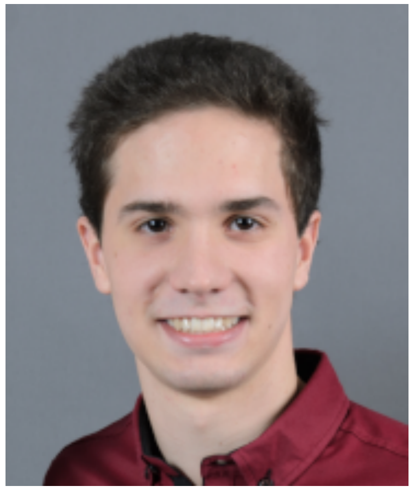
Conference on Fractionalization and Emergent Gauge Fields in Quantum Matter

ICTP

Crystalline phases and devil's staircase in qubit spin ice

Karlo Penc

HUN-REN Wigner Research Centre for Physics



M. Kondákor, K. Penc:
Phys. Rev. Research **5**, 043172 (2023).

HUN REN | wigner

supported by the Hungarian NKFIH Grant
Nos. K124176 and K142652

ice models

VOLUME 82, NUMBER 3 PHYSICAL REVIEW LETTERS 18 JANUARY 1999

Covalency of the Hydrogen Bond in Ice: A Direct X-Ray Measurement

E. D. Isaacs,[1] A. Shukla,[2] P. M. Platzman,[1] D. R. Hamann,[1] B. Barbiellini,[1] and C. A. Tulk[3]

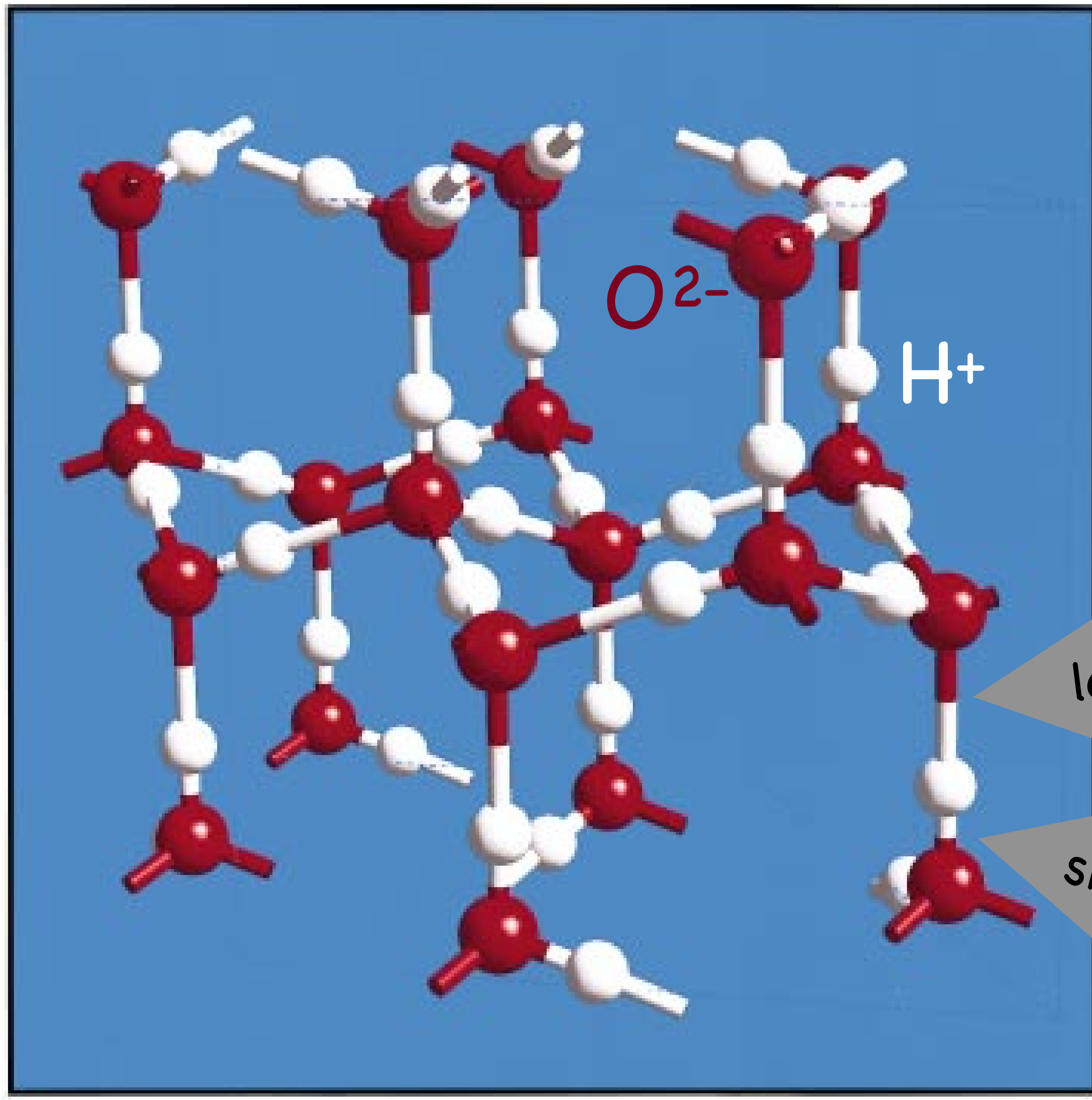


FIG. 1(color). Crystal structure of Bernal-Fowler ice I*h*. Red (white) balls give the positions of the oxygen (hydrogen). The crystallographic *c*-axis is in the vertical direction.

Bernal-Fowler ice rules (1933):

Each O^{2-} has four neighbouring H^+

Local charge neutrality ⇒ Only two H^+ are close to the O^{2-}

long O-H H-bond

short O-H covalent bond

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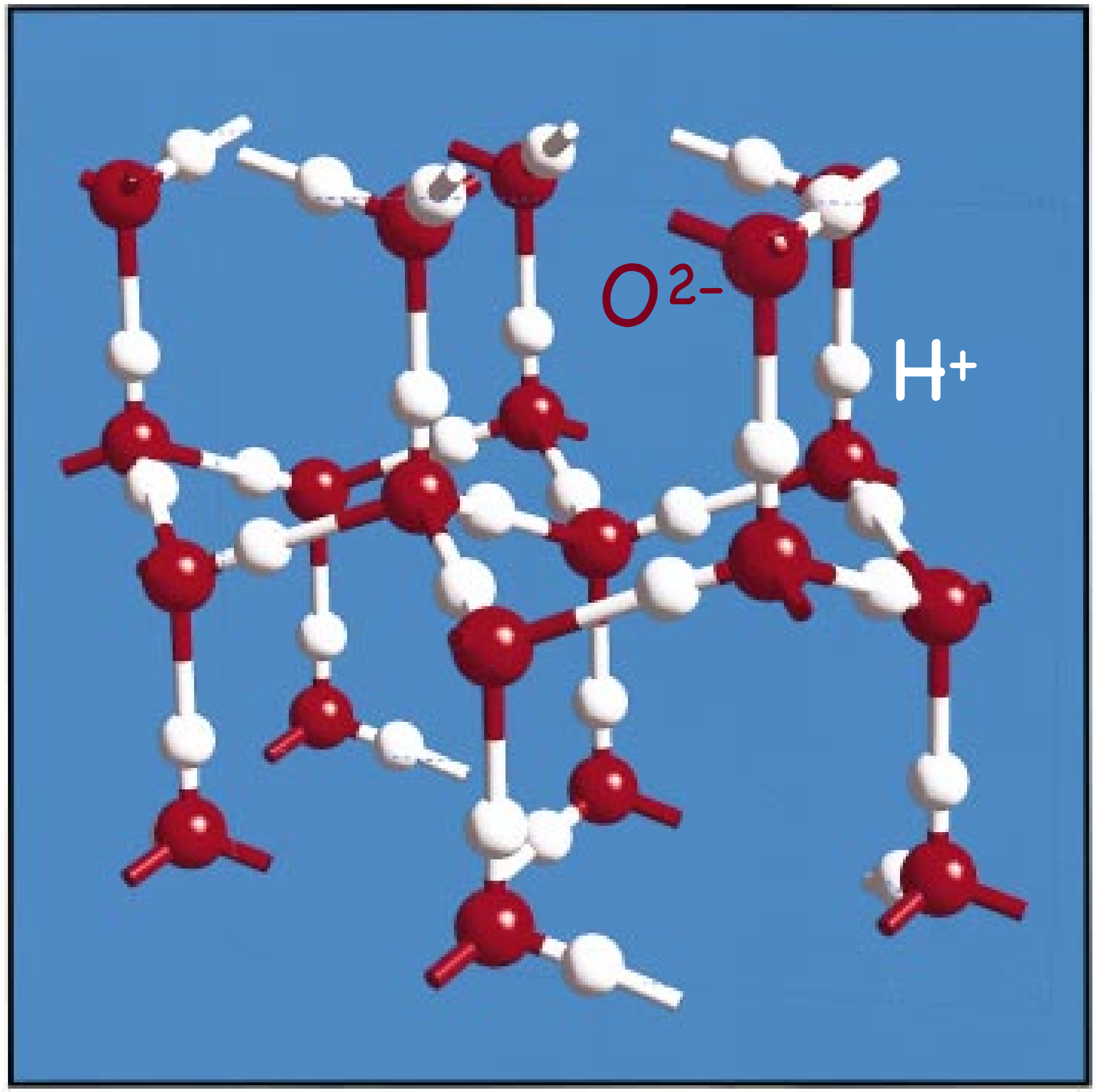

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Pauling ice degeneracy (1935):

$$Z \approx 2^{2N_O} \times \left(\frac{6}{16}\right)^{N_O} \approx 1.5^{N_O}$$

Each H has 2 possible positions on a bond.

Out of 16, only 6 configurations respect the ice rules.

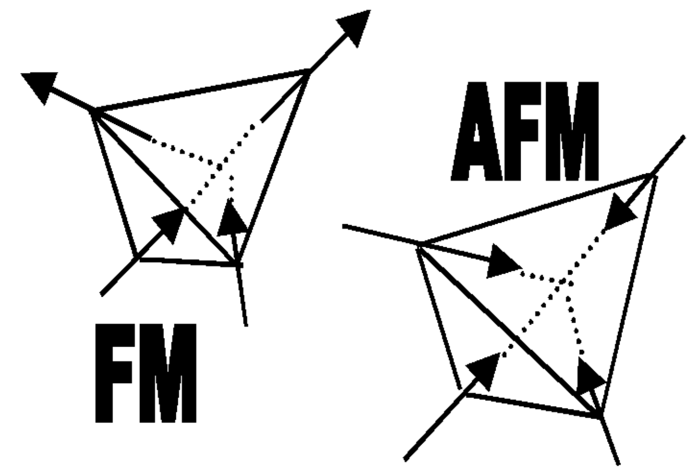
Nagle (1960's): $Z \approx 1.50685^{N_O}$

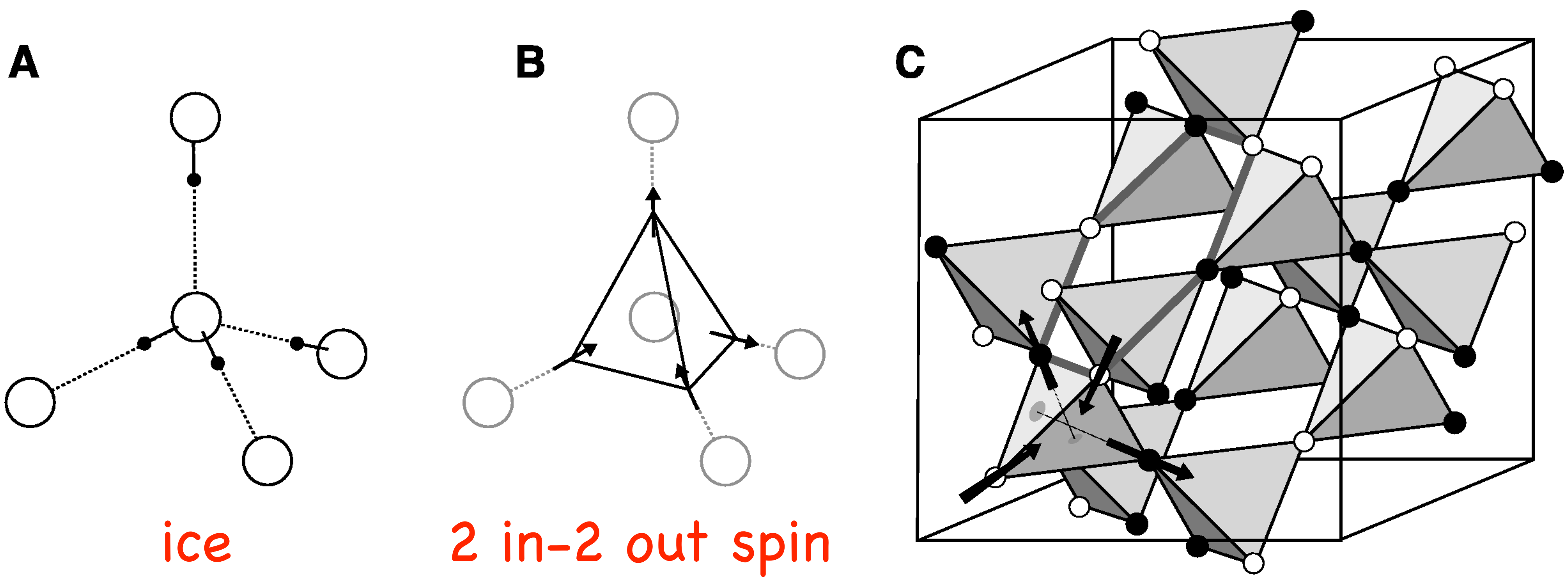
SCIENCE VOL 294 16 NOVEMBER 2001 1495

Spin Ice State in Frustrated Magnetic Pyrochlore Materials

Steven T. Bramwell[1] and Michel J. P. Gingras[2,3*]

$Dy_2Ti_2O_7$: frustrated "ferromagnet"





ice configuration

2 in-2 out spin configuration

PHYSICAL REVIEW VOLUME 102, NUMBER 4 MAY 15, 1956

Ordering and Antiferromagnetism in Ferrites

P. W. ANDERSON
Bell Telephone Laboratories, Murray Hill, New Jersey
(Received January 9, 1956)

The octahedral sites in the spinel structure form one of the anomalous lattices in which it is possible to achieve essentially perfect short-range order while maintaining a finite entropy. In such a lattice nearest-neighbor forces alone can never lead to long-range order, while calculations indicate that even the long-range Coulomb forces are only 5% effective in creating long-range order. This is shown to have many possible consequences both for antiferromagnetism in "normal" ferrites and for ordering in "inverse" ferrites.

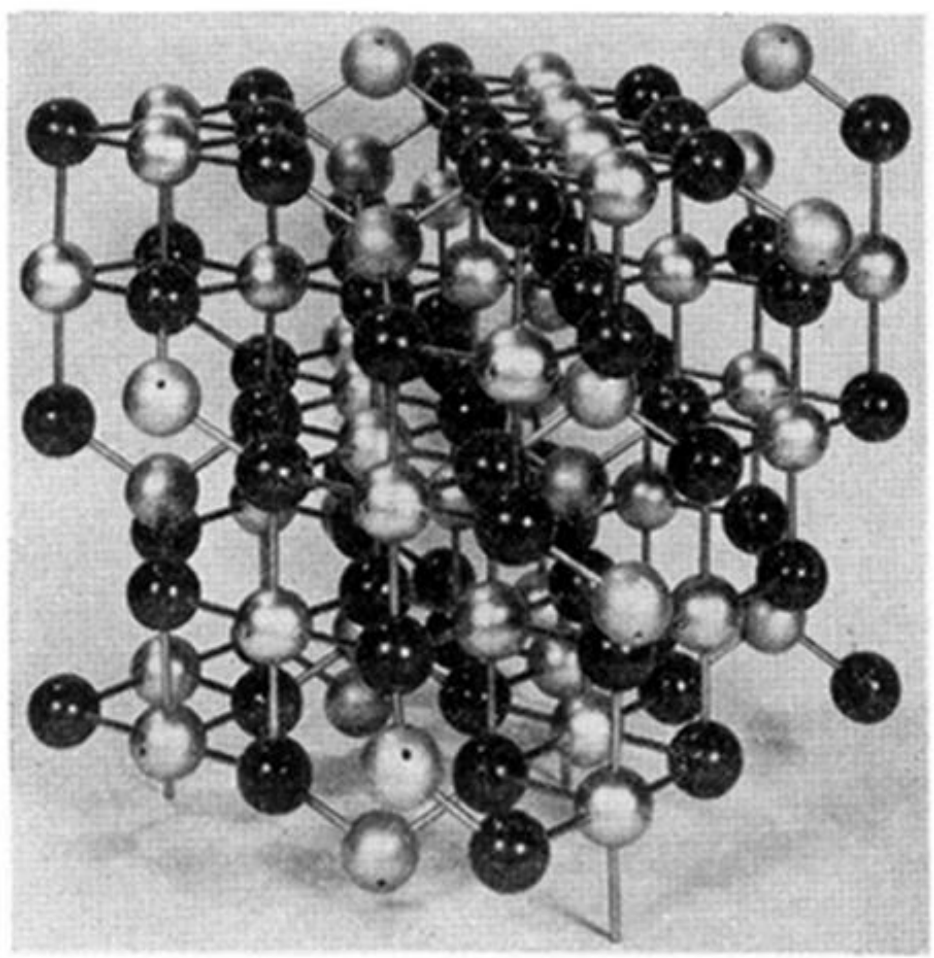


FIG. 1. Photograph of a model of the spinel lattice. The dark balls are oxygen; the tetrahedral sites are connected to their neighboring oxygens by four diagonal bonds, the octahedral by six vertical and horizontal ones.

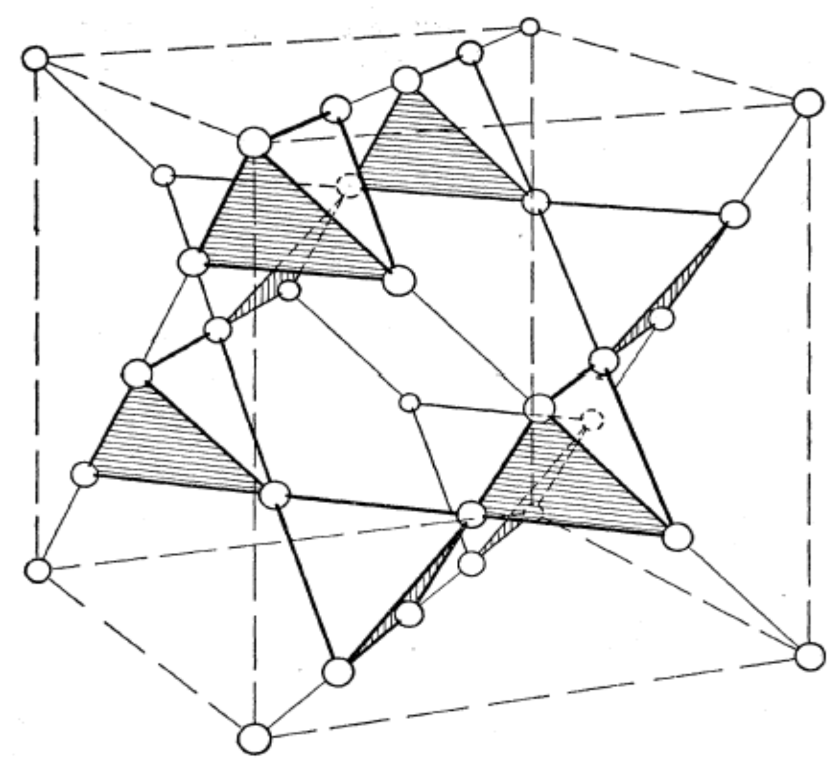
ice and correlated electrons

Ice and correlated electrons (Anderson 1953)

AB_2O_4 spinel, e.g. magnetite (Fe_3O_4) :

$(Fe^{3+}).(Fe^{2+}Fe^{3+}).(O^{2-}{}_4)$

B sublattice of (metal) cation sites form pyrochlore lattice of corner-sharing tetrahedra:



How do we arrange N charges on 2N sites of the pyrochlore lattice to minimize nearest-neighbour Coulomb repulsion?

$$\mathscr{H} = -t\sum_{\langle i,j\rangle} c_i^\dagger c_j + V\sum_{\langle i,j\rangle}\left(n_i - \frac{1}{2}\right)\left(n_j - \frac{1}{2}\right), \quad V \gg t$$

