Quantum spin liquids from quadrupolar magnets

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Collaborators

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Lovell

Pujari

Lang

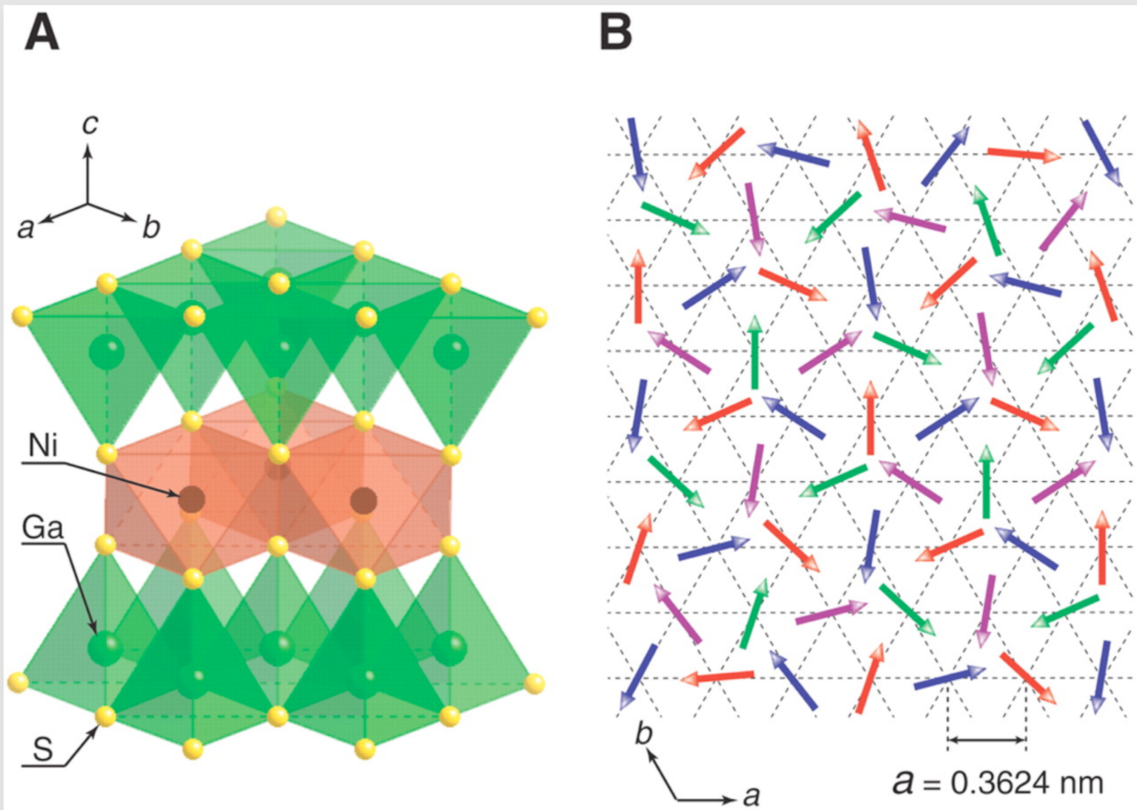
Murthy

Outline

- Quadrupolar magnets
  - Quantum Fluctuations : Spin Liquids
  - New percolation quantum criticality
- Quadratic band touchings in bilayer graphene

Motivation: $NiGa_2S_4$

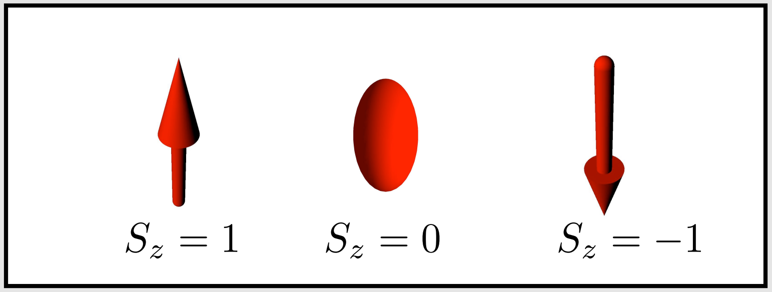
layered insulator, $\mathrm{Ni}^{2+} \rightarrow t_{2g}^6 e_g^2$ (S=1)



Nakatsuji *et al*, Science (2005)

Qudrapolar (Spin-nematic) order?

H. Tsunetsugu and M. Arikawa, Journal of the Physical Society of Japan 75, 083701 (2006).
A. Läuchli, F. Mila, and K. Penc, Phys.Rev.Lett.97,087205 (2006).
S. Bhattacharjee, V. B. Shenoy, and T. Senthil, Phys. Rev. B 74, 092406 (2006).



S=1 spin

A. F. Andreev and I. A. Grishchuk, Sov. Phys. JETP 60, 267 (1984).
A. Chubukov, J. Phys. Condens. Matter 2, 1593 (1990).

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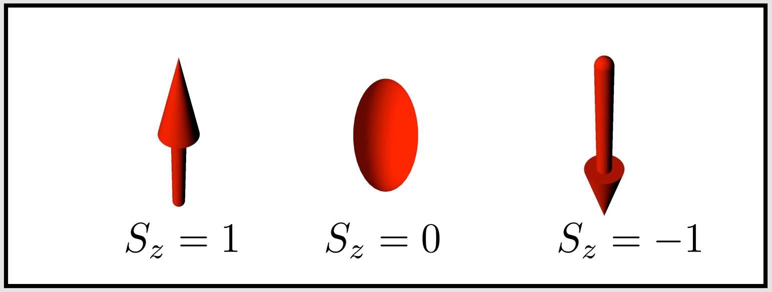
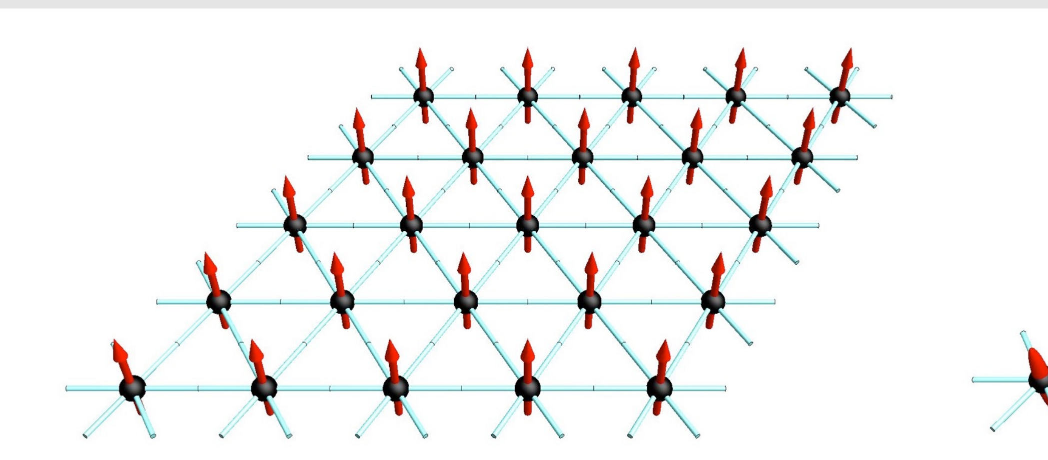
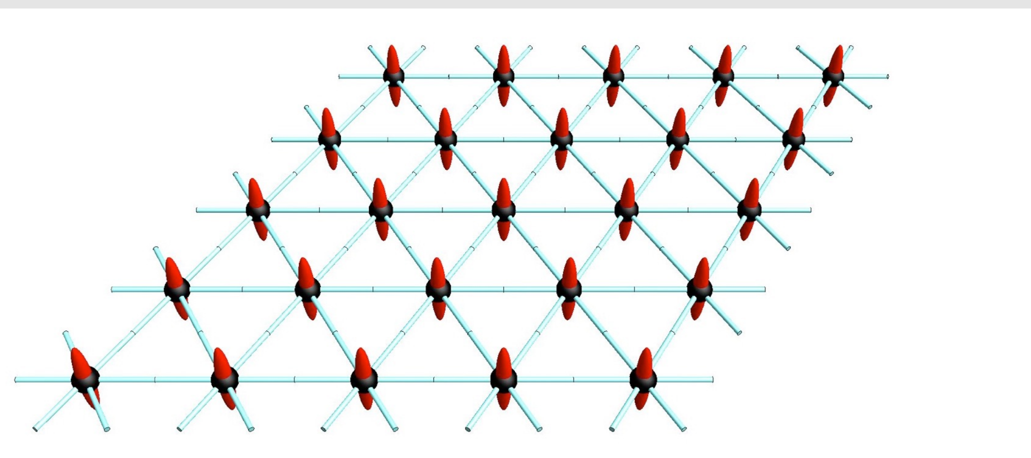


Dipolar order



Quadrupolar order



Order Parameter

$$\langle S_\alpha \rangle = 0$$

$$\langle Q_{\alpha\beta} \rangle \neq 0$$

$$Q_{\alpha\beta} \equiv \frac{S_\alpha S_\beta + S_\beta S_\alpha}{2} - \frac{2}{3}\delta_{\alpha\beta}$$

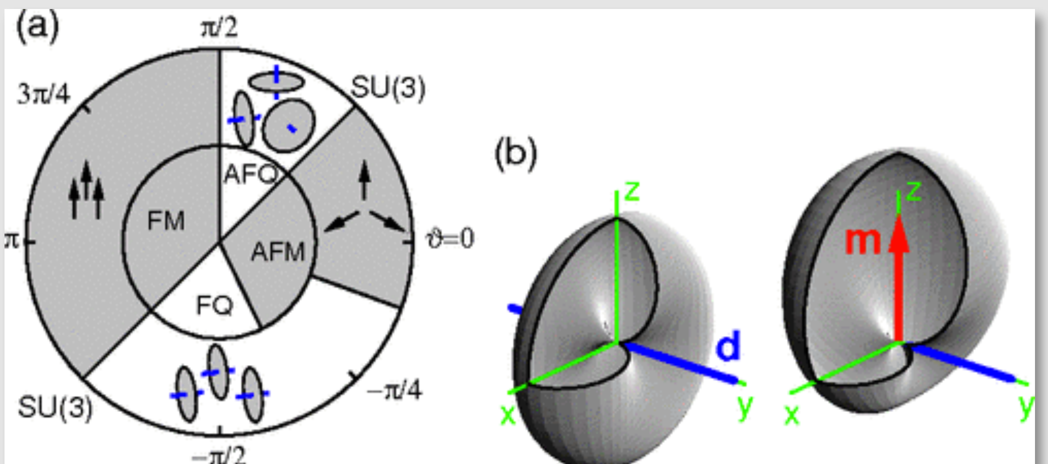
does not break TRS
but breaks spin-rotational symmetry
"Hidden Order"

Microscopics

What exchanges produce the "quadrupolar" order?

$$H = \sum_{\langle ij \rangle} \left[J_H \vec{S}_i \cdot \vec{S}_j + J(\vec{S}_i \cdot \vec{S}_j)^2 \right]$$

(SO(3) symmetry with *S=1*)



A.Läuchli, F. Mila, and K. Penc, Phys.Rev.Lett.97,087205 (2006).

Biquadratic model

R. K. Kaul, Phys, Rev. B, 86, 104411(2012)

Unbiased, high-precision simulations of quantum spin models, only possible with QMC w/o the sign problem

Surprisingly,

$$\hat{H}_J = -\frac{J}{3}\sum_{\langle ij\rangle}\left(\vec{S}_i\cdot\vec{S}_j\right)^2$$

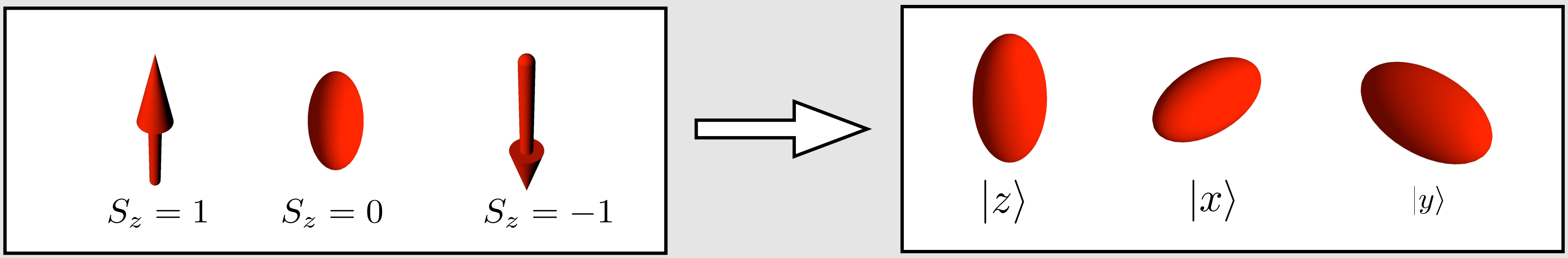
has no sign problem, even on non-bipartite lattices!

Unbiased methods with 10^5 spins
(numerically "exact" with controlled errors)

"Heisenberg model" of quadrupolar order

Biquadratic model

R. K. Kaul, Phys, Rev. B, 86, 104411(2012)



$$\left(\vec{S}_i \cdot \vec{S}_j\right)^2 - 1 = 3|\mathcal{S}\rangle\langle\mathcal{S}| \qquad |\mathcal{S}\rangle = \frac{|xx\rangle + |yy\rangle + |zz\rangle}{\sqrt{3}}$$

$$H_J = -J \sum_{\langle ij \rangle} |\mathcal{S}_{ij}\rangle\langle\mathcal{S}_{ij}|$$

Biquadratic model

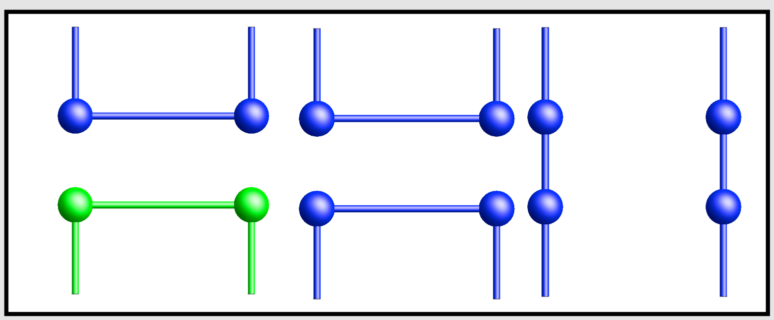
R. K. Kaul, Phys, Rev. B, 86, 104411(2012)

$$\mathcal{Z} = \mathrm{Tr}(e^{-\beta \hat{H}}) = \mathrm{Tr}(e^{-\epsilon \hat{H}} \ldots e^{-\epsilon \hat{H}})$$

$$H_J = -J \sum_{\langle ij \rangle} |\mathcal{S}_{ij}\rangle\langle\mathcal{S}_{ij}|$$

$$|\mathcal{S}\rangle = \frac{|xx\rangle + |yy\rangle + |zz\rangle}{\sqrt{3}}$$

$$\big(|xx\rangle + |yy\rangle + |zz\rangle\big)\big(\langle xx| + \langle yy| + \langle zz|\big)$$



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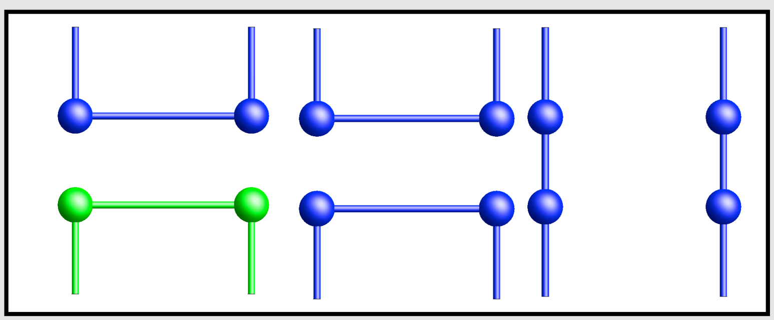
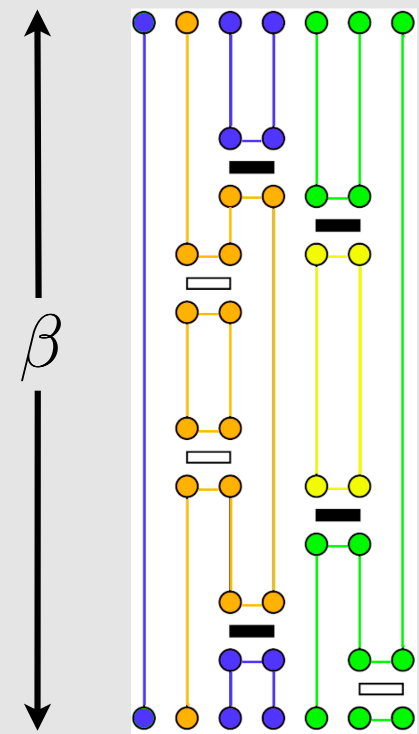


one-d example



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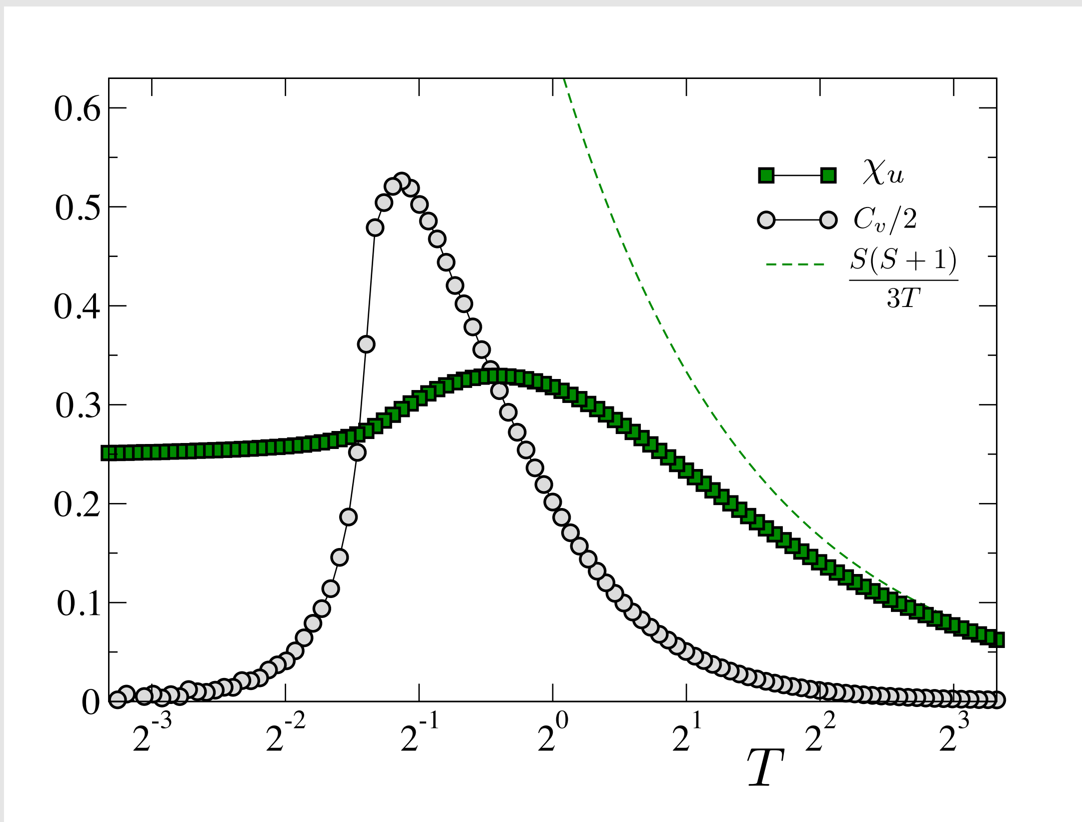
$$\hat{H}_J = -\frac{J}{3}\sum_{\langle ij\rangle}\left(\vec{S}_i\cdot\vec{S}_j\right)^2$$

