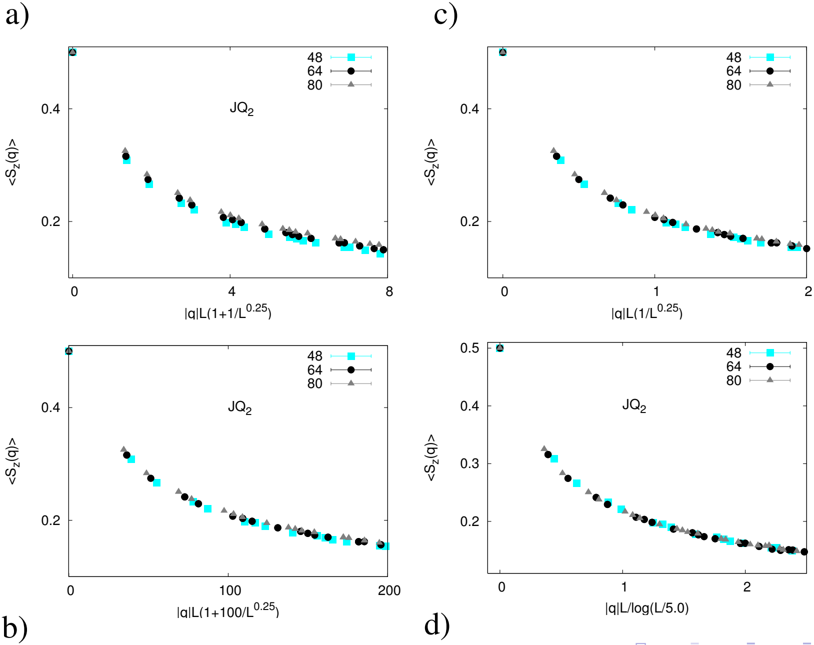
- $\langle S^z(\mathbf{q})\rangle = g_0(\mathbf{q}L/\log(L/l_0))$ for $|\mathbf{q}| \ll \pi/2$
- $\langle S^z(\mathbf{Q}+\mathbf{q})\rangle = L^{2-(1+\eta_n)/2} g_{\mathbf{Q}}(\mathbf{q}L/\log(L/l_{\mathbf{Q}}))$ for $|\mathbf{q}| \ll \pi/2$???

l_0 and $l_{\mathbf{Q}}$ some non-universal length scales.

Does this work?



Does this work?

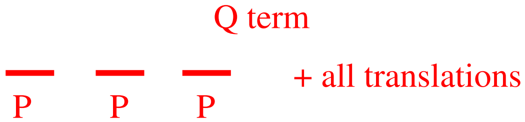


Taking stock

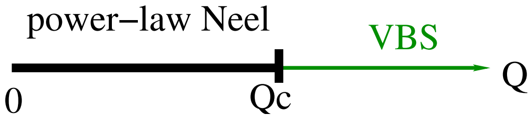
- $SU(2)$ deconfined critical point seems to have some logarithmic violations of scaling
- $SU(3)$ JQ_2 model seems to obey impurity scaling at deconfined critical point. (Banerjee, KD & Alet PRB 2011)
  Not settled yet: Kaul (arXiv 2010) finds SU(3) behaves a lot like SU(2) (?)

Tractable example of log violations:

- JQ_3 model in 1d
  $H = -\sum_i (JP_{i,i+1} + QP_{i,i+1}P_{i+2,i+3}P_{i+4,i+5})$



- $Q_c/4J \approx 0.04$ (projector QMC, Sanyal,Banerjee, KD (arXiv 2011)



consistent with parallel work: Tang and Sandvik (arXiv 2011)

Vacancy in power-law Neel phase

- Remove one site from periodic system with $N_{site} + 1$ sites (even)
- System with open boundaries and odd number of sites: Doublet ground state (focus on $S^z_{tot} = 1/2$ member).
- Study with projector QMC in $S_{tot} = S^z_{tot} = 1/2$ sector
- Bosonization:Free bosonic theory with marginal cosine interaction:

$$\frac{u}{2}\int_0^L dx\left[\left(\frac{d\phi}{dx}\right)^2 + \left(\frac{d\widetilde{\phi}}{dx}\right)^2\right] - \frac{u\epsilon_0}{r_0^2}\int_0^L dx\cos\left(\frac{2\phi(x)}{R}\right)$$

with

$$\frac{1}{2\pi R^2} = 1 - \pi\epsilon_0 \ .$$

- Expectation: ϵ_0 tuned to 0 as Q increased to Q_c.