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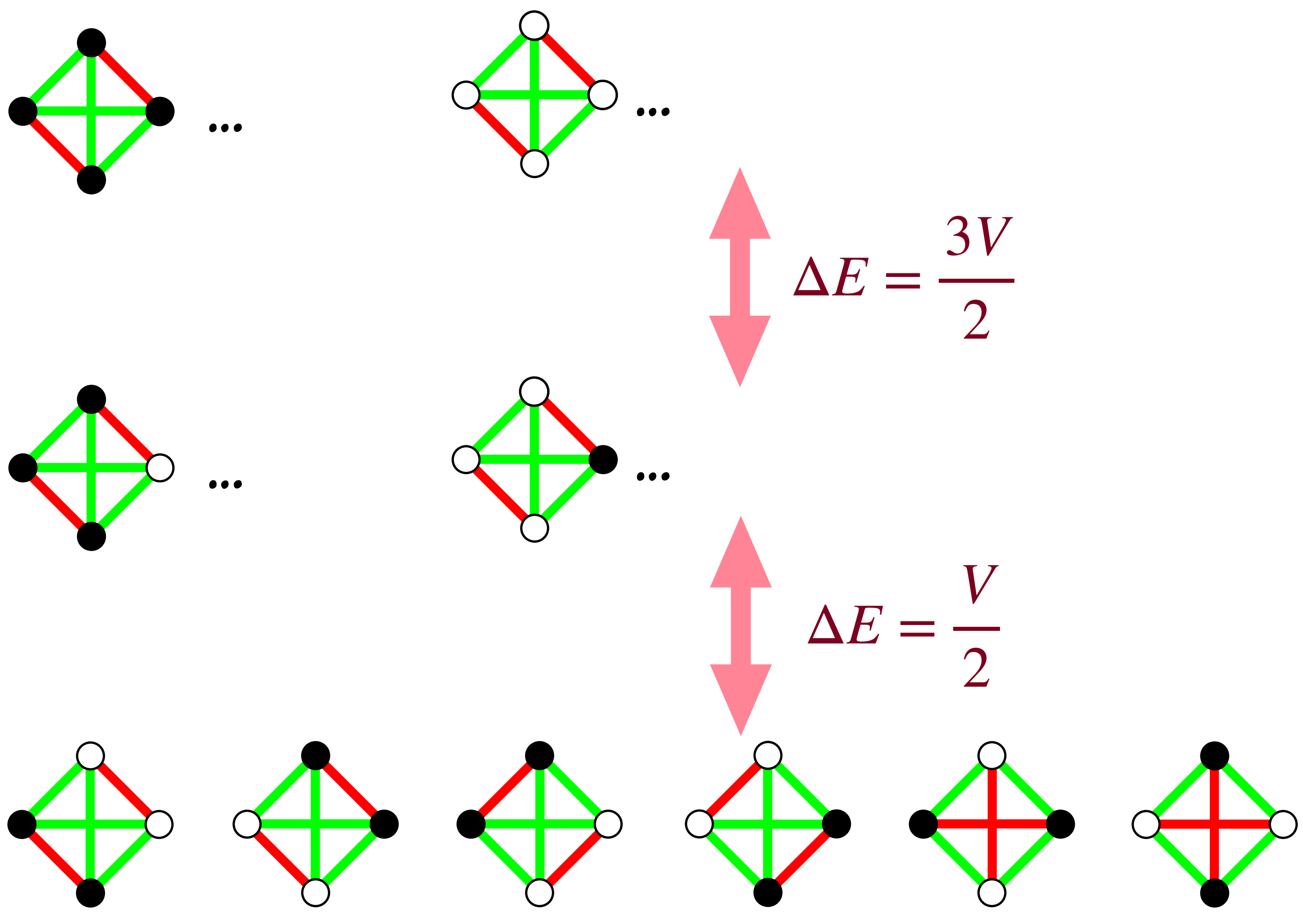

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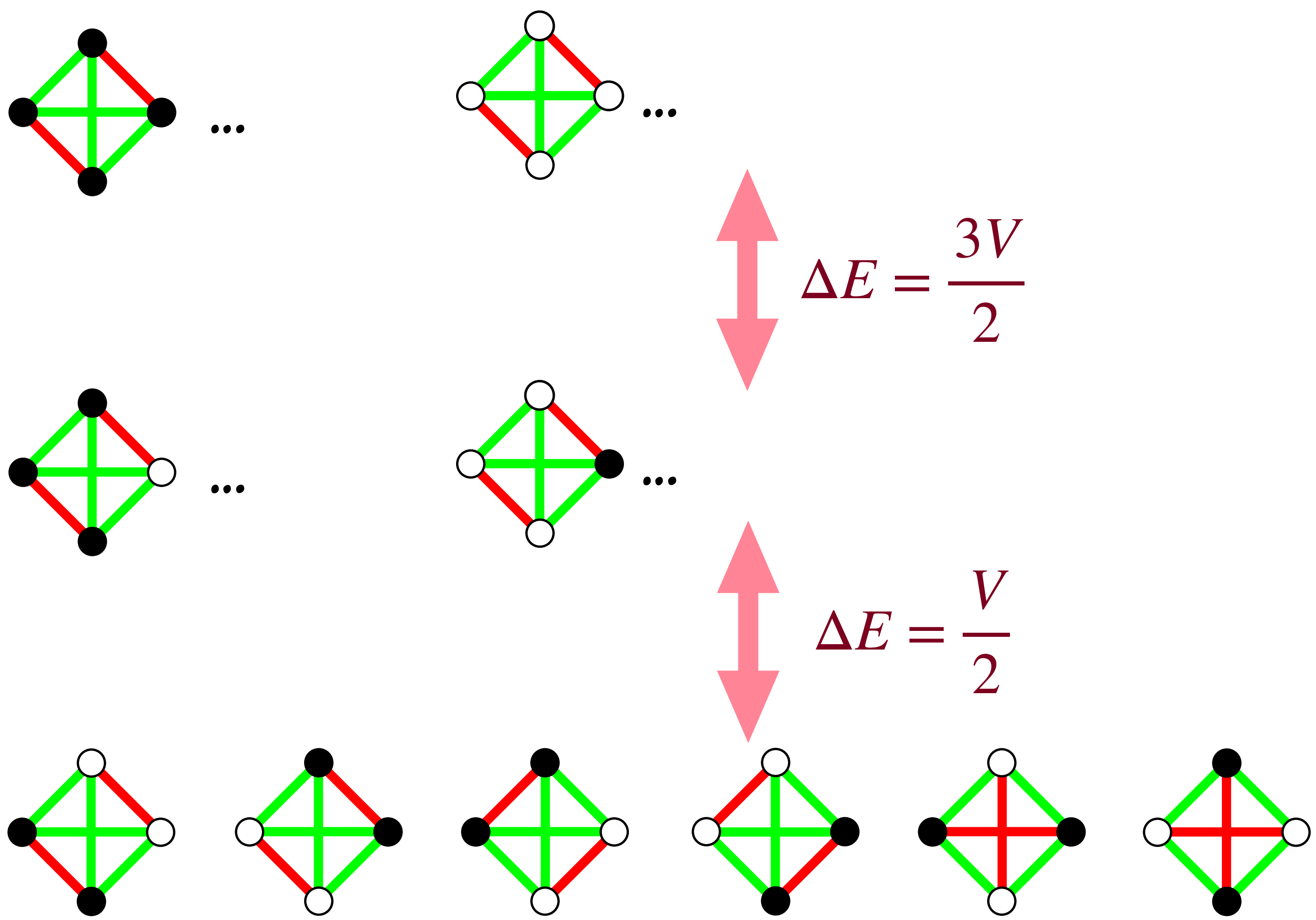
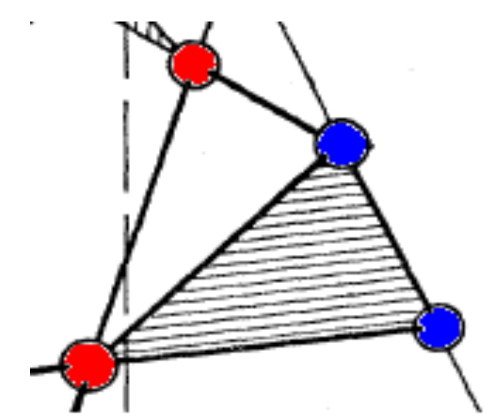


"Tetrahedron Rule"



Exactly two Fe^{3+} and two Fe^{4+} per tetrahedron

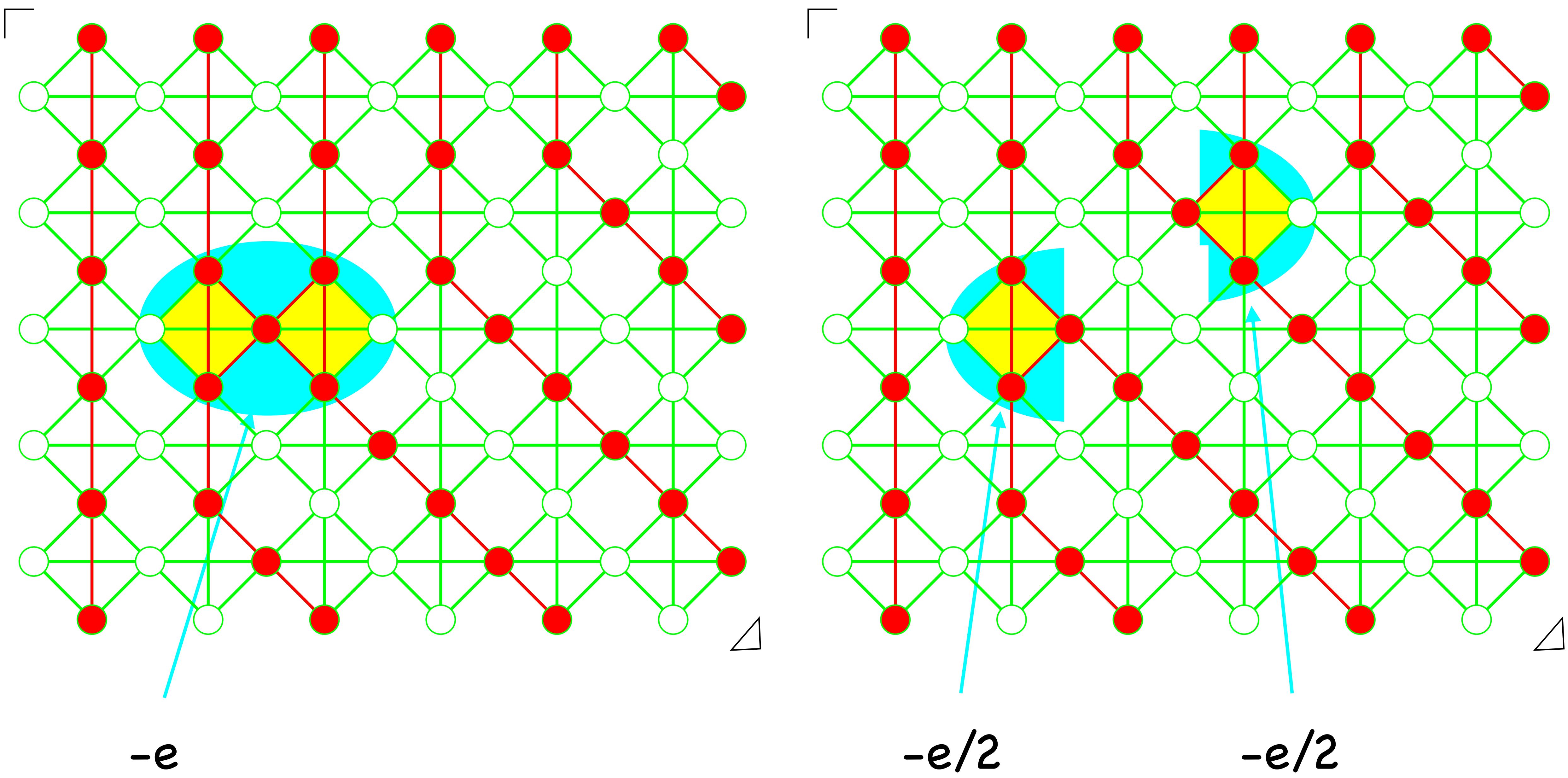
Ann. Phys. (Leipzig) **11** (2002) 12, 892 – 900

Fractional charges in pyrochlore lattices

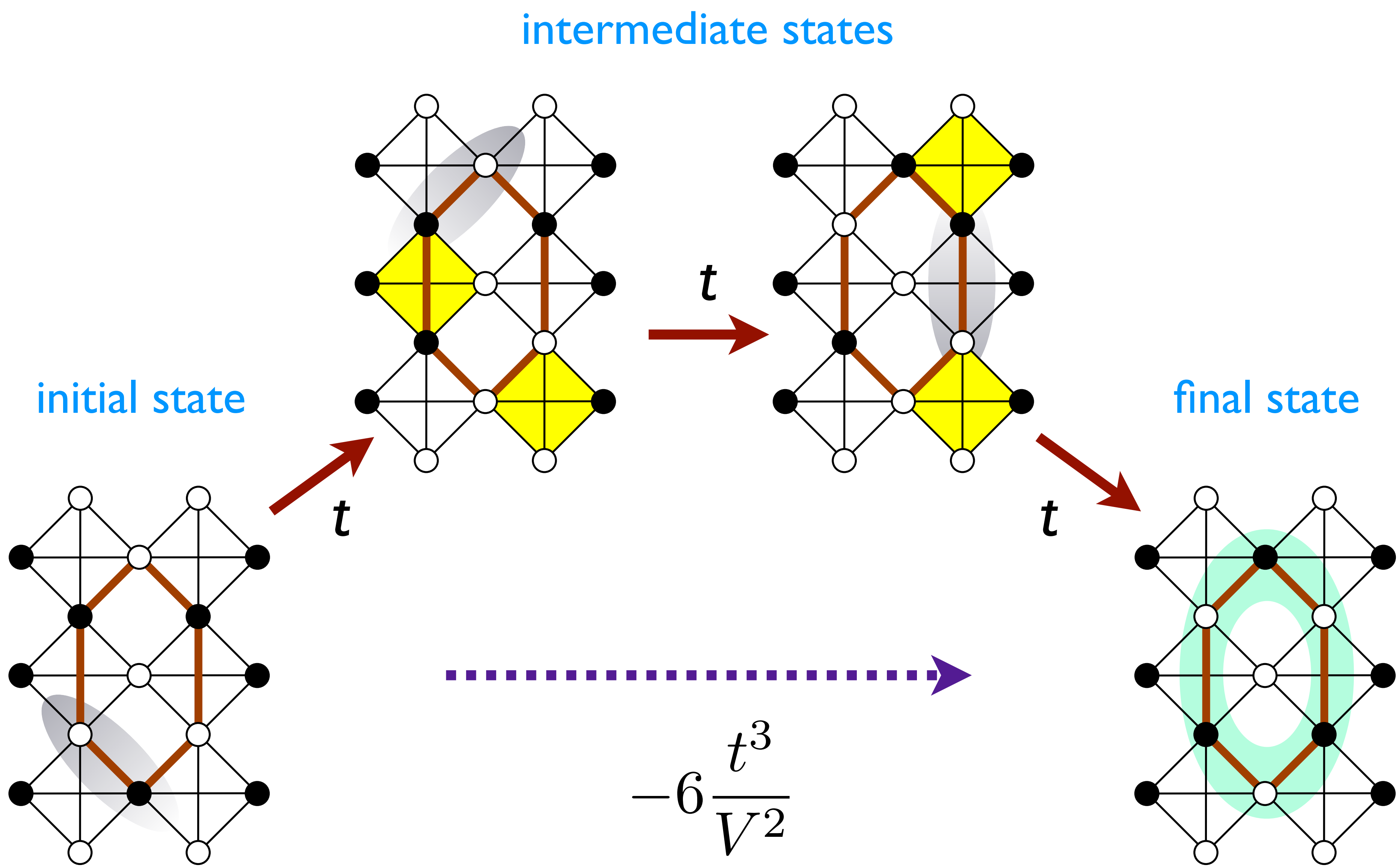
Peter Fulde[1,*], **Karlo Penc**[1,2], **and Nic Shannon**[1]

[1] Max-Planck-Institut für Physik komplexer Systeme, Nöthnitzer Straße 38, 01187 Dresden, Germany

[2] Research Institute for Solid State Physics and Optics, 1525 Budapest, P.O.B. 49, Hungary



Effective model of the insulator



Ring exchange splits the degeneracy of the ice manifold.

E. Runge and P. Fulde, Phys. Rev. B **70**, 245113 (2004);
F. Pollmann, J. J. Betouras, K. Shtengel, and P. Fulde, Phys. Rev. Lett. **97**, 170407 (2006).

t-V model on checkerboard lattice

$$\mathcal{H} = -t \sum_{\langle ij \rangle} c_i^\dagger c_j + V \sum_{\langle ij \rangle} n_i n_j$$

$$V \gg t$$

t-V model on checkerboard lattice

$$\mathcal{H} = -t \sum_{\langle ij \rangle} c_i^\dagger c_j + V \sum_{\langle ij \rangle} n_i n_j \qquad V \gg t$$

fermion model

charge ⟷ spin up

empty ⟷ spin down

hard-core boson model, no fermionic sign to worry

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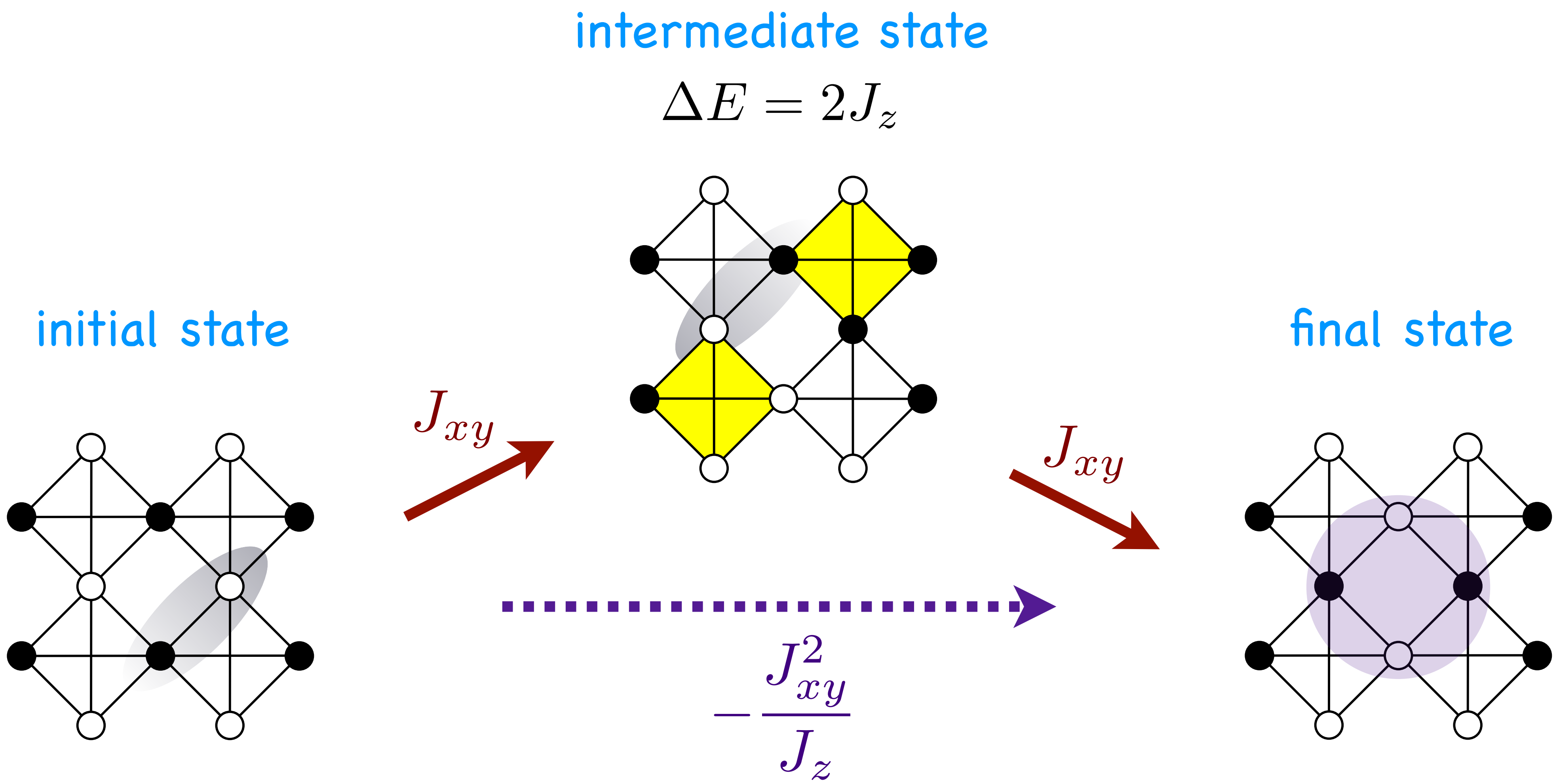
XXZ S=1/2 Heisenberg model on checkerboard lattice

$$\mathcal{H} = J_z \sum_{\langle ij \rangle} S_i^z S_j^z + \frac{J_{xy}}{2} \sum_{\langle ij \rangle} \left(S_i^+ S_j^- + S_i^- S_j^+ \right) \qquad J_z \gg J_{xy}$$