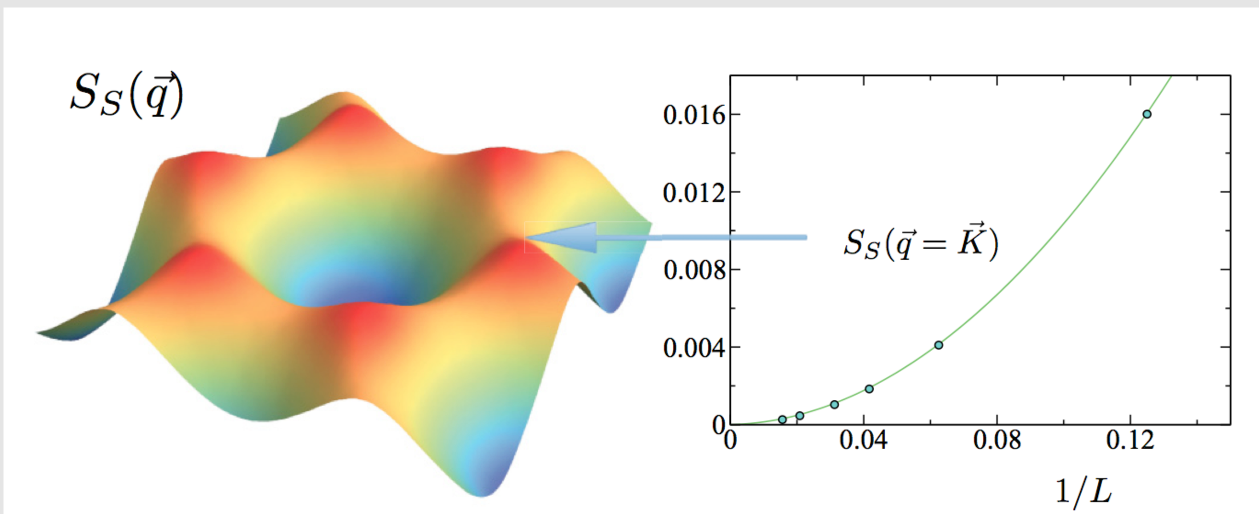


Biquadratic model

R. K. Kaul, Phys, Rev. B, 86, 104411(2012)

$$\hat{H}_J = -\frac{J}{3}\sum_{\langle ij \rangle}\left(\vec{S}_i \cdot \vec{S}_j\right)^2$$

spin structure factor shows absence of Bragg peaks and usual (dipolar) magnetism

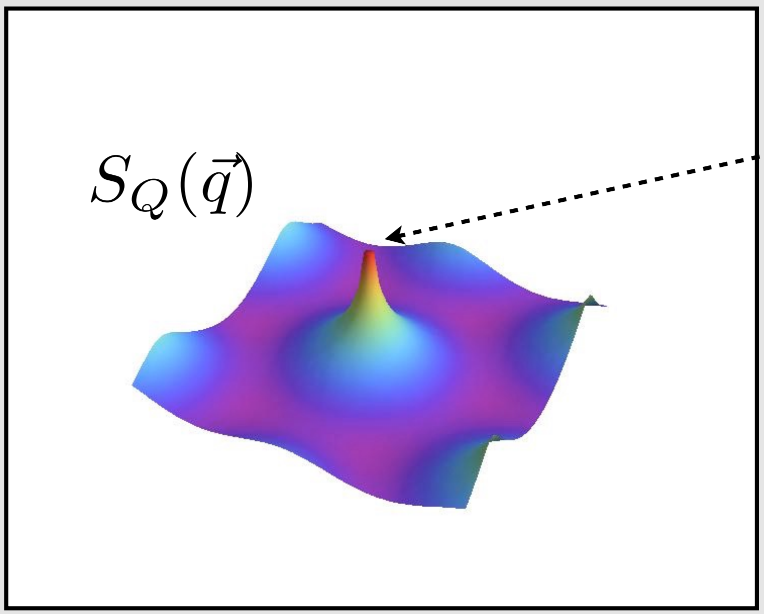


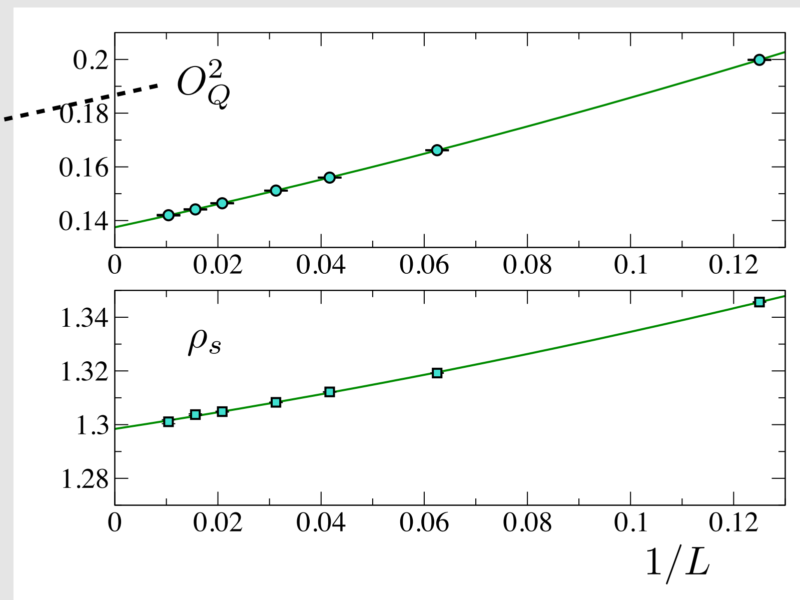
Biquadratic model

R. K. Kaul, Phys, Rev. B, 86, 104411(2012)

$$\hat{H}_J = -\frac{J}{3}\sum_{\langle ij \rangle}\left(\vec{S}_i \cdot \vec{S}_j\right)^2$$

Quadrupolar order parameter shows long-range order!

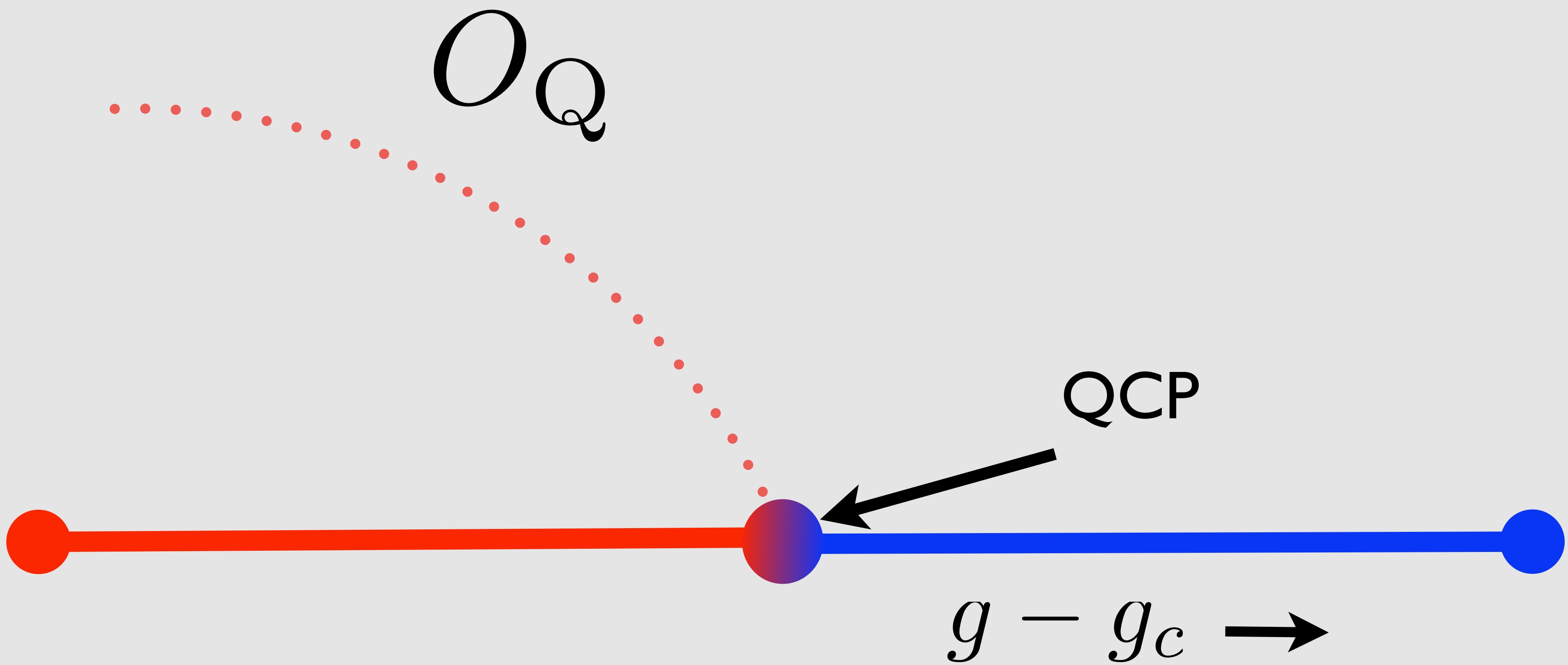




$$O_Q^2 = 0.1376(2) \quad \rho_s = 1.298(2) \; c = 1.869(4)$$

Quantum Criticality

Fundamental question:
what happens when you destroy quadrupolar order at T=0?



Outline

- Quadrupolar Order
    - Quantum Fluctuations : Spin Liquids
    - New percolation quantum criticality
- Quadratic band touchings in bilayer graphene

Destruction of Quadrupolar

Classical spin nematics $Q_{\alpha\beta}$

$$S = \sum_{\langle ij \rangle} \mathrm{Tr}[Q_i Q_j]$$

Landau Theory:

$$S = a\mathrm{Tr}[Q^2] + b\mathrm{Tr}[Q^3] + c_1\mathrm{Tr}[Q^4] + c_2\mathrm{Tr}[Q^2]^2$$

Nematic-Isotropic transition is first order

$\mathbb{Z}_2$ phase & Quadrupolar

Lammert, Rokhsar & Toner, *Phys. Rev. Lett. (1993)*

Re-write as Z_2 gauge theory

$$S = J \sum_{\langle ij \rangle} \sigma_{ij} \hat{n}_i \cdot \hat{n}_j + K \sum_{\square} \sigma\sigma\sigma\sigma$$

"half" vortices of director = Z_2 fluxes of IGT

increasing *K*, suppresses vortices!

$\mathbb{Z}_2$ phase & Quadrupolar

Lammert, Rokhsar & Toner, *Phys. Rev. Lett. (1993)*

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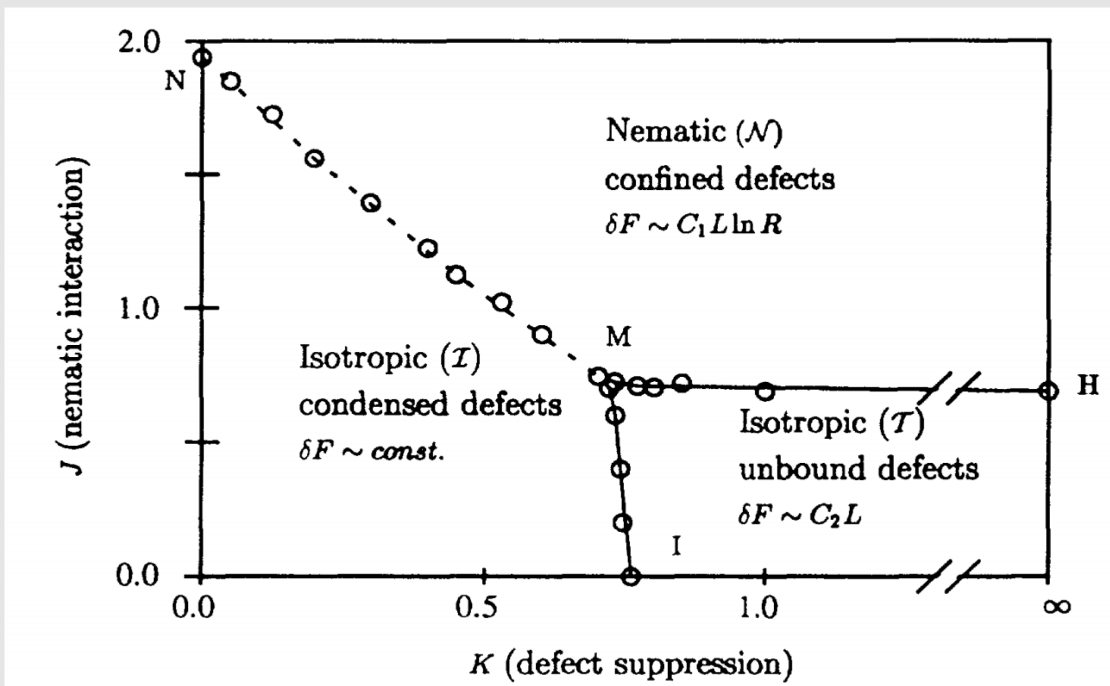

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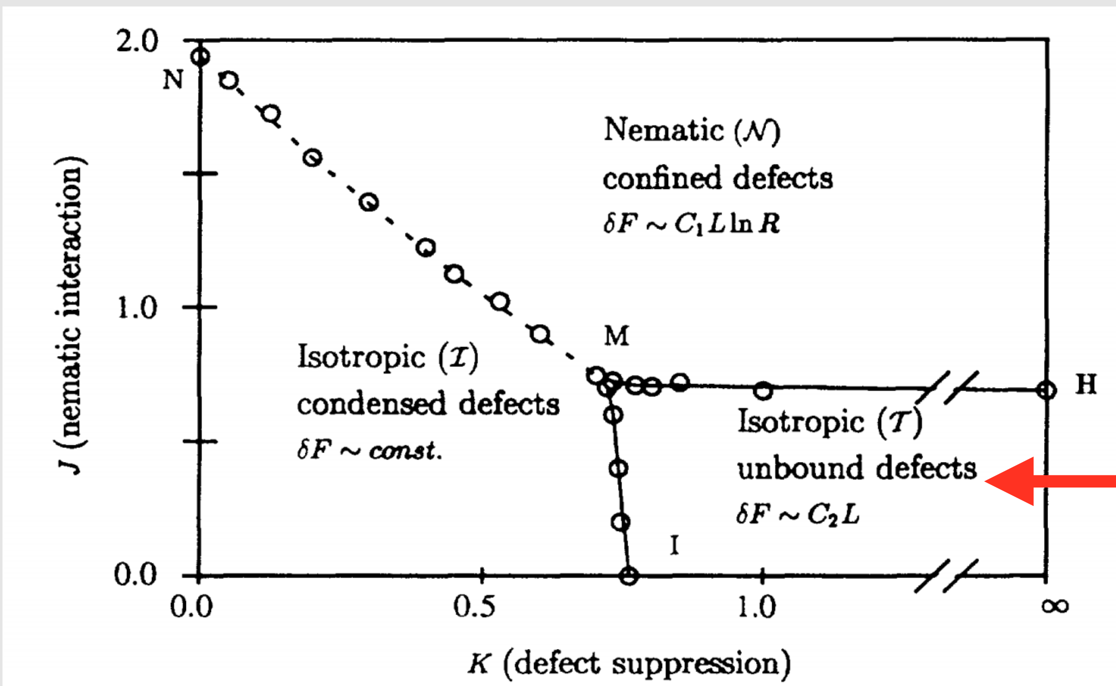


$\mathbb{Z}_2$ QSL

Search for $\mathbb{Z}_2$ phase

Lammert, Rokhsar & Toner, *Phys. Rev. Lett. (1993)*

Thermal transition out of quadrupolar can lead to $\mathbb{Z}_2$

Can we find a microscopic model where this happens?

thermal transitions in classical director models
(all cases known to me show first order N-I)

quantum transition in $d=2$ $S=1$ models
with quadrupolar order?

