Advanced School and Conference on Quantum Matter, ICTP, Trieste, 12/11/2025

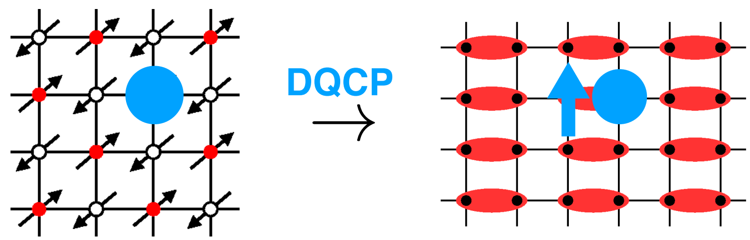
Single-hole Dynamics at the Deconfined quantum Critical Point

Anders W Sandvik, Boston University

Sibin Yang, Boston University

and help by former students Bowen Zhao, Gabe Schumm

ArXiv:2512.02962, ArXiv:2511.20447, manuscript in preparation



also discussing results on the quantum phase transition from

ArXiv:2405.06607

SO(5) multicriticality in two-dimensional quantum magnets

Jun Takahashi†,[1] Hui Shao†,[2] Bowen Zhao,[3] Wenan Guo,[4] and Anders W. Sandvik[3,5,*]

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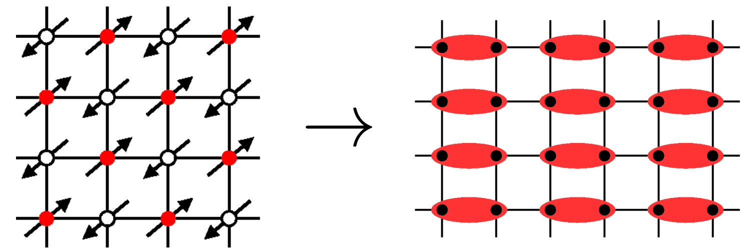
Outline

Deconfined quantum critical point (DQCP)
- original scenario for the AFM-VBS transition



J-Q models
- QMC amenable 2D “designer models” with AFM and VBS ground states

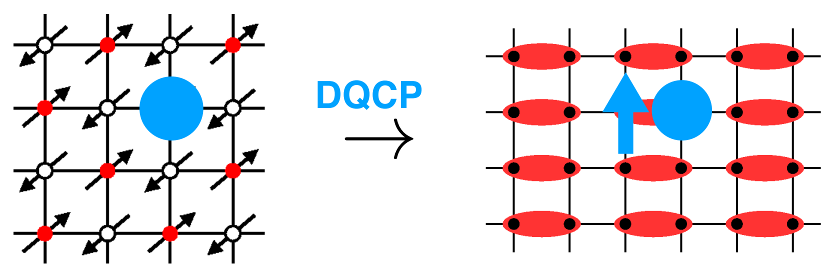
Weak first-order behavior and (likely) inaccessible critical point
- near-criticality at AFM-VBS transition

Modified DQCP scenario: SO(5) multi-critical point
- consistency with recent CFT calculations

Improved stochastic analytic continuation method for dynamics with QMC

Dynamic spin structure factor $S(k, \omega)$ at DQCP
$\rightarrow$ spinon deconfinement (π-flux model)

Single-hole spectral function $A(k, \omega)$
$\rightarrow$ spin-charge separation at DQCP

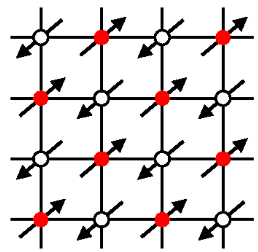


Deconfined quantum criticality in 2D quantum magnets

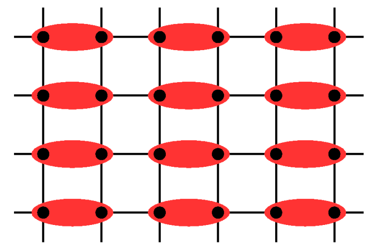
Senthil, Vishwanath, Balents, Sachdev, Fisher (Science 2004) + ….
(+ many previous works; Read & Sachdev, Sachdev & Murthy, Motrunich & Vishwanath….)

$$H = J\sum_{\langle ij \rangle} \mathbf{S}_i \cdot \mathbf{S}_j + g[\text{other symmetry preserving interactions}]$$

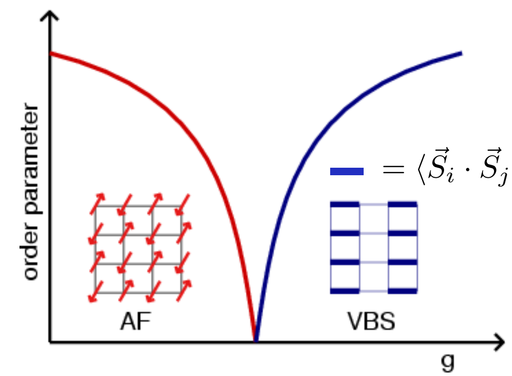
antiferromagnet for g=0
- breaks O(3) symmetry



$\rightarrow$



valence-bond (or plaquette) solid for $g > g_c$
- breaks Z_4 symmetry
- emergent U(1) symmetry close to the transition



Generic continuous T=0 transition proposed
- would be violation of Landau rule
- first-order would normally be expected

Later theories and numerics suggest emergent SO(5)

$\vec{O} = (n_x, n_y, n_z, d_x, d_y)$ Senthil & Fisher, Nahum et al.…

Convincing in SU(N) field theory
- QMC exponents agree for large N (Kaul, AWS 2012)
- not clear for small N (esp. N=2)

Numerics; J-Q models

2D Heisenberg exchange J
+ products of singlet projectors

Amenable to large-scale QMC studies

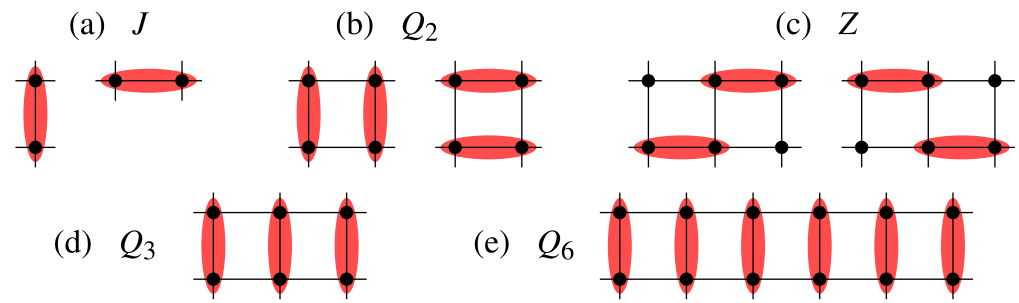
Likely critical point with emergent SO(5) symmetry (3 AFM, 2 VBS components)

Relevant perturbations of DQCP are
- SO(5) singlet (s) (previously assumed irrelevant)
- symmetry-changing (t) (driving AFM to VBS)

The J-Q models have weak first-order VBS-AFM transitions

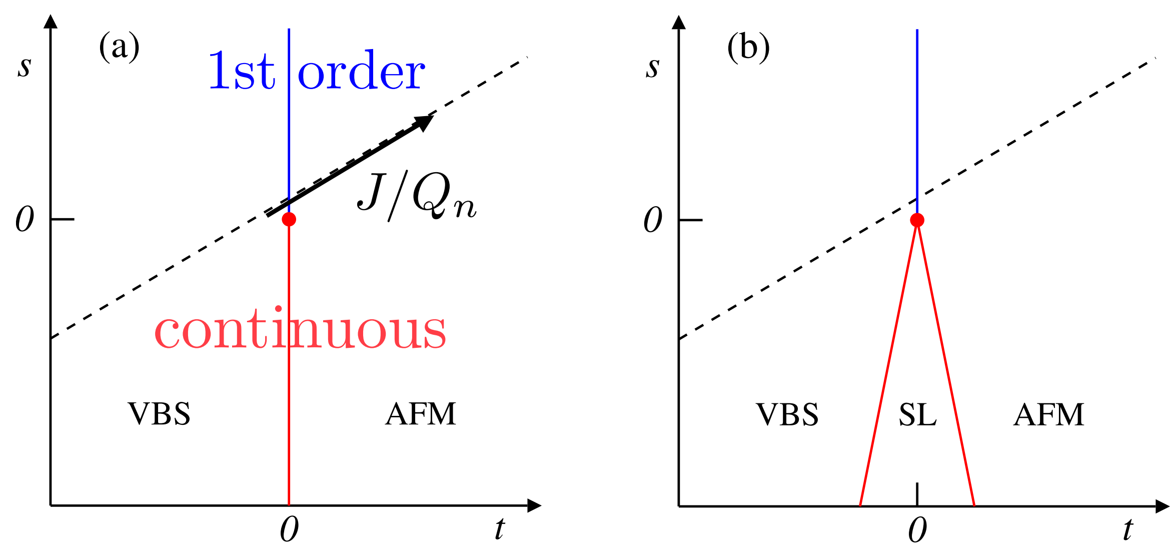
Crossing transition by tuning J/Q_n

J/Q_2 and J/Q_3 are near critical



$$H = -J\sum_{\langle ij\rangle} P_{ij} - Q_2 \sum_{\langle ijkl\rangle} P_{ij}P_{kl} - \ldots, \quad P_{ij} = \mathbf{S}_i \cdot \mathbf{S}_\mathbf{j}$$