Effective model



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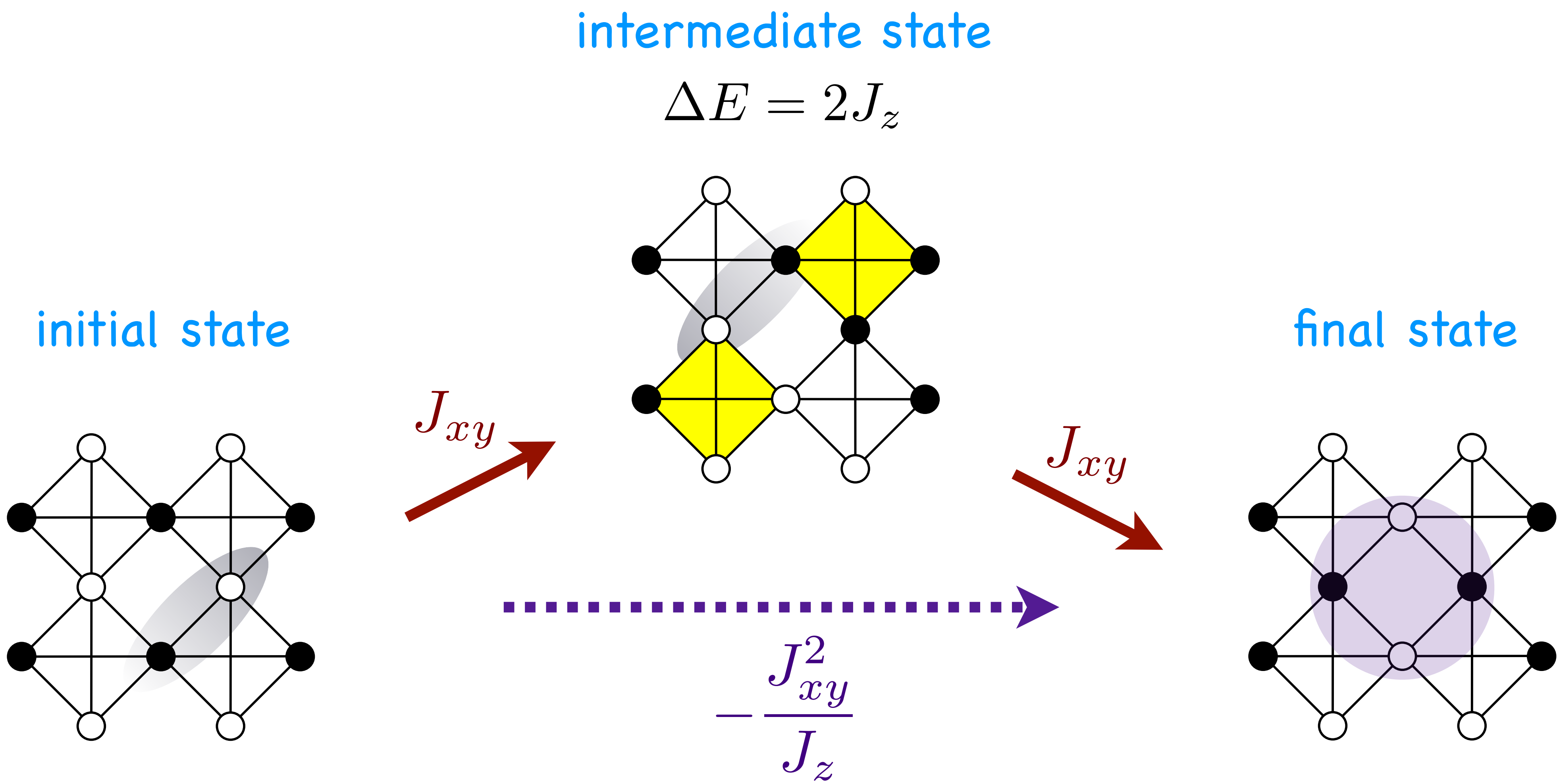
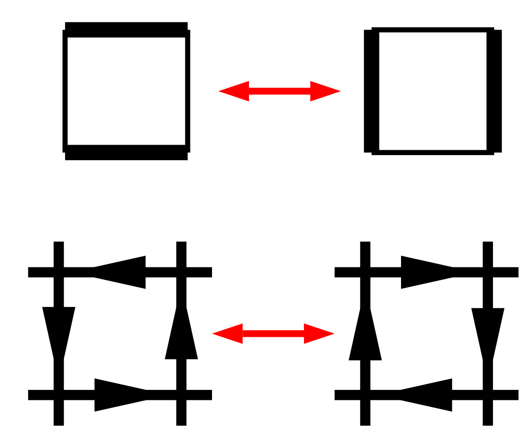


$$\mathcal{H}_{2\text{nd}} = -\frac{J_{xy}^2}{J_z} \sum_{\square} (S_1^+ S_2^- S_3^+ S_4^- + S_1^- S_2^+ S_3^- S_4^+)$$



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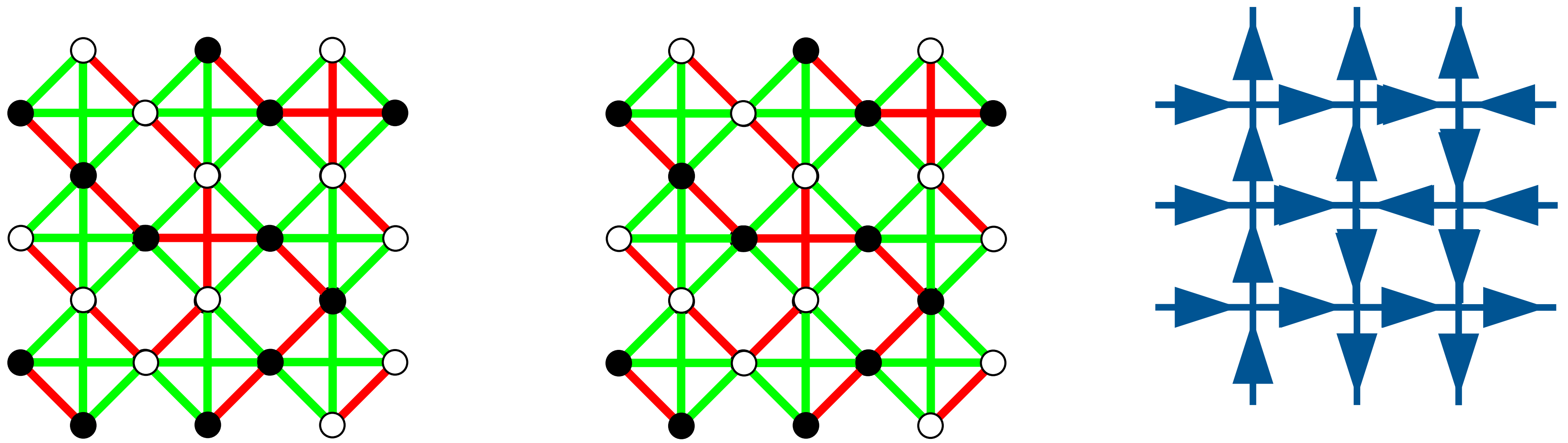
Ising model with transverse field

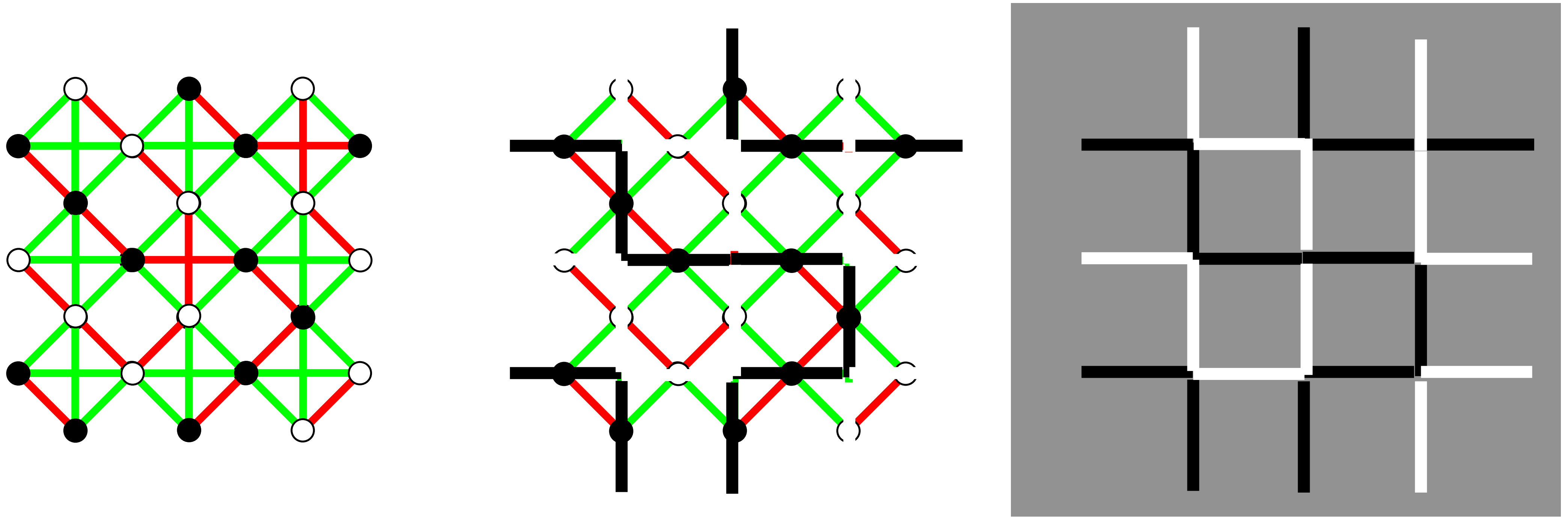
$$\mathscr{H} = J_z \sum_{\langle i,j \rangle} S_i^z S_j^z + h^x \sum_i S_i^x \qquad J_z \gg h^x$$

Mapping between different configurations

Mapping between Ising configurations and arrows:



Mapping between Ising configurations and fully packed loop model:



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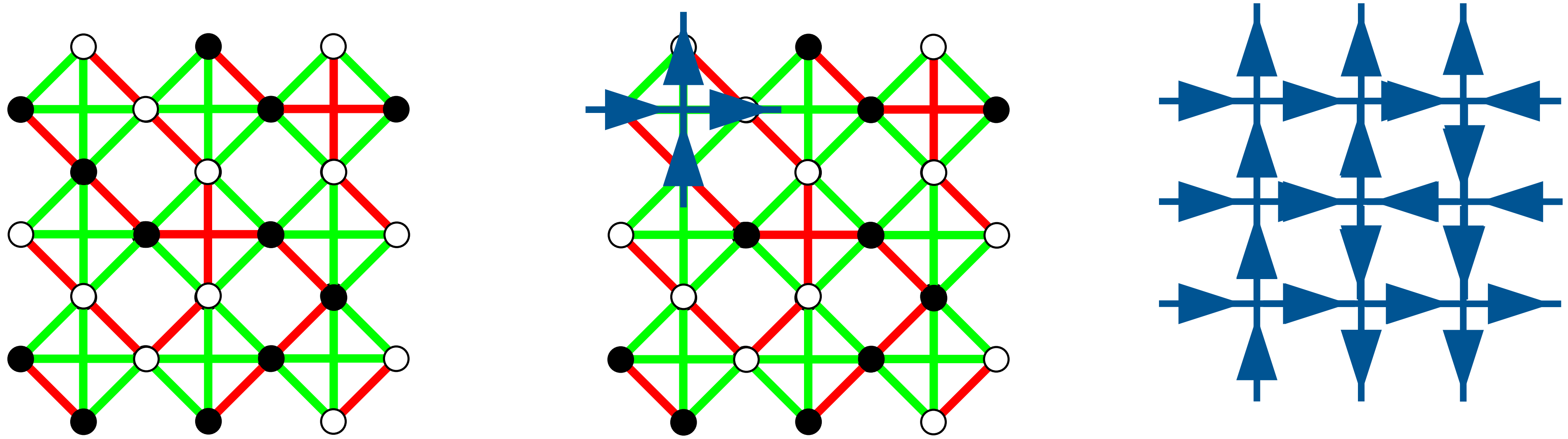

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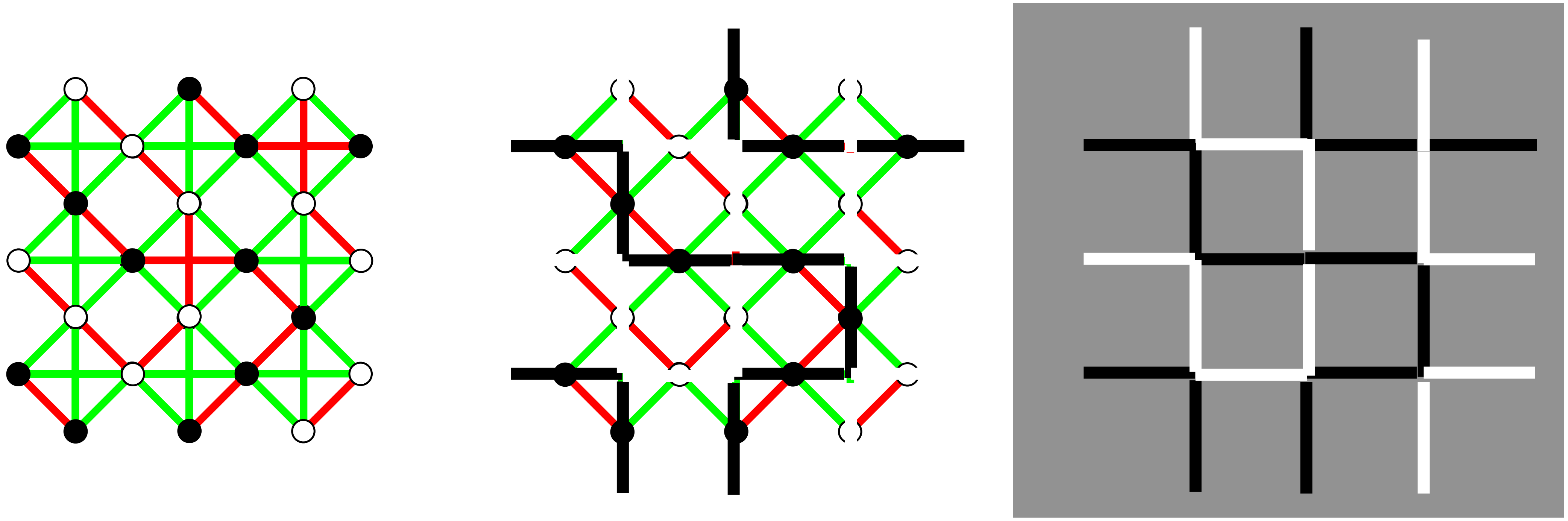

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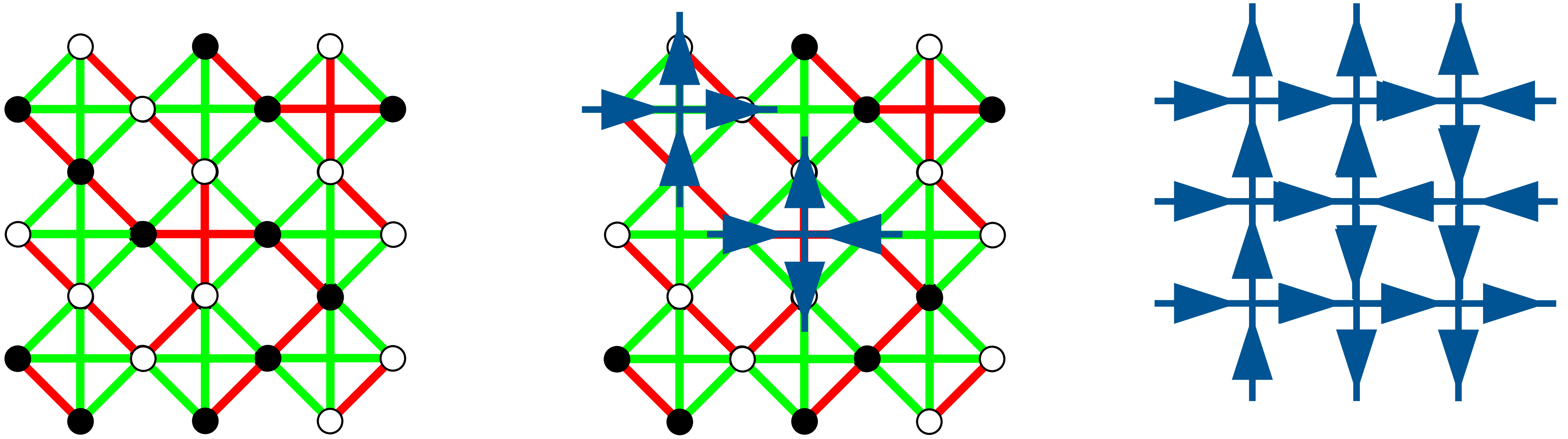

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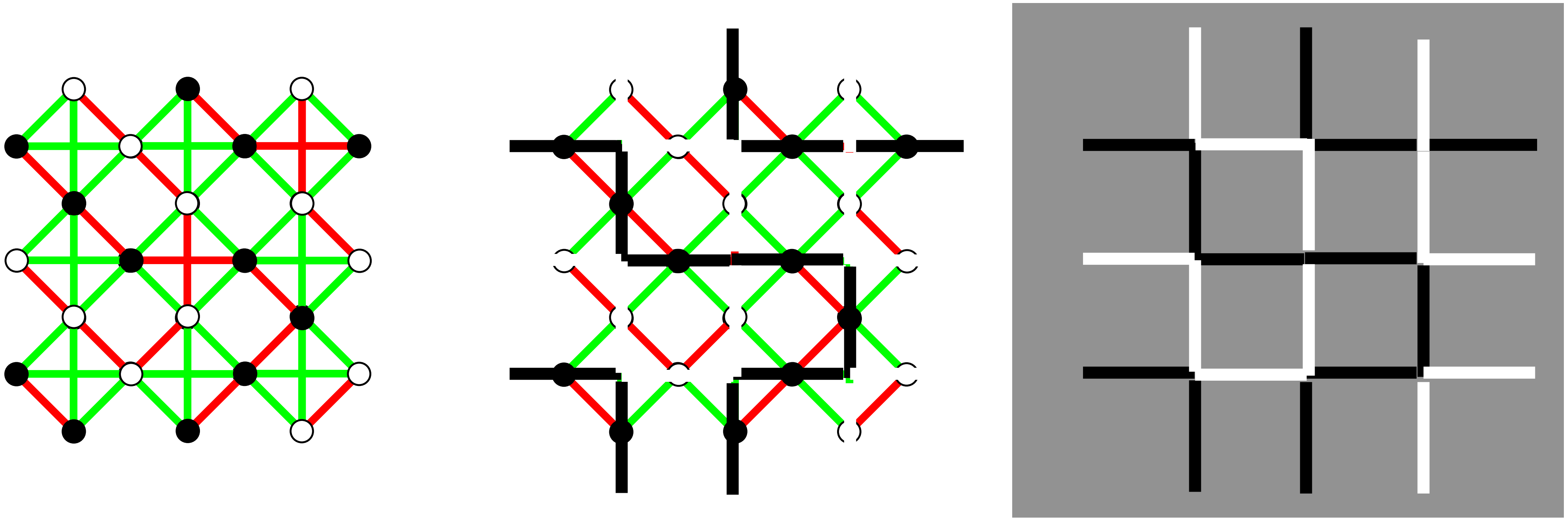

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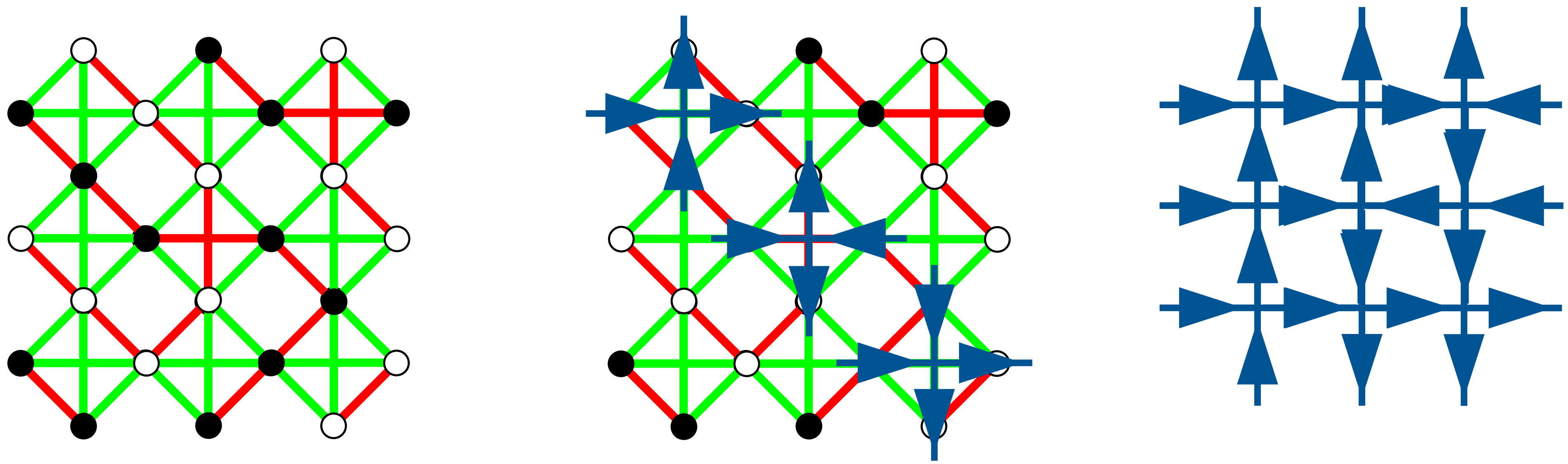

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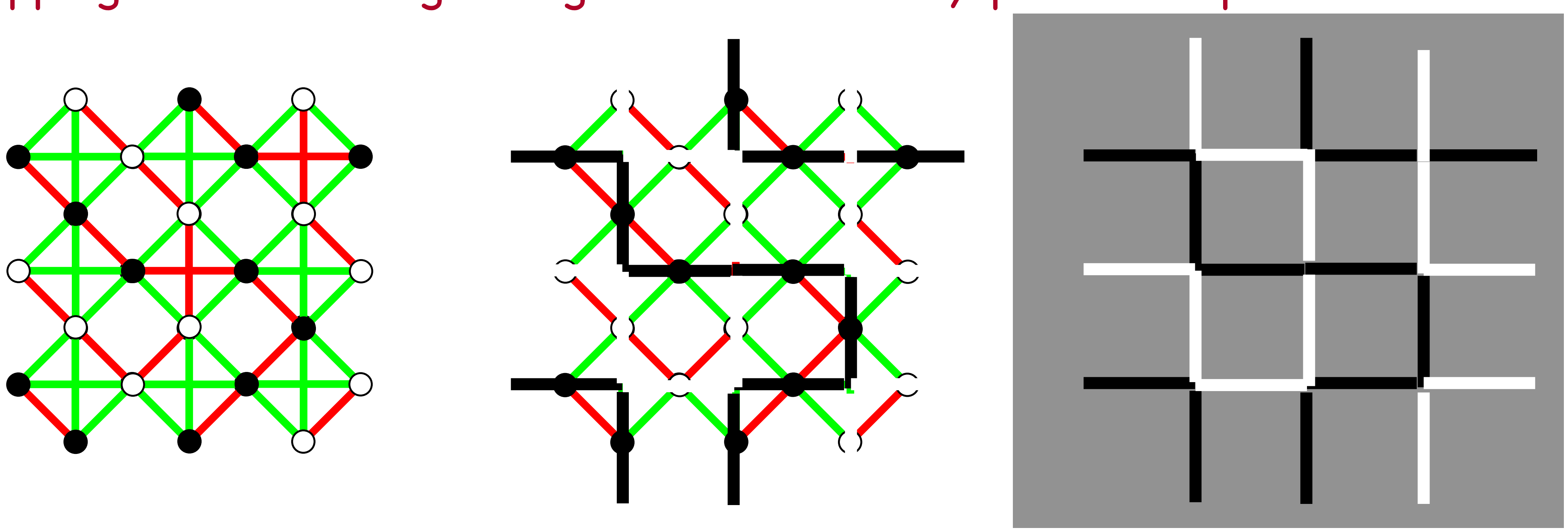