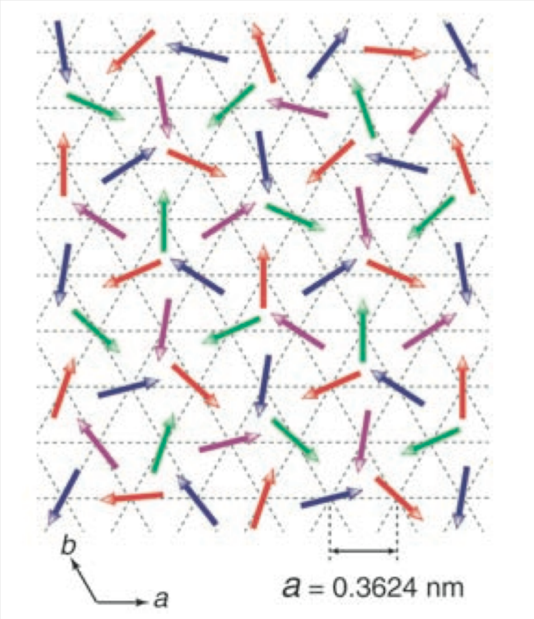
Quantum Fluctuations

$$\hat{H}_J = -\frac{J}{3}\sum_{\langle ij\rangle}\left(\vec{S}_i \cdot \vec{S}_j\right)^2$$

Quantum Fluctuations

Frustration

$$\hat{H}_J = -\frac{J}{3}\sum_{\langle ij\rangle}\left(\vec{S}_i\cdot\vec{S}_j\right)^2 + \dots$$



regular Heisenberg exchange (nn, 3-nn ...)

From SO(3) to SO(*N*)

R. K. Kaul PRL (2015)

$$H_J = -\frac{J}{3}\sum_{\langle ij\rangle}\left(\vec{S}_i\cdot\vec{S}_j\right)^2$$

$$\downarrow$$

$$H_J = -\frac{J}{N^2-2N}\sum_{\langle ij\rangle}(\hat{L}_i\cdot\hat{L}_j)^2$$

$$\hat{L}_j^{\alpha\beta}|\gamma\rangle_j = i\delta_{\beta\gamma}|\alpha\rangle_j - i\delta_{\alpha\gamma}|\beta\rangle_j \qquad N(N-1)/2$$

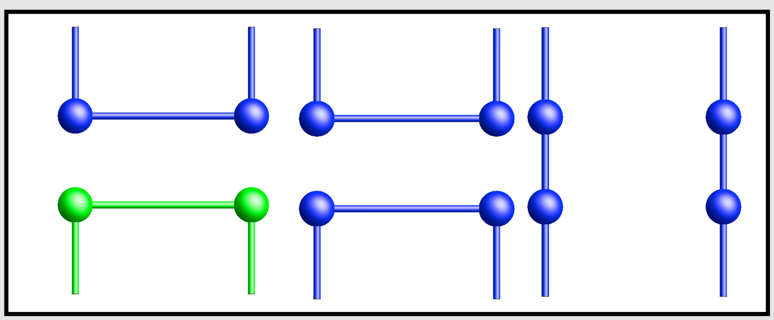
Remarkably, for all *N* this model is sign free on any lattice!

Projector Model

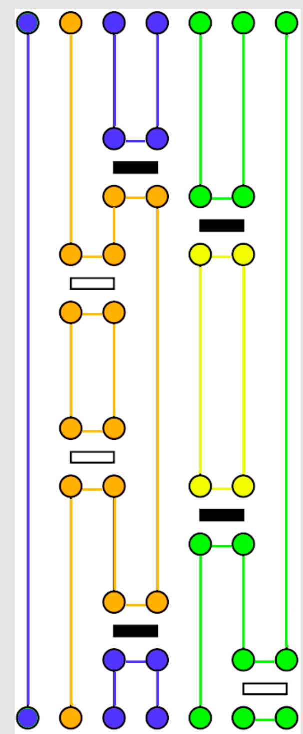
R. K. Kaul PRL (2015)

$$H_J = -J \sum_{\langle ij \rangle} |\mathcal{S}_{ij}\rangle\langle\mathcal{S}_{ij}|$$

$$|\mathcal{S}\rangle = \frac{1}{\sqrt{N}} \sum_{\alpha=1}^{N} |\alpha\alpha\rangle$$



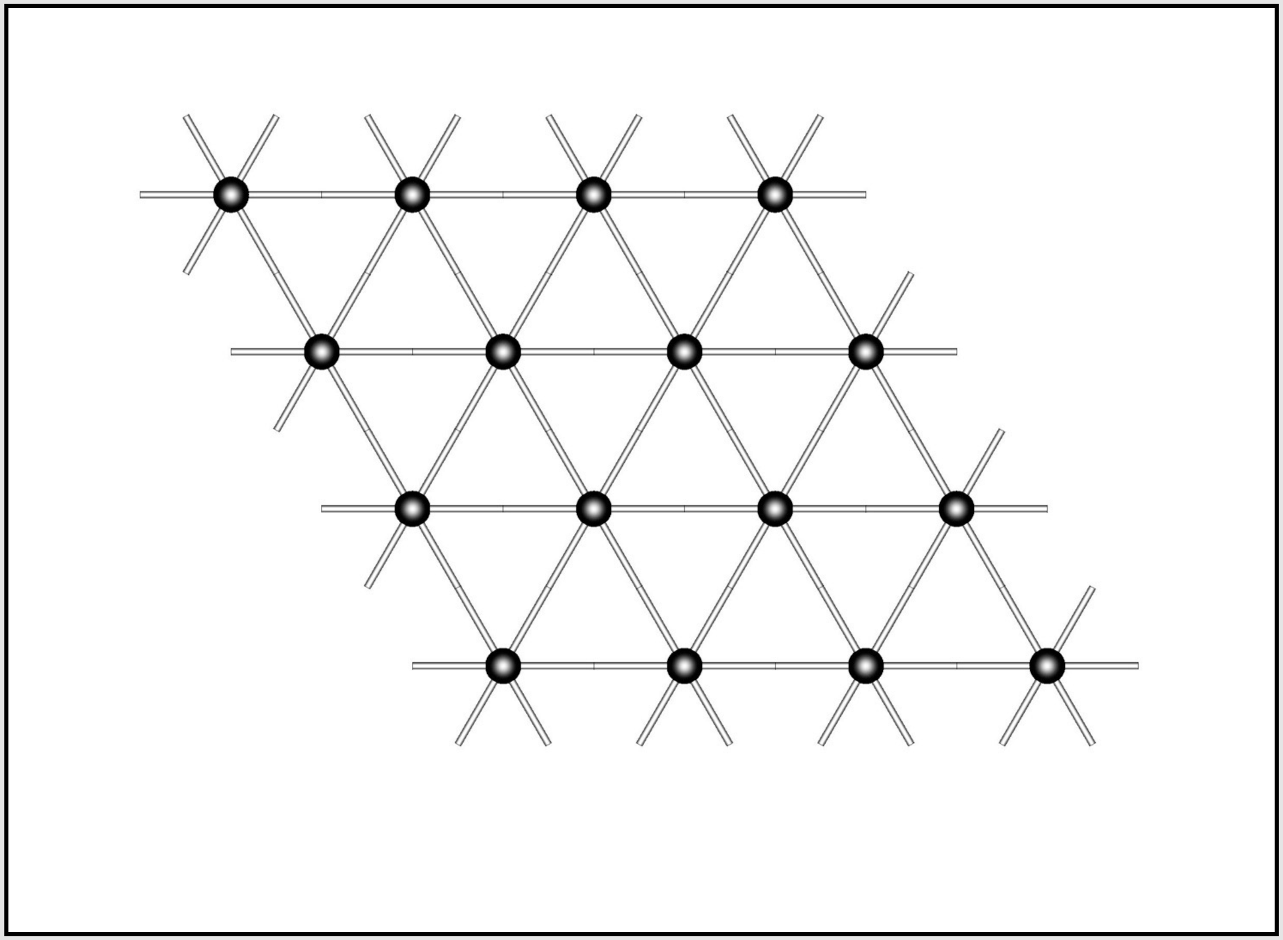
one-d example



Hilbert Space

R. K. Kaul PRL (2015)

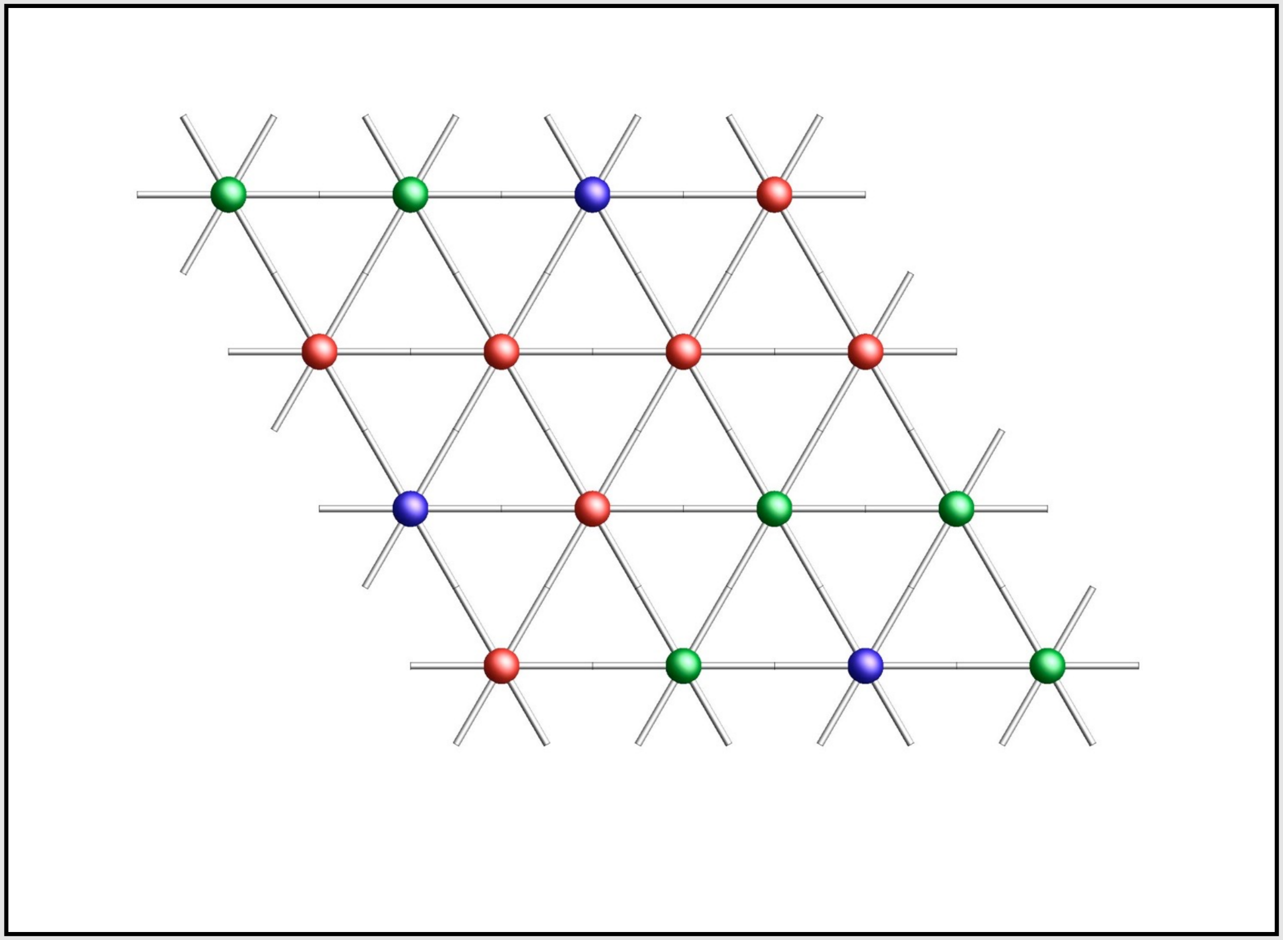
Consider any lattice



Hilbert Space

R. K. Kaul PRL (2015)

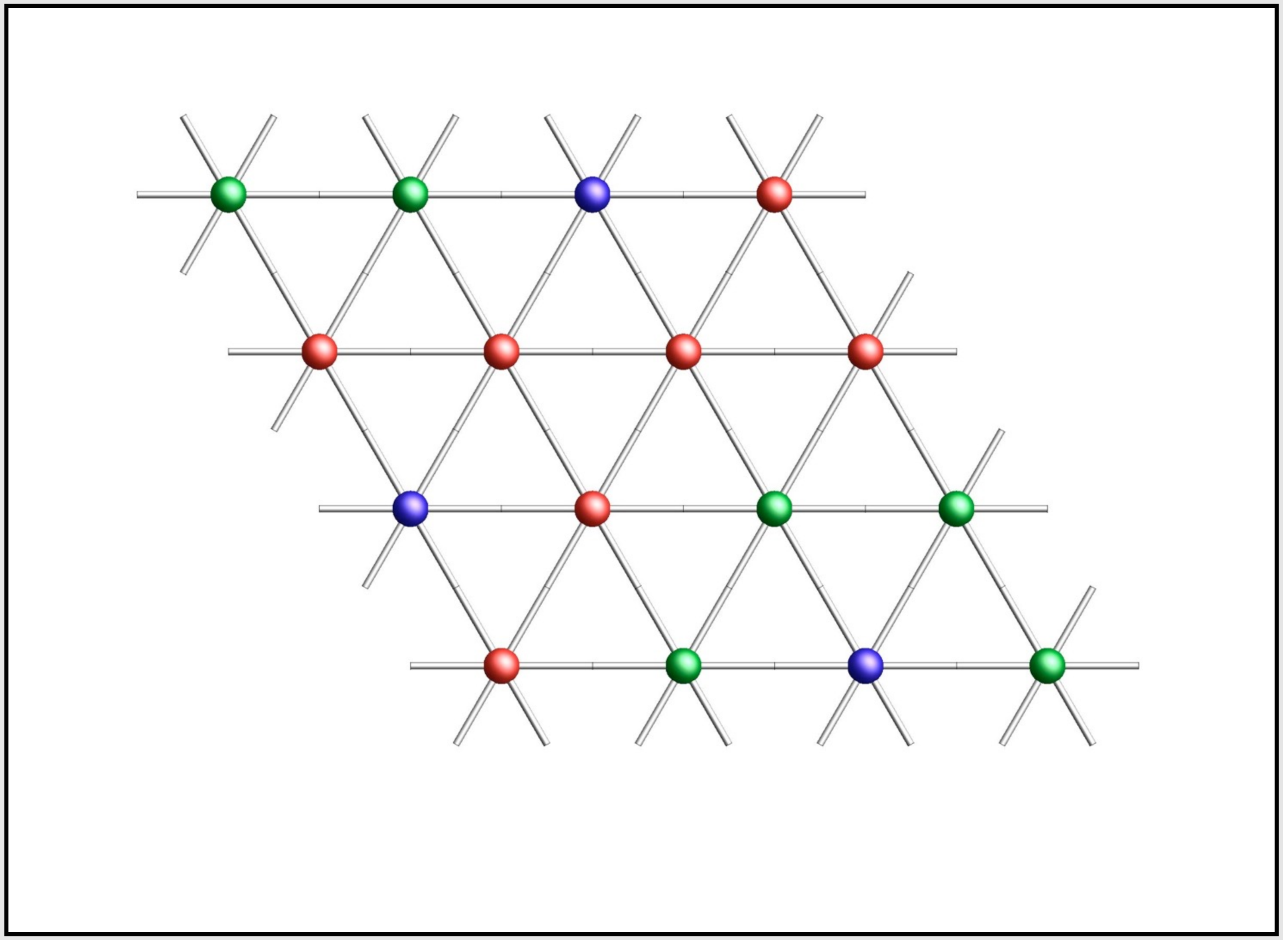
Assign one of *N* color to each site



Hilbert Space

R. K. Kaul PRL (2015)

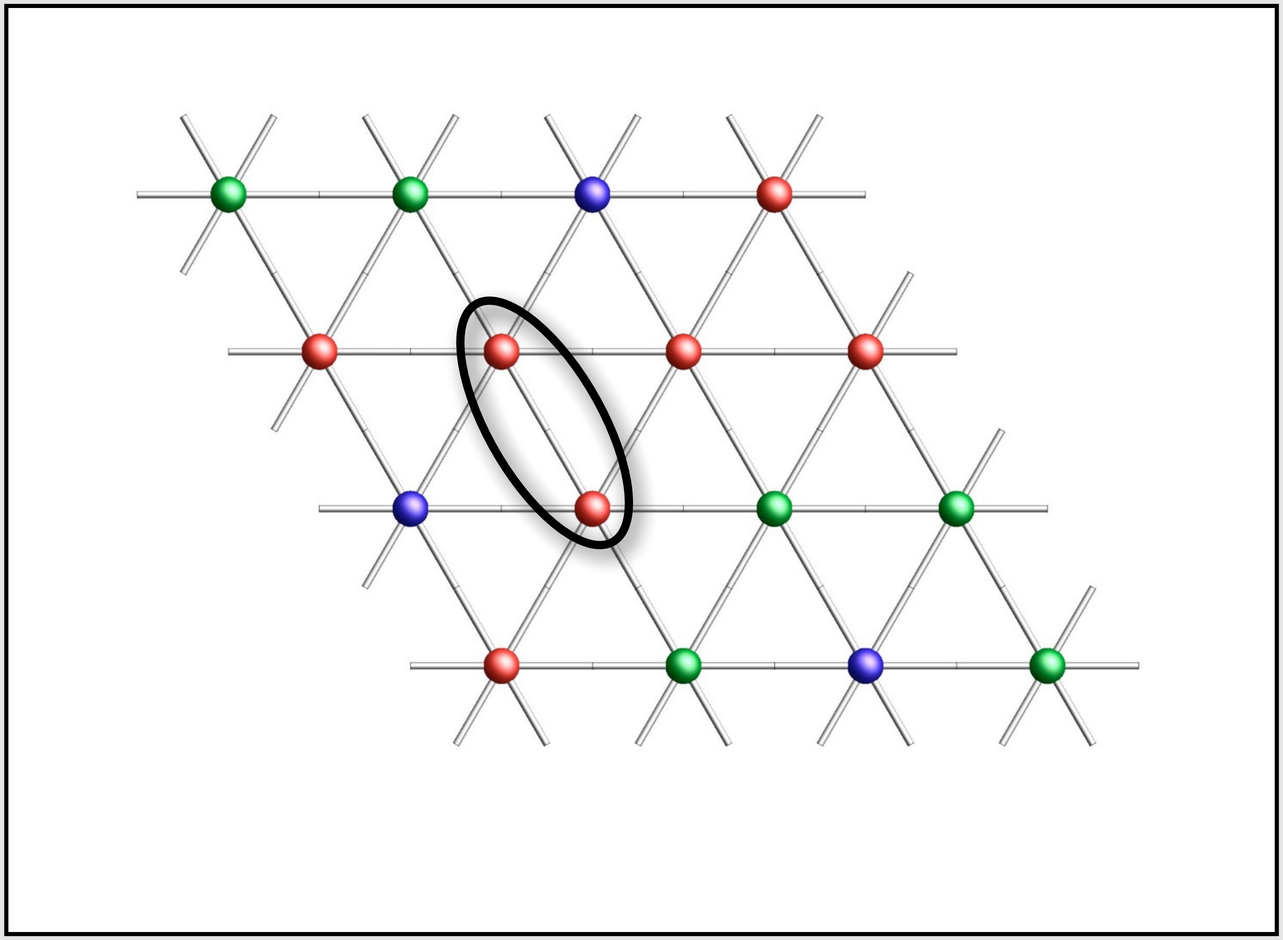
$$|\mathcal{S}\rangle\langle\mathcal{S}| = \frac{1}{N}\sum_{\alpha,\beta}|\alpha\alpha\rangle\langle\beta\beta|$$



