Emergent topological and fractional excitations in a two-dimensional valence-bond solid

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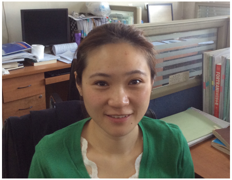
Collaborators



- Hui Shao (), Beijing Normal University (move to: CSRC and BU)
- Anders W. Sandvik, Boston University

outlines

Introduction

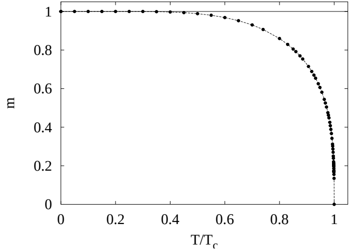
Emergent topological excitations in a valence-bond solid

Spinons and holons in a valence-bond solid

Conclusion

Thermal phase transitions

3D Ising FM-Paramagnetic transition (MC simulation)



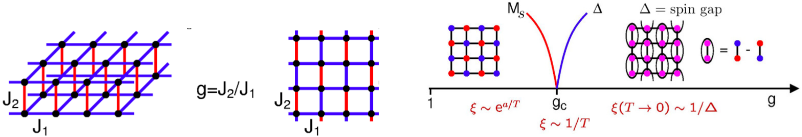
- At critical point, divergent length scale leads to singularity, which is the result of thermal fluctuations; temperature
- Quantum mechanics is largely irrelevant
- The coarse grained continuum field description: Landau-Ginzburg-Wilson Hamiltonian

$$H(\mathbf{m}) = \int \mathrm{d}V(t(\nabla\mathbf{m})^2 + c\mathbf{m}^2 + u\mathbf{m}^4); \quad Z = \int \mathcal{D}\mathbf{m} \;\; \mathrm{e}^{-H(\mathbf{m})}$$

  where $\mathbf{m}$ is the order parameter
- well understood within Wilson's RG framework
  - longrange order $\mathbf{m} \neq 0$: spontaneous symmetry breaking
  - universality class: symmetry and dimension

Quantum phase transitions

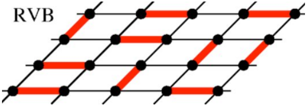
- happens at zero temperature, when adapt g in $H = H_0 + gH_I$; $[H_0, H_I] \neq 0$, continueous transition
- at g_c, the correlation length diverges, due to quantum fluctuations
- path integral maps D-dim quantum systems onto classical field theories in $D+1$-dim
- many of these transitions can be understood in the conventional Landau-Ginzburg-Wilson framework
- for example: AF Néel-Paramagnetic transition
  H_0 is AF Heisenberg Hamiltonian, $g = J_2/J_1$



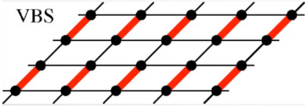
  - 3D classical Heisenberg universality class: confirmed by QMC
  - Experimental realized

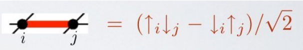
Non-trivial non-magnetic ground state

- resonating valence-bond (RVB) spin liquid
  exotic state without any long-range order

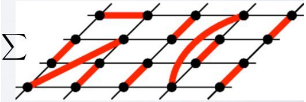


- valence-bond solid (VBS)
  breaking the translation and rotation symmetry of the lattice



  - Valence bond 

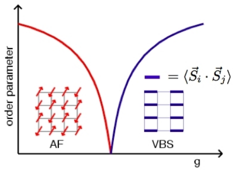
  - valence-bond state: the overcomplete basis



$$\langle \mathbf{m}_s \rangle = \langle \frac{1}{N} \sum_i \mathbf{S}_i (-1)^{x_i+y_i} \rangle = 0$$

Deconfined quantum criticality: Néel-VBS transition in 2D

Read and Sachdev, 1989; Senthil, Vishwanath, Balents, Sachdev, Fisher (2004)



- Berry phase related interference effect in path integral, complex statistical weight in the field theories, NOT like classical statistical systems

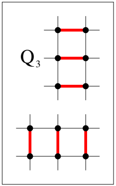
- Order parameters of the Néel state and the VBS state are NOT the fundamental objects, they are composites of fractional quasiparticles carrying $S = 1/2$
- Bind together in the VBS state (confinement) and condensate the Néel state, deconfine at the critical point leading to a continuous phase transition
- Violate the LGW paradigm: phase transition separates states with different broken symmetries should be first order

- The most natural physical realization of the Néel-VBS transition for SU(2) spins is in frustrated quantum magnets
- however, notoriously difficult to study numerically: sign problem in QMC

Designer Hamiltonian: J-Q model

Sandvik designs the J-Q model

$$H = -J \sum_{\langle ij \rangle} P_{ij} - Q \sum_{\langle ijklmn \rangle} P_{ij} P_{kl} P_{mn}, \quad P_{ij} = (\frac{1}{4} - \mathbf{S}_i \cdot \mathbf{S}_j)$$