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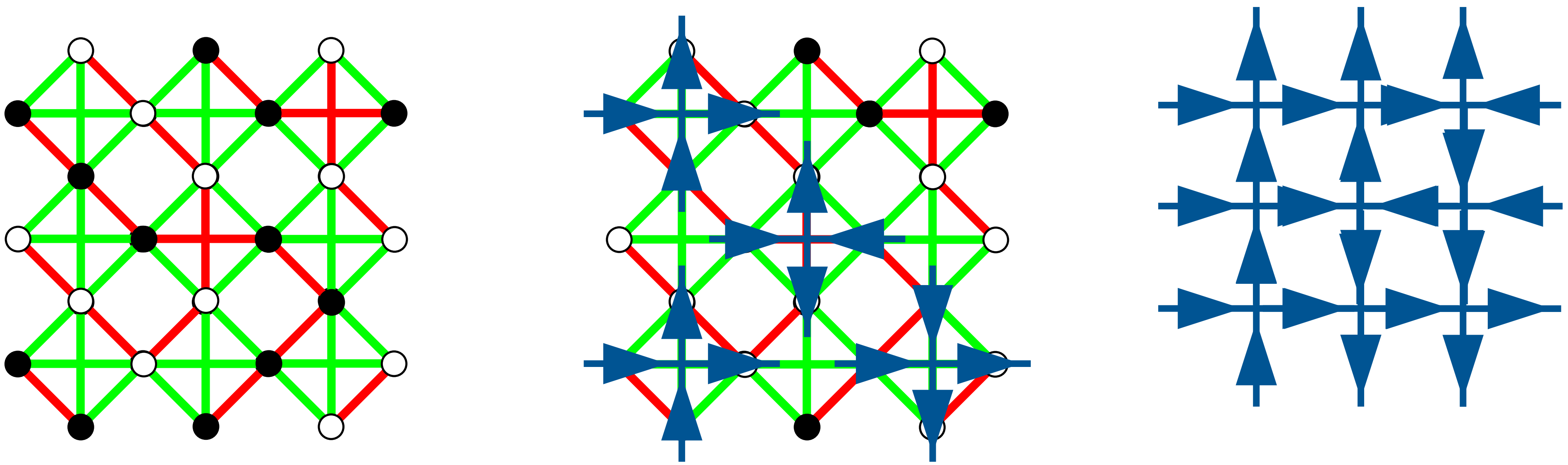

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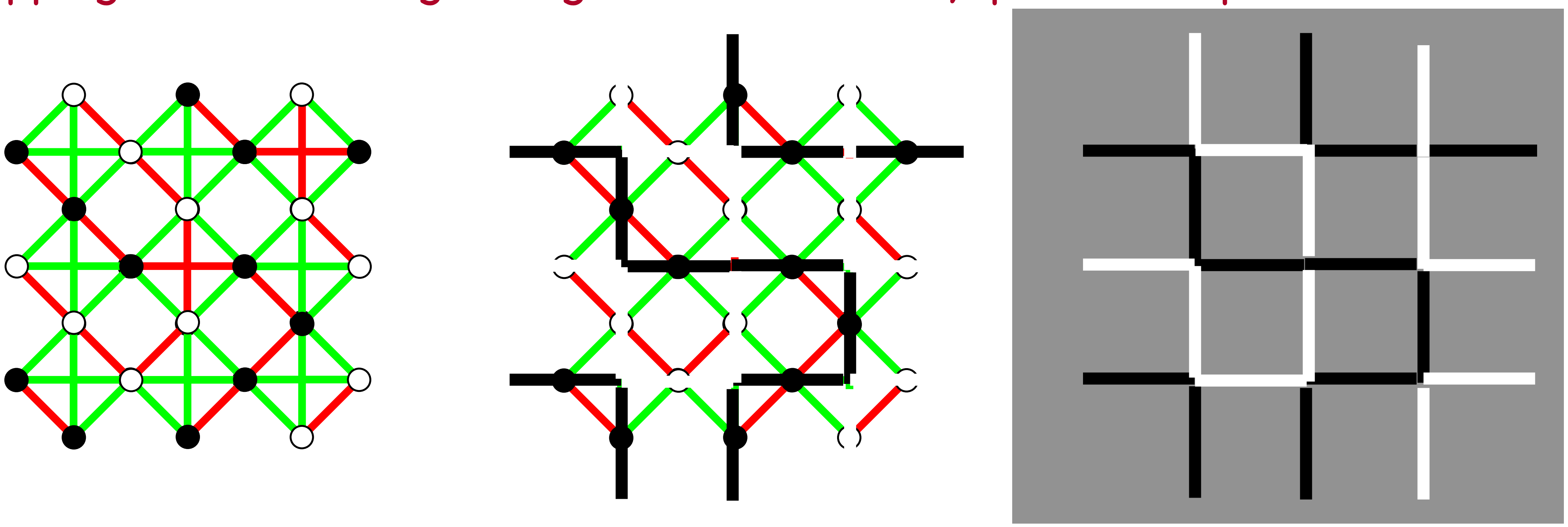

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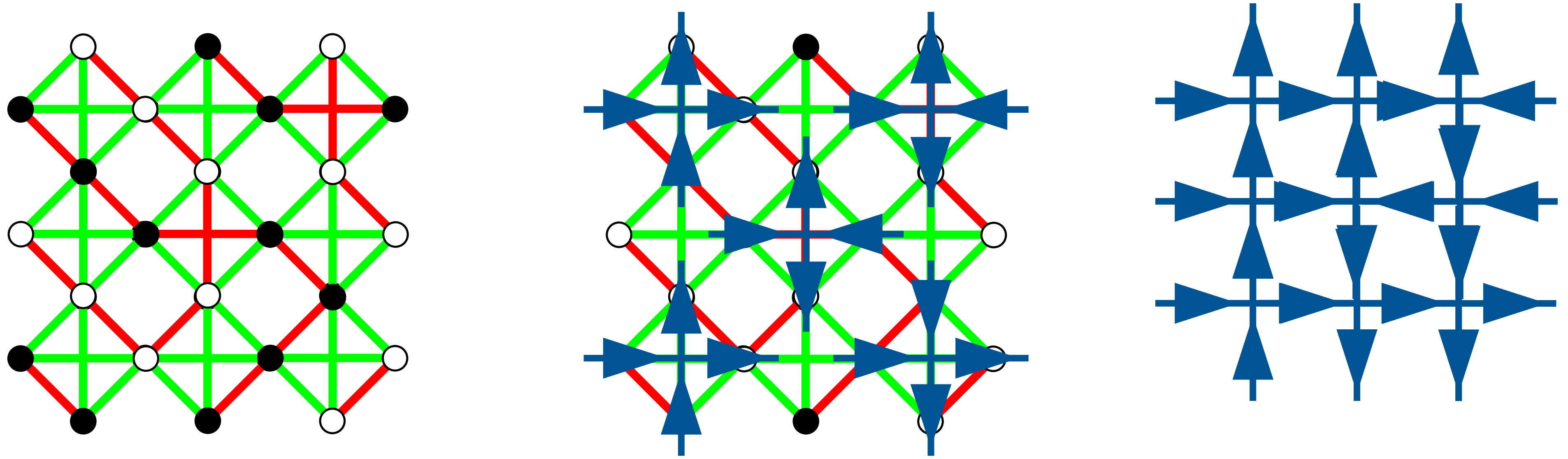

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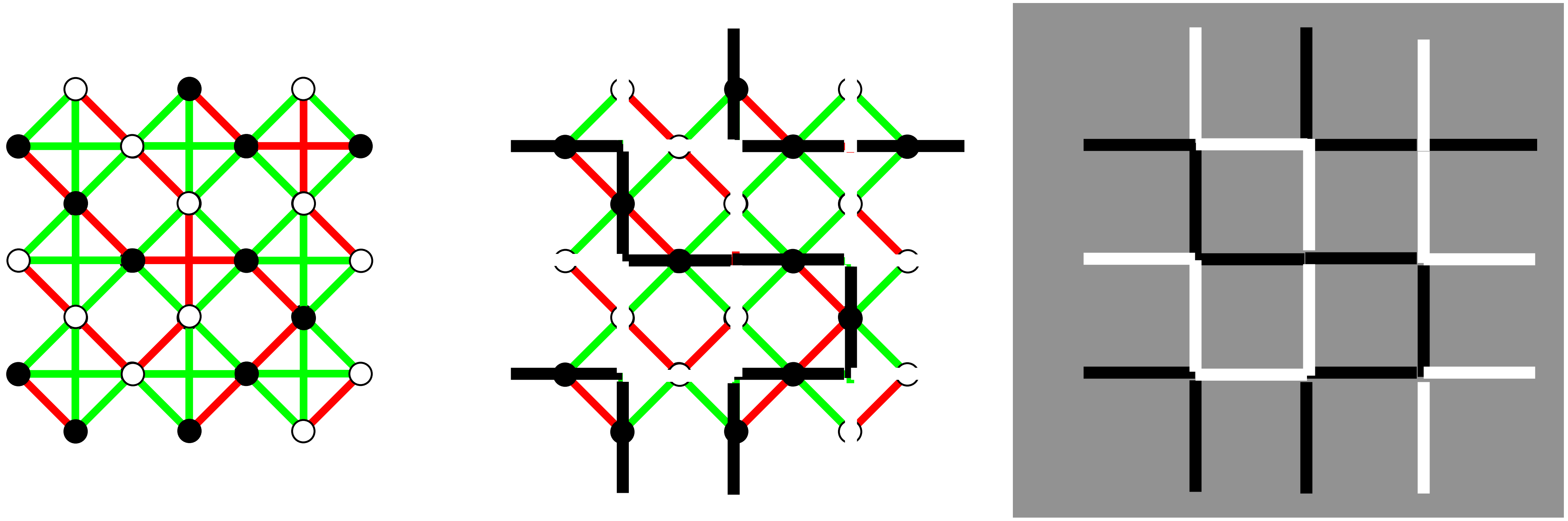

PHYSICAL REVIEW B **69**, 220403(R) (2004)

Cyclic exchange, isolated states, and spinon deconfinement in an *XXZ* Heisenberg model on the checkerboard lattice

Nic Shannon,[1,2] Grégoire Misguich,[3] and Karlo Penc[4]

$$\mathcal{H} = J_z \sum_{\langle ij \rangle} S_i^z S_j^z + \frac{J_{xy}}{2} \sum_{\langle ij \rangle} (S_i^+ S_j^- + S_i^- S_j^+)$$

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tunneling between ice-configurations

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effective model

also S. Chakravarty, PRB **66**, 224505 (2002).

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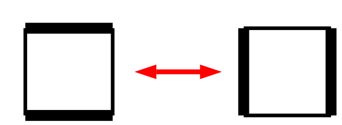
add a Rokhsar-Kivelson-like diagonal term

$$\mathcal{H} = \sum_{\square} [V(|\circlearrowleft\rangle\langle\circlearrowleft| + |\circlearrowright\rangle\langle\circlearrowright|) - t(|\circlearrowleft\rangle\langle\circlearrowright| + |\circlearrowright\rangle\langle\circlearrowleft|)],$$

Quantum 6-vertex model

cf. Quantum-dimer model



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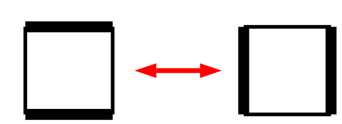
cf. Quantum-dimer model 

The model is also known as the (2+1)-dimensional U(1) quantum link model

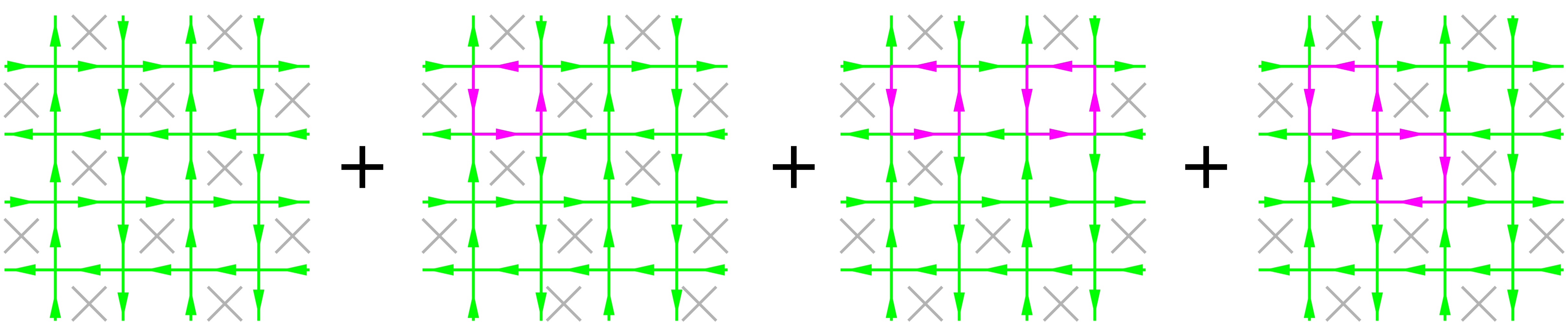
Why did Rokhsar-Kivelson add the V term?

$$\mathcal{H} = \sum_{\square} [V(|\circlearrowleft\rangle\langle\circlearrowleft| + |\circlearrowright\rangle\langle\circlearrowright|) - t(|\circlearrowleft\rangle\langle\circlearrowright| + |\circlearrowright\rangle\langle\circlearrowleft|)],$$

For V=t the Hamiltonian is a sum of projectors:

$$\mathscr{H}_{V=t=1} = \sum_{\square} \left(|\circlearrowleft\rangle - |\circlearrowright\rangle \right)\left(\langle\circlearrowleft| - \langle\circlearrowright| \right)$$

The ground state wave function is an equal amplitude superposition of all configurations:



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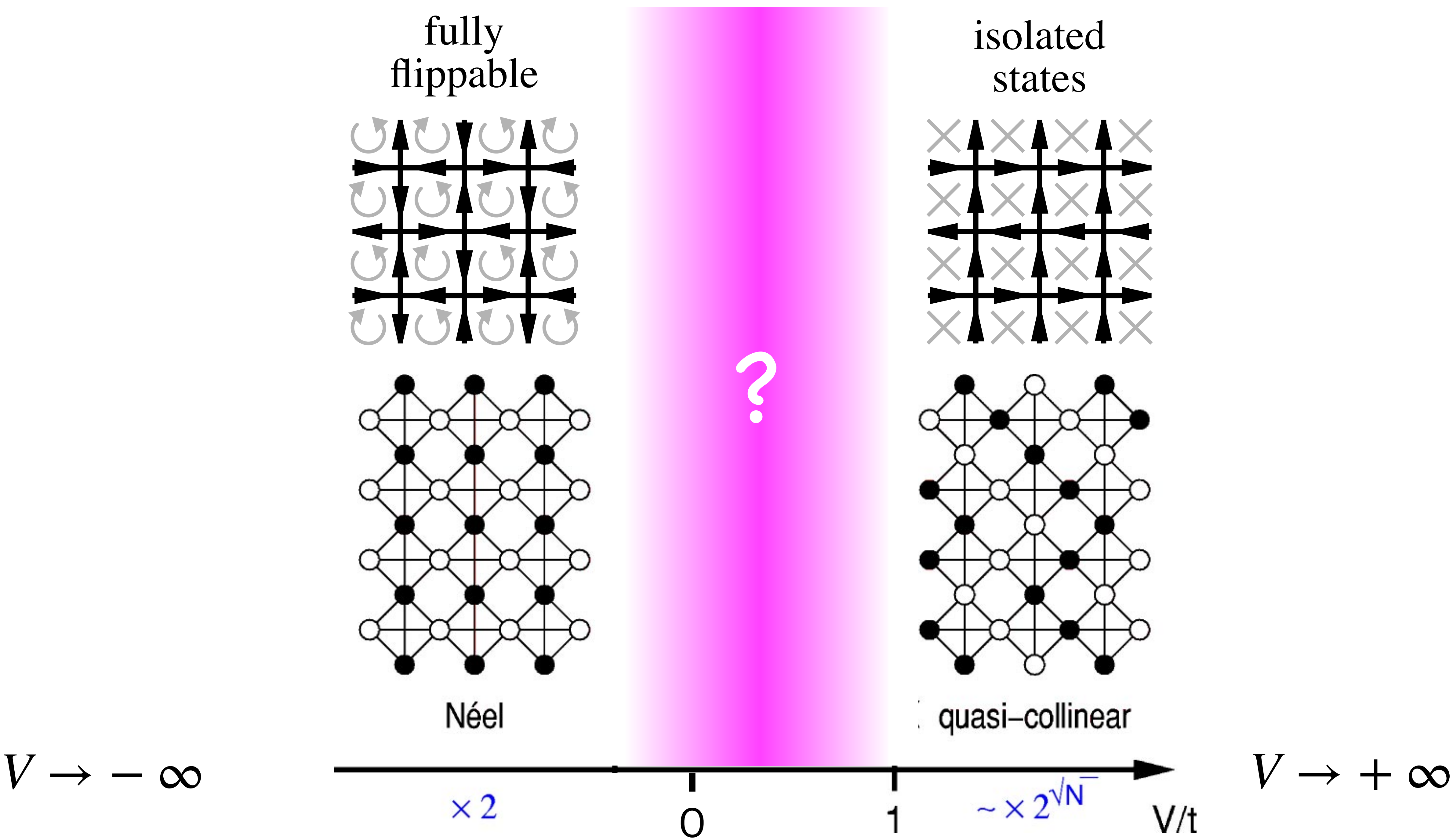
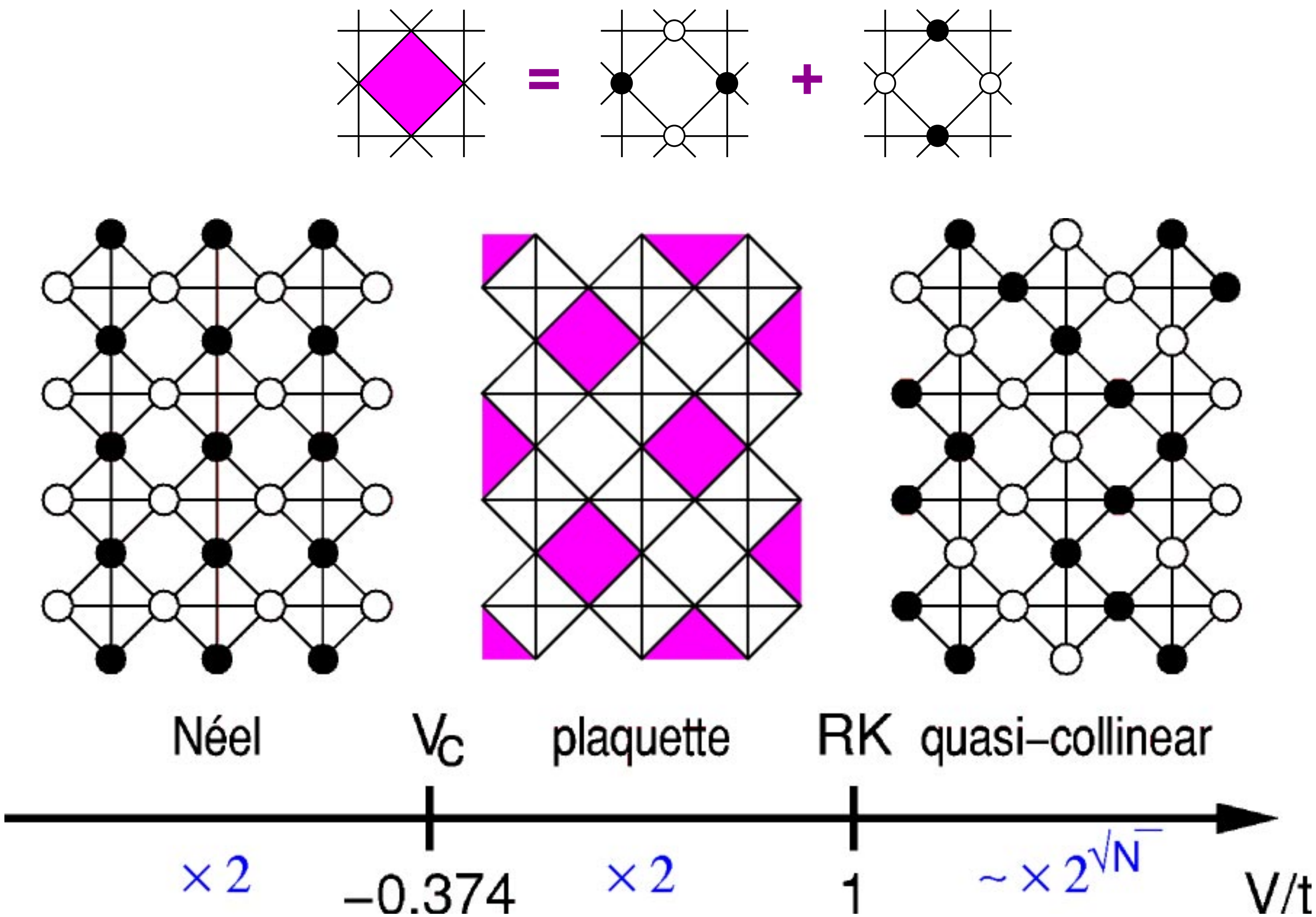