Quantum Dynamics

R. K. Kaul PRL (2015)

$$|\mathcal{S}\rangle\langle\mathcal{S}| = \frac{1}{N}\sum_{\alpha,\beta}|\alpha\alpha\rangle\langle\beta\beta|$$



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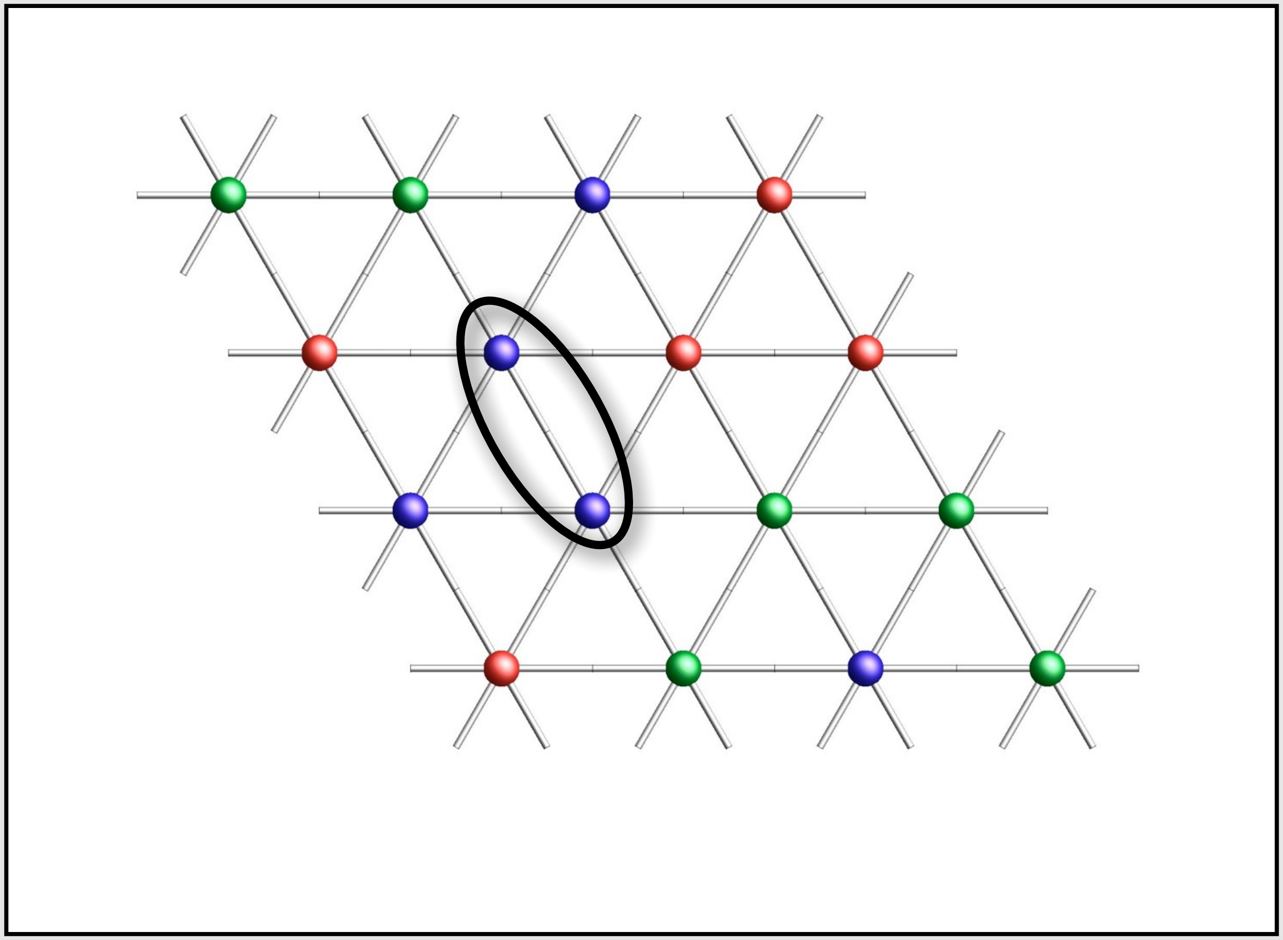

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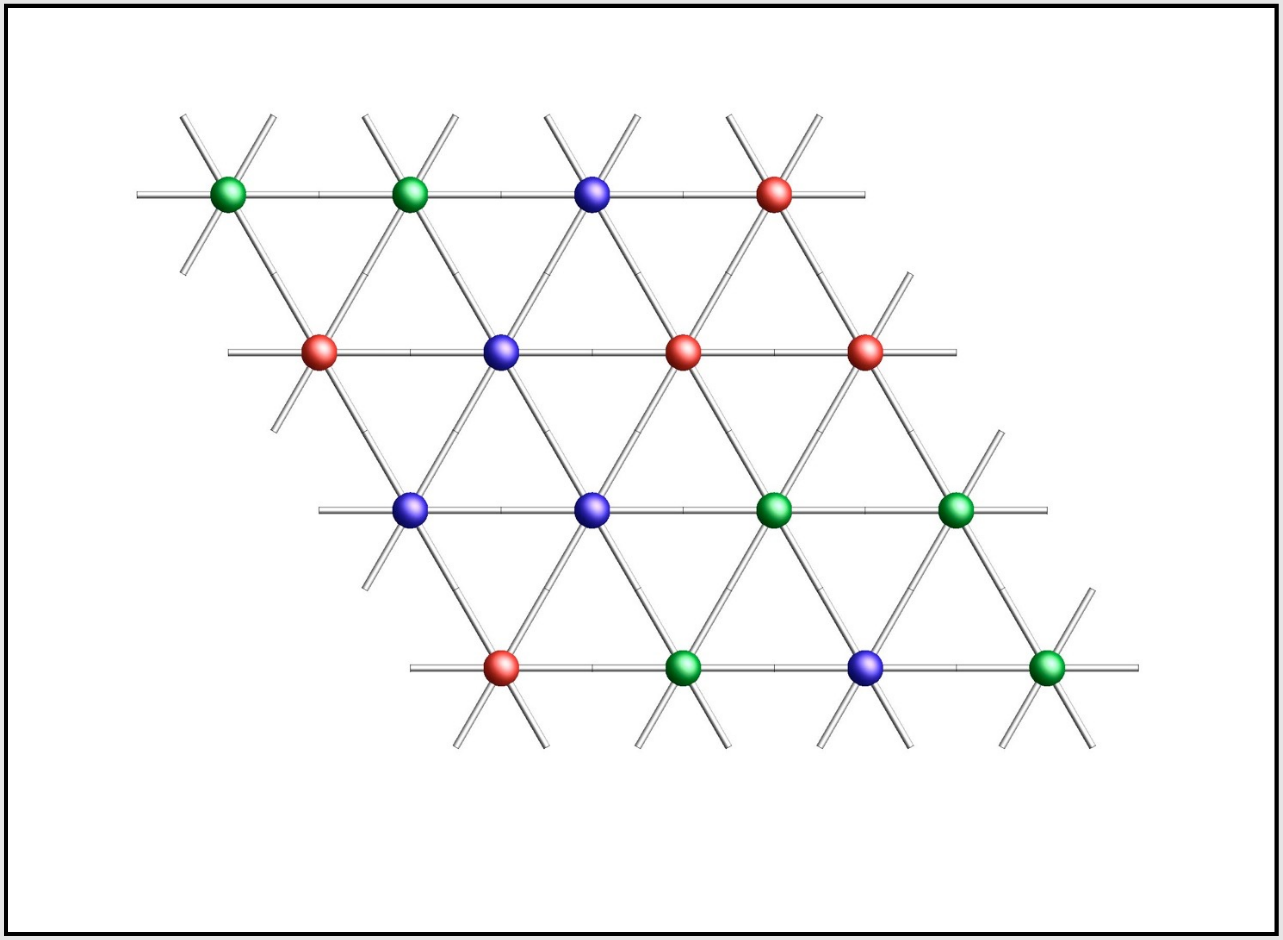
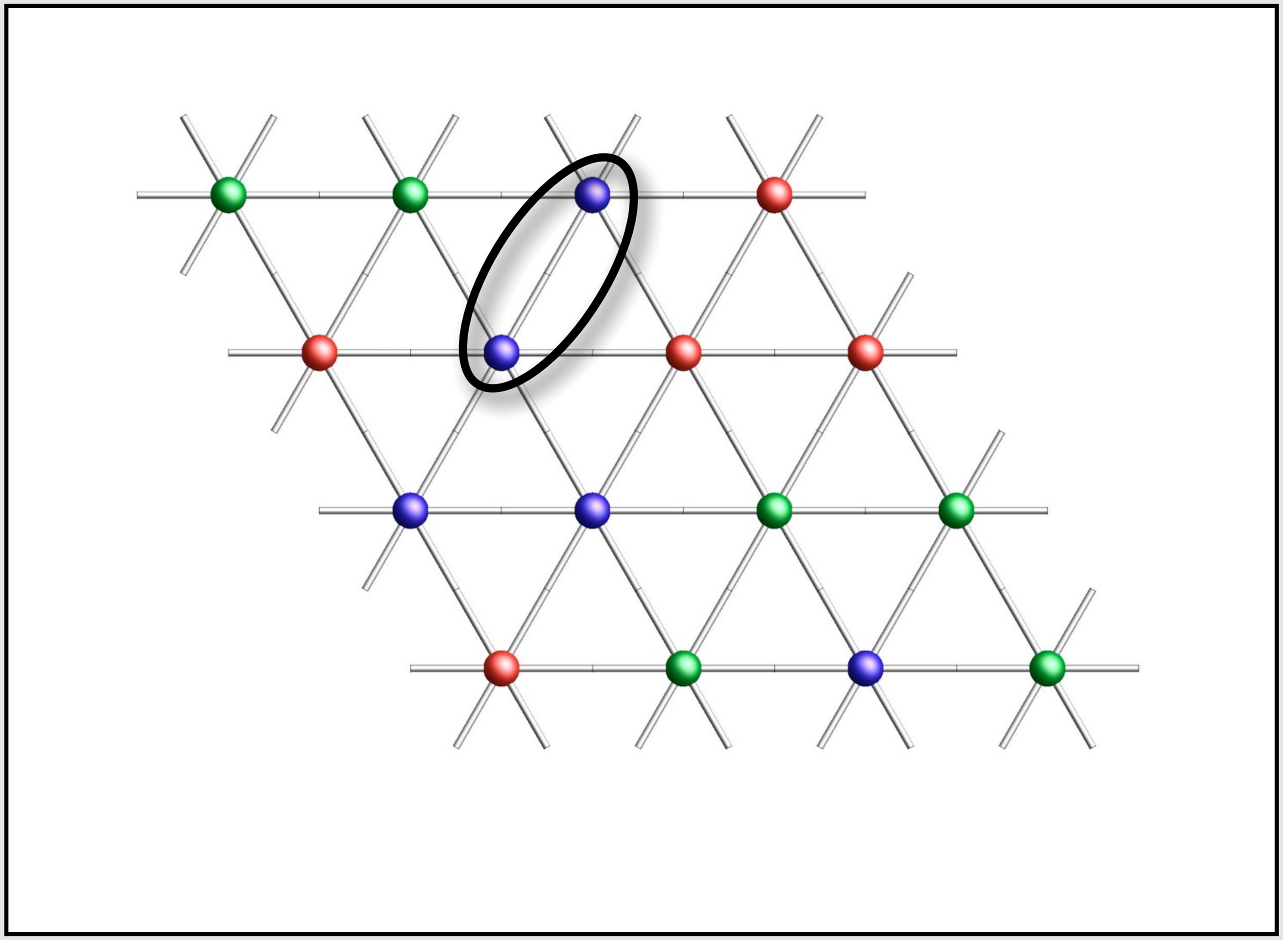


Quantum Dynamics

R. K. Kaul PRL (2015)

$$|\mathcal{S}\rangle\langle\mathcal{S}| = \frac{1}{N}\sum_{\alpha,\beta} |\alpha\alpha\rangle\langle\beta\beta|$$



SO(N) Projector Hamiltonian

R. K. Kaul PRL (2015)

$$H_J = -J \sum_{\langle ij \rangle} |\mathcal{S}_{ij}\rangle\langle\mathcal{S}_{ij}|$$

$N = 3$ ground state has quadrupolar order.

what is the ground state as N is varied?

Large-*N*: quantum dimer model

R. K. Kaul PRL (2015)

$$H_J = -J \sum_{\langle ij \rangle} |\mathcal{S}_{ij}\rangle\langle\mathcal{S}_{ij}|$$

$$\hat{H}_{\mathrm{QDM}} = -t \sum_{\mathrm{plaq}} \Big\{ \Big(|\,=\,\rangle_i \langle\,\|\,|_i + h.c. \Big)$$

At large-*N* $\hat{H}_J$ maps to a QDM, which has a valence bond-solid ground state.

Affleck; Read & Sachdev.
Moessner & Sondhi, PRB, PRL (2004)

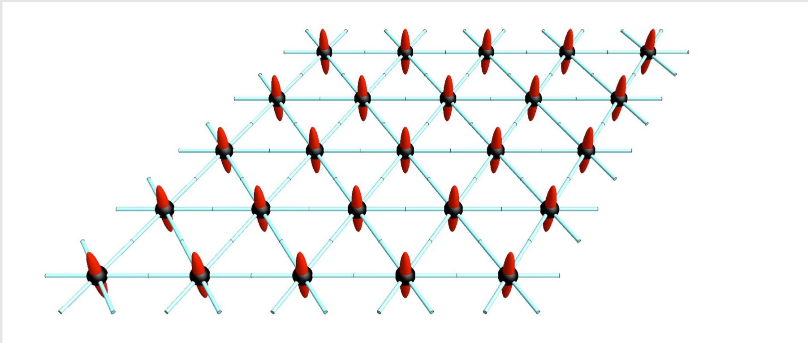
QMC Simulations

SSE method, A. W. Sandvik AIP (2011)
Loop, H. G. Evertz. Adv Phys (2003)

Finite-T. Efficient loop algorithm. Unbiased.