Possible (t,s) phase diagrams



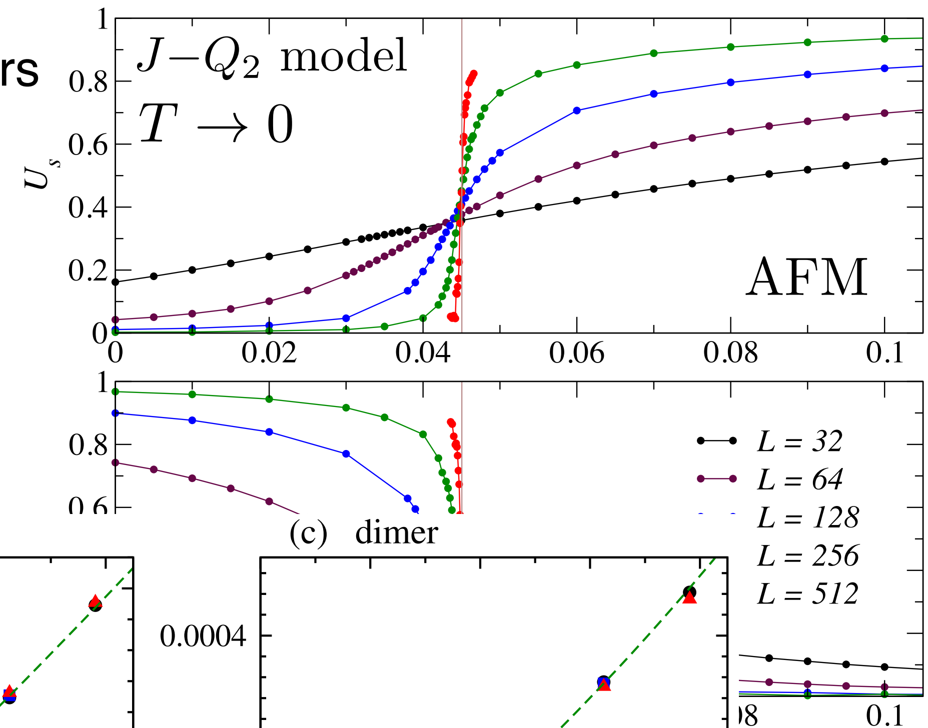
Transition point of J-Q_2 model (QMC)

Binder cumulants of AFM and VBS order parameters

$$U_s = \frac{5}{2}\left(1 - \frac{1}{3}\frac{\langle M_z^4\rangle}{\langle M_z^2\rangle^2}\right) \quad U_d = 2\left(1 - \frac{1}{2}\frac{\langle D^4\rangle}{\langle D^2\rangle^2}\right)$$

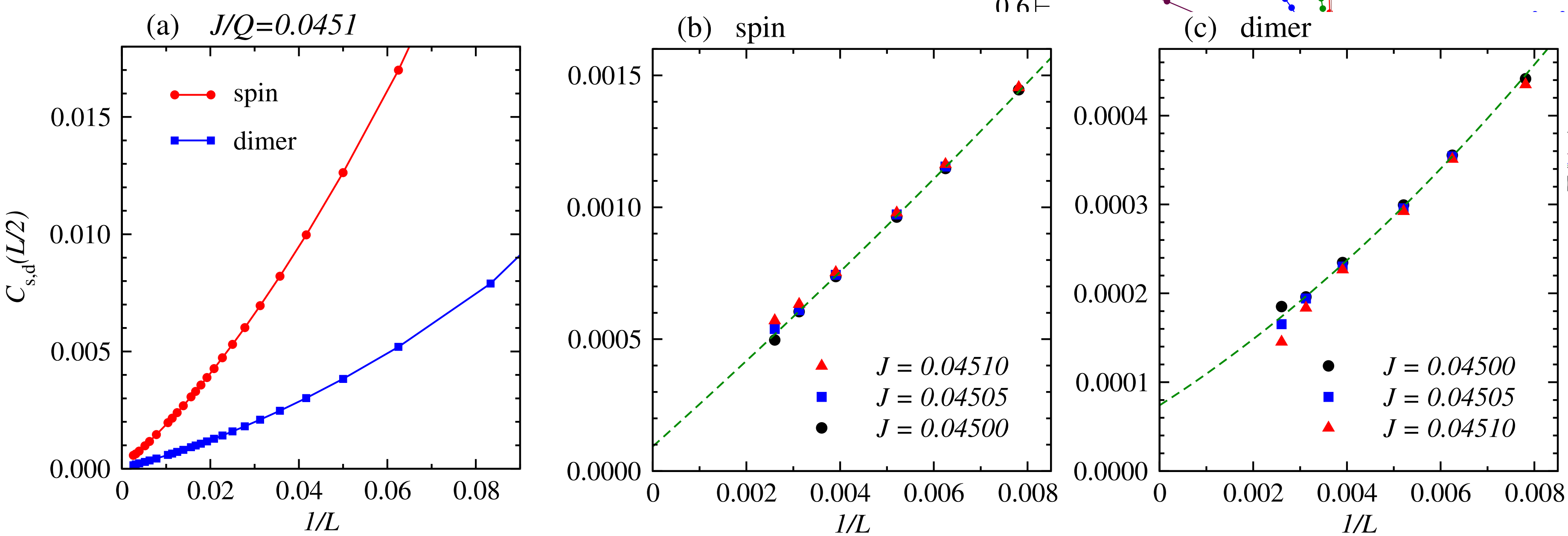
$U_s \to 1$, $U_d \to 0$ in AFM phase

$U_s \to 0$, $U_d \to 1$ in VBS phase



Long-distance (r=L/2) correlations

→ weak coexisting order parameters at $(J/Q)_c$



Scaling dimensions from large-scale QMC simulations ArXiv:2405.06607

- compare with SO(5) CFT bootstrap and fuzzy sphere calculations

	Δ_ϕ	Δ_s	Δ_t	Δ_j	Δ_4
This work	0.607(4)	2.273(4)	1.417(7)	2.01(3)	3.723(11)
SO(5) CFT	0.630*	2.359	1.519	2*	3.884
Fuzzy sphere	0.585	2.831	1.458	2*	3.895

S. M. Chester and N. Su, Bootstrapping Deconfined Quantum Tricriticality, Phys. Rev. Lett. **132**, 111601 (2024).

Zhou, Z., Hu, L., Zhu, W. & He, Y.-C. SO(5) deconfined phase transition under the fuzzy-sphere microscope: approximate conformal symmetry, pseudo-criticality, and operator spectrum. Phys. Rev. X 14, 021044 (2024).

Whatever the ultimate nature is of the DQCP, the J/Q_2 and J/Q_3 models are sufficiently nearby to reliably study it.