Plaquette phase



$$\mathcal{H} = \sum_{\square} [V(|\circlearrowleft\rangle\langle\circlearrowleft| + |\circlearrowright\rangle\langle\circlearrowright|) - t(|\circlearrowleft\rangle\langle\circlearrowright| + |\circlearrowright\rangle\langle\circlearrowleft|)],$$

N. Shannon, G. Misguich and K. Penc, PRB **69**, 220403(R) (2004),
O. F. Syljuåsen and S. Chakravarty, PRL **96**, 147004 (2006).

qubit quantum spin ice

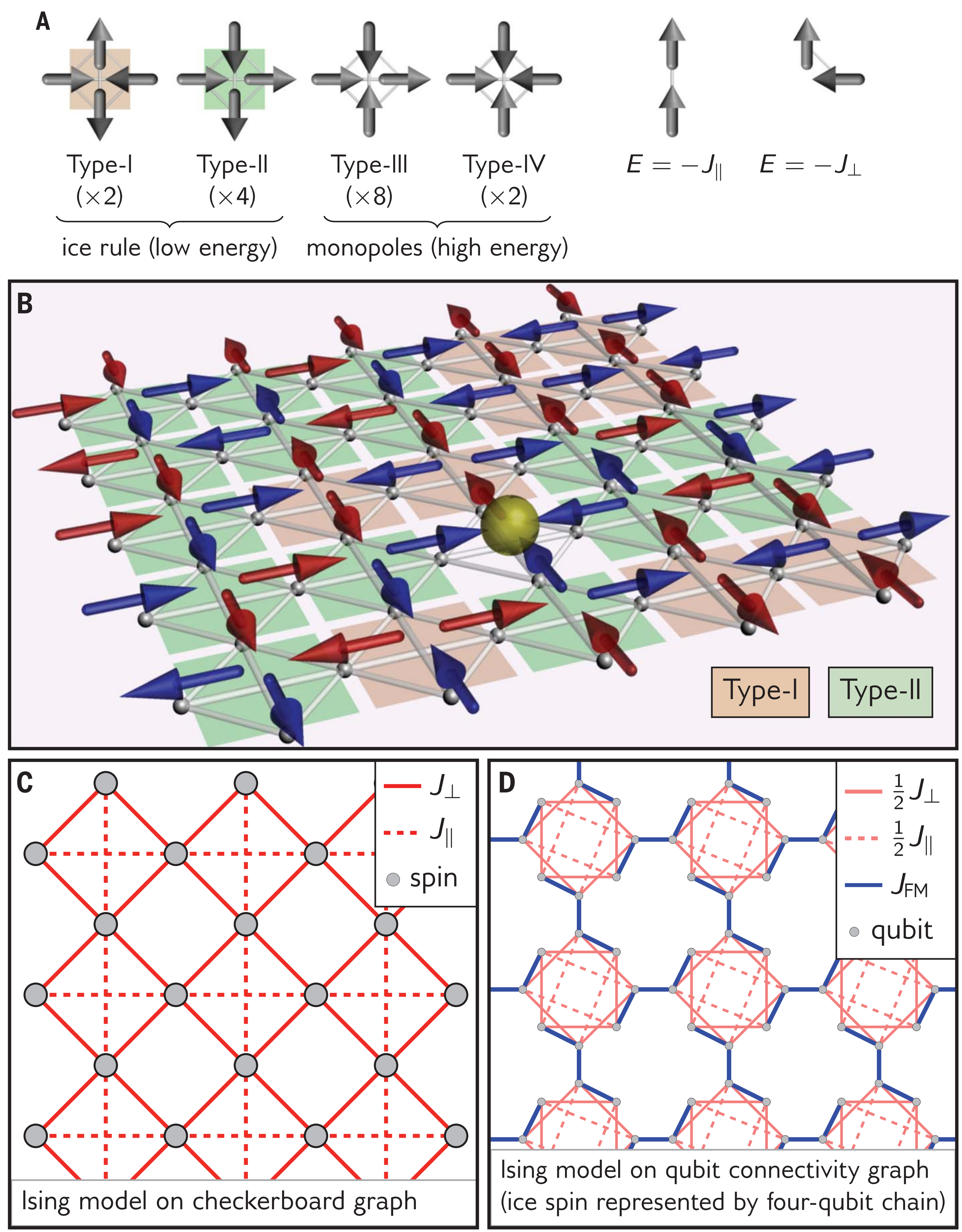
Science **373**, 576–580 (2021)

MAGNETISM

Qubit spin ice

Andrew D. King[1]*, Cristiano Nisoli[2]*, Edward D. Dahl[1,3], Gabriel Poulin-Lamarre[1], Alejandro Lopez-Bezanilla[2]

$$\mathcal{H} = \mathcal{J}\left(\sum_{\langle ij\rangle} J_{ij}\hat{\sigma}_i^z\hat{\sigma}_j^z + \sum_i h_i\hat{\sigma}_i^z\right) - \Gamma\sum_i \hat{\sigma}_i^x$$



MAGNETISM

Qubit spin ice

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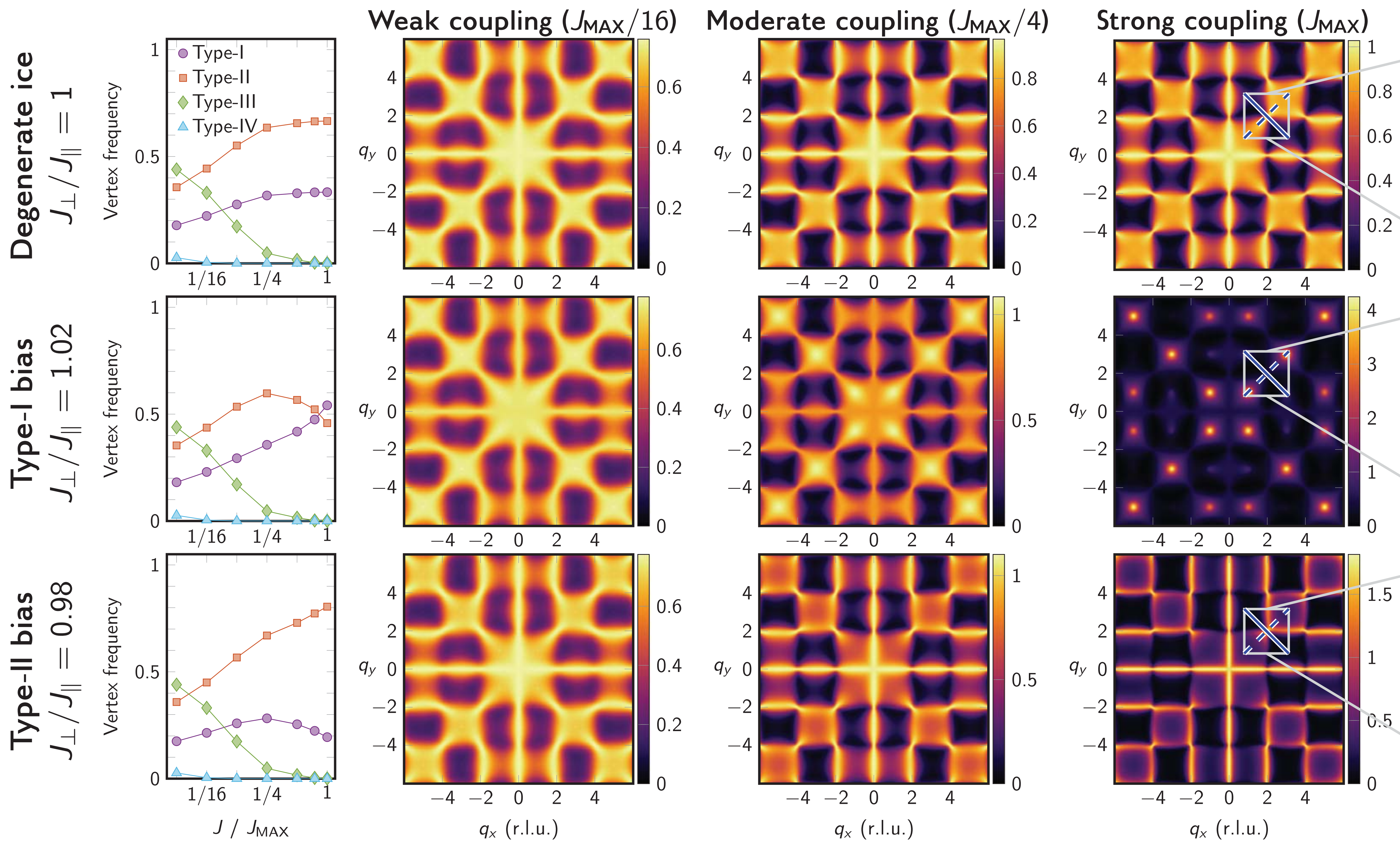
Structure factor S(**q**) for varying couplings, in reciprocal lattice space.

14×14 ice system



MAGNETISM

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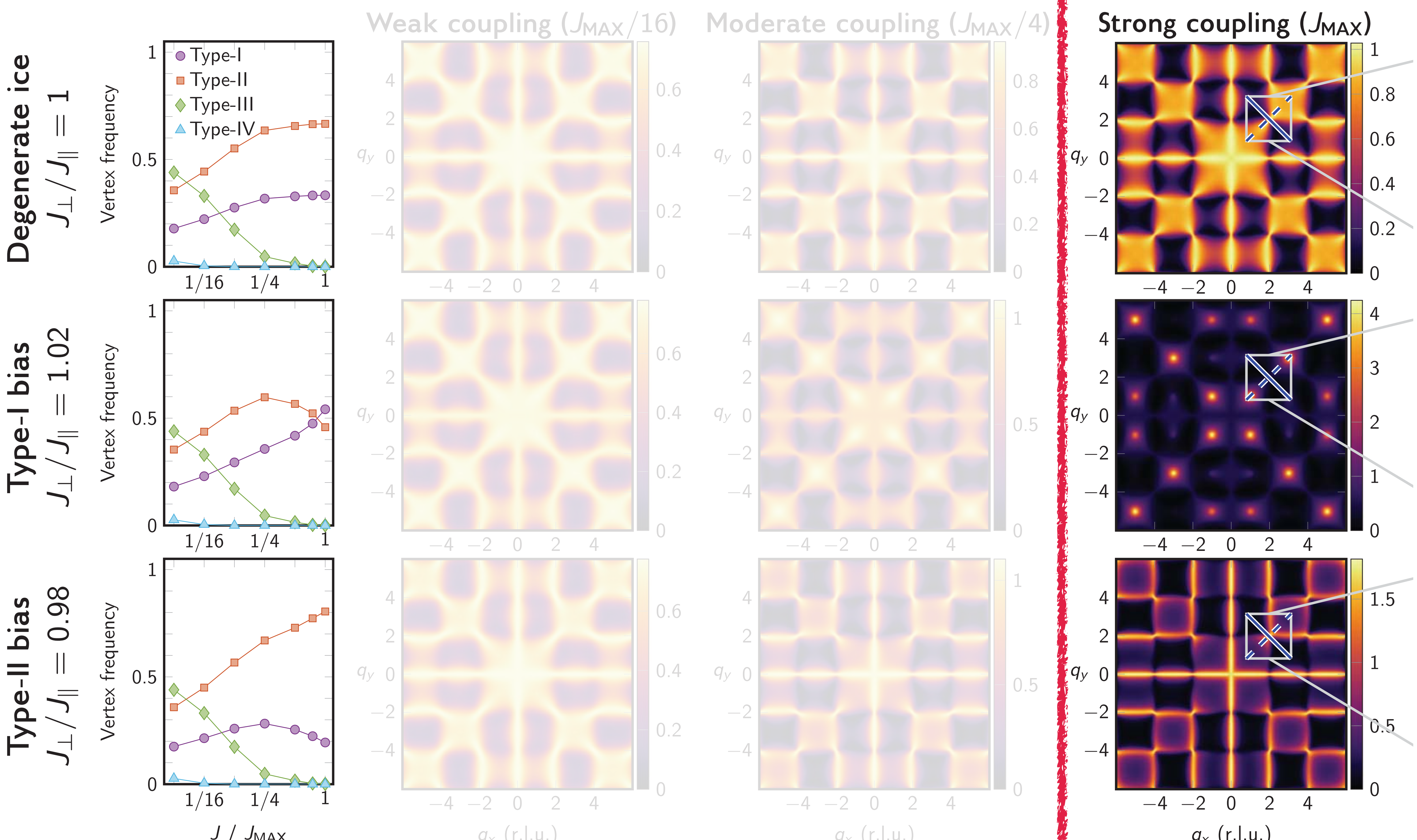
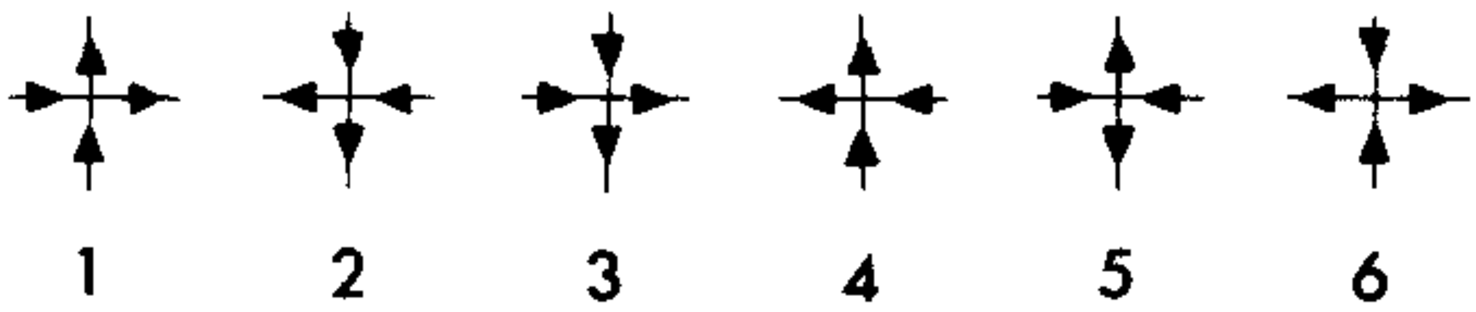
Quantum 6-vertex model



type-I and II vertices

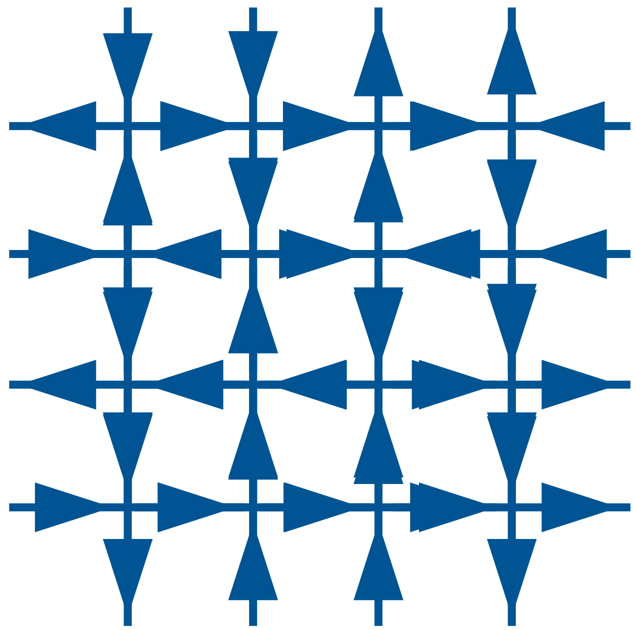
classical ice models (Baxter book)



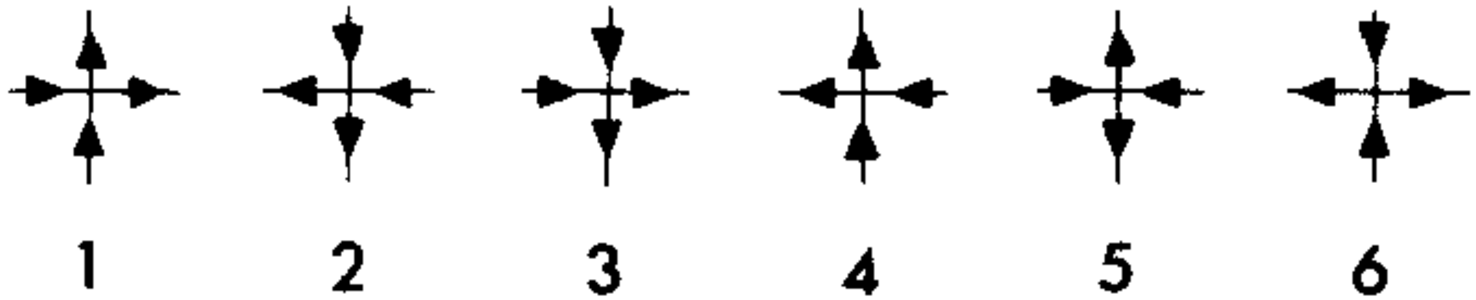
Ice

As was remarked above, the ice model is obtained by taking all energies to be zero, i.e.

$$\varepsilon_1 = \varepsilon_2 = \ldots = \varepsilon_6 = 0\,. \tag{8.1.4}$$



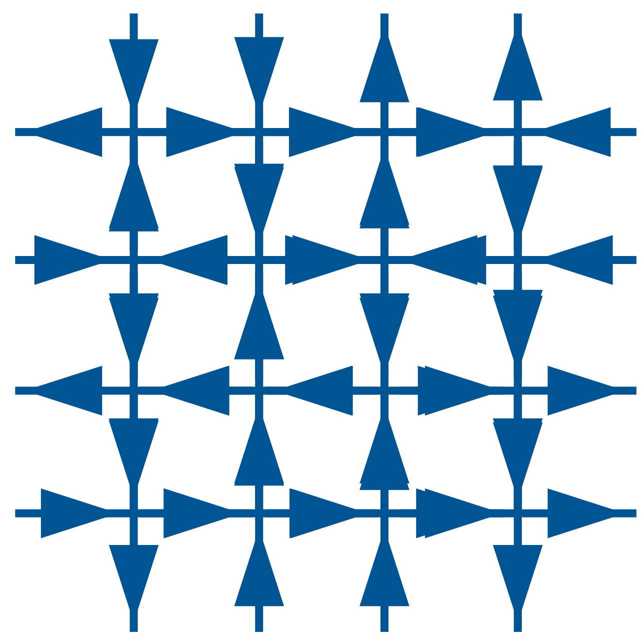
classical ice models (Baxter book)



Ice

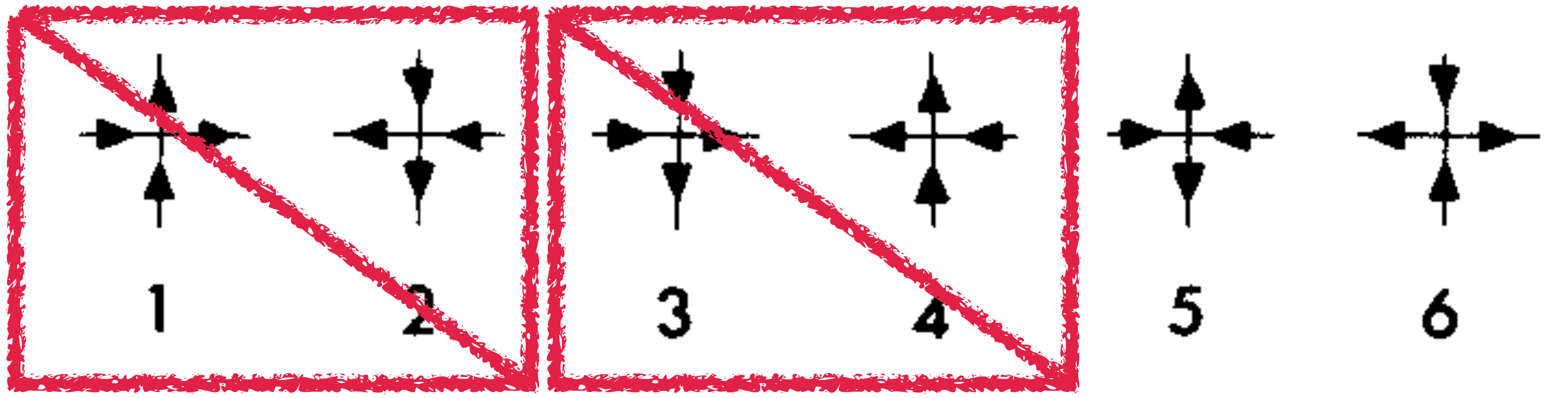
As was remarked above, the ice model is obtained by taking all energies to be zero, i.e.