$$\beta = L$$

Triangular lattice



Quadrupolar order

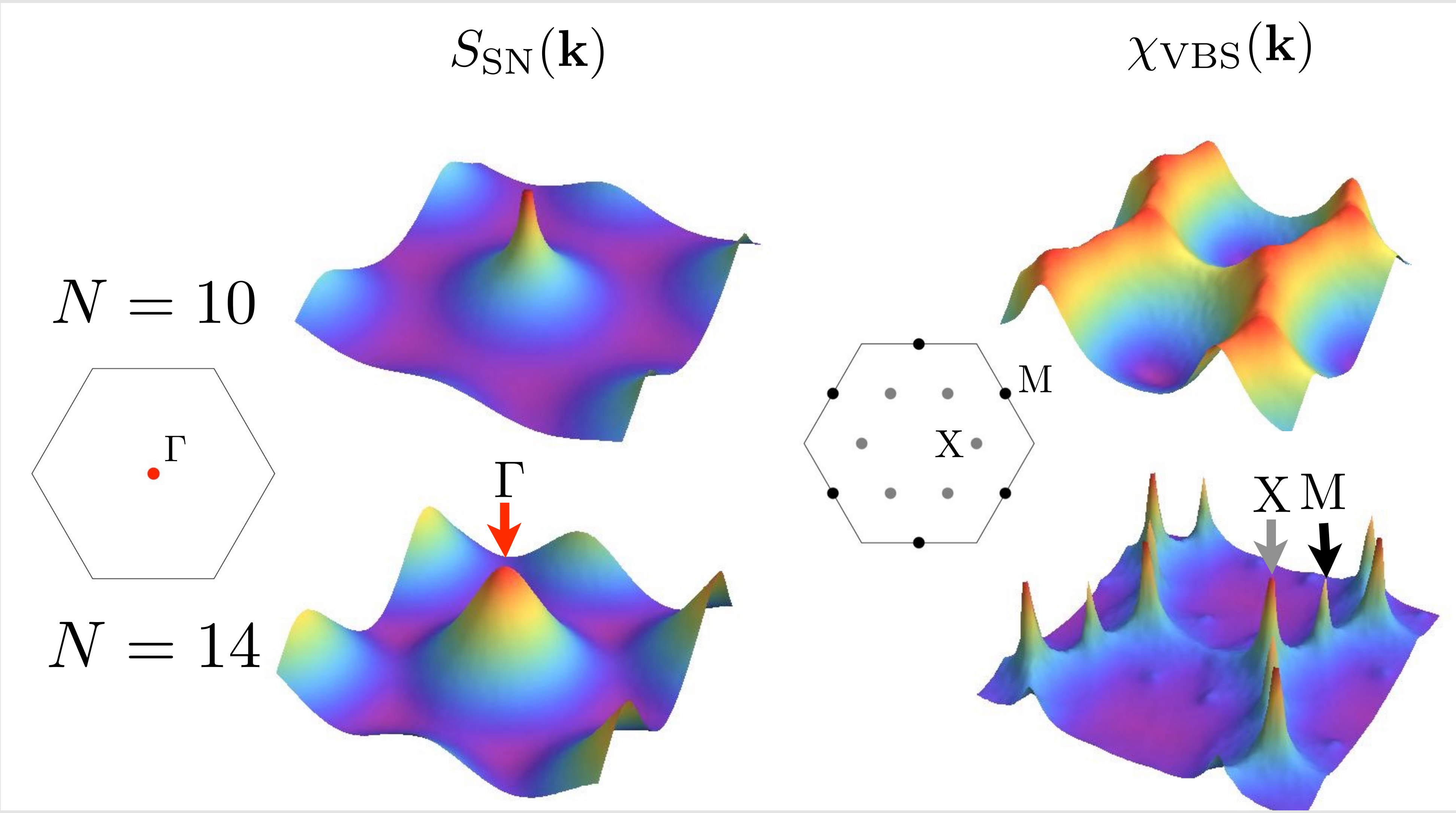
$$S_{\mathrm{SN}}(\mathbf{k}) = \frac{1}{N_{\mathrm{site}}} \sum_{ij} e^{i\mathbf{k}\cdot(\mathbf{r}_i - \mathbf{r}_j)} \langle \hat{Q}_{\alpha\alpha}(i) \hat{Q}_{\alpha\alpha}(j) \rangle$$

VBS order

$$\chi_{\mathrm{VBS}}(\mathbf{k}) = \frac{1}{N_{\mathrm{site}}} \sum_{ij} e^{i\mathbf{k}\cdot(\mathbf{r}_i - \mathbf{r}_j)} \frac{1}{\beta} \int d\tau \langle \hat{P}_{\mathbf{r}_i,\mathbf{r}_i+\hat{x}}(\tau) \hat{P}_{\mathbf{r}_j,\mathbf{r}_j+\hat{x}}(0) \rangle$$

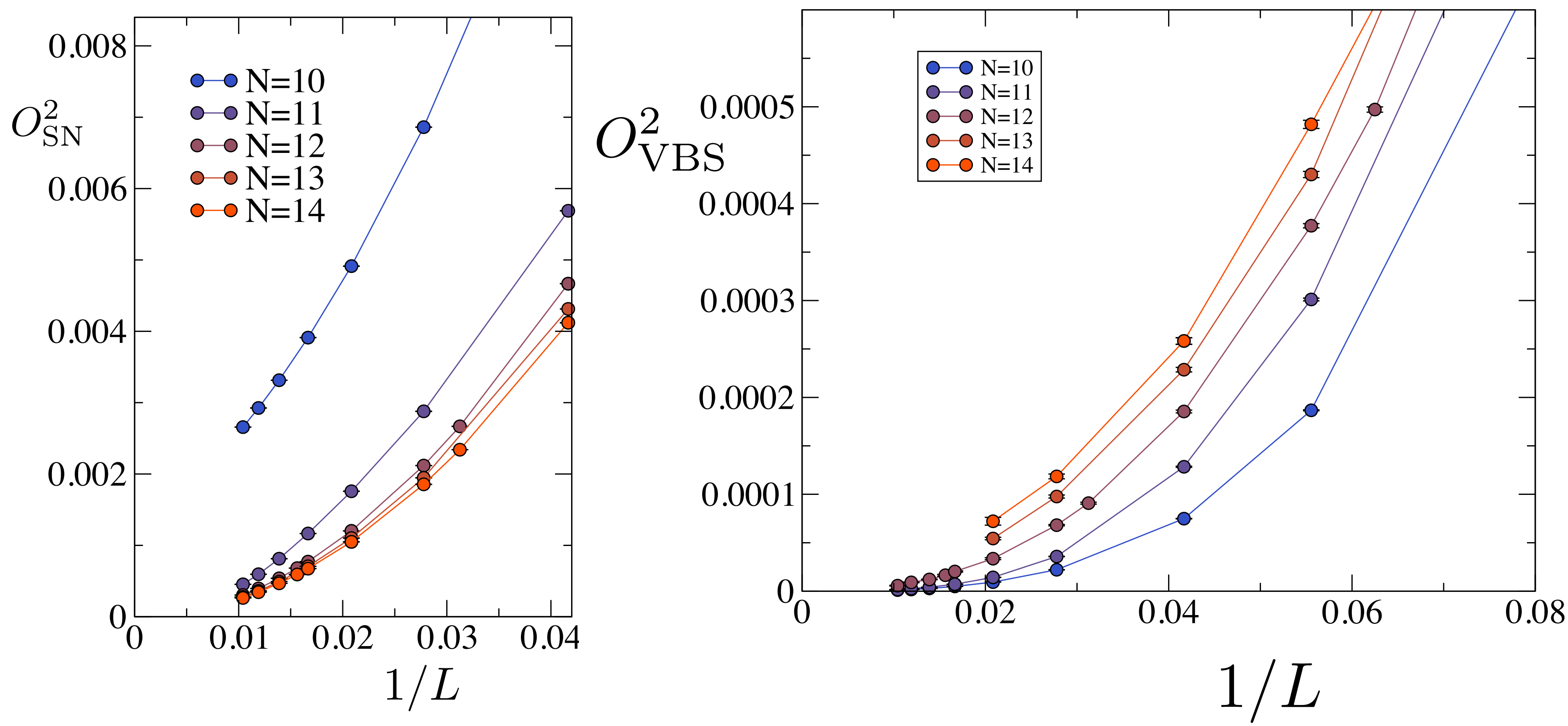
Correlation Functions

R. K. Kaul PRL (2015)



cf. Ralko, Ferrero, Becca, Ivanov & Mila (2006)

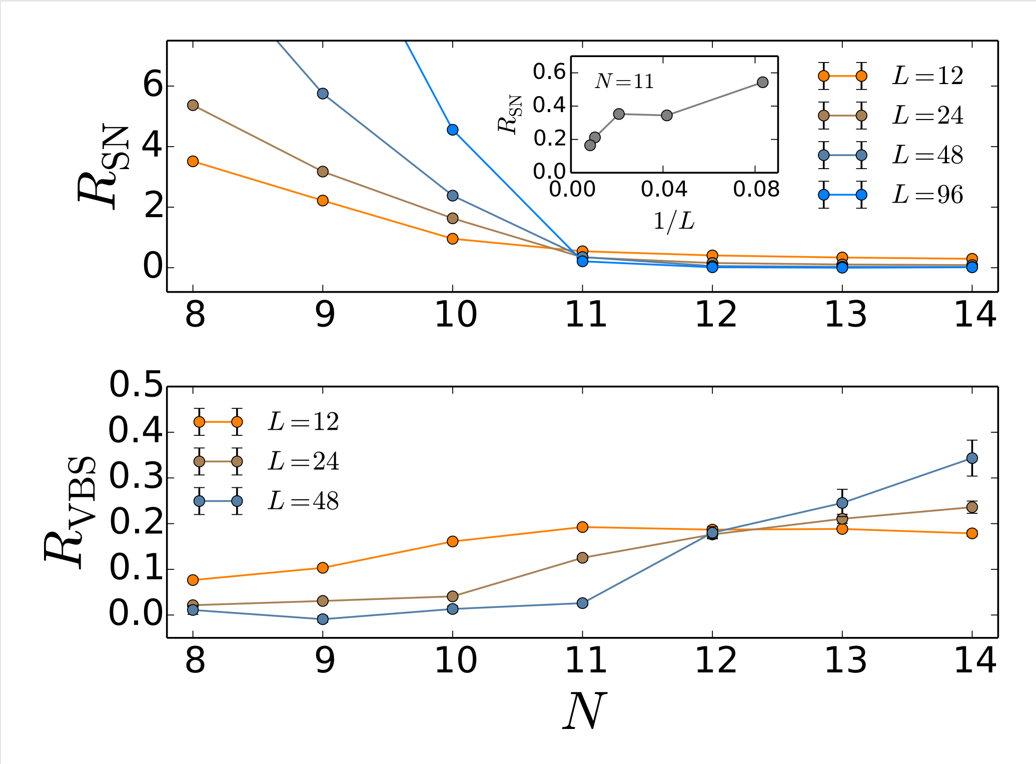
Extrapolation of Order



Q-VBS for H_J.

R. K. Kaul PRL (2015)

$$R_{\mathrm{SN}} = 1 - \frac{S_{\mathrm{SN}}(\mathbf{\Gamma}+\mathbf{a}2\pi/L)}{S_{\mathrm{SN}}(\mathbf{\Gamma})} \quad (\text{where } \mathbf{a} \equiv \mathbf{x} - \mathbf{y}/\sqrt{3})$$



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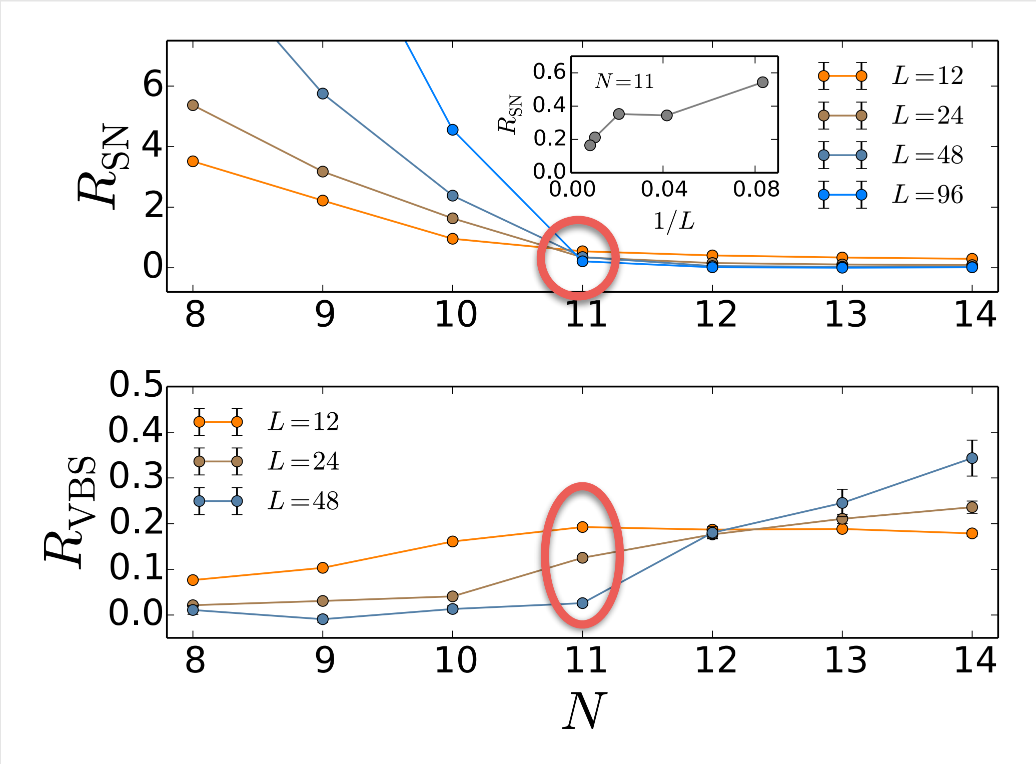
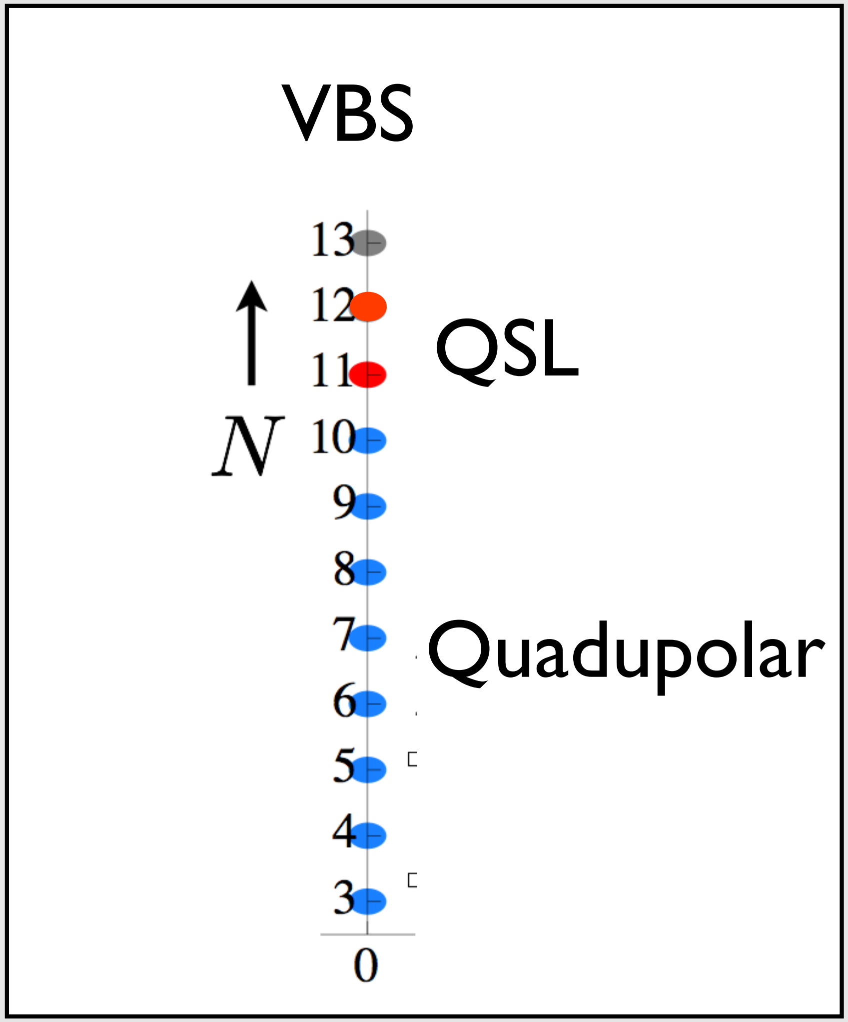


Phase Diagram

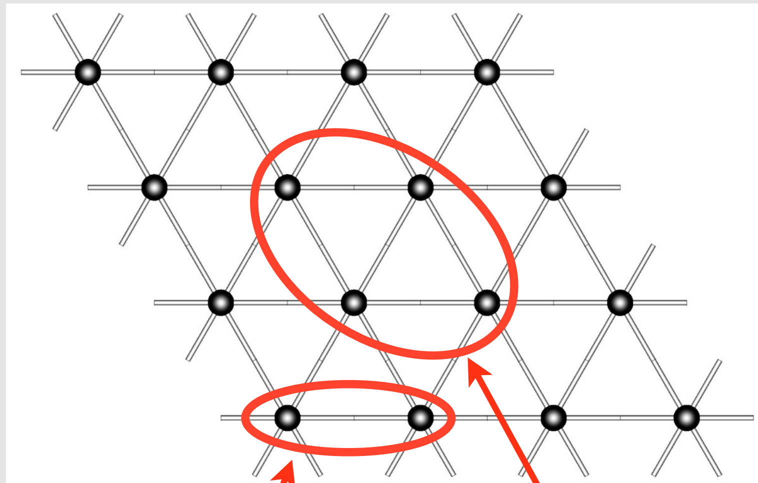


what is the nature of the QSL phase?