Nature of excitations

- spectral functions
- here at T=0

Spin structure factor (neutrons): $S(k,\omega) = \sum_n |\langle n | S^z_k | 0\rangle | \delta(\omega - [E_n - E_0])$

Single-hole spectral fktn (ARPES): $A(k,\omega) = \sum_n |\langle n | c_{\sigma,k} | 0\rangle | \delta(\omega - [E_n - E_0])$

QMC + numerical analytic continuation

Stochastic Analytic Contiunuation (SAC)

H. Shao, AWS, Phys. Rep. (2023)

Spectral function of operator O

$$S(\omega) = \frac{\pi}{Z} \sum_{m,n} \mathrm{e}^{-\beta E_n} |\langle m|O|n\rangle|^2 \delta(\omega - [E_m - E_n])$$

Imaginary-time correlation from QMC

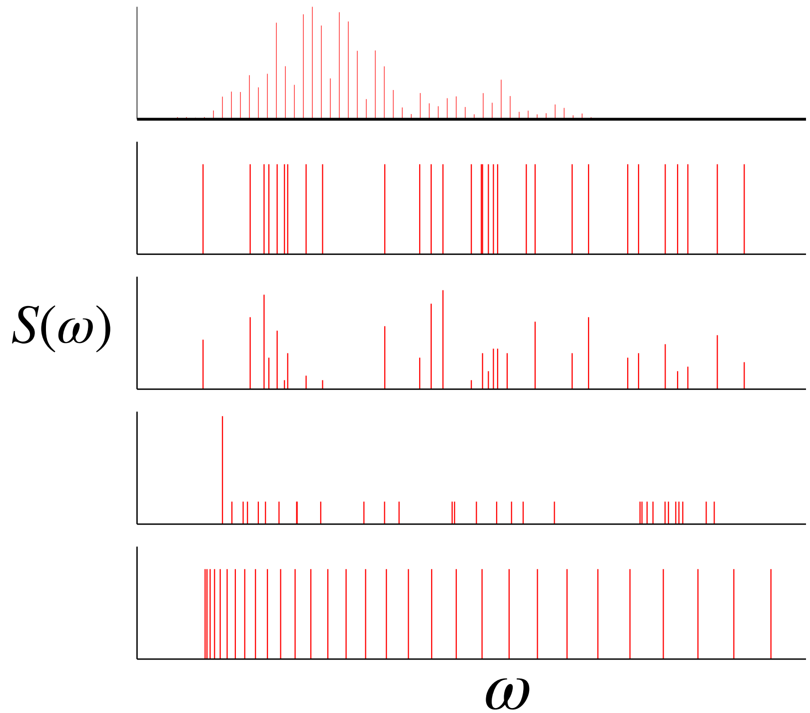
$$G(\tau) = \langle O^\dagger(\tau) O(0)\rangle$$

Related to spectral function by

$$G(\tau) = \frac{1}{\pi}\int_{-\infty}^{\infty} d\omega S(\omega) \mathrm{e}^{-\tau\omega}$$

Solve inverse problem by sampling $S(\omega)$

- parametrized in some suitable way
- here with large number of δ-functions



$$P(S|\bar{G}) \propto \exp\left(-\frac{\chi^2(S)}{2\Theta}\right) \qquad \chi^2 = \sum_{i=1}^{N_\tau}\sum_{j=1}^{N_\tau} (G_i - \bar{G}_i) C^{-1}_{ij} (G_j - \bar{G}_j)$$

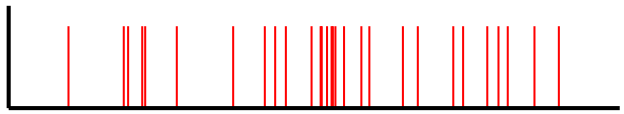
$\rightarrow \langle S(\omega)\rangle$ average spectral density

Sampling temperature Θ chosen optimally to avoid over-fitting

Each parametrization is associated with an entropy E(S), affecting the average spectrum

- constraints can be used to resolve sharp features

Example: L=16 Heisenberg chain, S(π/2,ω), T/J=0.5



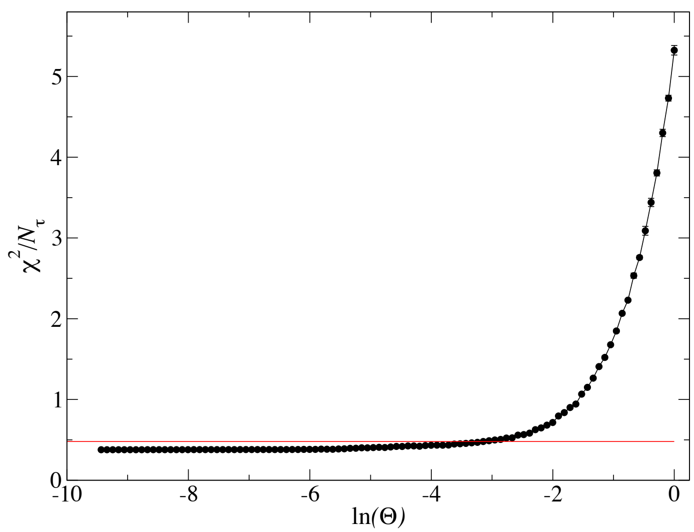
Dependence on the sampling temperature,;

θ = 10/1.1^n, n=0,1,2,…

Criterion for optimal Θ (to avoid over-fitting)

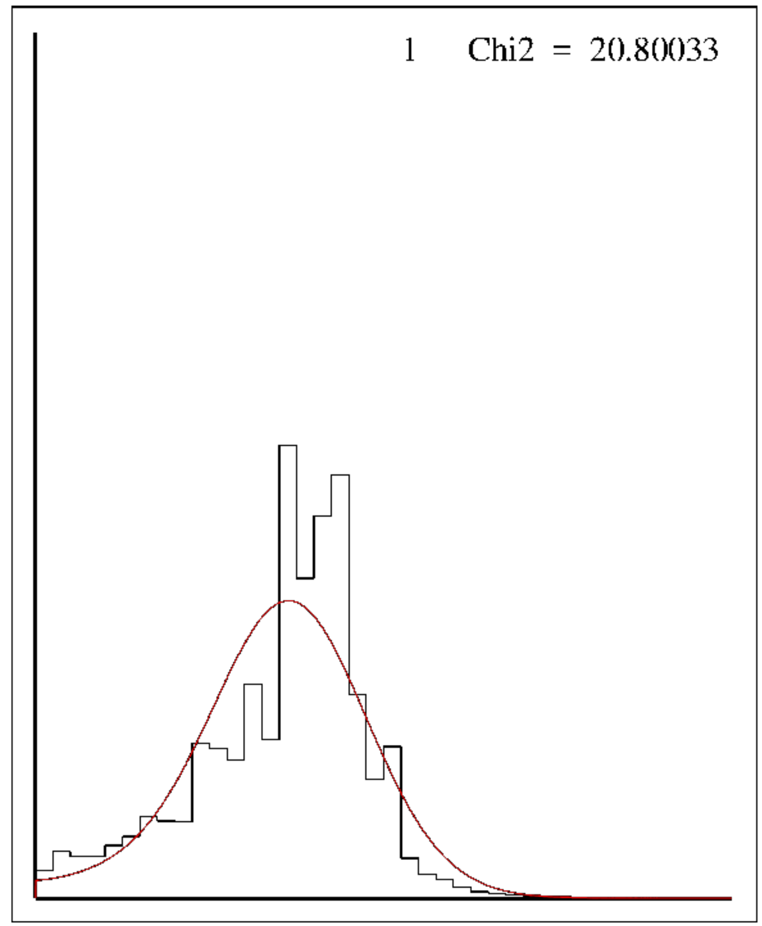
$$\langle \chi^2(\Theta) \rangle \approx \chi^2_{\min} + a\sqrt{2\chi^2_{\min}} \qquad a \sim 0.5$$

corresponds to $\langle \chi^2 \rangle$ exceeding $\chi^2_{\min}$ by of the order the standard distribution of χ^2 distribution



$$S(k,\omega) = \sum_n |\langle n|S^z_k|0\rangle|\delta(\omega - [E_n - E_0])$$

shown as histogram



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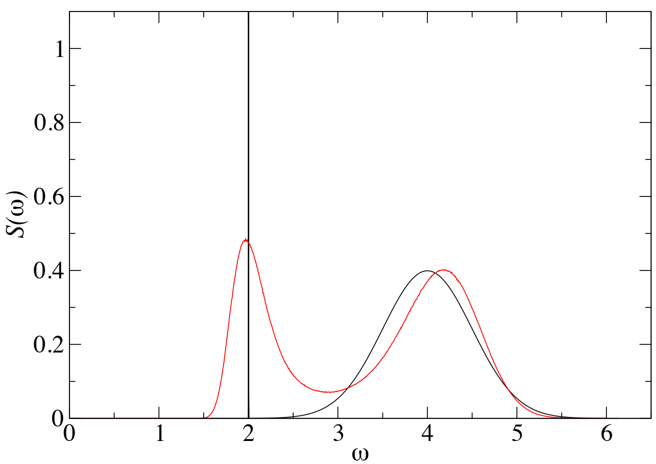
Spectra with sharp quasi-particle peak