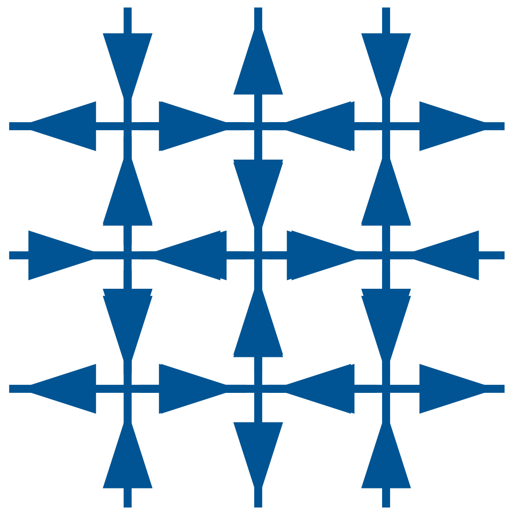
$$\varepsilon_1 = \varepsilon_2 = \ldots = \varepsilon_6 = 0\,. \tag{8.1.4}$$



Lieb's Bethe-ansatz solution: $Z = \left(\frac{4}{3}\right)^{3N/2} \approx 1.5396^N$

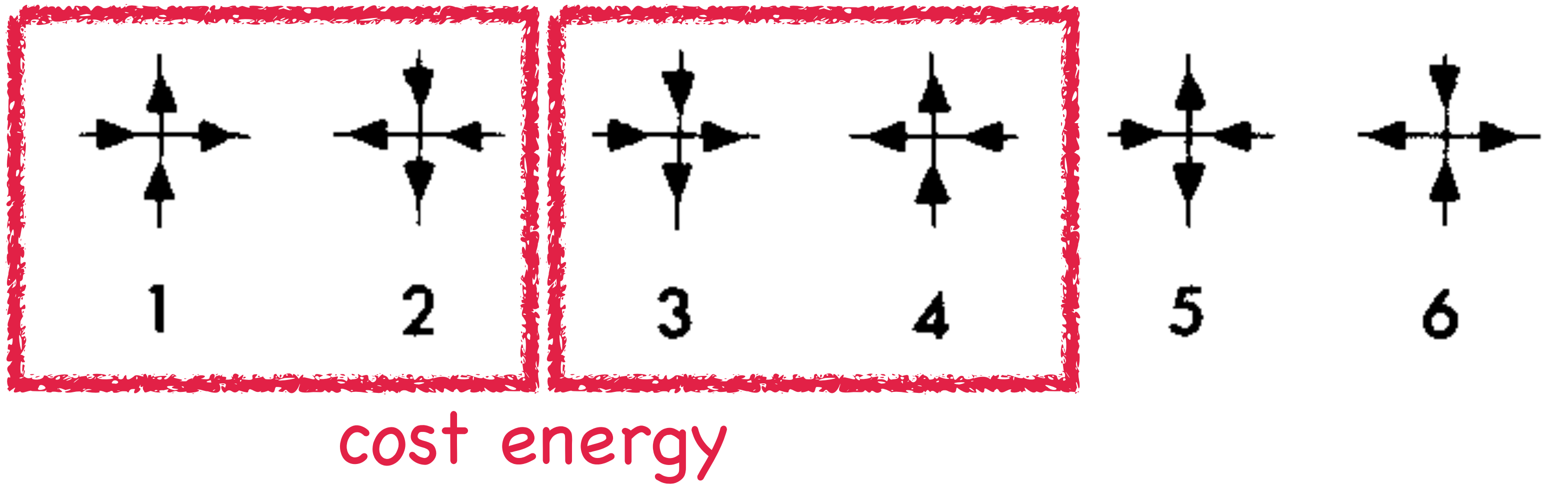
classical ice models (Baxter book)





degeneracy: 2x

classical ice models (Baxter book)



F Model

Rys (1963) suggested that a model of anti-ferroelectrics could be obtained by choosing

$$\varepsilon_1 = \varepsilon_2 = \varepsilon_3 = \varepsilon_4 > 0, \varepsilon_5 = \varepsilon_6 = 0 . \qquad (8.1.6)$$

The ground state is then one in which only vertex arrangements 5 and 6 occur. There are only two ways of doing this. One is shown in Fig. 8.3,

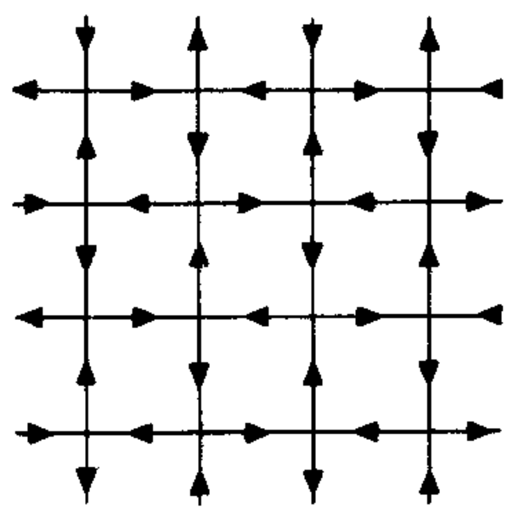
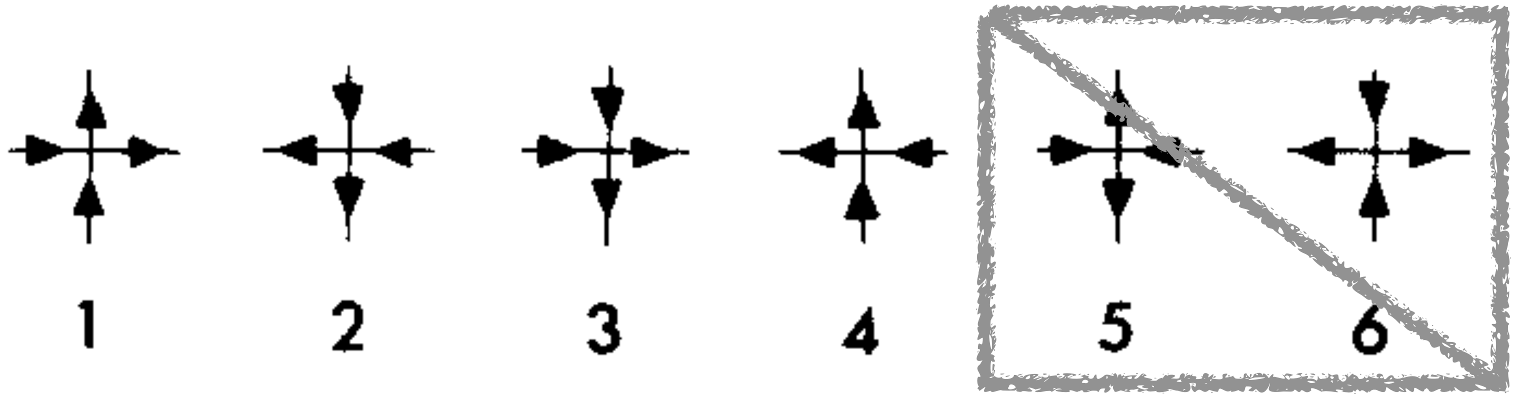
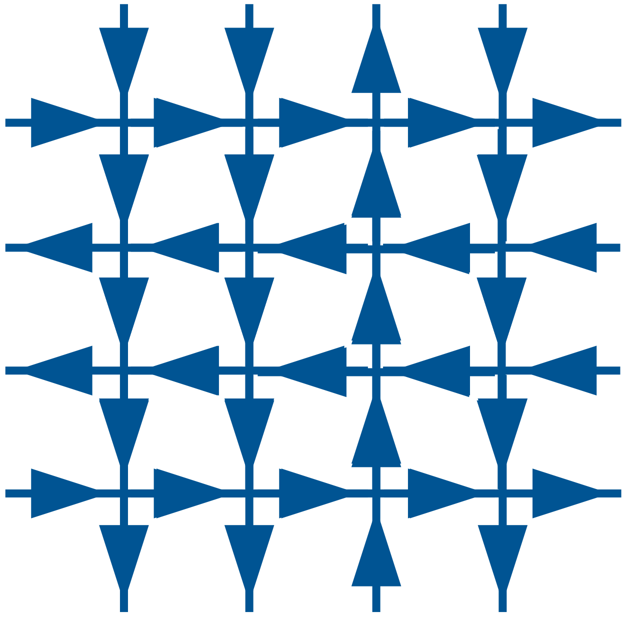


Fig. 8.3. One of the two ground-state energy configurations of the anti-ferroelectric ice-type model. Only vertex configurations 5 and 6 occur.

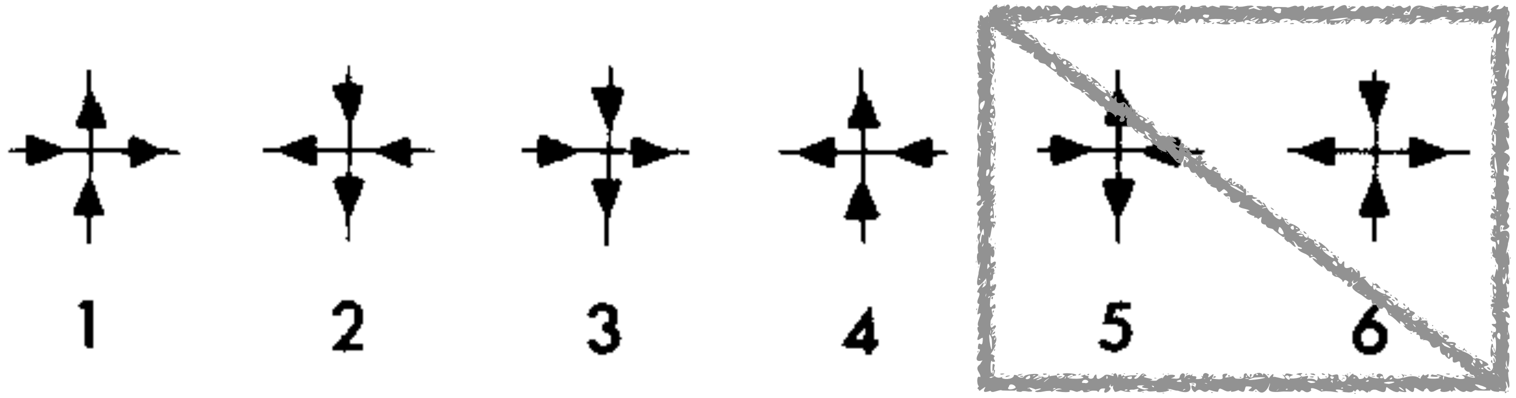
classical ice models (Baxter book)

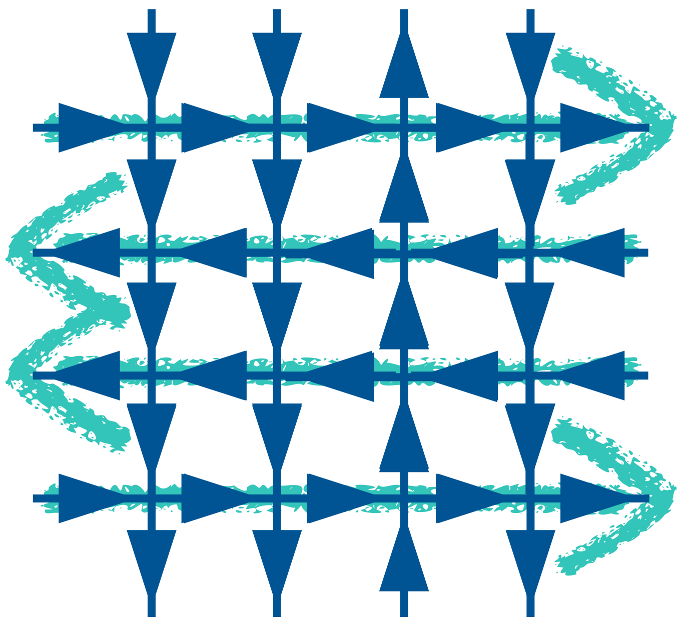




E. H. Lieb, Phys. Rev. Lett. **18**, 1046 (1967)
B. Sutherland, Phys. Rev. Lett. **19**, 103 (1967)

classical ice models (Baxter book)





E. H. Lieb, Phys. Rev. Lett. **18**, 1046 (1967)
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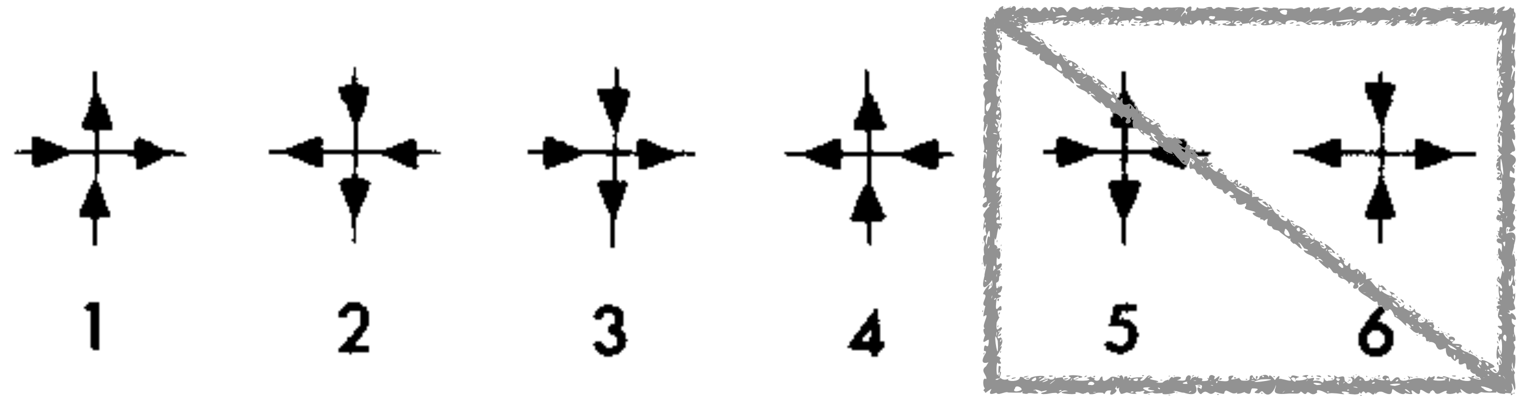
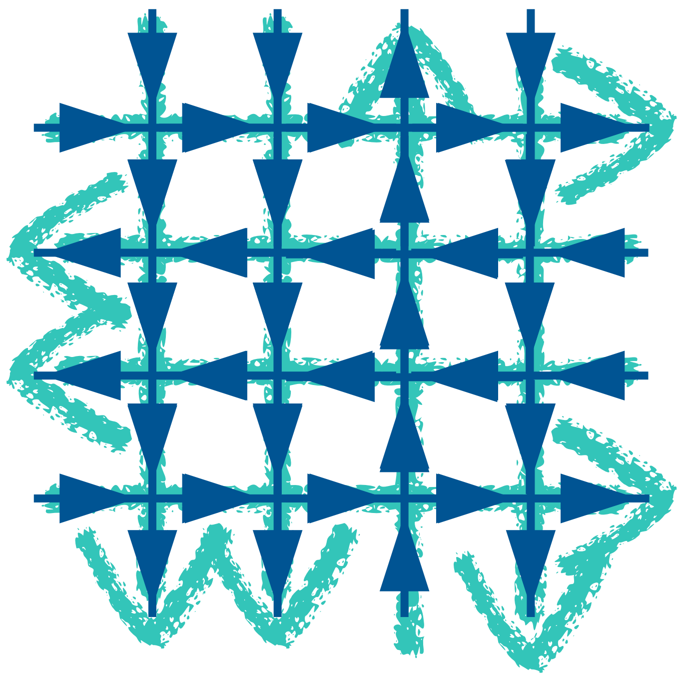
classical ice models (Baxter book)

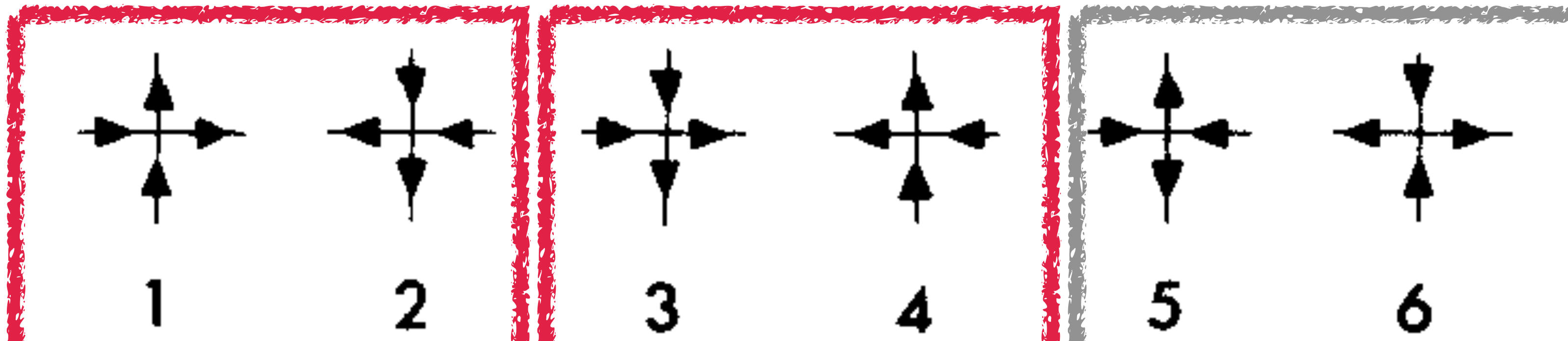




degeneracy: subextensive $\propto 2^L$

E. H. Lieb, Phys. Rev. Lett. **18**, 1046 (1967)
B. Sutherland, Phys. Rev. Lett. **19**, 103 (1967)

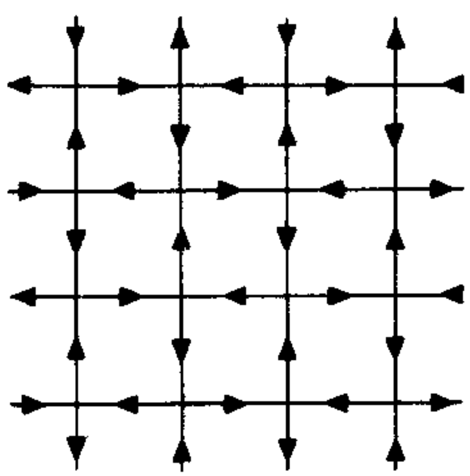
classical ice models (Baxter book)



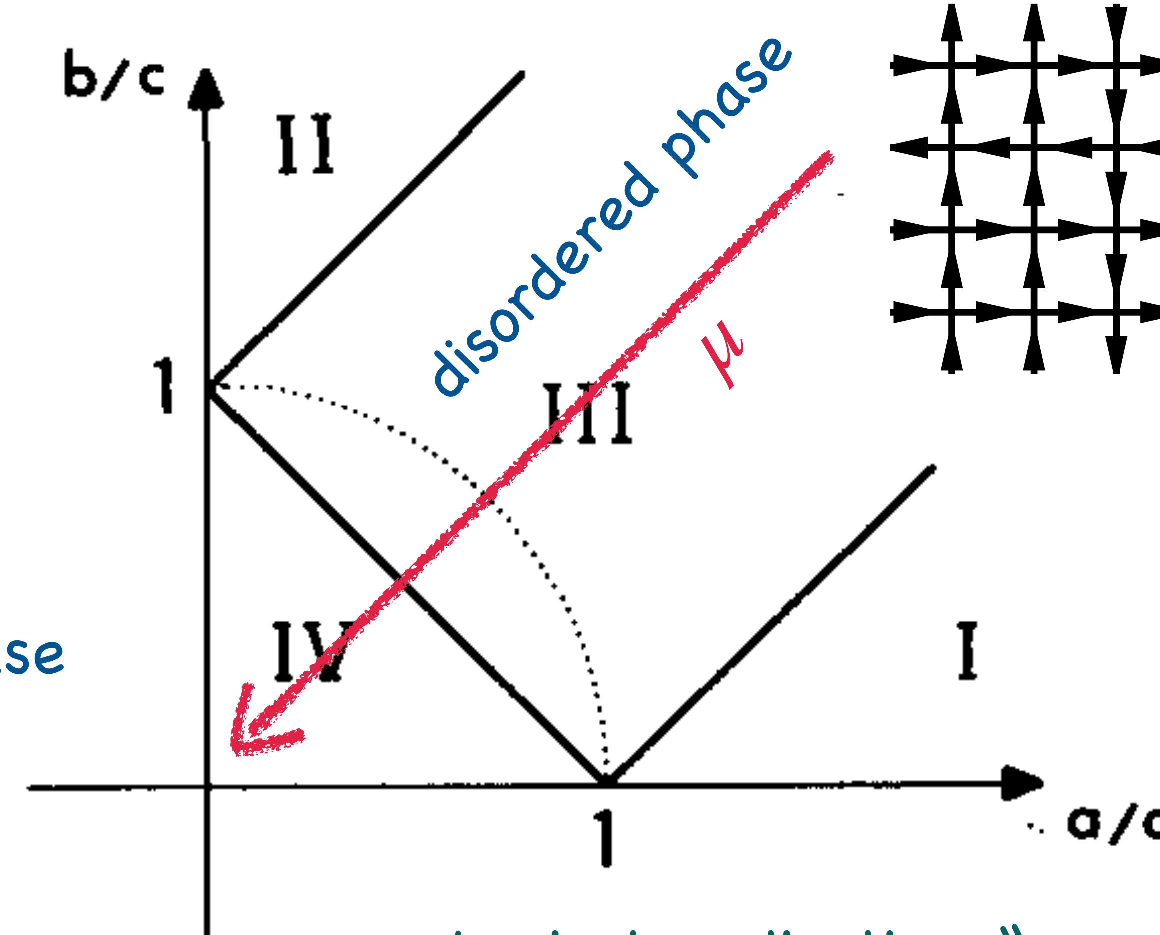
$\varepsilon_1 = \varepsilon_2 = \mu$ $\quad \varepsilon_3 = \varepsilon_4 = \mu$ $\quad \varepsilon_5 = \varepsilon_6 = 0$