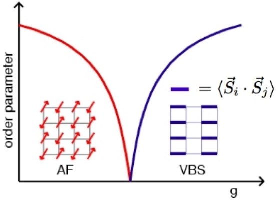


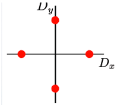
Lattice symmetries are kept

- large Q, columnar VBS

VBS order parameter

$$D_x = \frac{1}{N} \sum_{i=1}^{N} (-1)^{x_i} \mathbf{S}_i \cdot \mathbf{S}_{i+\hat{x}},$$
$$D_y = \frac{1}{N} \sum_{i=1}^{N} (-1)^{y_i} \mathbf{S}_i \cdot \mathbf{S}_{i+\hat{y}}$$





- small Q, Néel

Néel order parameter

$$\mathbf{m}_s = \frac{1}{N} \sum_i \mathbf{S}_i (-1)^{x_i + y_i}$$

- No sign problem for QMC simulations,
- ideal for QMC study of the DQC physics

Sandvik, PRL 98, 227202(2007)

Finite-size scaling: a critical **squared order parameter(A)** scales

$$A(q,L) = L^{-(1+\eta)} f[(q-q_c)L^{1/\nu}], \qquad q = Q/(J+Q)$$

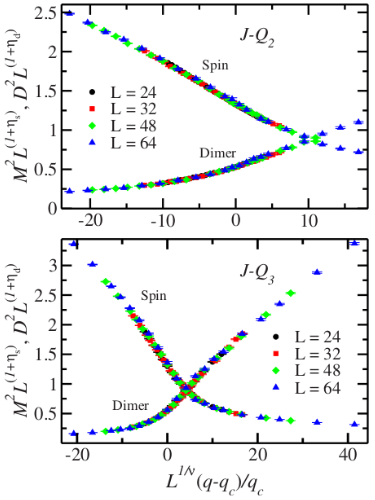
Data "collapse" for **different systems**:

- J-Q_2 model; $q_c = 0.961(1)$
  $\eta_s = 0.35(2); \eta_d = 0.20(2);$
  $\nu = 0.67(1)$
- J-Q_3 model; $q_c = 0.600(3)$
  $\eta_s = 0.33(2); \eta_d = 0.20(2);$
  $\nu = 0.69(2)$ Lou,Sandvik and Kawashima, PRB 2009
- Comparable results for honeycomb J-Q model

  Alet and Damle, PRB 2013 Kaul et al., PRL 2014
- **Exponents drift** for large L

  Kawashima et al. PRB 2013

  - weak first-order transition?
  - or large scaling corrections?



other ways to study the QDC?

- Study the topological excitations in the VBS state
  - Although topological order has mainly been discussed in the context of exotic states without any long-range order such as quantum spin liquids, topological excitations can also arise in the VBS state, e.g. quantum dimer model
  - and the consequence to the deconfine criticality
- Direct study the confinement/deconfinement:

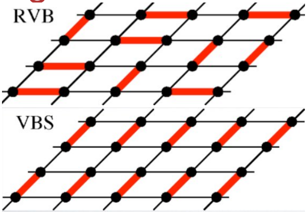
  spinons and holons in VBS phase and at criticality

emergent topological excitations

refs:

1. PRB 91, 094426 (2015) (arXiv:1502.01085)
2. arXiv1501.00237

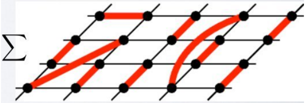
Quantum dimer model and winding number



- RVB spin liquid

- valence-bond solid (VBS)

Non-trivial non-magnetic ground states can be expressed with short valence-bond singlet(VBs) motivates the introduction of Quantum dimer model



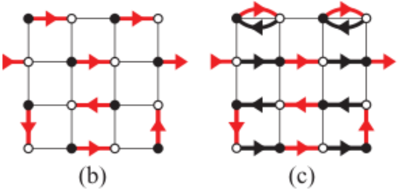
Square lattice Hamiltonian

$$H_{dimer} = \sum_{\square} -J(|\ \|\ \rangle\langle = | + H.c.) + V(| = \rangle\langle = | + |\ \|\ \rangle\langle\ \|\ |)$$

Rokhsar and Kivelson, PRL, 1988

Quantum dimer model and winding number

- Topological order has been discussed in the quantum dimer model
  the winding number
- The definition of the winding number



reference state (B $\rightarrow$ A) | a valence-bond state (A $\rightarrow$ B) | transition graph, $W = (0, 1)$

Tang et al PRB 2011

Winding number conservation

- W is a good quantum number in Quantum dimer model:

The Hilbert space can be separated to sectors with different winding numbers.