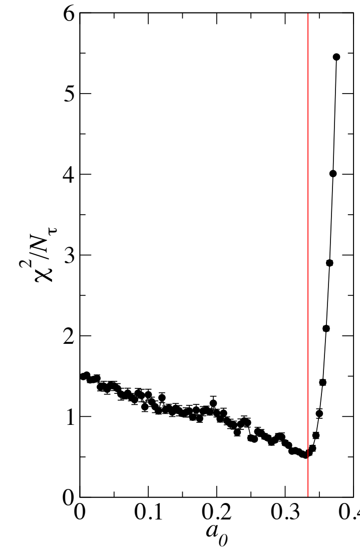
Example: δ-function and continuum, synthetic data

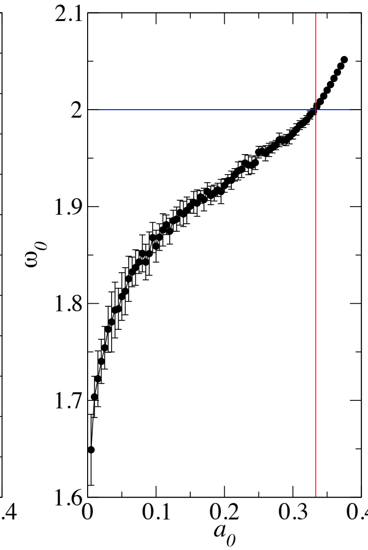
- noise level $2*10^{-5}$ (20 τ points, $\Delta\tau$=0.1)



Find optimal a_0 by scanning

1+500 δs: quasi-particle weigh affects the sampling entropy
- detected in <χ^2>

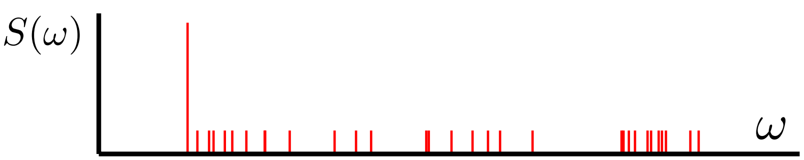




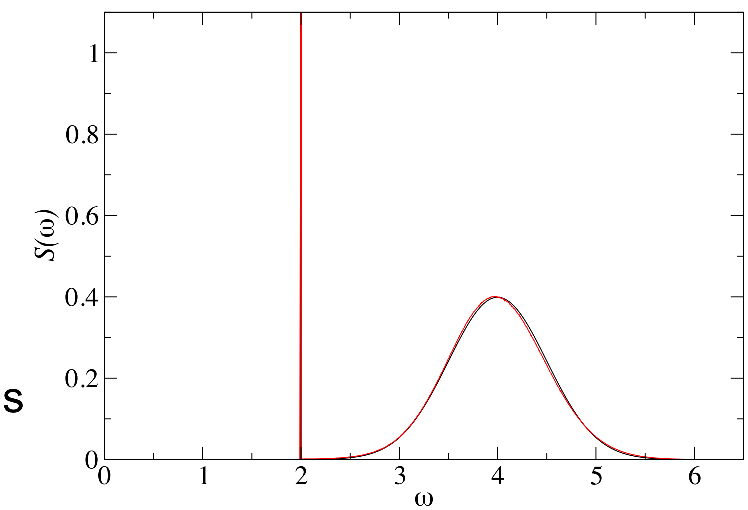
Unrestricted sampling cannot resolve the δ-function
- second broad peak is also distorted

Solution: use one "macroscopic" δ-function

- fixed weight a_0 at sampled ω_0
- other delta-functions cannot go below ω_0



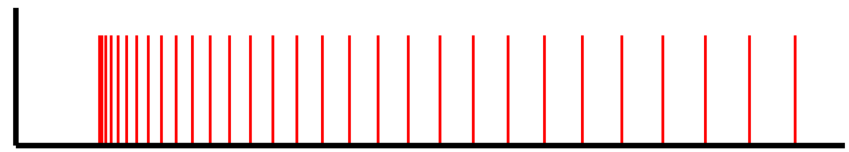
with better edge, entire spectrum is well reproduced



Spectrum with continuous edge divergence

Constraint of monotonically increasing distances

- no constraint on lower and upper bounds
- entropy favors divergent lower edge continuum



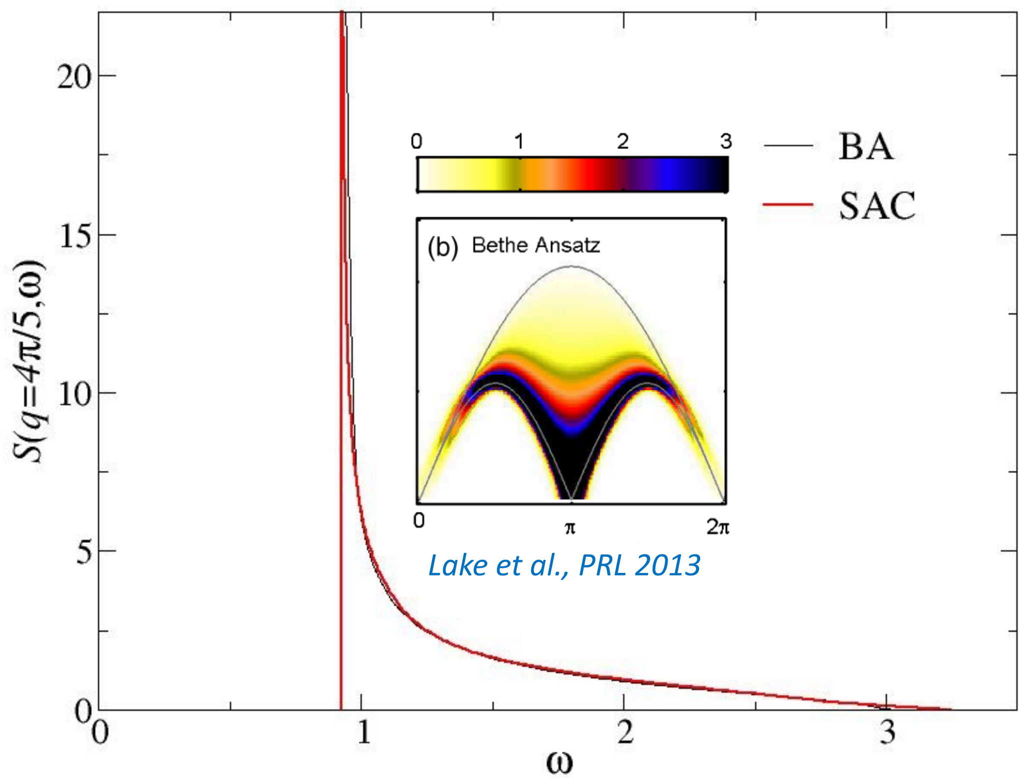
Example:
Heisenberg chain (L=500, T→0)

200 δ-functions

- Sampling done with cluster update

- Lower edge is good to ~0.2%

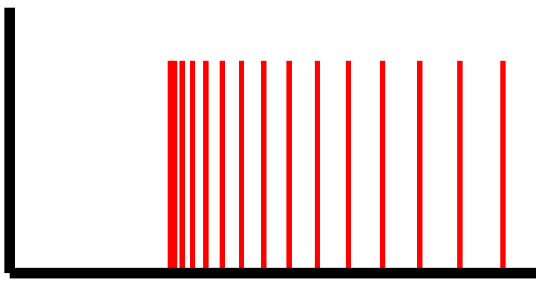
- Very close to known $(\omega-\omega_0)^{-1/2}$ singularity



Comparing with numerical Bethe Ansatz, same system size (J.-S. Caux)

The monotonicity constraint results in entropic pressure to a sharp peak at the edge
- good if the spectrum sought has such an edge