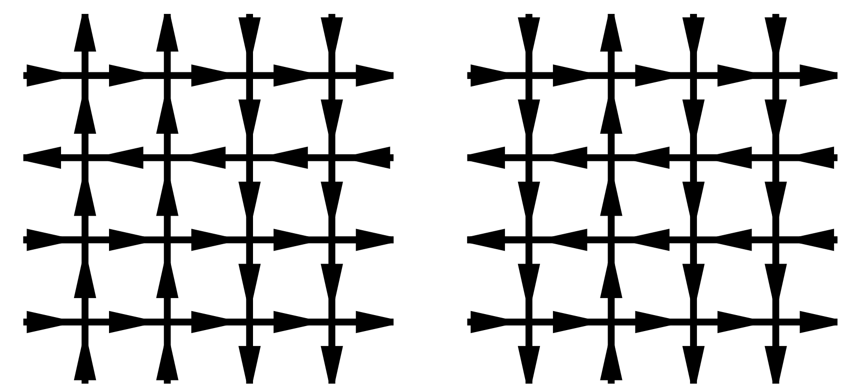
$$\omega_j = \exp(-\varepsilon_j/k_B T), \quad j = 1, \ldots, 6\,,$$

$$a = \omega_1 = \omega_2, \quad b = \omega_3 = \omega_4, \quad c = \omega_5 = \omega_6 . = 1$$



anti-ferroelectric phase
=
fully flippable

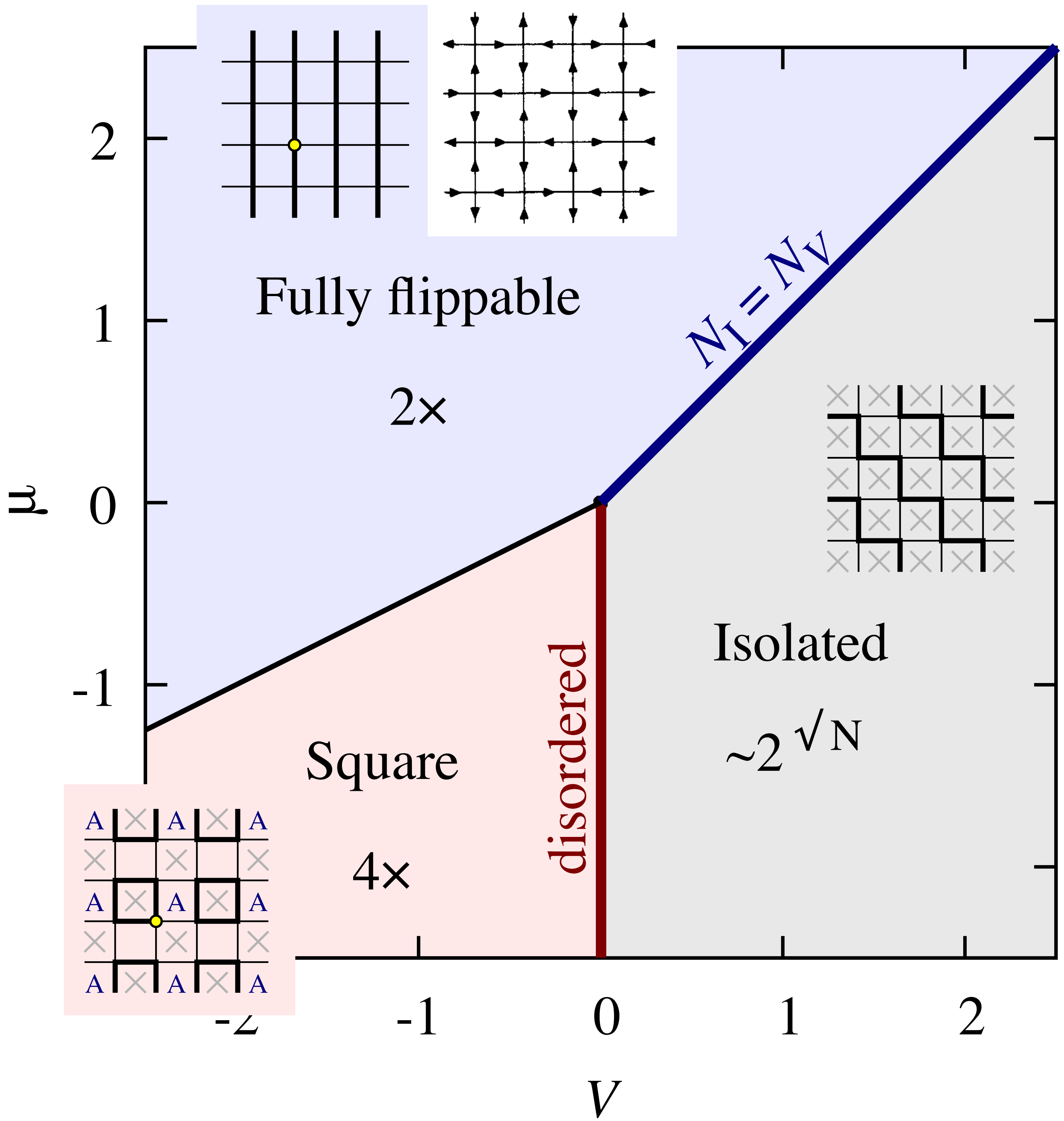




physical realisation: “square ice”, KH_2PO_4

Classical Phase Diagram

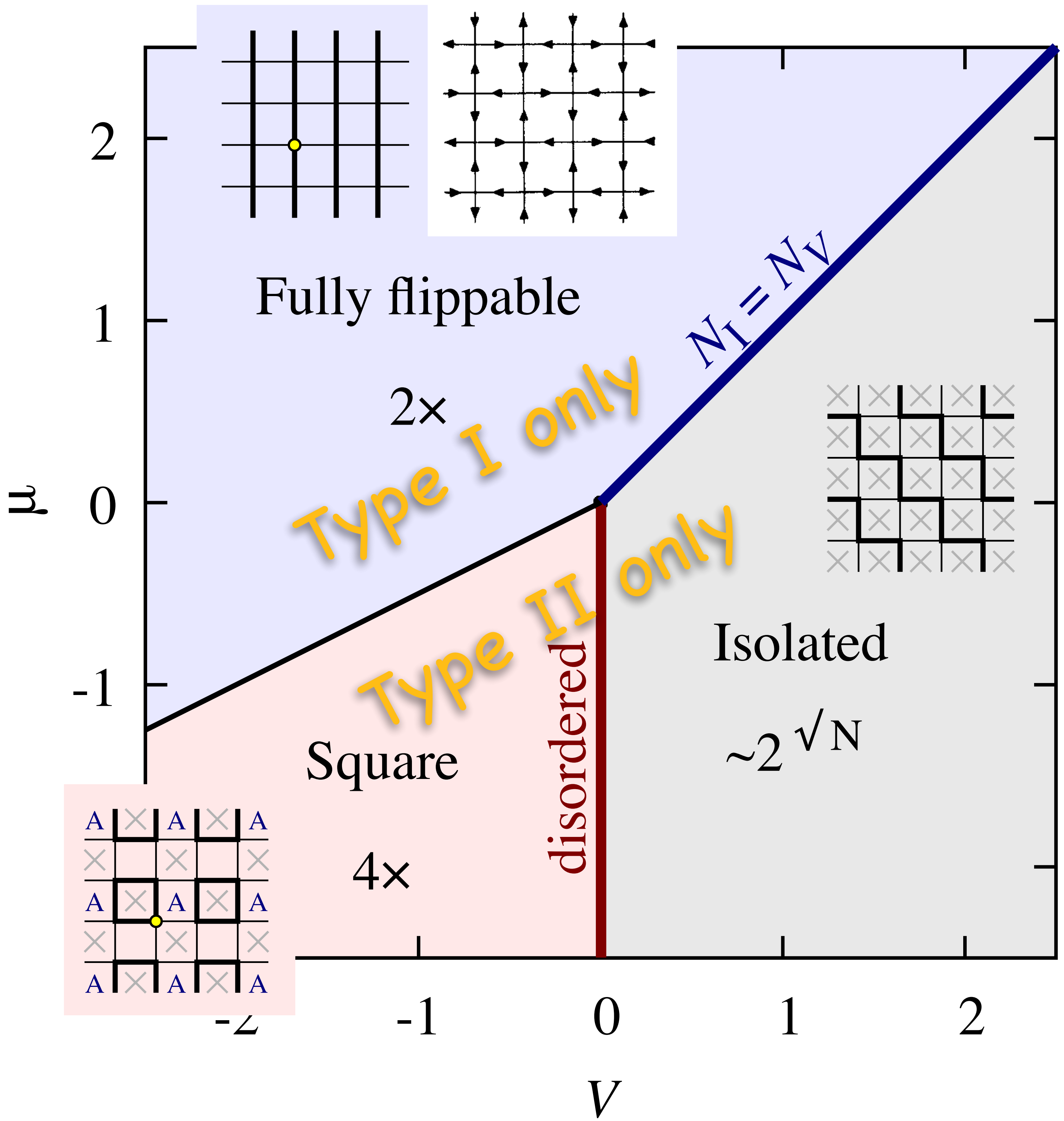
$$\mathcal{H}_t = \mu N_{\rm II} + V \sum_{\rm plaq.} \left(|\circlearrowleft\rangle\langle\circlearrowleft| + |\circlearrowright\rangle\langle\circlearrowright| \right)$$

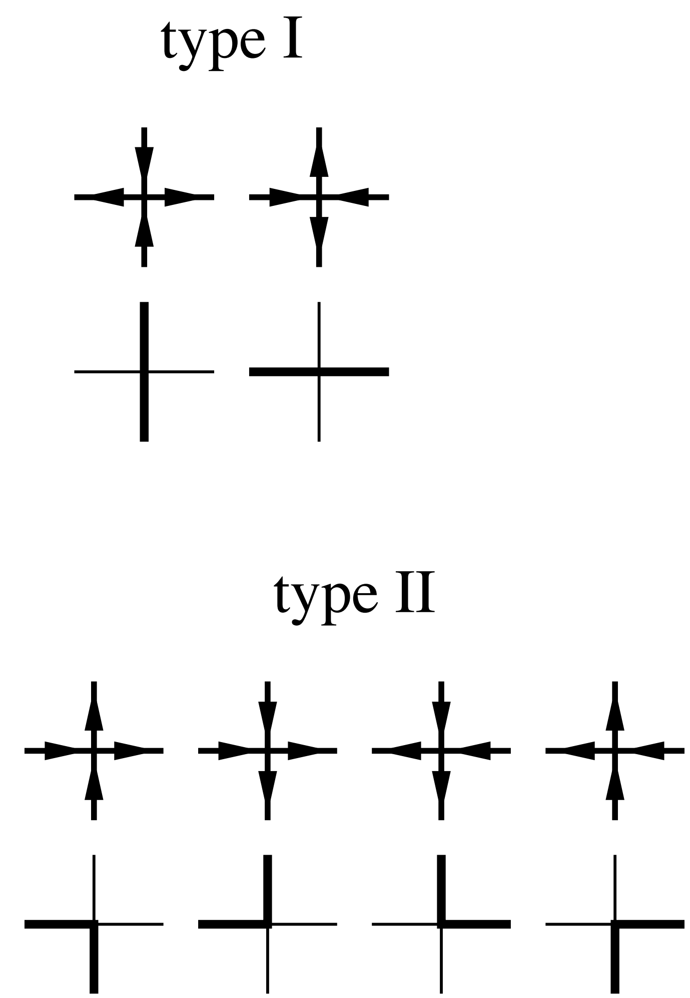


M. Kondákor, K. Penc:
Phys. Rev. Research **5**, 043172 (2023)

Classical Phase Diagram

$$\mathcal{H}_t = \mu N_{\mathrm{II}} + V \sum_{\mathrm{plaq.}} \left(|\circlearrowleft\rangle\langle\circlearrowleft| + |\circlearrowright\rangle\langle\circlearrowright| \right)$$

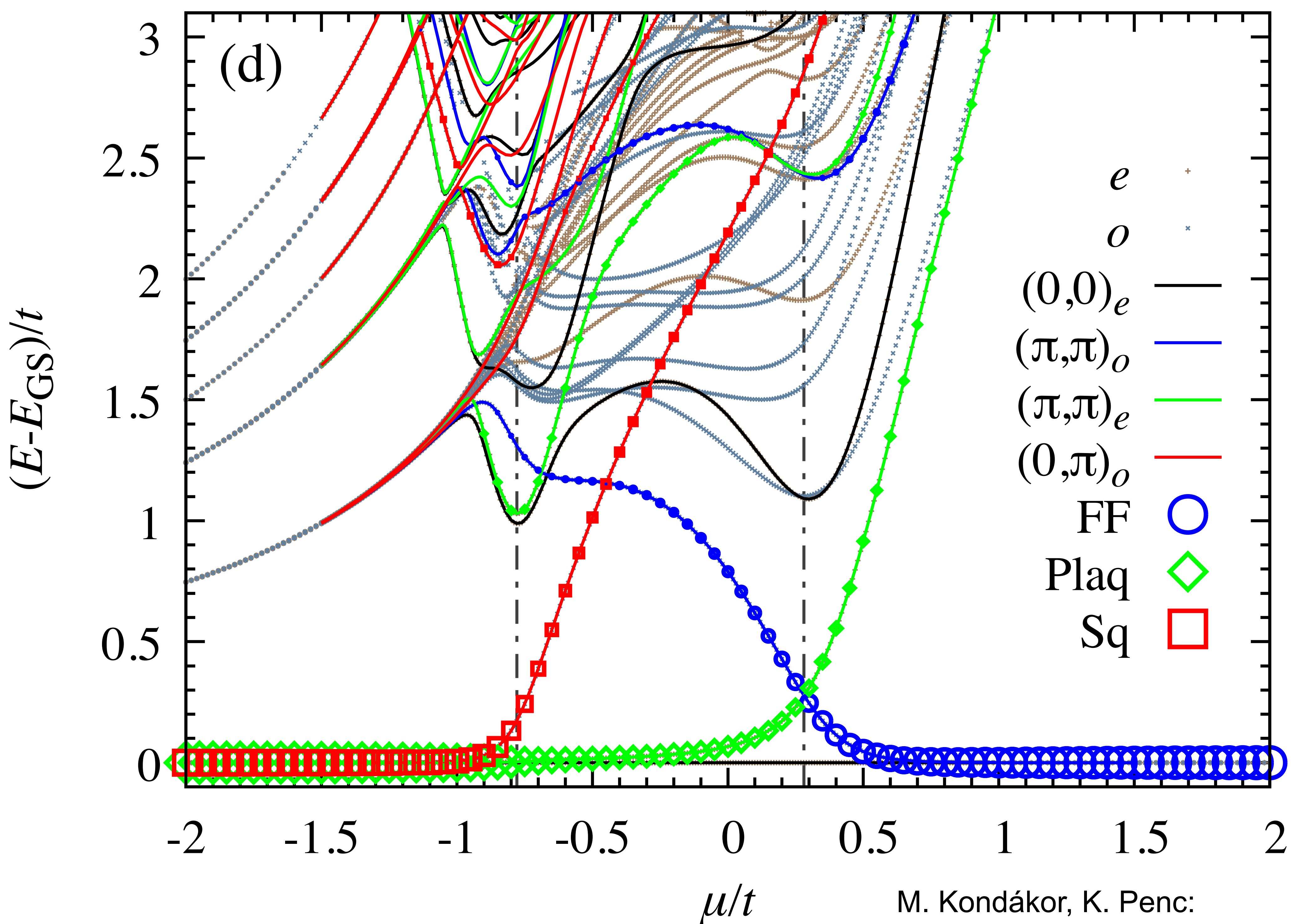




M. Kondákor, K. Penc:
Phys. Rev. Research **5**, 043172 (2023)

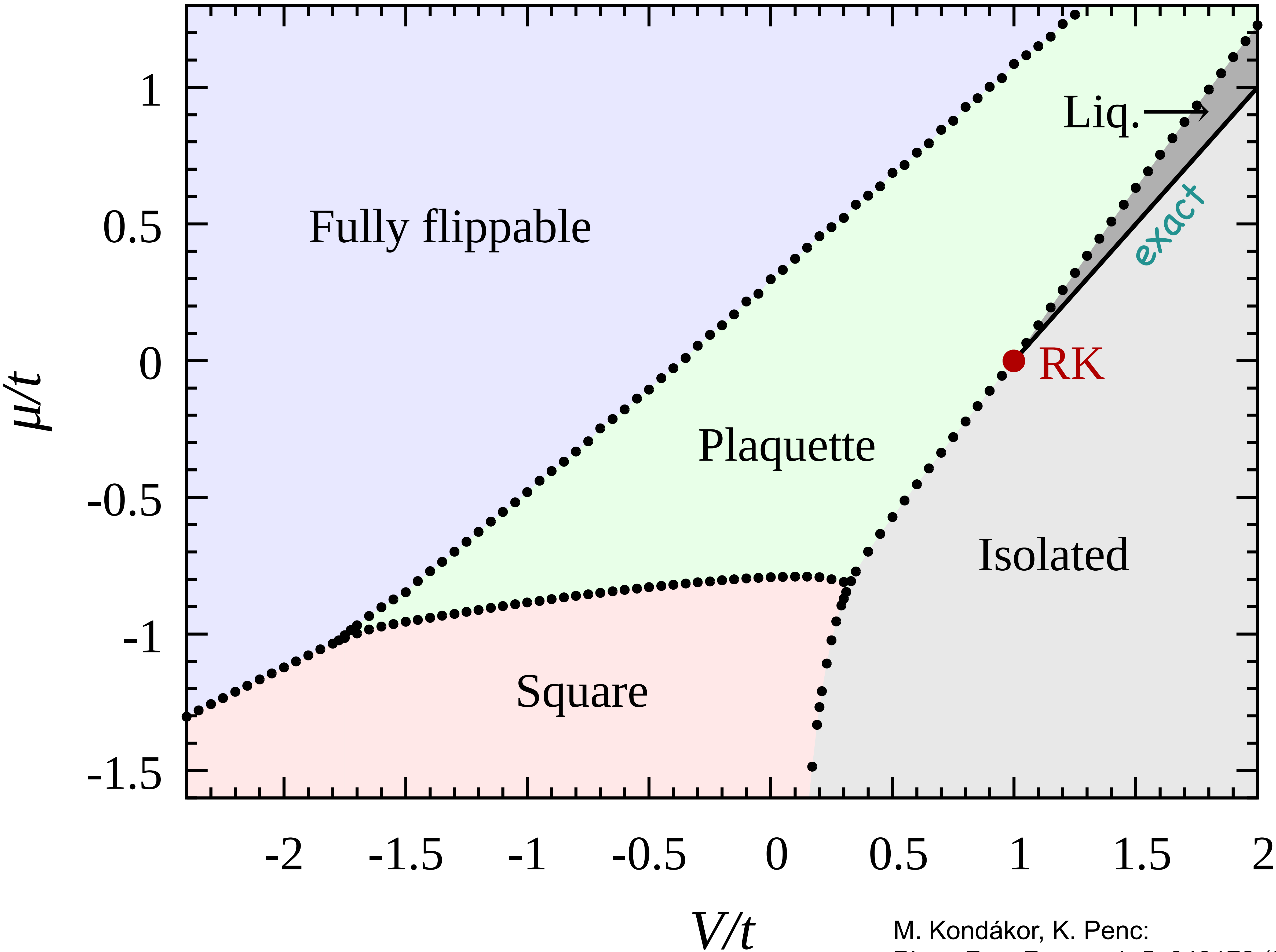
Quantum Phase Diagram: Level spectroscopy

$$\mathcal{H}_t = -t \sum_{\text{plaq.}} \left(|\circlearrowleft\rangle\langle\circlearrowright| + |\circlearrowright\rangle\langle\circlearrowleft| \right) + V \sum_{\text{plaq.}} \left(|\circlearrowleft\rangle\langle\circlearrowleft| + |\circlearrowright\rangle\langle\circlearrowright| \right) + \mu N_{\mathrm{II}}$$



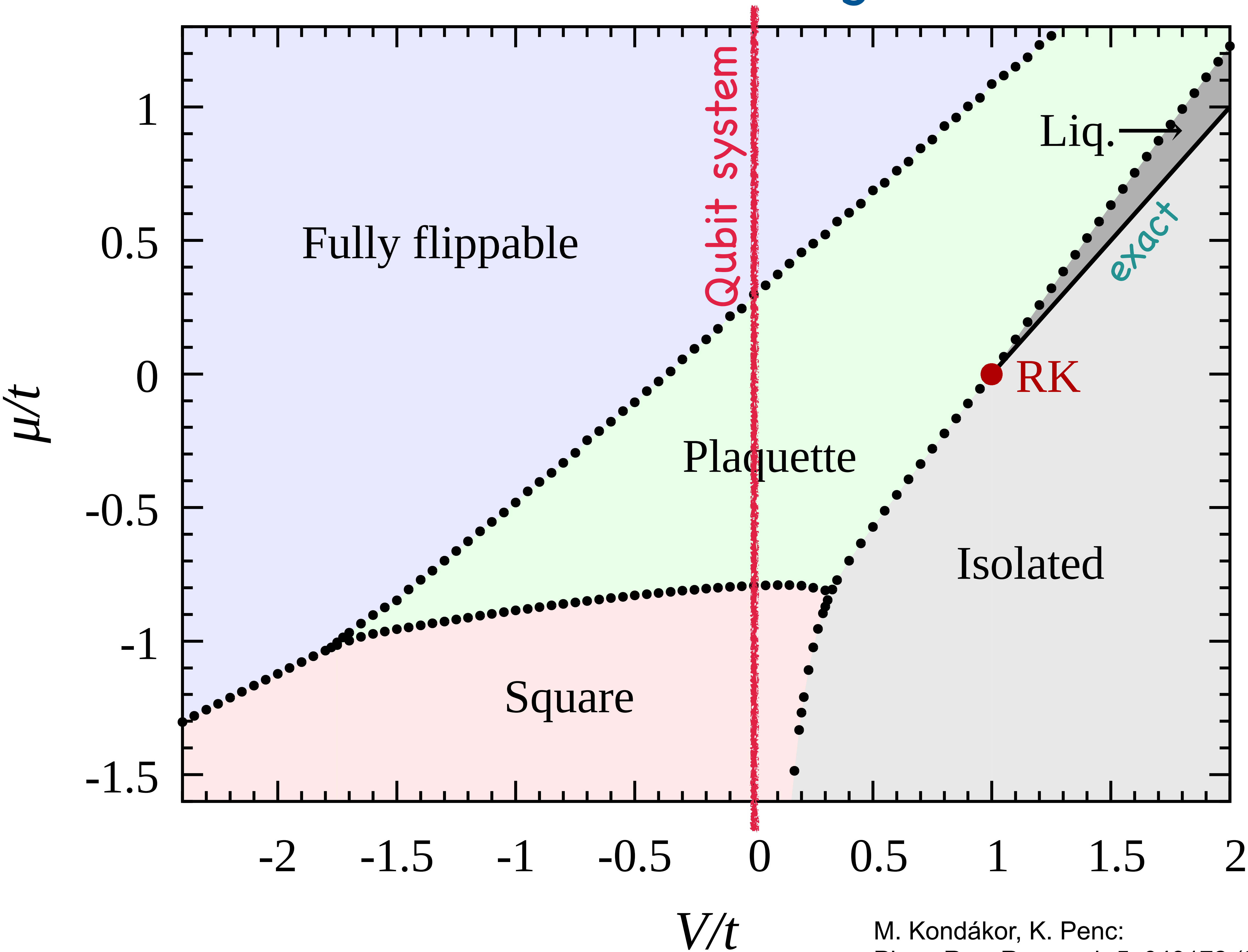
M. Kondákor, K. Penc:
Phys. Rev. Research **5**, 043172 (2023)