$$\langle W_1|H_{dimer}|W_2\rangle = 0, \quad \text{if } W_1 \neq W_2$$

short bond only and the off-diagonal terms being local, W can not be changed

- Find the lowest energy eigenstate in different sector by applying the imaginary time evolution operator to an initial state

$$\boxed{|\Psi_\tau\rangle = U(\tau)|\Psi_0(W)\rangle = \mathrm{e}^{-\tau H}|\Psi_0(W)\rangle}$$

For $\tau \to \infty$

$$\boxed{|\Psi_\tau\rangle \to |0, W\rangle}$$

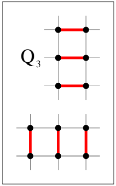
$|0, W\rangle$ is the lowest eigenstate state in the W sector.

Quantum spin model

- The VBS ground states hosted by the J-Q model

Consider the J-Q_3 model

$$H = -J \sum_{\langle ij \rangle} P_{ij} - Q \sum_{\langle ijklmn \rangle} P_{ij} P_{kl} P_{mn}$$



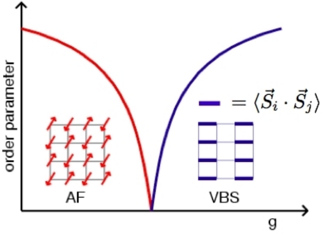
singlet projector $P_{ij} = (\frac{1}{4} - \mathbf{S}_i \cdot \mathbf{S}_j)$
large Q limit, strongly ordered columnar VBS

Néel order parameter

$$\mathbf{m}_s = \frac{1}{N} \sum_i \mathbf{s}(-1)^{x_i + y_i}$$

VBS vector order parameter

$$D_x = \frac{1}{N} \sum_{i=1}^{N} (-1)^{x_i} \mathbf{S}_i \cdot \mathbf{S}_{i+\hat{x}},$$
$$D_y = \frac{1}{N} \sum_{i=1}^{N} (-1)^{y_i} \mathbf{S}_i \cdot \mathbf{S}_{i+\hat{y}}$$



Project to the ground state

- Crucial difference from QDM:

  Long bonds exist in the J-Q model

$$\boxed{\langle W_1|H_{\mathrm{JQ}}|W_2\rangle \neq 0, \quad \text{if } W_1 \neq W_2}$$

Apply the imaginary time evolution operator to an initial state

$$\boxed{|\Psi_\tau\rangle = U(\tau)|\Psi_0(W)\rangle = \mathrm{e}^{-\tau H}|\Psi_0(W)\rangle}$$

For $\tau \to \infty$, and a finite size, winding number is not conserved

$$\boxed{|\Psi_\tau\rangle \to |0\rangle}$$

$|0\rangle$ is the ground state.

Projector Quantum Monte Carlo method

General idea of QMC :

- rewrite a quantum-mechanical expectation value into a classical form

$$\langle A \rangle = \frac{\mathrm{Tr}\{A e^{-\beta H}\}}{\mathrm{Tr}\, e^{-\beta H}} \quad \text{or} \quad \frac{\langle \Psi | A | \Psi \rangle}{\langle \Psi | \Psi \rangle} \rightarrow \frac{\sum_c A_c W_c}{\sum_c W_c}$$

A_c is the estimator of A.

- There are many different ways of doing it:
  Worldline (worm), SSE, Fermion determinant, $\cdots$

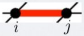
For ground state calculations

$$\boxed{\langle A \rangle = \frac{\langle \Psi_0 | U(\tau) A U(\tau) | \Psi_0 \rangle}{\langle \Psi_0 | U(\tau) U(\tau) | \Psi_0 \rangle} \rightarrow \frac{\sum_c A_c W_c}{\sum_c W_c}}$$

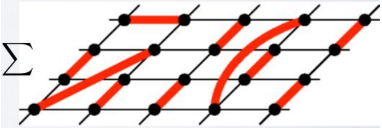
Projector Quantum Monte Carlo method

- using VB basis (in the singlet sector)

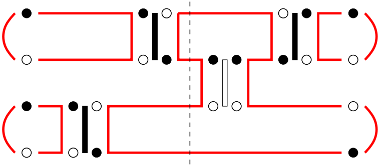
$$|\Psi\rangle = \sum_v f_v |v\rangle, \qquad |v\rangle = |(a_1, b_1)\cdots(a_{N/2}, b_{N/2})\rangle$$



$= (\uparrow_i\downarrow_j - \downarrow_i\uparrow_j)/\sqrt{2}$



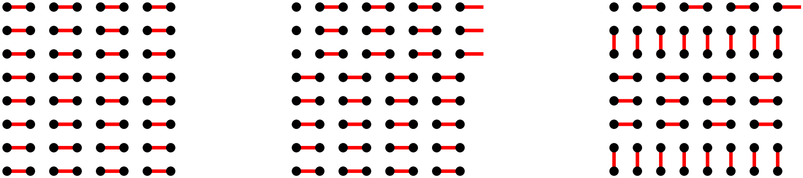
- SSE representation $\rightarrow Z = \sum_c W_c$
- loop update algorithm are used



- energy estimator n: number of operators, $\langle H\rangle = -\langle n\rangle/(2\tau)$.