Non-divergent edge: optimize by constraining smallest spacing

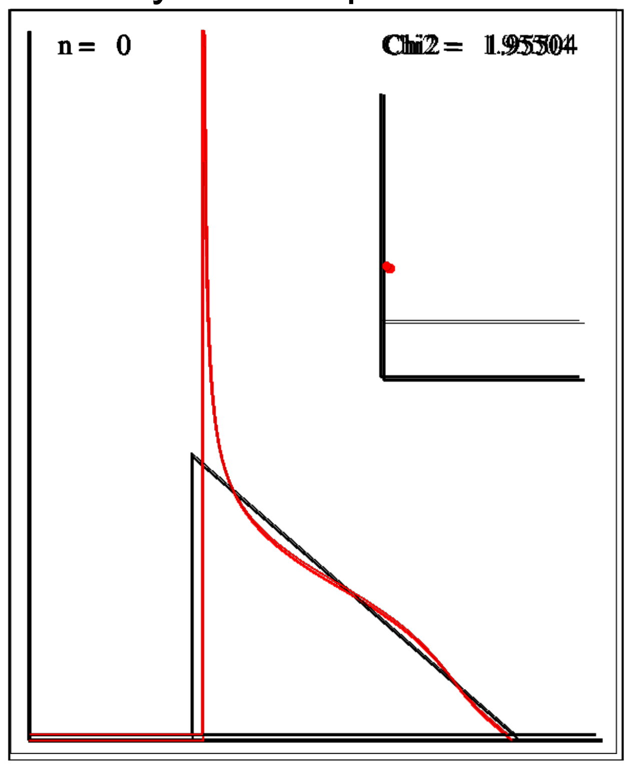


$\Delta\omega_0 = \omega_1 - \omega_0$

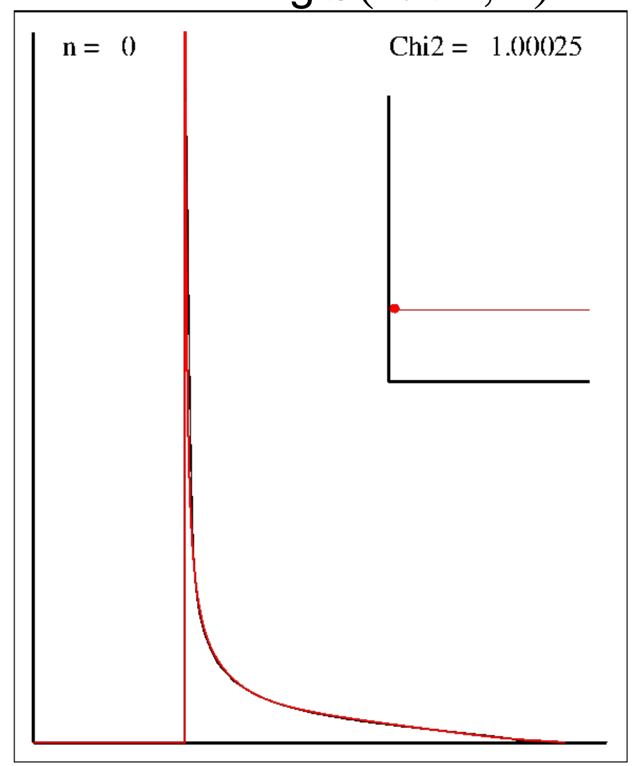
- scan over

$$\Delta\omega_0 = n\Delta_\delta,\ n = 0, 1, 2, \ldots$$

synthetic spectrum



Heisenberg $S(4\pi/5,\omega)$



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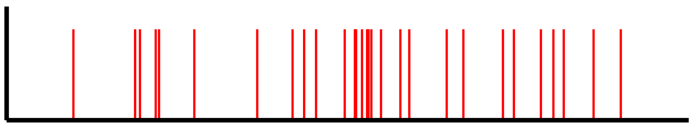
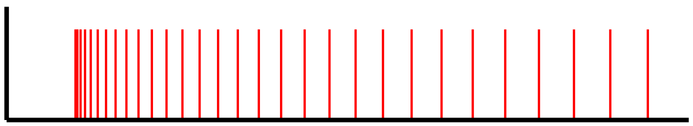
How about non-monotonic spectrum following edge?

Mix these two parametrizations:



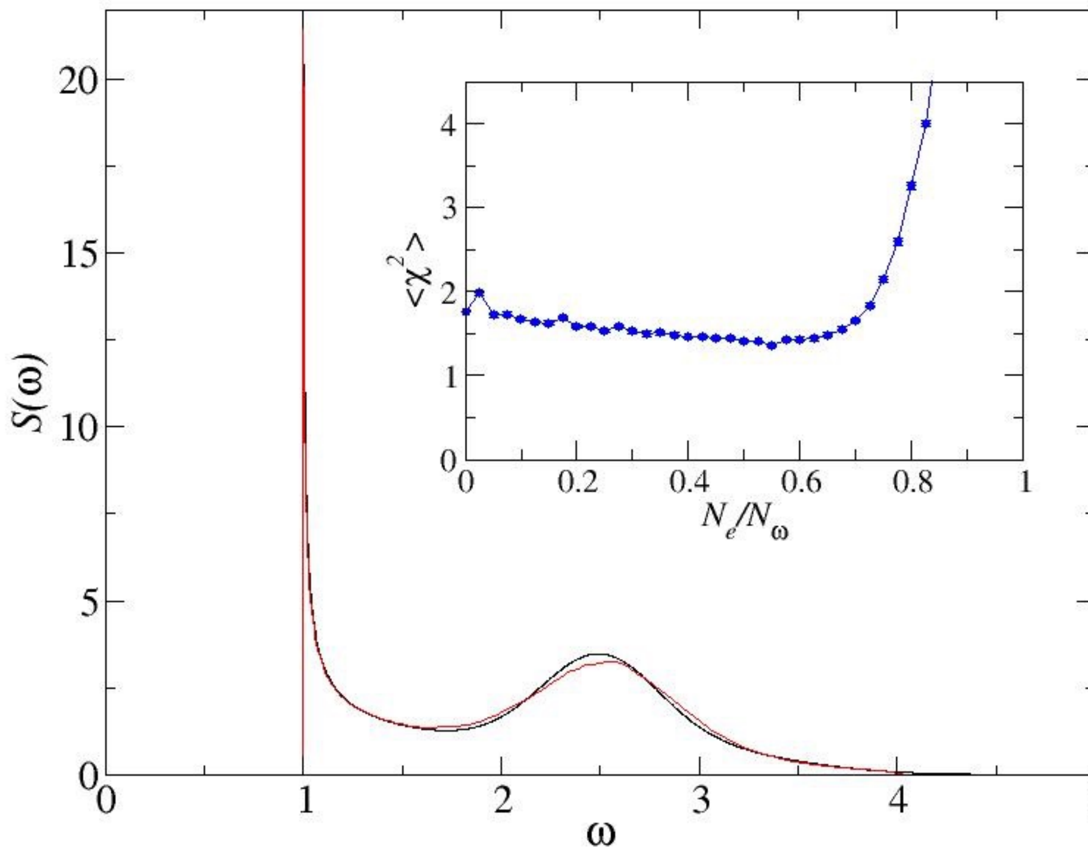


Out of N_ω deltas, use

N_e for “edge”

$N_\omega - N_e$ for “background”

background cannot go below the edge



QMC calculation of single-particle Green's function (imaginary time)

Example: t-J model

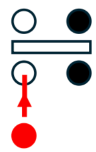
- using canonical transformation (Angelucci 1995)

$$|\eta_i\rangle = |n_i, z_i\rangle \in \{|0,\uparrow\rangle_i, |0,\downarrow\rangle_i, |1,\uparrow\rangle_i\} = \{ \uparrow_i , \downarrow_i , 0_i\}$$

in Stochastic Series QMC *(S. Yang, G. Schumm, B. Zhao, AWS, arXiv: 2511.20447)*

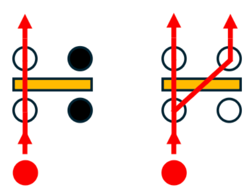
$$H = -\sum_{a=1}^{3} \sum_{\langle i,j \rangle} (-H_{a,ij})$$

$$-H_{1,ij} = J\Delta_{ij}(1 - \sigma_i^z \sigma_j^z)/4$$



$$-H_{2,ij} = -(\sigma_j^+ \sigma_i^- + \sigma_j^- \sigma_i^+) \times \left[J\Delta_{ij}/2 + t(f_i^\dagger f_j + f_j^\dagger f_i)\right]$$