$\mathbb{Z}_2$ topological order?

phase transitions

A.W. Sandvik, PRL (2007)

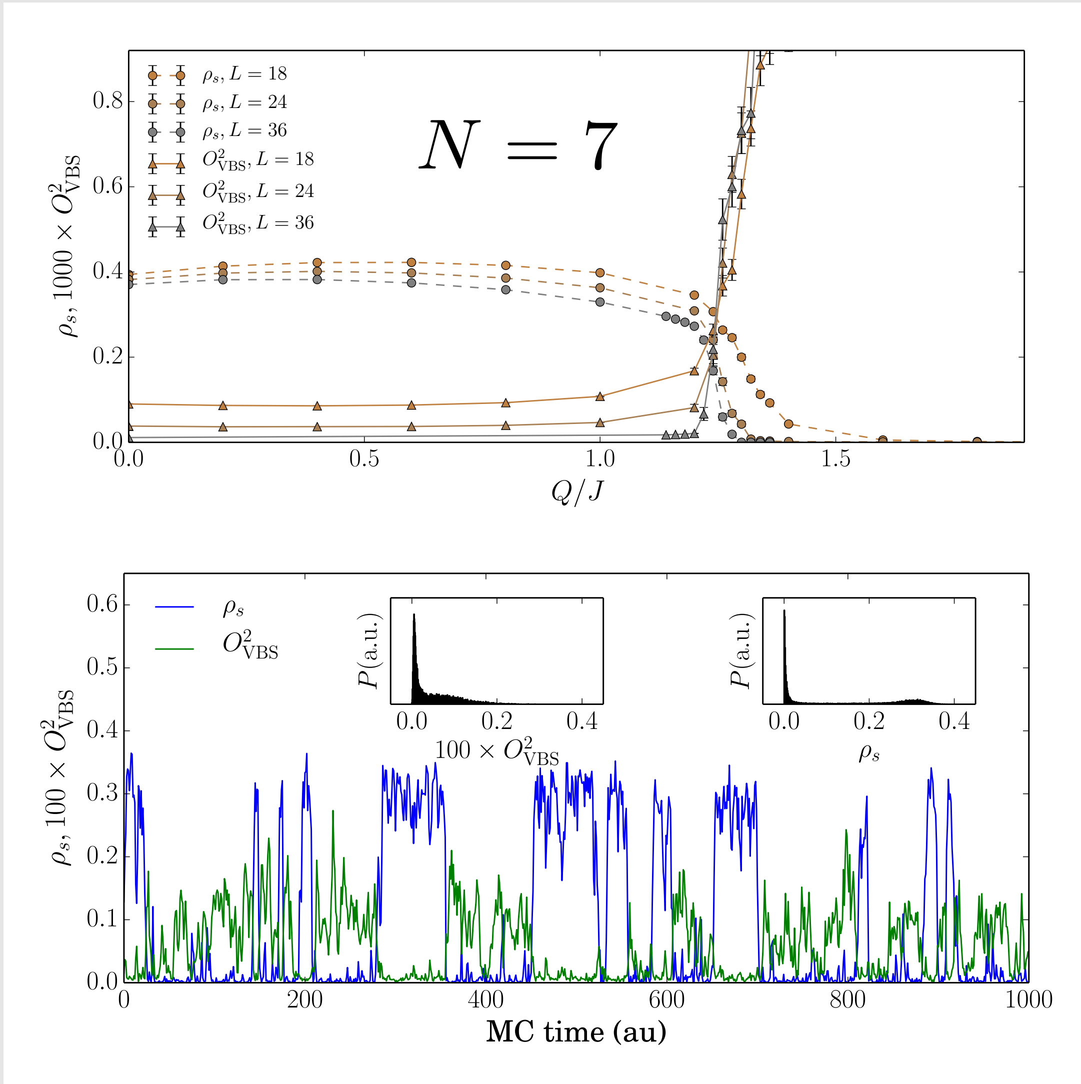


$$H_{J-Q} = -J \sum_{\langle ij \rangle} P_{ij} - Q \sum_{\langle ijkl \rangle} P_{ij} P_{kl}$$

Sign-free way to tune from magnetic to VBS at fixed N!

Evidence for 1st order Q-VBS

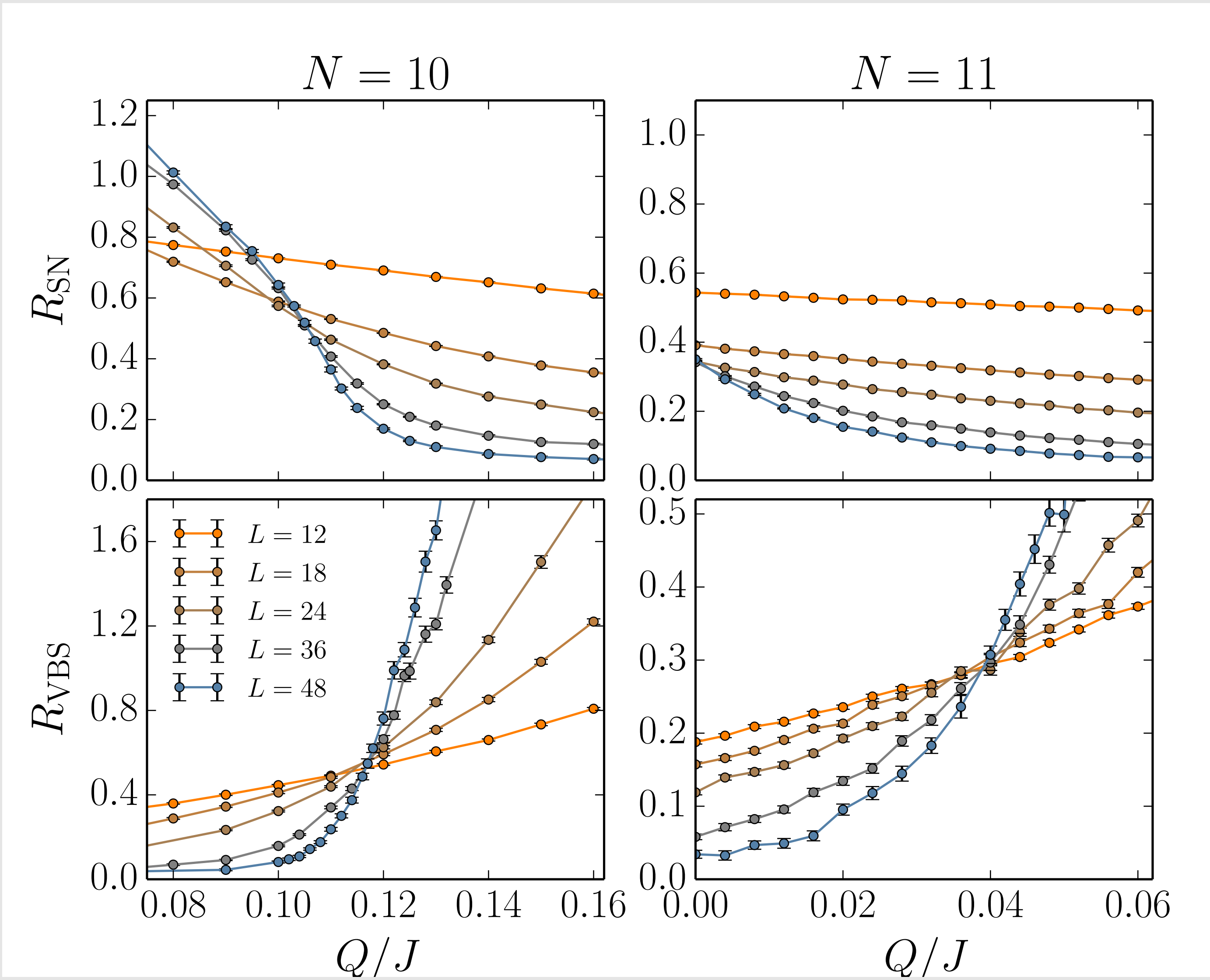
R. K. Kaul PRL (2015)



$Q/J = 1.26$

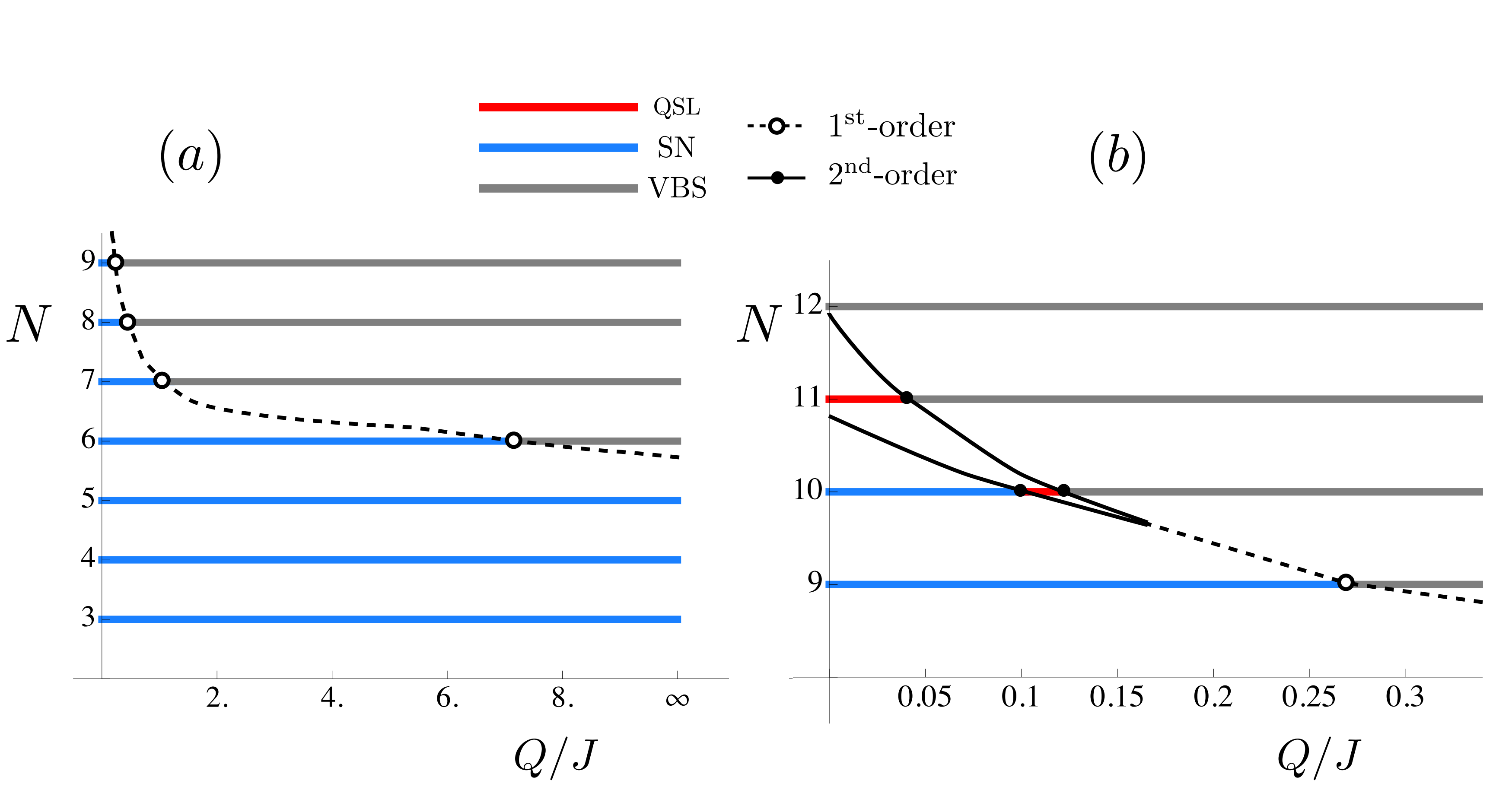
Intermediate QSL

R. K. Kaul PRL (2015)



J-Q Phase Diagram

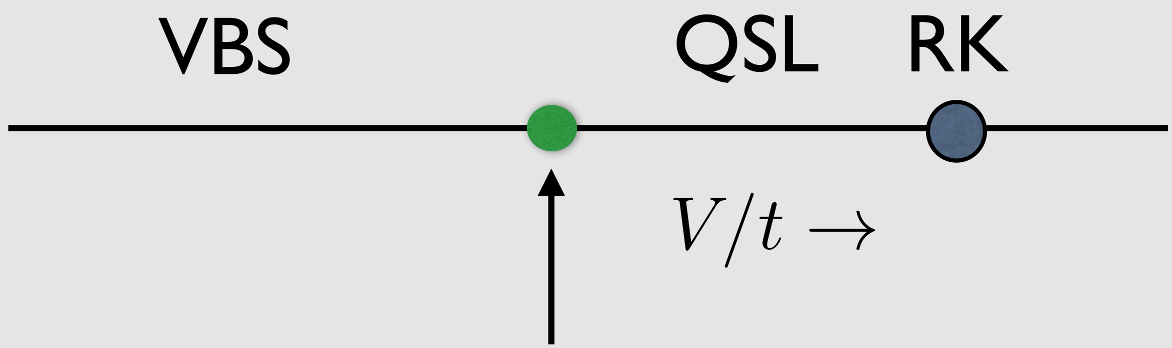
R. K. Kaul PRL (2015)



QSL-VBS transition

Moessner & Sondhi, PRB, PRL (2004)

Triangular Quantum Dimer Model



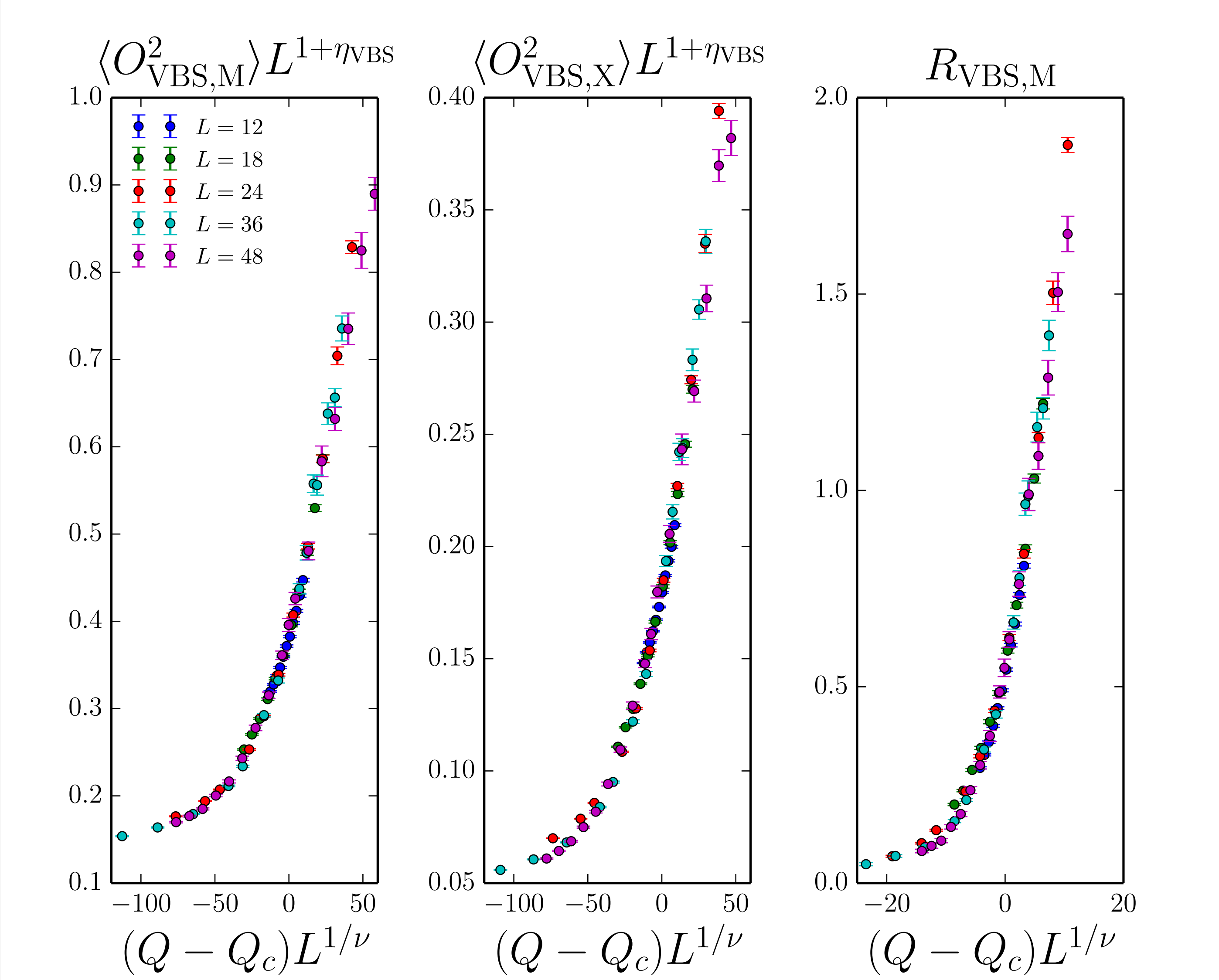
O(4)* transition.

VBS order parameter is bilinear in O(4) theory

Hypothesis has never been tested!

QSL-VBS: O(4)*?

R. K. Kaul PRL (2015)



Critical Universality?

R. K. Kaul PRL (2015)

$$\eta_{\mathrm{VBS}} = 1.3(2)$$

$$\nu_{\mathrm{VBS}} = 0.65(20)$$ **(?)**

Large η_{VBS} is direct evidence of fractionalization!

Critical Universality?

R. K. Kaul PRL (2015)

$$\eta_{\mathrm{VBS}} = 1.3(2)$$

$$\nu_{\mathrm{VBS}} = 0.65(20)$$ **(?)**

Large η_{VBS} is direct evidence of fractionalization!

$$\eta^{(2)}_{O(4)} = 1.375(5) \qquad \eta^{(1)}_{O(4)} = 0.0359(9)$$

$$\nu_{O(4)} = 0.7525(10)$$

Quantum Effective Theory

Grover & Senthil (2007); Moessner, Sondhi, Fradkin (2001); Senthil, Fisher (2000)

$$S = J \sum_{\langle ij \rangle} \sigma_{ij} \hat{n}_i \cdot \hat{n}_j + K \sum_{\square} \sigma\sigma\sigma\sigma$$

$$Z = \sum_{c} e^{-S - i\frac{\pi}{2} \sum_r (f_{r\tau} - 1)}$$

If director fluctuations are gapped: "odd-Ising gauge theory"

$$H_{IGT} = -K\sigma^z\sigma^z\sigma^z\sigma^z - h_\perp \sigma^x$$

$$\prod_{+} \sigma^x = -1$$

On triangular lattice get QSL or VBS. Trivial "I" absent!