Set initial states

Initial state with only short bonds and a winding number $|\Psi_0(w_x)\rangle$

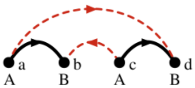


$W = (0, 0)$ $\quad$ $W = (1, 0)$ $\quad$ locally rotated $W = (1, 0)$

- the ground state is dominated by the $w_x = 0$ sector
- local rotations of dimers do not change the winding number
- Winding number can be changed due to long bonds in VBS

How does the presence of long bonds lead to non-conservation of W?

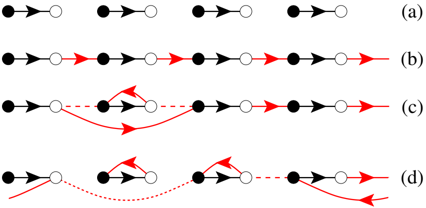
How long bonds leads to non-conservation of W?



$$P_{ab}|(a,b)\cdots(c,d)\rangle = |(a,b)\cdots(c,d)\rangle$$

$$P_{bc}|(a,b)\cdots(c,d)\rangle = \frac{1}{2}|(a,d)\cdots(c,b)\rangle$$

- A simple one-dimensional example

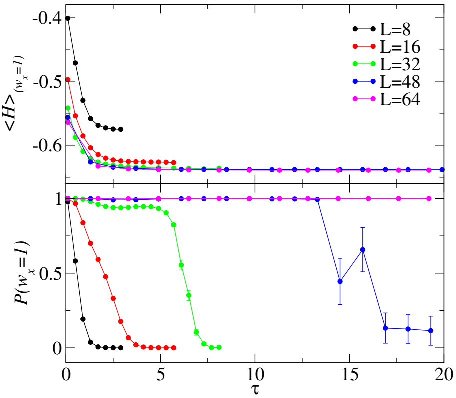


- reference conf.
- transition graph with $W = 1$
- a single projector has acted and produce a long bond!
- a second operation leads to a bond which would have length 5, but has length $L - 5 = 3$, and $W \to 0$.

- The maximum bond length to conserve W is $L/4$

Finite-size scaling of the projection

- Check the winding number of the configurations at τ: $P(w_x, \tau)$
- Calculate energy density $\langle H \rangle (w_x)$ only in the initial w_x sector



- For finite L, the state evolves to a "quasi-eigenstate" before w_x decays to lower values, with a "quasi-eigenenergy" $\langle H \rangle (w = 1) > \langle H \rangle (w = 0)$
- $L \to \infty$, the projected state $U(\tau)|\Psi_0(w_x)\rangle$ evolves toward the lowest eigenstate with winding number w_x.

Emergence of the topological quantum number

Relate the energy gap to domain-wall energy

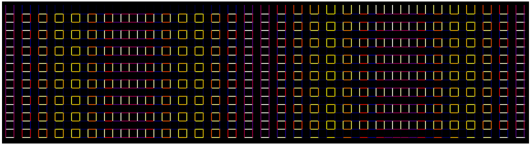
- How to understand the emergent ’quasi eigenenergy’ of the topological state?

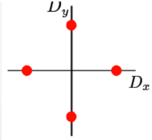
  The winding number effectively counts the number of domain walls

Relate the energy gap to domain-wall energy

snapshot of the pattern $\langle B_\alpha(\mathbf{r})\rangle = \langle \mathbf{S}(\mathbf{r})\cdot\mathbf{S}(\mathbf{r}+\alpha)\rangle$, domain walls