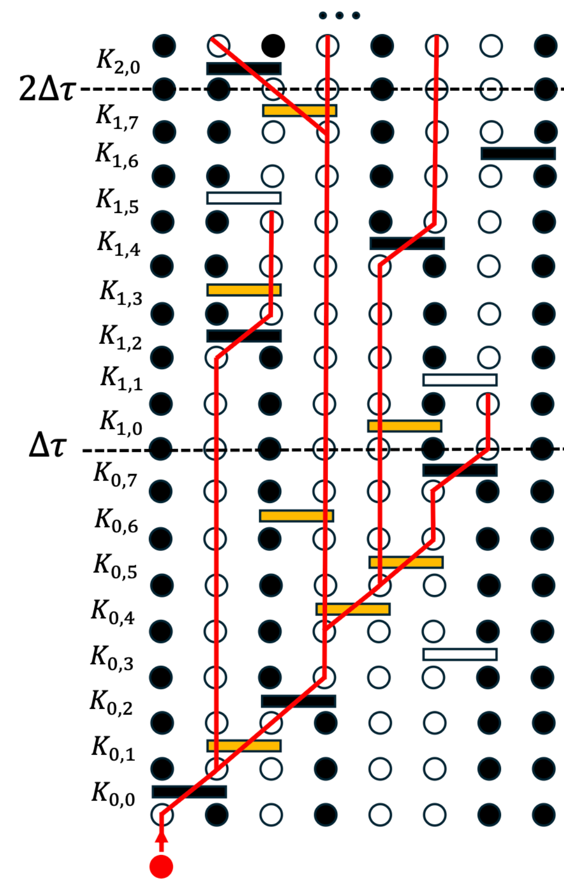
$$-H_{3,ij} = -(t/2)(1 + \sigma_i^z \sigma_j^z)(f_i^\dagger f_j + f_j^\dagger f_i) + tI_{ij}$$



$$\mathrm{e}^{-\beta H} = \left(\mathrm{e}^{-\Delta_\tau H}\right)^L$$

$$= \sum_K \left[\prod_{l=1}^{L} \frac{\Delta_\tau^{n_l}}{n_l!}\right] \prod_{l=1}^{L} \prod_{s=1}^{n_l} K_{l,s}$$

$$K_{l,s} \in \{-H_{a,ij}\}$$



1D example, N=8

Spin configurations sampled (no sign problem)

- all hole paths consistent with spin configuration are summed up exactly
- (no sign problem in practice even though some path cancelations)

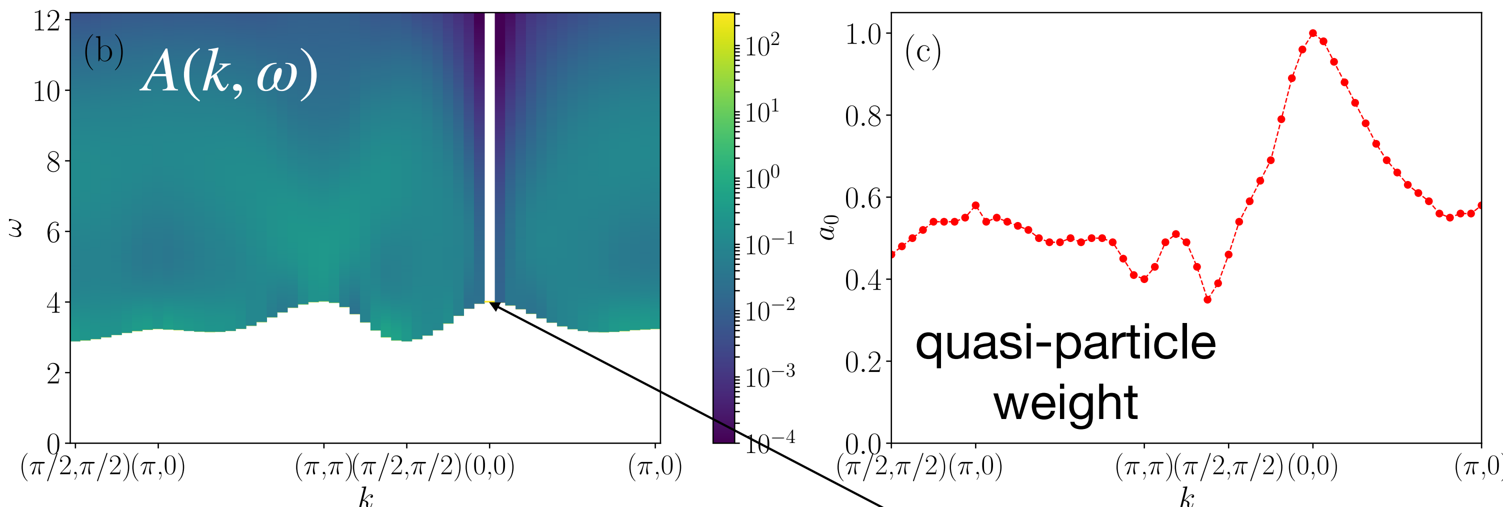
Single-hole dynamics in the AFM phase

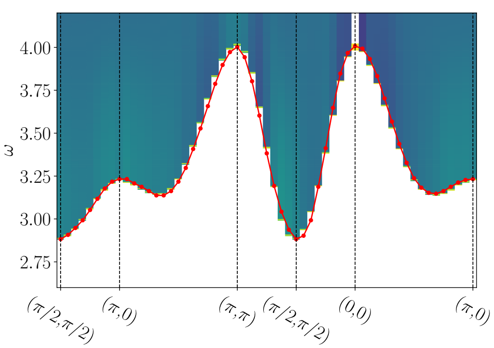
Electron ejected (hole injected); now a manifestly fermionic problem

- the J-Q model supplemented by hopping; t-J-Q model

$$H = H_{JQ} - t \sum_{\langle ij \rangle,\sigma} (c^{\dagger}_{\sigma,j} c_{\sigma,i} + c^{\dagger}_{\sigma,i} c_{\sigma,j})$$

Test on standard 2D t-J model (Q=0) at "supersymmetric" point t/J=1/2 (δ-function edge)





Expected with AFM order:

$$\omega_{\mathbf{k}} = \omega_{(\pi,\pi)-\mathbf{k}}$$

well satisfied (red line)

- Exact result at k=0 reproduced; $A(k=0,\omega) = \delta(\omega - 4)$
- Dispersion minimum at $k = (\pi/2,\pi/2)$
- Almost flat band (close to quartic) around $k = (\pi,0)$

"ledge + peak" DOS as in 2D Hubbard model [Schumm, Zhang, Sandvik, PRB 2025]

Dynamic signatures of DQCP (1) spin excitations

PHYSICAL REVIEW B **98**, 174421 (2018)

Editors' Suggestion

Dynamical signature of fractionalization at a deconfined quantum critical point

Nvsen Ma,[1] Guang-Yu Sun,[1,2] Yi-Zhuang You,[3,4] Cenke Xu,[5] Ashvin Vishwanath,[3] Anders W. Sandvik,[1,6] and Zi Yang Meng[1,7,8]

Planar J-Q model: $H_{\mathrm{JQ}} = -J \sum_{\langle ij \rangle} (P_{ij} + \Delta S_i^z S_j^z) - Q \sum_{\langle ijklmn \rangle} P_{ij} P_{kl} P_{mn}$

QMC + SAC for spin structure factor $S(q,\omega)$

Compare with fermion parton theory;

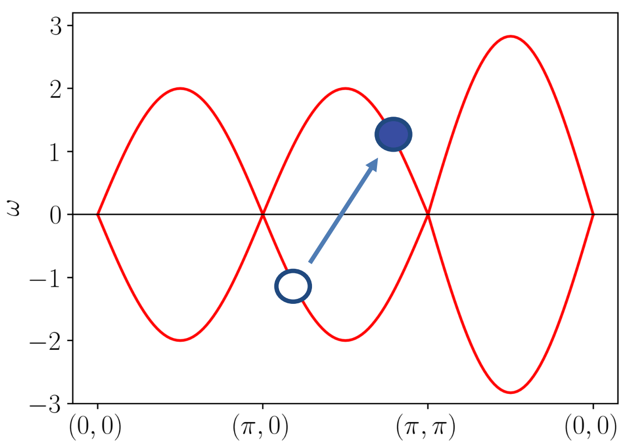
- N_f=4 compact QED_3, π-flux square-lattice model