SO(N) representation

Arovas, Auerbach; Demidio, Murthy, Kaul (unpublished)

$$H_J = -J \sum_{\langle ij \rangle} |\mathcal{S}_{ij}\rangle\langle\mathcal{S}_{ij}|$$

$$H_b = -\frac{J}{N} \sum_{\langle ij \rangle} \left(b^\dagger_{i\alpha} b^\dagger_{j\alpha} \right) \left(b_{j\beta} b_{i\beta} \right) \qquad n_b = 1$$

With $n_b \neq 1$ forms new SO(N) spin "bosonic" representations

Large-N, SO(N)

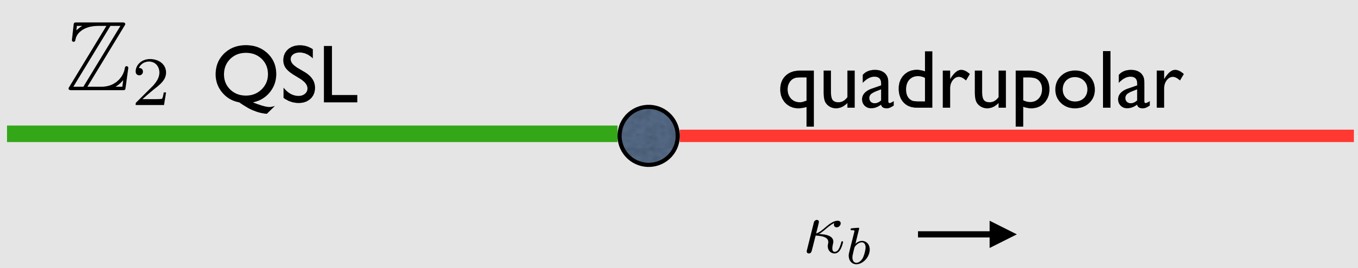
Demidio, Murthy, Kaul (unpublished)

Access saddle with $n_b = \kappa_b N$

$$\mathcal{L}_b = b^*_{i\alpha}\partial_\tau b_{i\alpha} + \frac{N}{J}|Q_{ij}|^2 + Q^*_{ij} b_{i\alpha} b_{j\alpha} + \mathrm{c.c.} + \lambda_i (b^\dagger_{i\alpha} b_{i\alpha} - \kappa_b N)$$

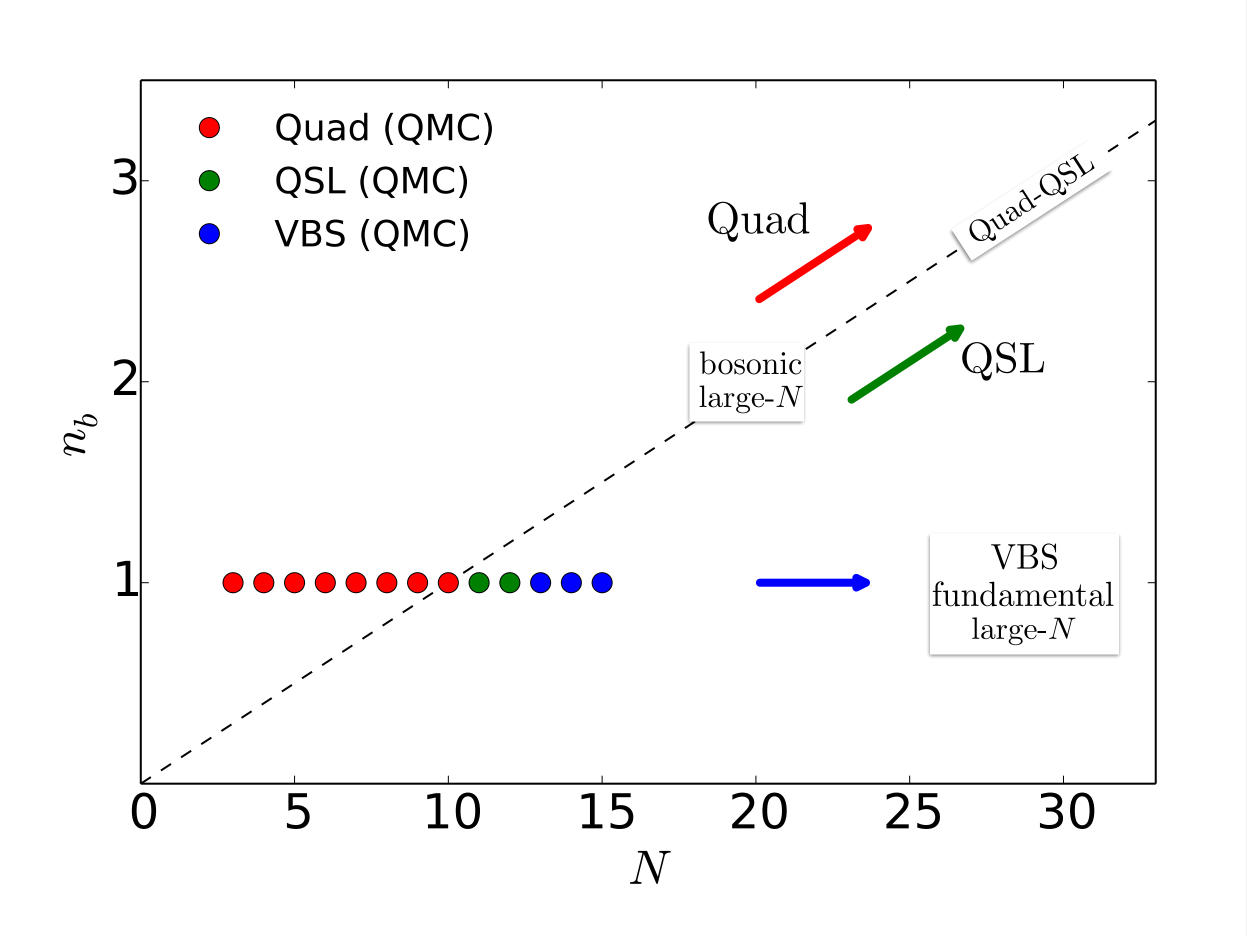
$(2\kappa_b^c + 1) \approx 1.20\ldots$ (triangular lattice)

Uniform saddle : only $\mathbb{Z}_2$ gauge fluctuations!
Stable to confinement.

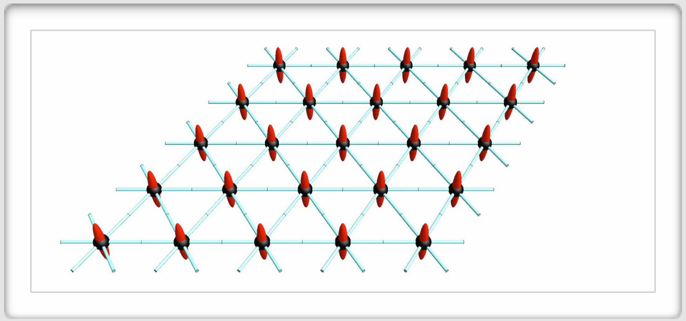


SO(N) phase diagram

$$H_b = -\frac{J}{N}\sum_{\langle ij\rangle}\left(b^\dagger_{i\alpha}b^\dagger_{j\alpha}\right)\left(b_{j\beta}b_{i\beta}\right) \qquad (n_b \ \& \ N)$$



Conclusions



- disordering *S=1* quadrupolar insulators, a natural route to access $\mathbb{Z}_2$ phases.
- sign-free study of phase transitions
- nature of QSL?
- studies of QSLs in *d=3*?
- QSL physics with quenched disorder?

Outline

- Quadrupolar magnets
    - Quantum Fluctuations : Spin Liquids
    - **New percolation quantum criticality**
- Quadratic band touchings in bilayer graphene

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- Quadrupolar magnets
    - Quantum Fluctuations : Spin Liquids
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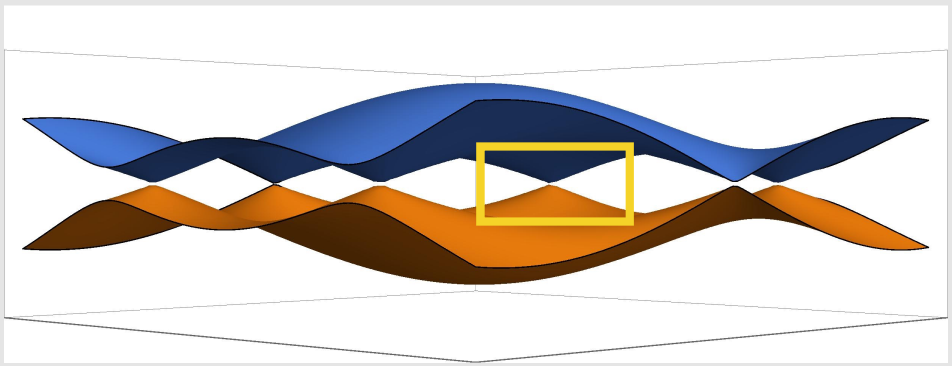
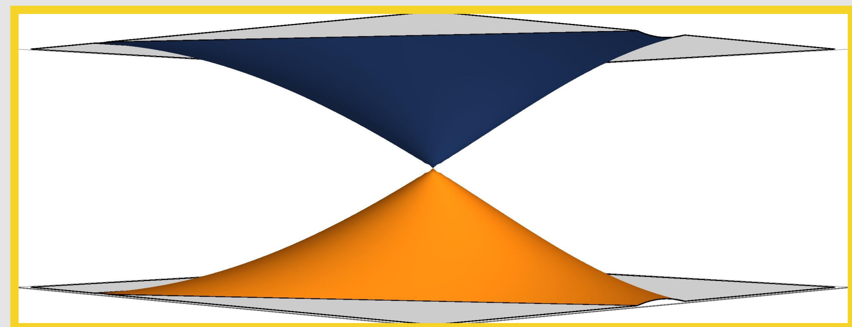
Question

What is the effect of local quartic interactions on graphene's band structure?

Single Layer Graphene

$$H_{\mathrm{SL}} = -t \sum_{\langle ij \rangle} a^\dagger_{i\sigma} b_{j\sigma}$$

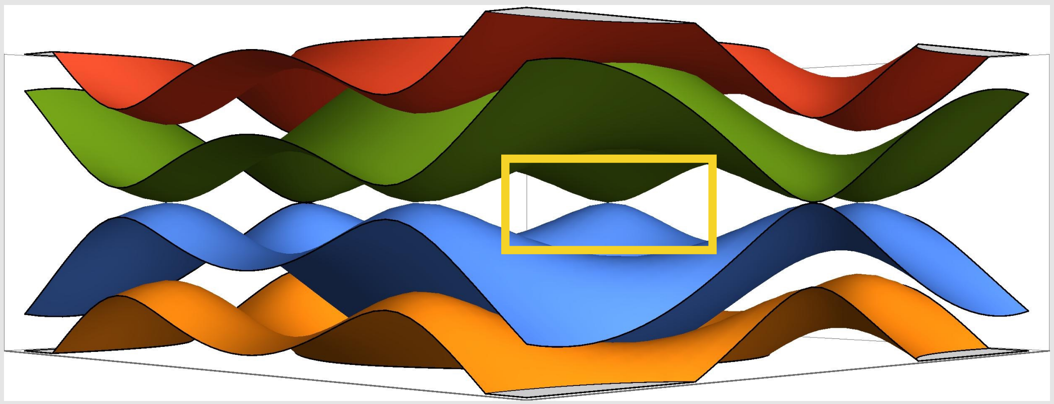


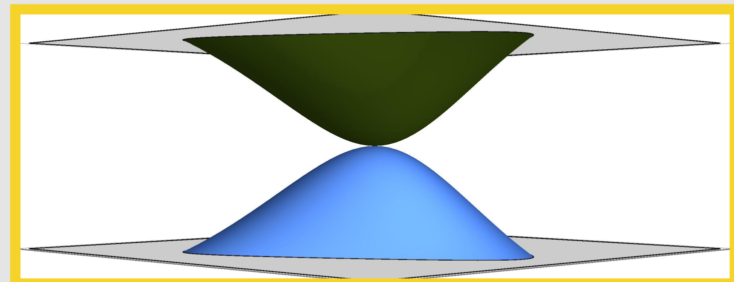


local quartic interactions *irrelevant*

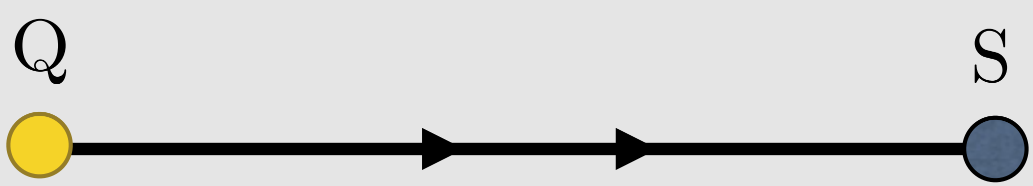
Bilayer Graphene

$$H_{\mathrm{BSB}} = -t \sum_{\langle ij \rangle \ell} a^{\dagger}_{i\sigma\ell} b_{j\sigma\ell} - t_{\perp} \sum_{i} a^{\dagger}_{i\sigma 2} b_{i\sigma 1} + \mathrm{h.c.}$$





local quartic interactions *marginally relevant*



Hubbard Model Expectation

any short-range quartic interaction …

$$H_U = U n_{i\uparrow} n_{i\downarrow} \qquad U \to \infty \quad \text{Néel phase.}$$

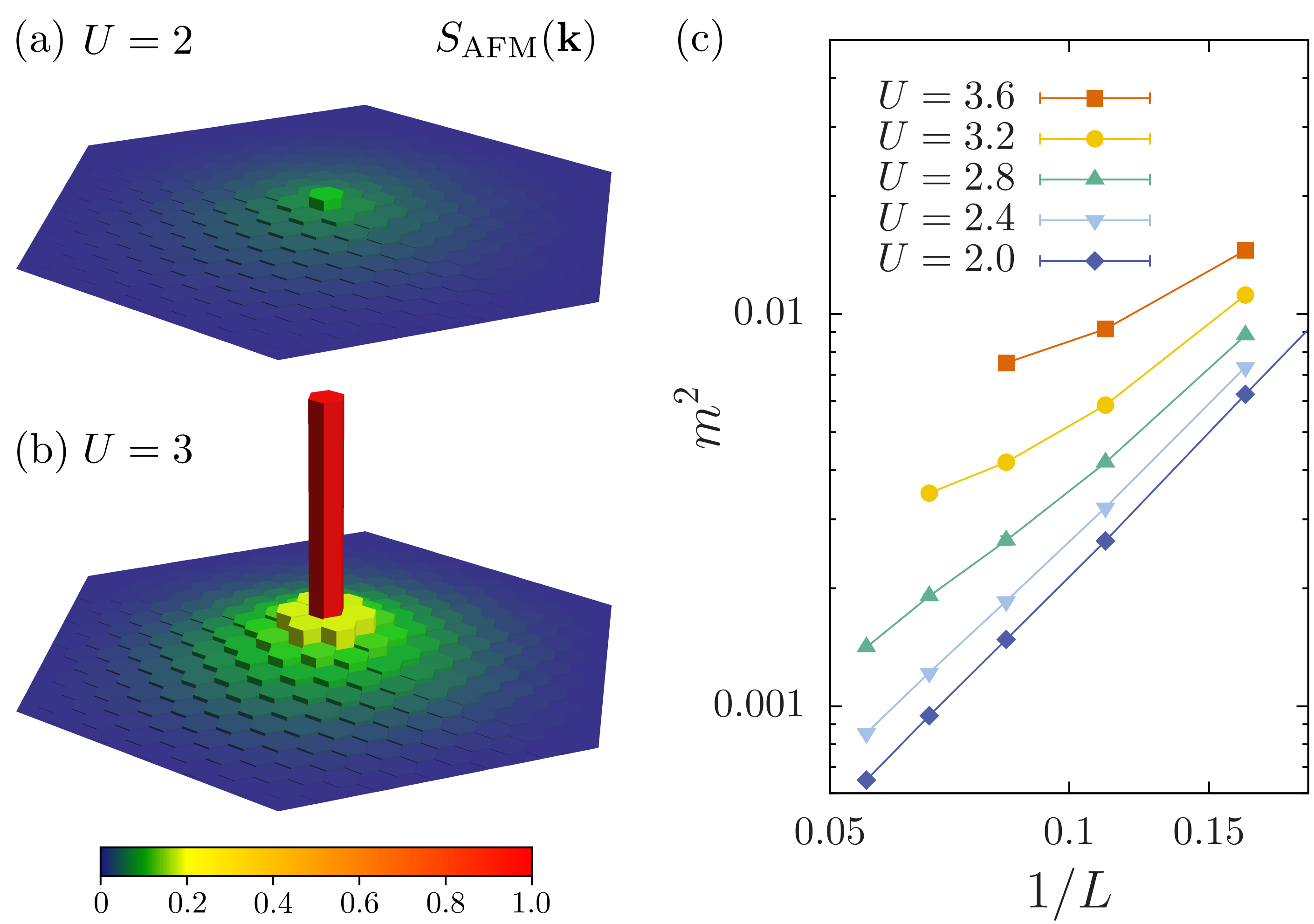
single layer

bernal bilayer

O. Vafek and K. Yang, Phys. Rev. B 81, 041401 (2010)
O. Vafek, Phys. Rev. B 82, 205106 (2010)
F. Zhang, H. Min, M. Polini, and A. H. MacDonald, Phys. Rev. B 81, 041402 (2010)
R. Nandkishore and L. Levitov, Phys. Rev. Lett. 104, 156803 (2010)
Y. Lemonik, I. L. Aleiner, C. Toke, and V. I. Fal'ko, Phys. Rev. B 82, 201408 (2010)
T. C. Lang, Z. Y. Meng, M. M. Scherer, S. Uebelacker, F. F. Assaad, A. Muramatsu, C. Honerkamp, and S. Wessel, Phys. Rev. Lett. 109, 126402 (2012)
…