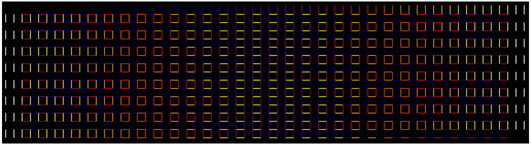
- periodic system with $W = 1$

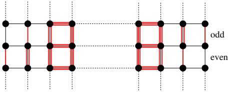




$\phi = \Delta\theta = 2\pi$

- open boundaries to enforce domain wall





$\phi = \Delta\theta = \pi$

- describe the domain wall, local order parameter

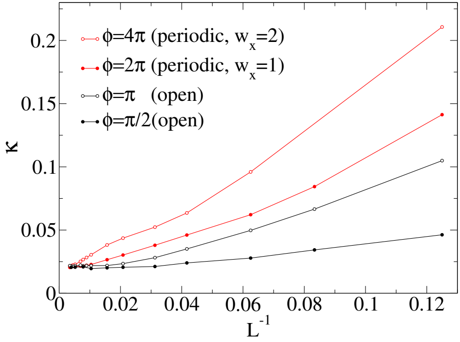
$$D_x(x) = [\langle B_{\hat{x}}(x,y)\rangle - \tfrac{1}{2}\langle B_{\hat{x}}(x-1,y)\rangle - \tfrac{1}{2}\langle B_{\hat{x}}(x+1,y)\rangle](-1)^x$$
$$D_y(x) = [\langle B_{\hat{y}}(x,y)\rangle - \langle B_{\hat{y}}(x,y+1)\rangle](-1)^y.$$

The VBS angle $\theta(x) = \mathrm{atan}\left[\frac{D_y(x)+D_y(x+1)}{2D_x(x)}\right]$

Domain wall energy

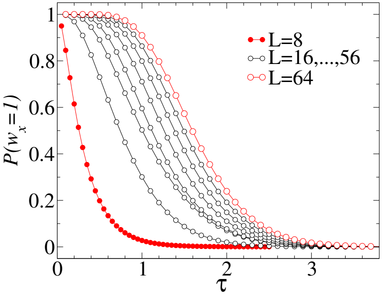
- (Effective) Winding number and VBS angle change $w_x = \phi/(2\pi)$.
- Define the domain wall energy

$$\kappa(w_x, L) = (\langle H \rangle_{w_x} - \langle H \rangle_0)/(w_x 4L)$$

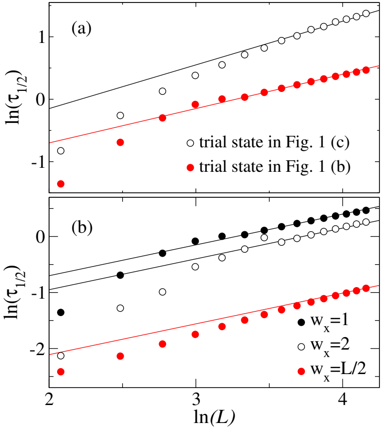


- Different calculations give consistent results for $L \to \infty$

Imaginary-time life time of the quasi-eigenstate



- $\tau_{1/2}$ is the life time at which $P(w_x) = 1/2$

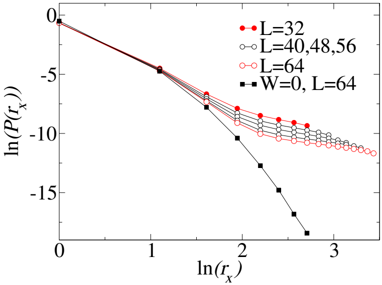


- Take a long total time $\beta = M\Delta_\tau$, $U(\beta)|\Psi_0(w_x)\rangle$
- $\tau = m\Delta_\tau$ is the "time slice"
- Measure $P(w_x)$ at τ

life time grows asymptotically as L^α

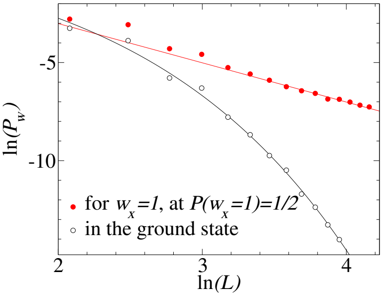
Why the life time so short?

- bond-length distribution at $\tau_{1/2}$



Lots of long bonds are generated in the transient states

- Comparing P_W of bond-length $> L/4$ in the ground state and in the $w_x = 1$ states at $\tau_{1/2}$



- $w_x = 1$ sector, $P_W \propto L^{-2}$
- Ground state, $P_W \propto \exp(-aL^{0.7})$

Real-time evolution

So far, the lifetime is actually the ’time’ that the state staying in W after projecting time.

Not the real time that the state staying in the initial state in the real evolving of state.

They can be connected using a simplified model.

Real-time evolution: a two-state model

We consider a very simplified two-state model:

- $|\downarrow\rangle$ and $|\uparrow\rangle$ correspond to $w_x = 0, 1$ sectors, respectively
- with energies $-\epsilon, \epsilon$
- perturbed by an off-diagonal matrix element $x \ll \epsilon$

$$H_2 = \begin{pmatrix} -\epsilon, & x \\ x, & \epsilon \end{pmatrix}$$

- Imaginary time evolving: $|\langle\uparrow|\psi(\tau)\rangle|^2 = 1/2$ leads to