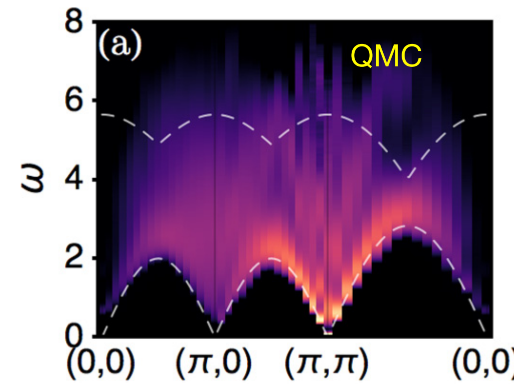
$$H_{\mathrm{MF}} = \sum_i \mathrm{i}(f_{i+\hat{x}}^\dagger f_i + (-)^x f_{i+\hat{y}}^\dagger f_i) + \mathrm{H.c.}$$

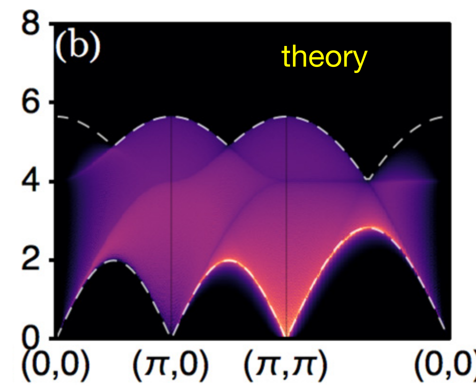
$$\boldsymbol{S}_i = \frac{1}{2} f_i^\dagger \boldsymbol{\sigma} f_i$$

$$\epsilon_s(\mathbf{k}) = \pm\sqrt{+\sin^2(\mathbf{k}_x) + \sin^2(\mathbf{k}_y)}$$

negative states filled



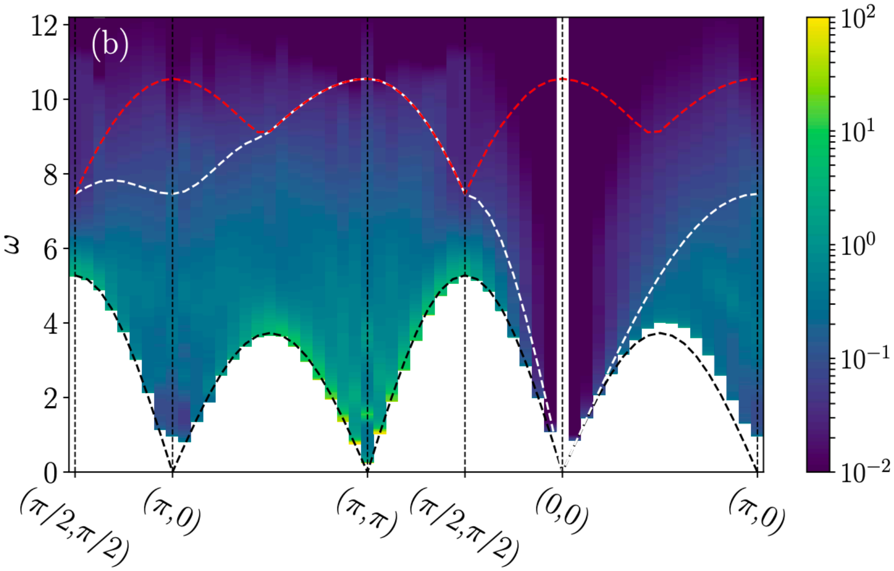


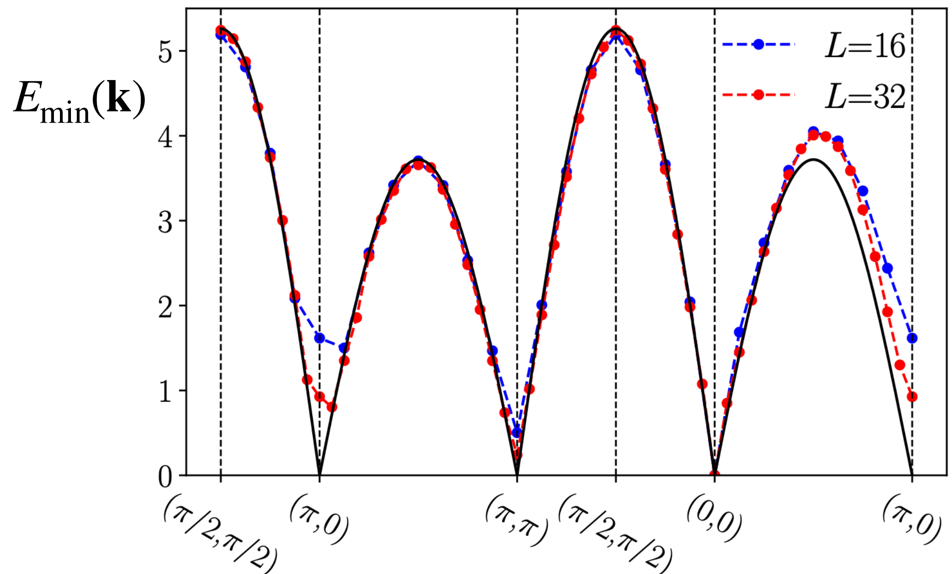


Spinon deconfinment on large length scales close to the critical point

At the transition point of the isotropic J-Q model (Q=1,J=0.667,t=1,L=32)

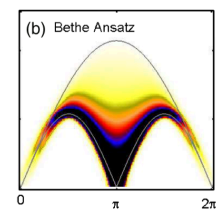
- an edge followed by continuum (no quasi-particle peak); use constraints discussed





Different unit cells for phases (gauge) can be chosen in the π-flux model

- the dispersion relation is gauge invariant
- but the two-particle continuum depends on the gauge



Upper bound of the 2-spinon continuum: $E_{\max}(\mathbf{k}) = \max[\epsilon_s(\mathbf{k}_1) + [\epsilon_s(\mathbf{k}_2)], \quad \mathbf{k} = \mathbf{k}_1 + \mathbf{k}_2$

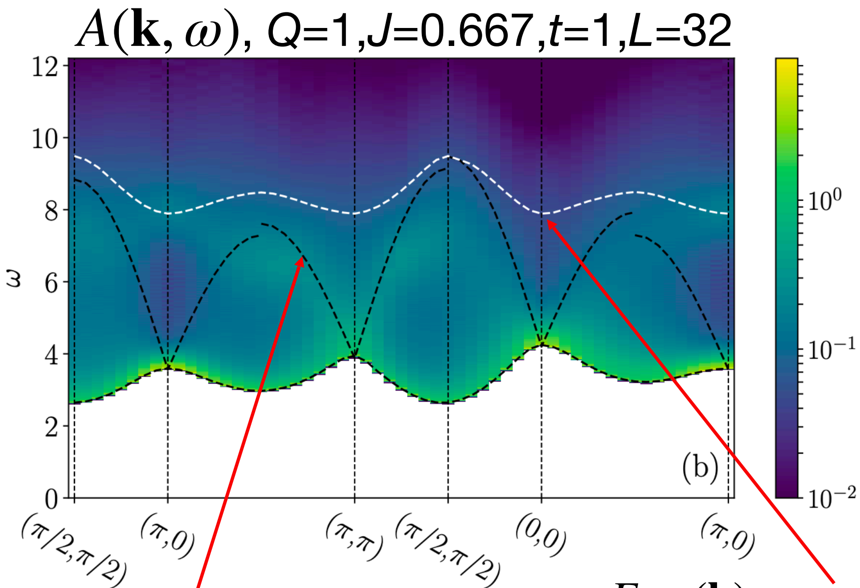
red: $|k_x| + |k_y| \leq \pi$ (similar to previous work)