Calculating the spin texture

- Calculate alternating part of $\langle S^z(r)$ in bosonization

$$S^z(r) = \frac{a}{2\pi R}\frac{d\phi}{dr} + \frac{\mathcal{A}}{\sqrt{r_0}}(-1)^{\frac{r}{a}} \sin\left(\frac{\phi(r)}{R}\right) \ .$$

- Compare with projector QMC numerics. (define alternating part by coarse-graining)

Focus: Effect of marginal operator on alternating part of spin texture

Prediction ("RG improved" perturbation theory)

$$N_z(r) = c\sqrt{a}\frac{F_0}{\sqrt{L}}\left(\frac{\epsilon_0}{\epsilon(L)}\right)^{\frac{1}{4}}(1-\epsilon(L)R)\ ,$$

with

$$F_0(\frac{r}{L}) = \sqrt{\frac{\pi\sin\theta_r}{2}}\ ,$$

and

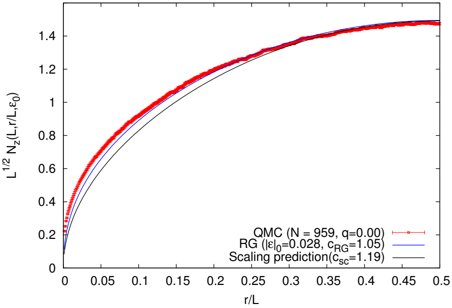
$$R(\frac{r}{L}) = \frac{\pi}{2}\log\frac{2\pi}{\sin\theta_r} + 2\left(\int_0^{\theta_r} + \int_0^{\pi-\theta_r}\right)\phi\cot\phi d\phi\ ,$$

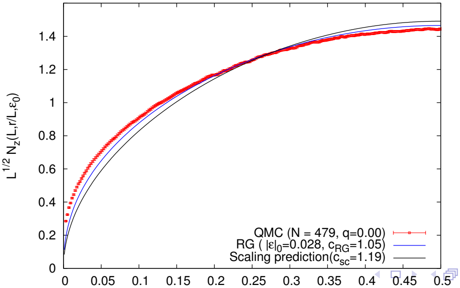
with

$$\epsilon(L) = -\frac{|\epsilon_0|}{1+2\pi|\epsilon_0|\left\{\log\left(\frac{L}{r_0}\right)+\frac{1}{2}\log\left(\log\left(\frac{L}{r_0}\right)\right)\right\}}\ ,$$

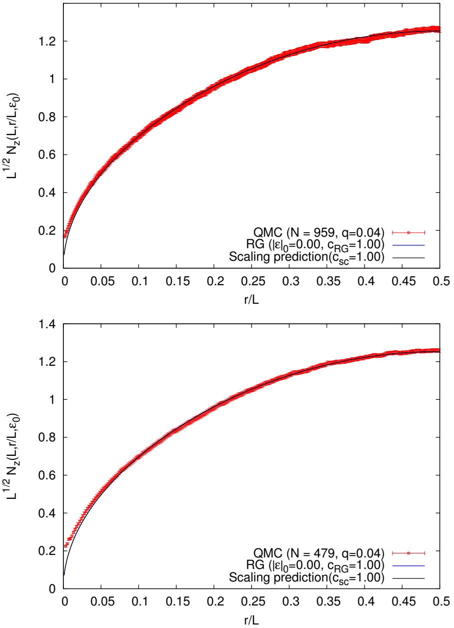
and $\theta_r \equiv \frac{\pi r}{L}$, $L = N_{site}+1$, $r_0 = a$.

Are multiplicative logarithmic violations seen in texture?

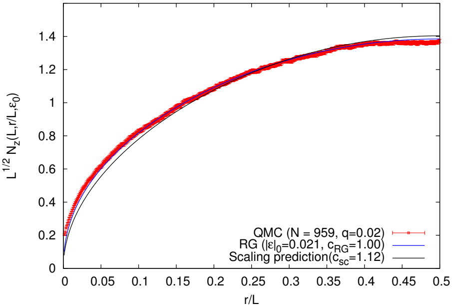


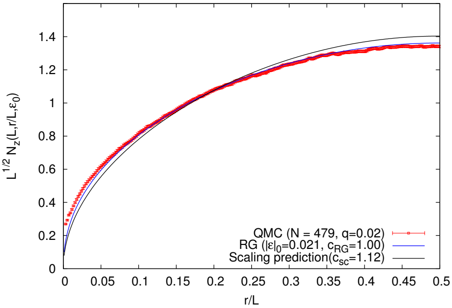


Compare with pure scaling at Q_c



And half-way to Q_c:





Wrapping up

- $SU(2)$ deconfined critical point seems to have some logarithmic violations of scaling
- $SU(3)$ JQ_2 model seems to obey impurity scaling at deconfined critical point. (Banerjee, KD & Alet PRB 2011)
  Although Kaul (arXiv 2010) finds that SU(3) looks similar to SU(2) (?)
- Marginal operator at $N = 2$ becomes irrelevant for $N > 2$ in $SU(N)$ deconfined critical points?
- Simple tractable 1d case gives concrete example of log violations arising from marginally irrelevant interaction.

Acknowledgements

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