$$\exp(-2\tau_{1/2}\epsilon) = \frac{x}{2\epsilon}$$

- together with the scaling $\epsilon \sim L$ and $\tau_{1/2} \sim L^\alpha$

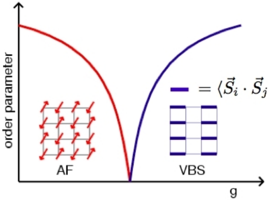
$$x \sim L \exp(-L^{1+\alpha})$$

- Real time decay rate

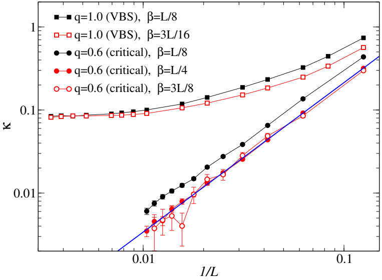
$$P(\downarrow) \propto \frac{x^2}{x^2+\epsilon^2} \sin^2(t\sqrt{\epsilon^2+x^2}), \qquad \nu = \frac{2x^2}{\pi\epsilon} \propto L e^{-2L^{1+\alpha}}$$

At deconfined critical point

At $q = Q/(J+Q) = 0.6$, critical point between VBS and Néel.



FSS of VB domain-wall energy, $\kappa \propto L^{-b}, b \approx 1.80(1)$



$\beta = L/4$ is long enough to converge the energy.

At deconfined critical point

- there are two diverging length scales

$$\xi \propto (q - q_c)^{-\nu}, \qquad \xi_{DW} \propto (q - q_c)^{-\nu'}, \nu' > \nu$$

- domain-wall energy can be expressed as $\kappa = K/\Lambda$
  K is a stiffness: energy cost of a twist of the VB order
  Λ is the width of the region over which the twist distributes.
- According to DQC theory, $K \propto 1/\xi$, $\Lambda \propto \xi_{DW}$

$$\kappa \propto \frac{1}{\xi \xi_{DW}} \propto (q - q_c)^{\nu + \nu'}$$

- translate to finite size at q_c: $\xi_{DW} = L, \xi = \xi_{DW}^{\nu/\nu'}$

$$\kappa(q_c) \propto L^{-(1+\nu/\nu')}$$

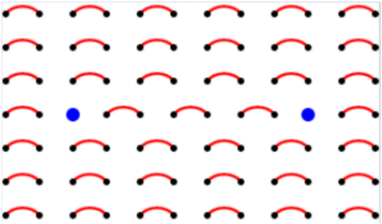
  we have $b = 1 + \nu/\nu'$, and $\nu/\nu' = 0.80(1)$
- The only other estimate from analysis of the emergent U(1) symmetry: $\nu/\nu' = 0.83((4)$, J. Lou et al PRB 80, 180414(R)(2009)

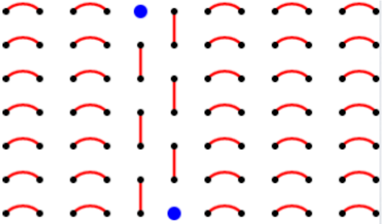
Spinons and holons in the VBS and at deconfined critical point

work in progress

Spinons and holons in the VBS and at DQC

- Intuitive picture of spinon confinement in the VBS phase
  - The VBS ground state is a product of singlets if fluctuations are neglected
  - A spinon is an $S = 1/2$ excitations
  - An $S = 1$ (triplon) excitation can be regarded as a bound state of two spinons
    - confined spinons
    - confinement due to 'string' in VBS background

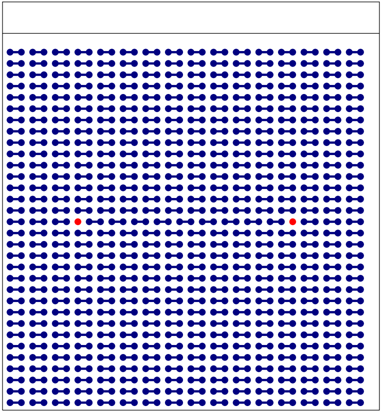




Holons and spinons in the VBS and at critical point

- what really happens in the VBS?

Create two defects (spinons or holons), e.g. ‘dig two holes’, try to separate them

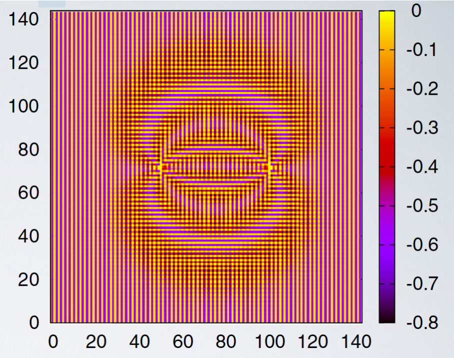


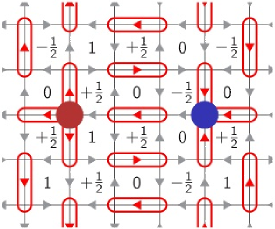
- The intuitive picture:
  linear confining potential due to ‘string’ of VBS mismatches