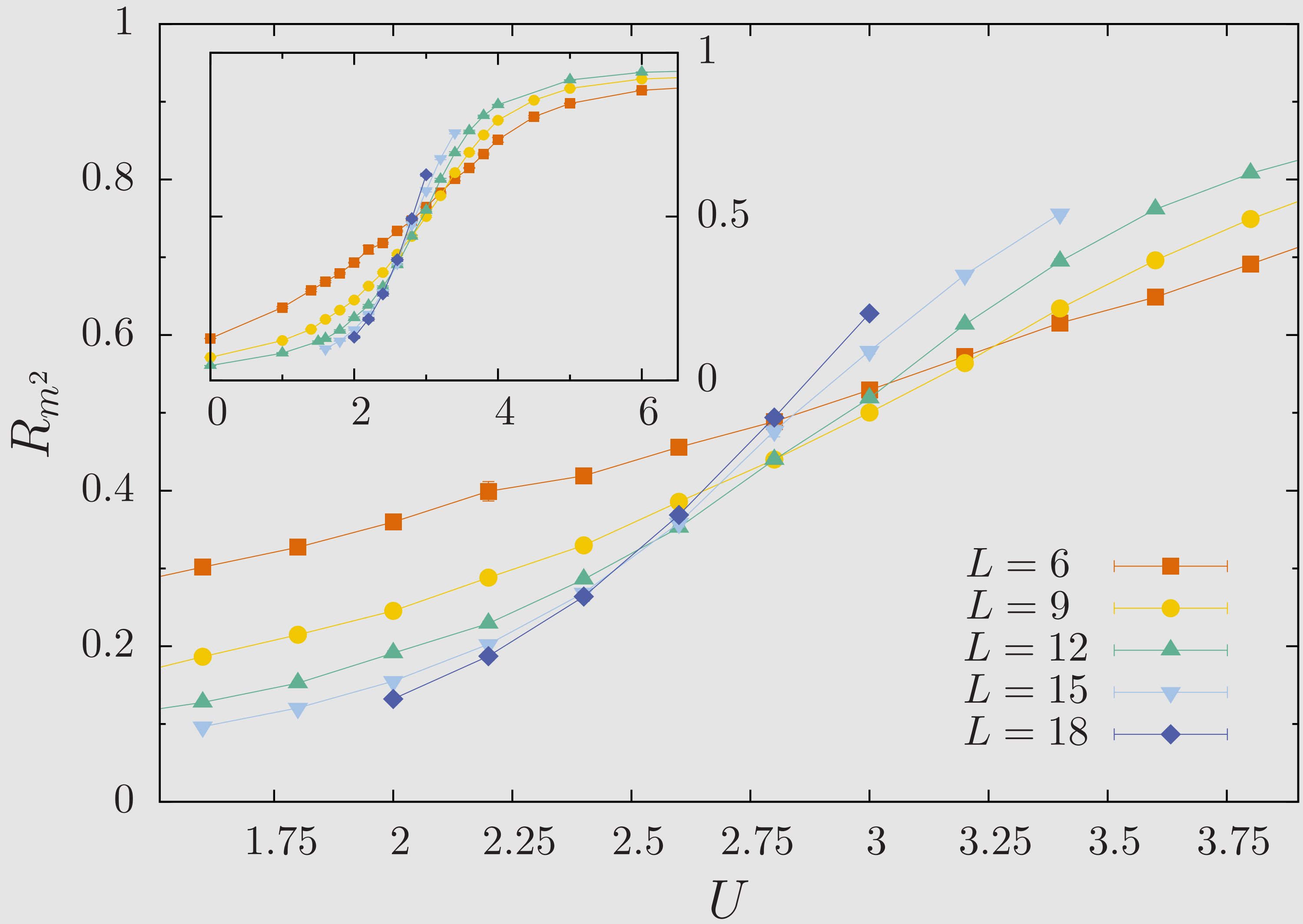
QMC of Bernal-Hubbard

S. Pujari, T.C. Lang, G. Murthy, R.K. Kaul, *Phys. Rev Lett. (2016)*



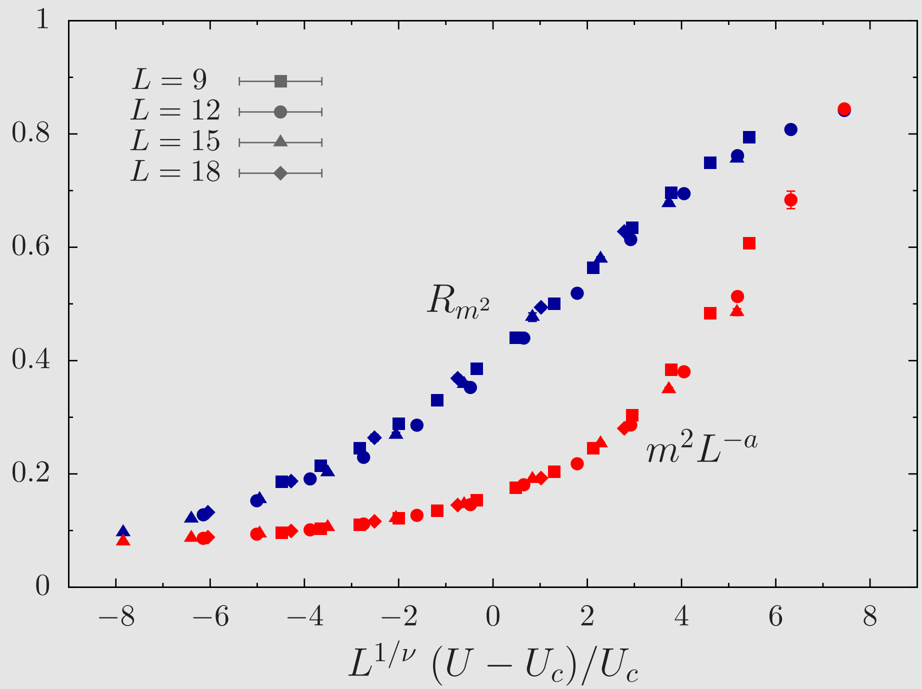
Finite Coupling Phase Transition

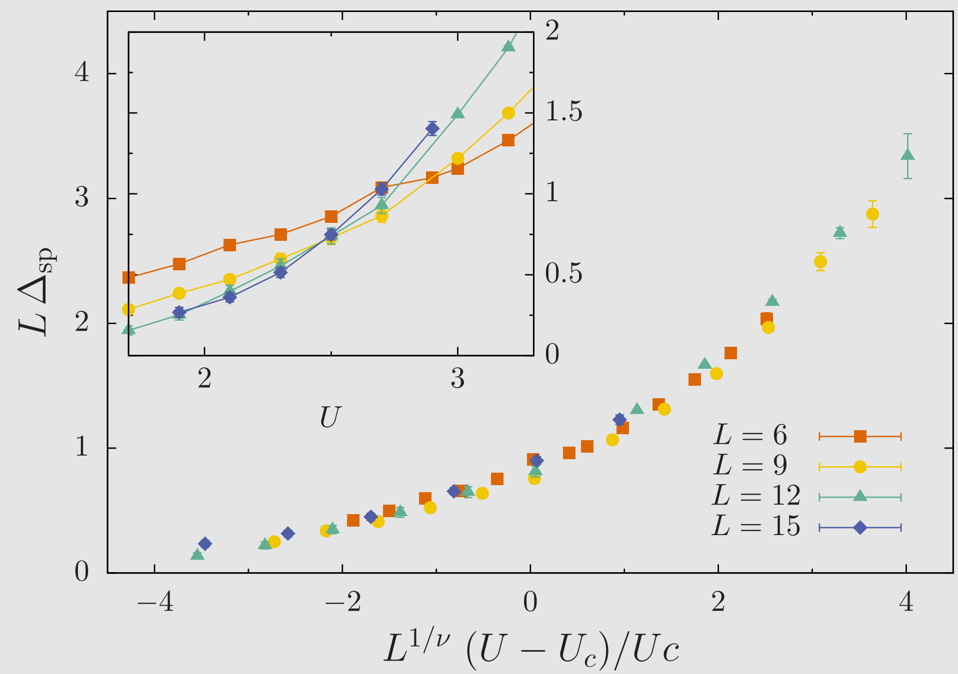
S. Pujari, T.C. Lang, G. Murthy, R.K. Kaul, *Phys. Rev Lett. (2016)*



Critical Collapse

S. Pujari, T.C. Lang, G. Murthy, R.K. Kaul, *Phys. Rev Lett. (2016)*





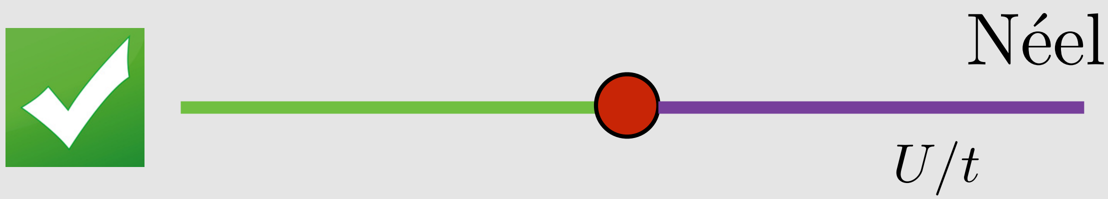
All our data is consistent with a quantum critical point

$$z = 0.9(2) \qquad U_c = 2.5(2)$$

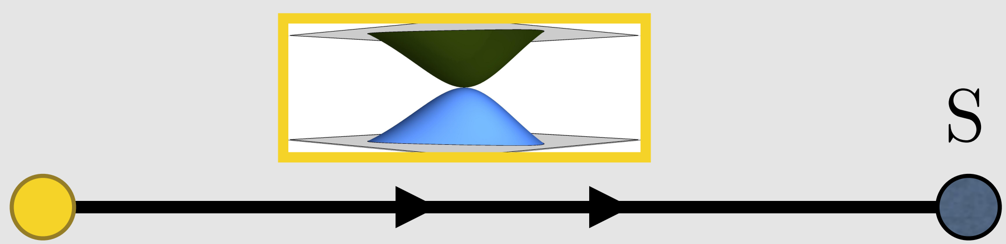
Revised Phase Diagram

bernal bilayer

bernal bilayer



What is the nature of weak coupling phase?
Quantum phase transition?
RG-flow?



Bernal: QBT

S. Pujari, T.C. Lang, G. Murthy, R.K. Kaul, *Phys. Rev Lett. (2016)*

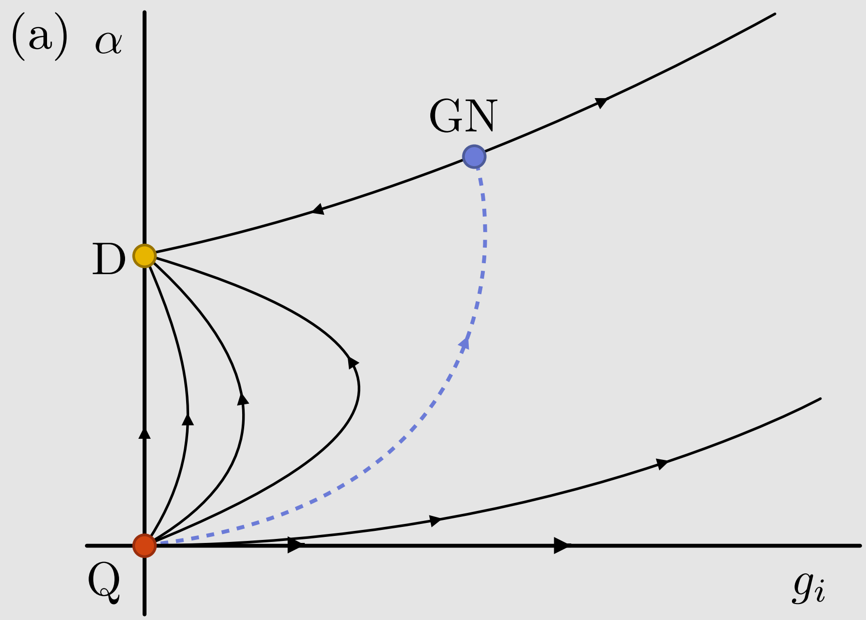
effective theory for quadratic part

$$H^{(2)} = \Psi^{\dagger}_{\mathbf{K}+\mathbf{k}} \left(\mathrm{Re}[\phi(\mathbf{k})]\sigma^x + \mathrm{Im}[\phi(\mathbf{k})]\sigma^y \right) \Psi_{\mathbf{K}+\mathbf{k}}$$

$$\phi(\mathbf{k}) \equiv \alpha(k_x + ik_y) + \beta(k_x - ik_y)^2 + \mathcal{O}(k^3).$$

RG-flow

S. Pujari, T.C. Lang, G. Murthy, R.K. Kaul, *Phys. Rev Lett. (2016)*



$$\frac{dg}{d\ln b} = c_1 g^2$$

$$\frac{d\alpha}{d\ln b} = \alpha$$

Bernal: QBT

S. Pujari, T.C. Lang, G. Murthy, R.K. Kaul, *Phys. Rev Lett. (2016)*

effective theory for quadratic part

$$H^{(2)} = \Psi^\dagger_{\mathbf{K}+\mathbf{k}} \left(\mathrm{Re}[\phi(\mathbf{k})]\sigma^x + \mathrm{Im}[\phi(\mathbf{k})]\sigma^y \right) \Psi_{\mathbf{K}+\mathbf{k}}$$

$$\phi(\mathbf{k}) \equiv \alpha(k_x + ik_y) + \beta(k_x - ik_y)^2 + \mathcal{O}(k^3).$$

nearest neighbor model on bilayer is finely tuned

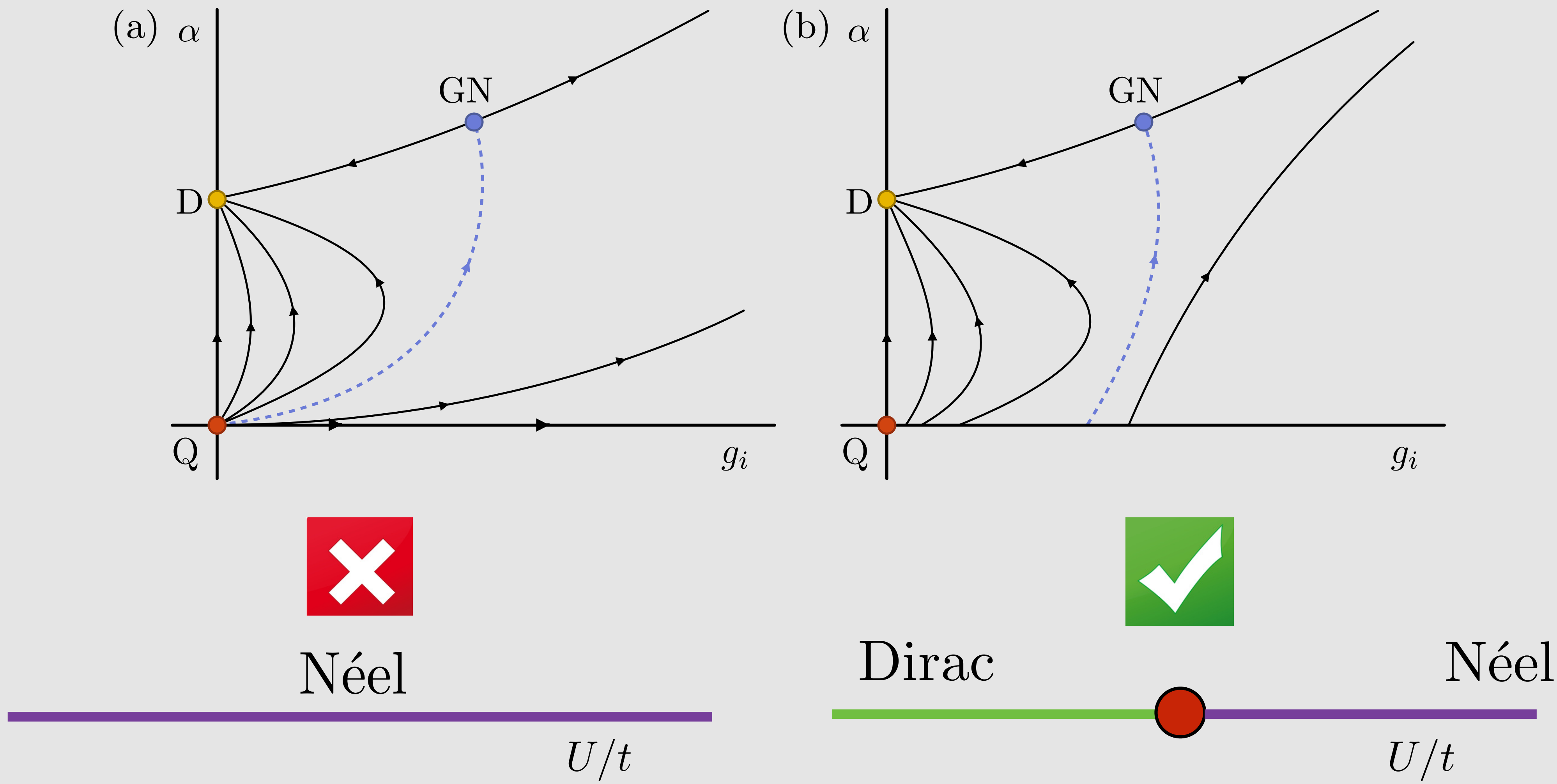
$$\alpha = 0$$

Quadratic band touching is not symmetry protected!

$$\frac{dg}{d\ln b} = c_1 g^2 \qquad \frac{d\alpha}{d\ln b} = \alpha + c_2 g^2$$

RG-flow

S. Pujari, T.C. Lang, G. Murthy, R.K. Kaul, *Phys. Rev Lett. (2016)*



Summary

- weak interaction cause Dirac dispersion to emerge
- no weak coupling symmetry breaking (short-range)
- Gross-Neveu quantum criticality

phase diagram of Hubbard model with trigonal warping?
symmetry breaking with Coulomb interactions? (experiments?)