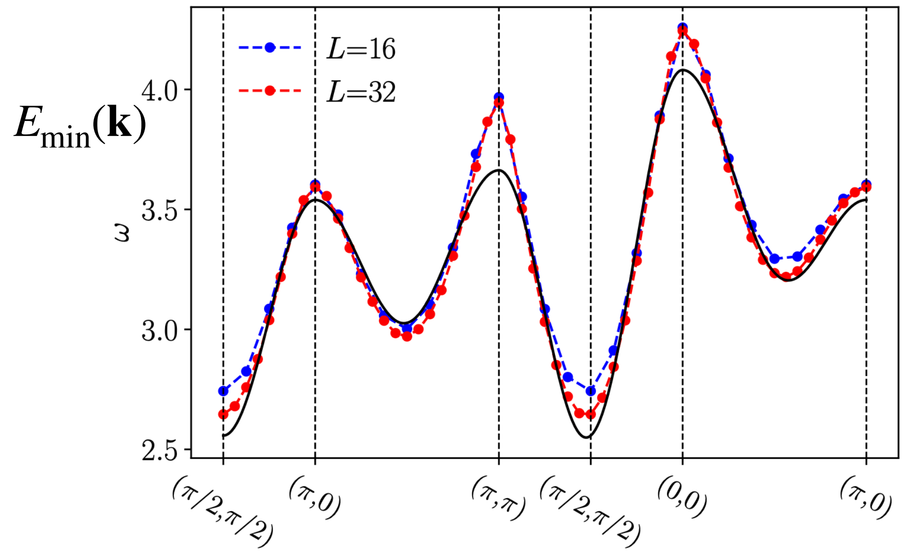
white: $k_x, k_y \in [0,\pi]$ (motivated by spinons in Heisenberg chain)

The smaller BZ seems to work better

- not completely clear…

Dynamic signatures of DQCP (2) spin-charge separation





$E_{\max}(\mathbf{k}) = \max[\epsilon_s(\mathbf{k}_1) + [\epsilon_h(\mathbf{k}_2)]$

Spinon added to holon at local max

$$\epsilon_h(\mathbf{k}) = t_1[\cos(k_x)+\cos(k_y)] + t_2[\cos(k_x+k_y)+\cos(k_x-k_y)] + t_3[\cos(2k_x)+\cos(2k_y)] + \mu,$$

If spin-charge separation:

independently propagating spinon and holon, $\epsilon_{s+h}(k) \in \{\epsilon_s(k-q)+\epsilon_h(q)\}, \quad q \in \mathrm{BZ}$

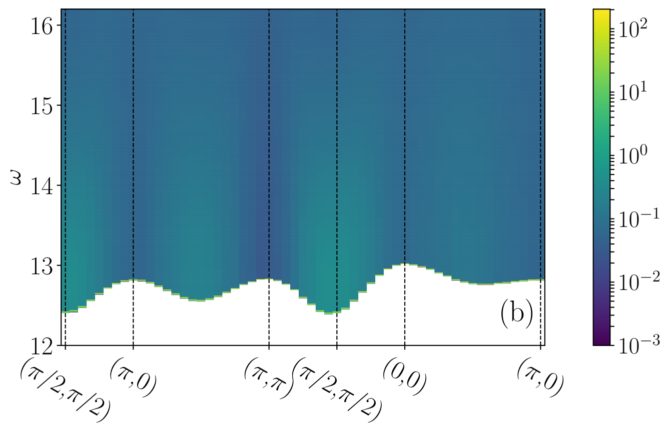
We have $\min[\epsilon_{s+h}(k)]$ and $\epsilon_s(k)$; solve for $\epsilon_h(k)$ and $\max[\epsilon_{s+h}(k)]$

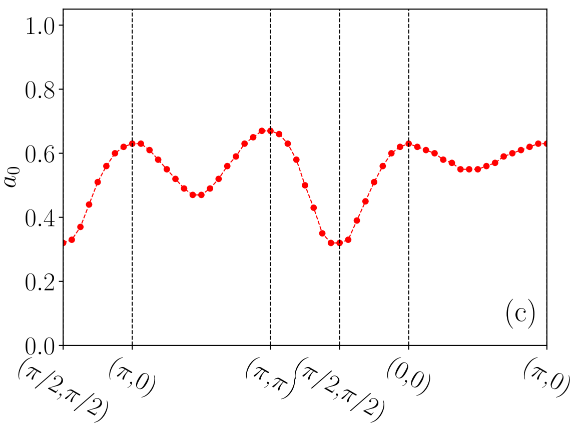
- consistent solution if spinon $k_x, k_y \in [-\pi/2, \pi/2]$; then holon dispersion = lower bound

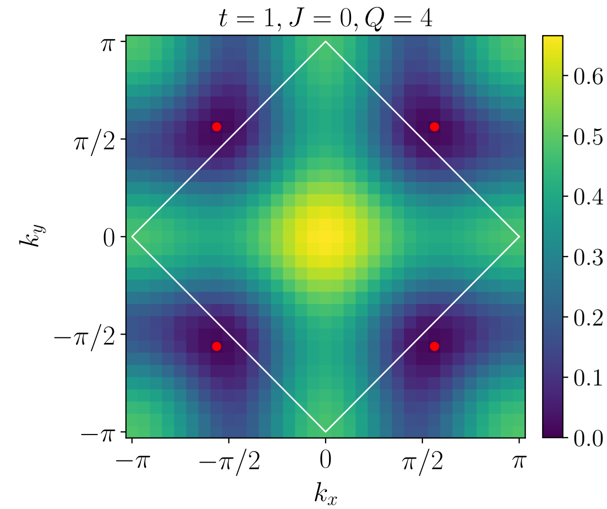
Shifted BZ for spinon similar to spin-charge separation in 1D

In the VBS phase: spin-poloaron (spinon-holon bound state) expected

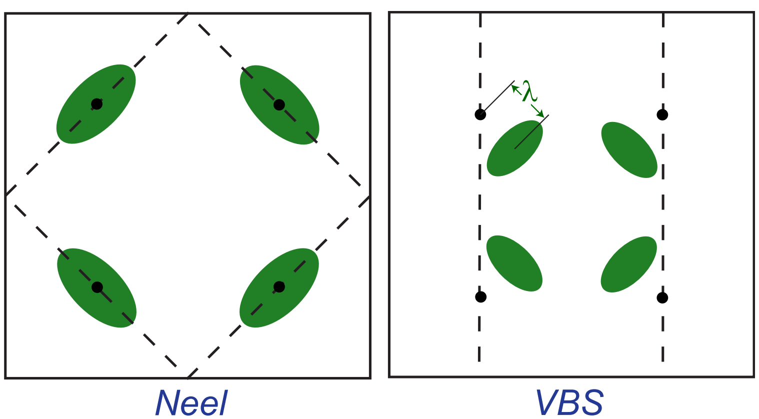
- impose δ-function quasi-particle peak





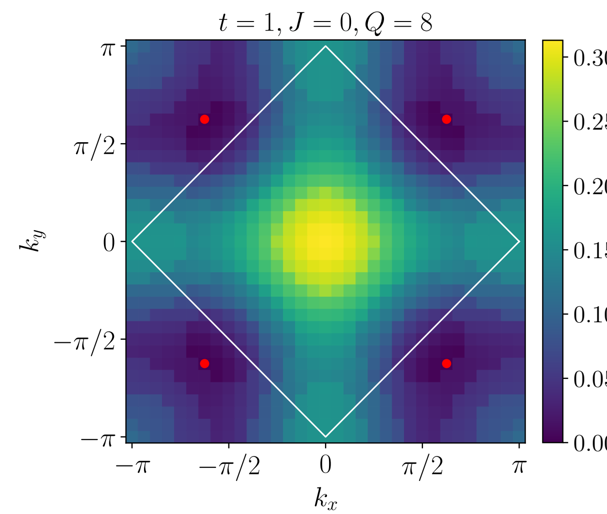


Kaul et al.: dispersion minimum moves away from $(\pi/2,\pi/2)$



- sign and magnitude of shift λ not determined

QMC results in qualitative agreement



Summary & Conclusions

Deconfined quantum criticality is still not fully understood
(but we are getting very close)

Role of J-Q models studied by QMC and numerical analytic continuation
- reliable results on large lattices
- advances in analytic continuation offer more spectral details

Deconfined spinons seem to be described by π-flux model with $k_x, k_y \in [0,\pi]$

Gives consistent holon dispersion, spinon-holon continuum
- if spinon BZ shifted to $k_x, k_y \in [-\pi/2,\pi/2]$

Similar to spinon deconfinement and spin-charge separation in 1D