This picture assumes only short bonds

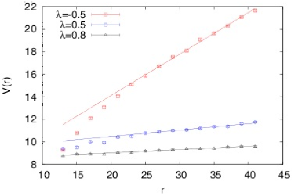
Holons and spinons in the VBS and at critical point

- Quantum dimer Banerjee *et al*, PRB 90, 245143 (2014) linear potential





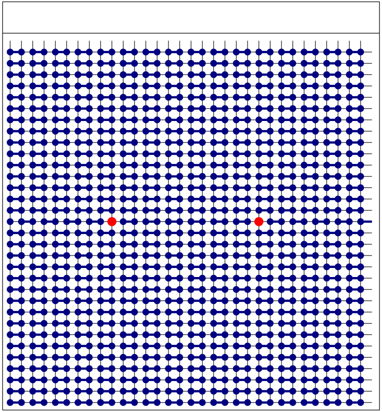
Potential between two static charge



Holons and spinons in the VBS and at critical point

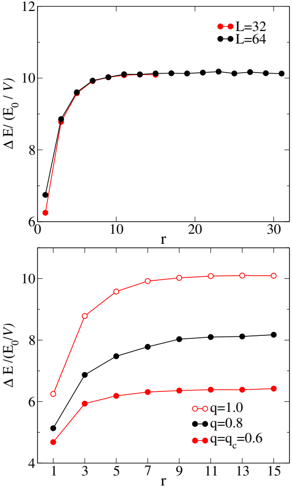
Generate two holons, expect confinement: linear potential

- We find the potential is short-ranged

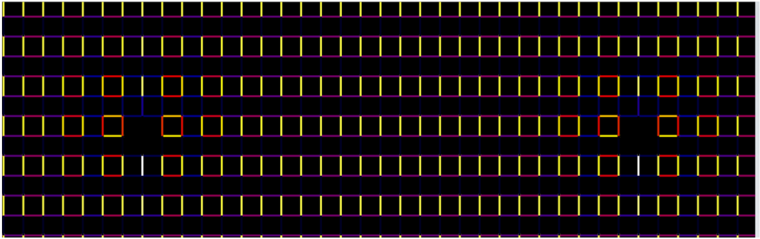


$q = Q/(J+Q)$, E_0/V: ground state energy density

$$V(r) = \Delta E/(E_0/V)$$

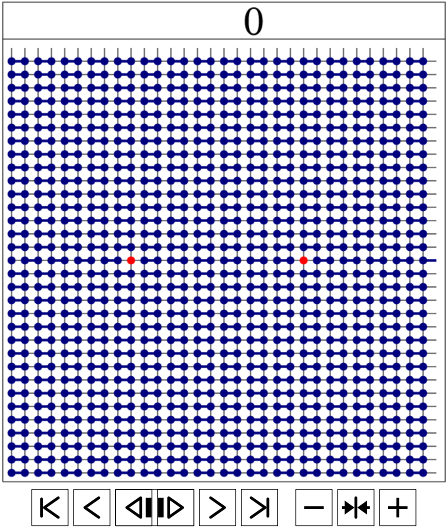


Snapshot of the bond pattern $\langle B_x \rangle, \langle B_y \rangle$



No global change, no confining string observed, why?

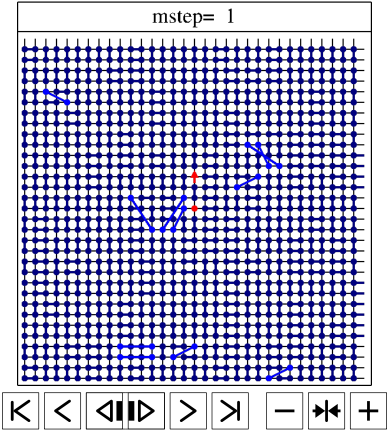
Visualize the generation of long bond



- A very long bond forms with ends close to the holons, corresponds to two spinons forming a singlet
- holon+spinon forming two composite particles (full electron).
- the cost of separating the two particles is very small

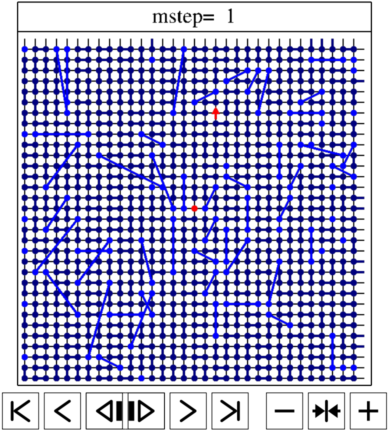
The spinon-holon composite particle

- deep VBS phase



- bound state of holon-spinon pair

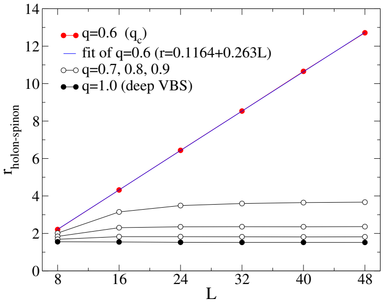
- at Q_c

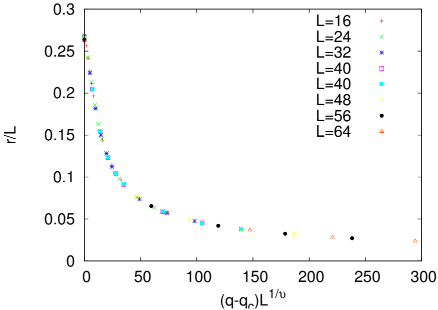


- average distance diverges as the deconfined quantum critical point is approaching

Direct measure the holon-spinon distance

The size of the composite particle can be characterized by the spinon-holon mean distance

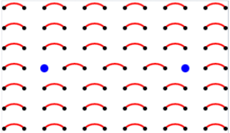




- As $q = Q_3/(J + Q_3)$ approaches the deconfined critical point, the average distance of the holon-spinon pair diverges with system size linearly.
- dimensionless ratio $\langle r \rangle / L$
- data collapsing: $q_c = 0.6, \nu = 0.63$
  - no log correction is needed, unlike in studies of the magnetization distribution Banerjee, Damle and Alet, PRB, 2010 .

The two-spinon distance in the J-Q_2 model

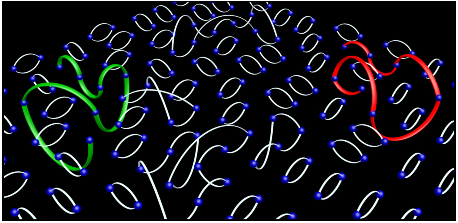
- a $S = 1$ state



$$\langle \psi_L(0, S = 1)|U(\tau)U(\tau)|\psi_R(0, S = 1)\rangle$$

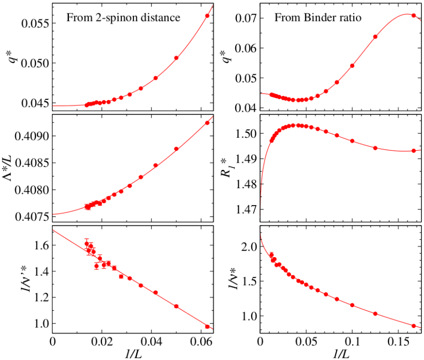
A QMC transition graph representing $\langle \psi_L|\psi_R \rangle$ of $S = 1$ states

- two strings (spinons) in a background of loops formed by valence bonds.
- Archs above and below the plane represent $|\psi_R\rangle$ and $\langle \psi_L|$, respectively.



Tang and Sandvik, PRL 2011; Banerjee and Damle, J. Stat. Mech 2010

The two-spinon distance in the J-Q_2 model



- The two-spinon distance $\langle\Lambda\rangle/L$ is also universal, like the Binder ratio of Néel order parameter.
- Solving the crossing points of $\langle\Lambda(L)\rangle/L$ and $\langle\Lambda(2L)\rangle/2L$ versus q

$$g^* - q_c \propto L^{-(1/\nu' + \omega)}, \quad \Lambda^*(L)/L - R \propto L^{-\omega}$$

and $1/\nu'$ can be extracted from slopes at the crossing point

- we find $q_c = 0.04463(4), \nu' = 0.58(2)$ (here we take $q = Q_2/J$)
- ν' is the domain wall width exponent!
- From Binder ratio, we have $\nu = 0.446$ which controls the correlation.
- $\nu/\nu' = 0.77(3)$ agrees with the result obtained from the VBS domain-Wall energy

Conclusion

- We have studied that the topological excitations in the VB state
  - demonstrated a mechanism of the decay of winding numbers in a VBS; different from the quantum dimer model
  - imaginary life time of winding state diverges as a power of the system size L.
  - The winding number effectively counts the number of domain walls, the energy gap is the domain wall energy
  - A simplified two-states model shows the real-time life time of the topological excitation is exponentially long in L: a well-defined conserved quantum number for large systems
  - At DQC, the domain-wall energy turns to zero; we found $\nu/\nu' = 0.80(1)$, support the DQC theory
- Preliminary results of the confinement of spinons/holons
  - In the VBS, the confining potential is not linear, due to quantum fluctuations of VBS background (long bonds)
  - Critical region, NO logarithmic corrections in the FSS of spinon/holon pair distance.
  - We obtained ν' and $\nu/\nu' = 0.8$ in supporting of the DQC theory