Quantum Phase Diagram



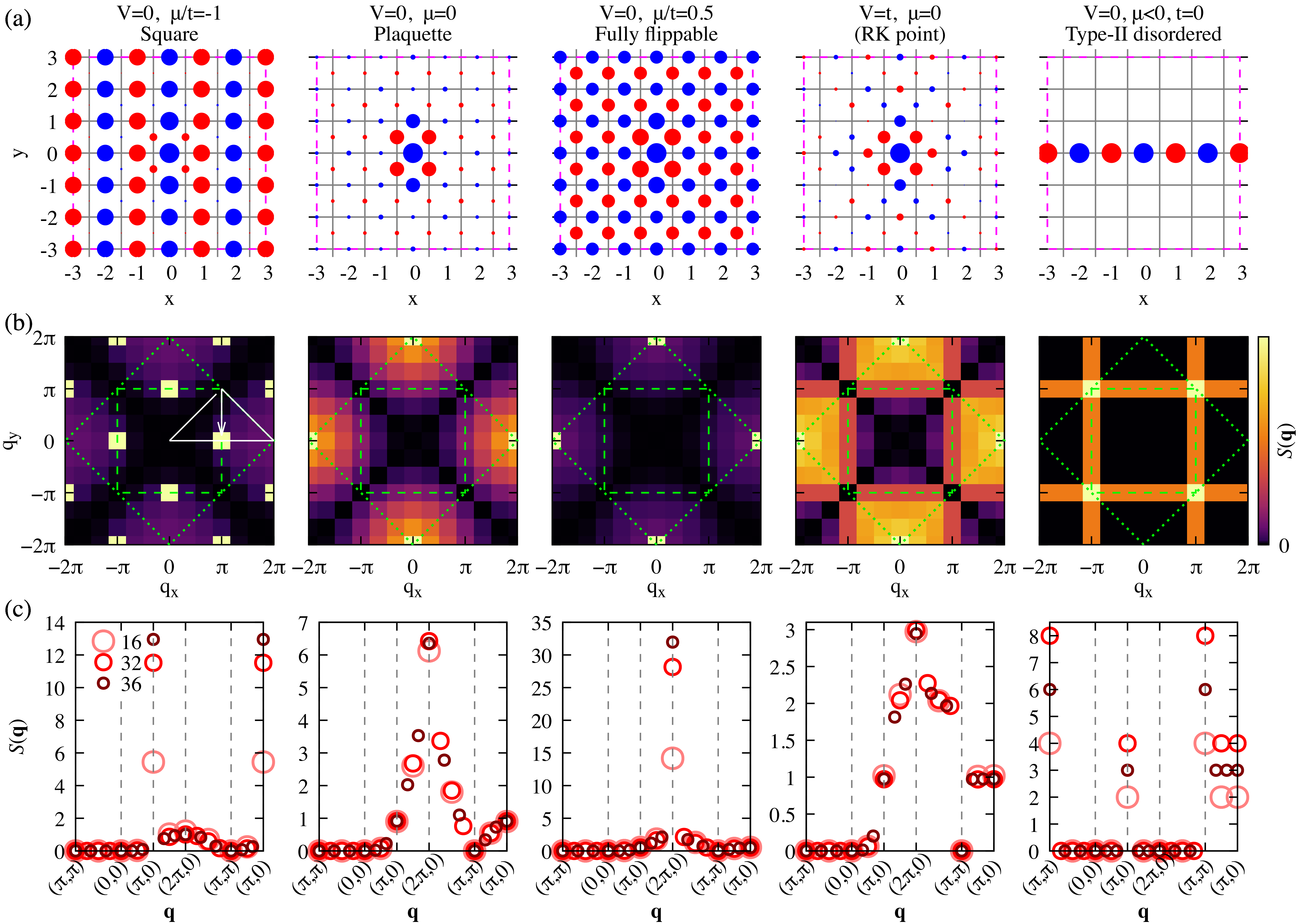
M. Kondákor, K. Penc:
Phys. Rev. Research **5**, 043172 (2023)

Quantum Phase Diagram



M. Kondákor, K. Penc:
Phys. Rev. Research **5**, 043172 (2023)

Density-density Structure factors



MAGNETISM

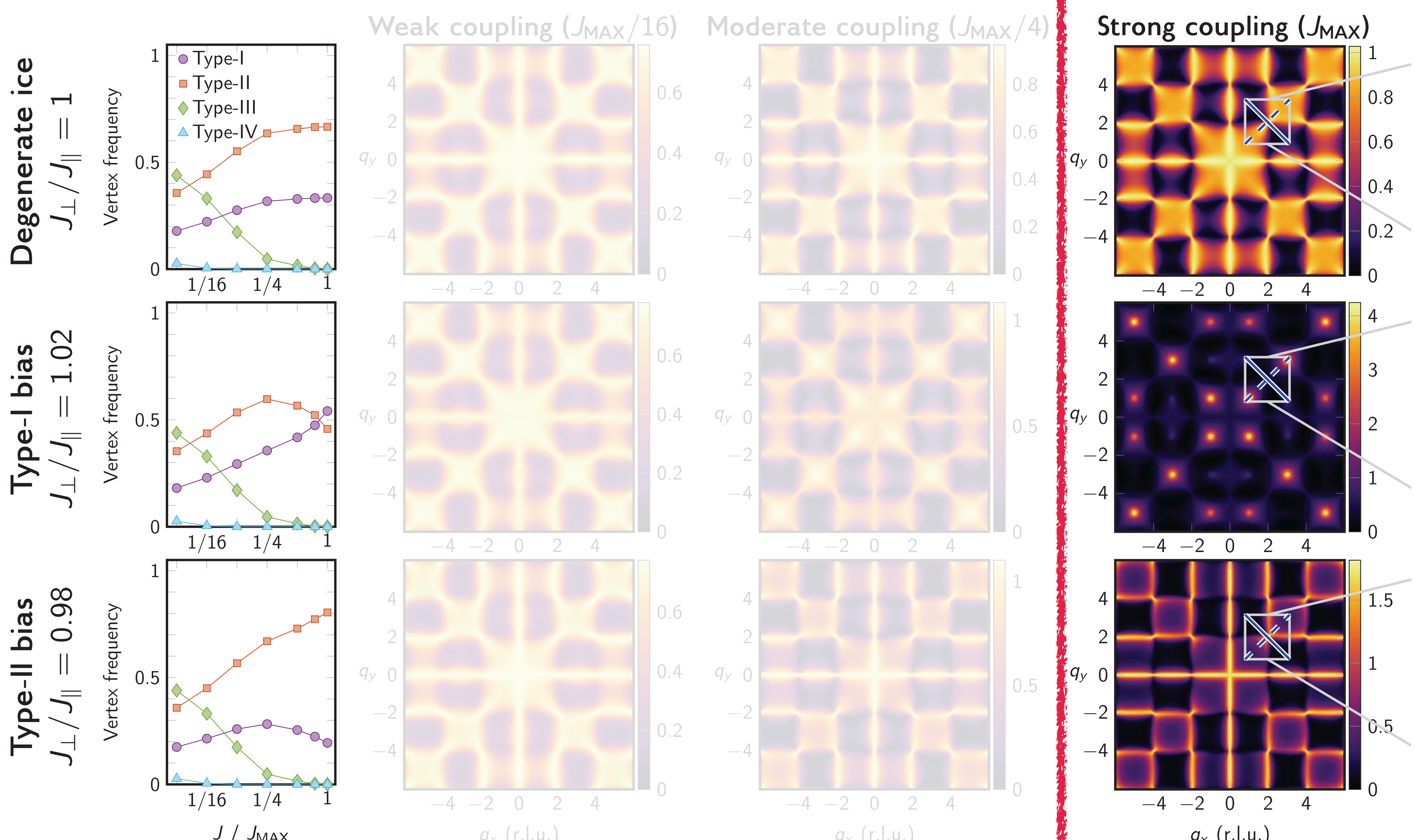
Qubit spin ice

Andrew D. King[1]*, Cristiano Nisoli[2]*, Edward D. Dahl[1,3], Gabriel Poulin-Lamarre[1], Alejandro Lopez-Bezanilla[2]

Structure factor S(**q**) for varying couplings, in reciprocal lattice space.

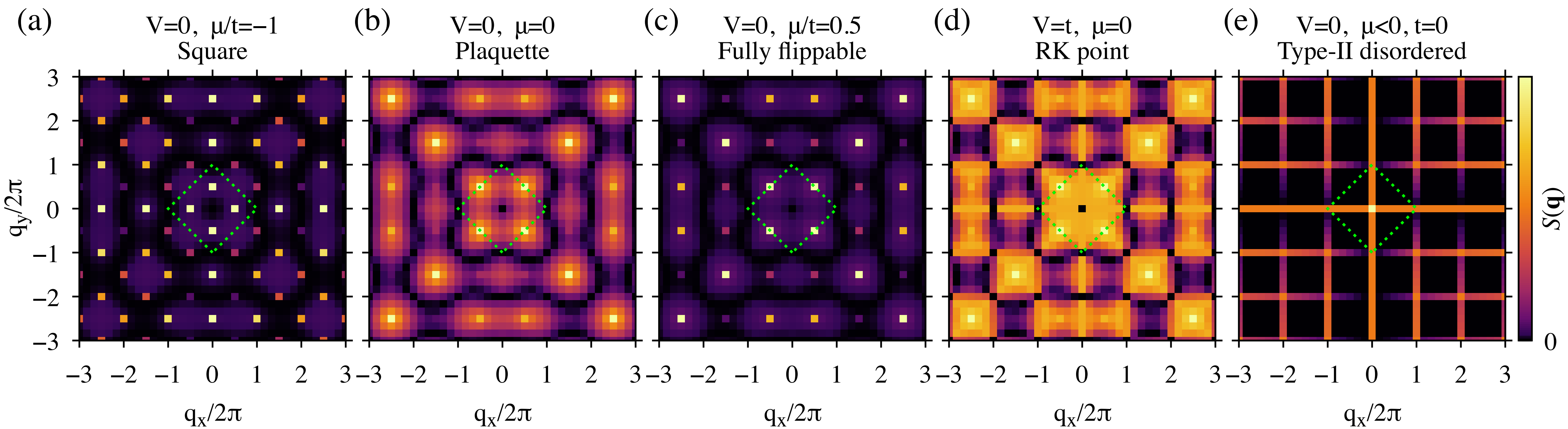
14×14 ice system

Quantum 6-vertex model

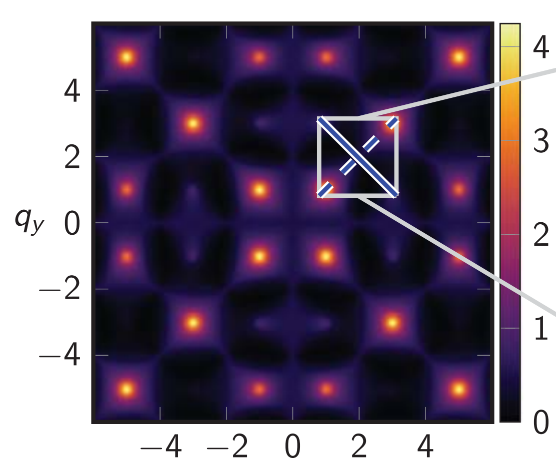


Comparison between Q6M and qubit spin ice

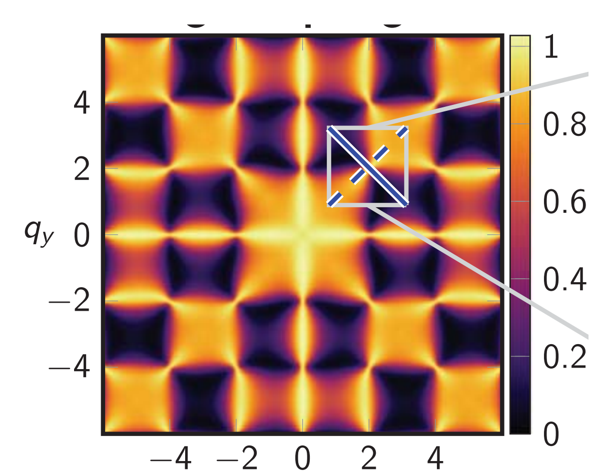
quantum 6-vertex model:



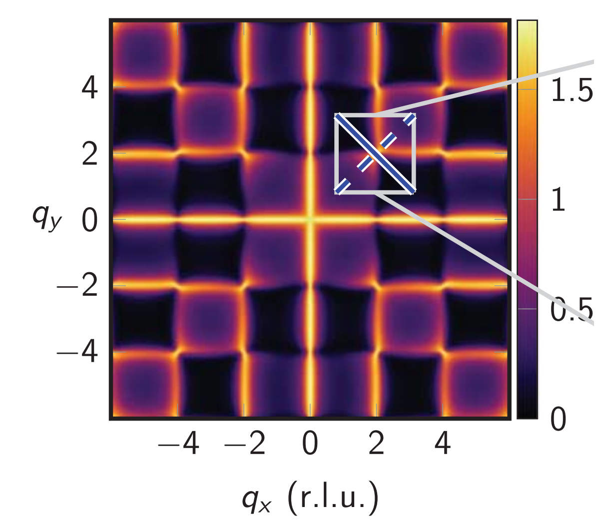
qubit spin ice:



Type-I bias



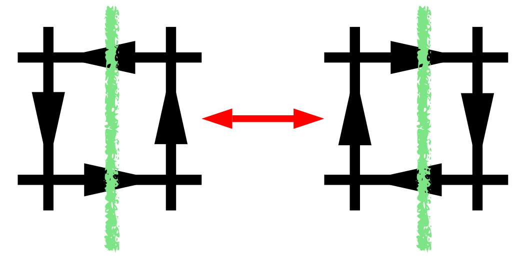
Degenerate ice



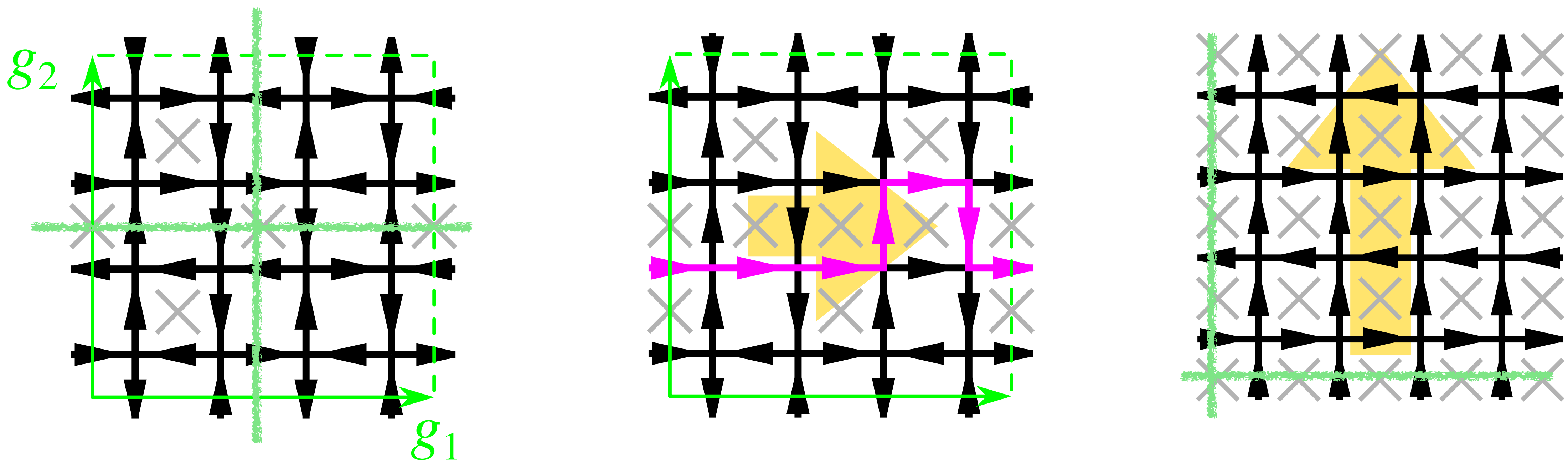
Type-II bias

flux sectors

flux is invariant under dynamics



isolated state

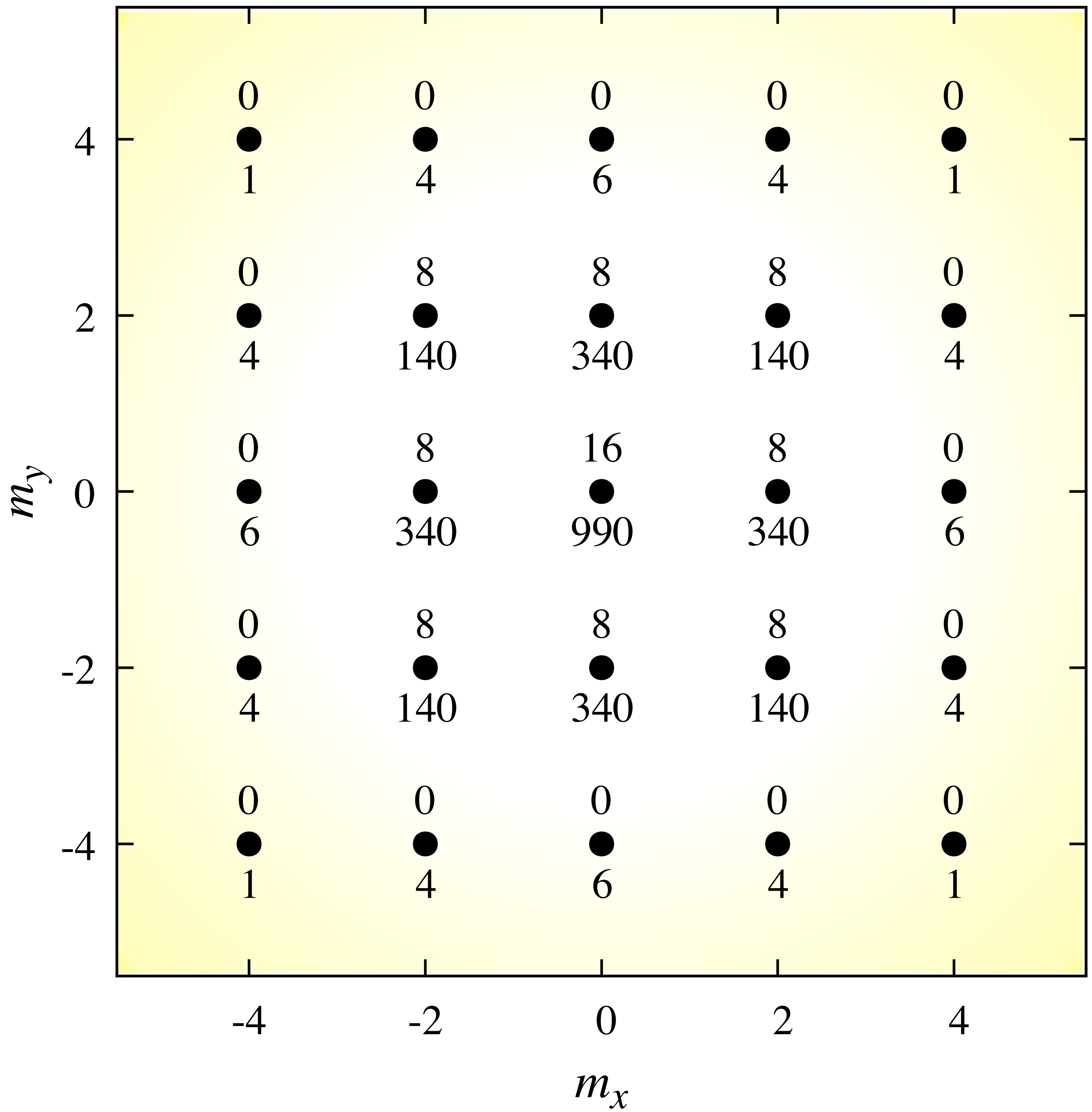


$\mathbf{m} = (0,0)$ $\mathbf{m} = (2,0)$ $\mathbf{m} = (0,4)$

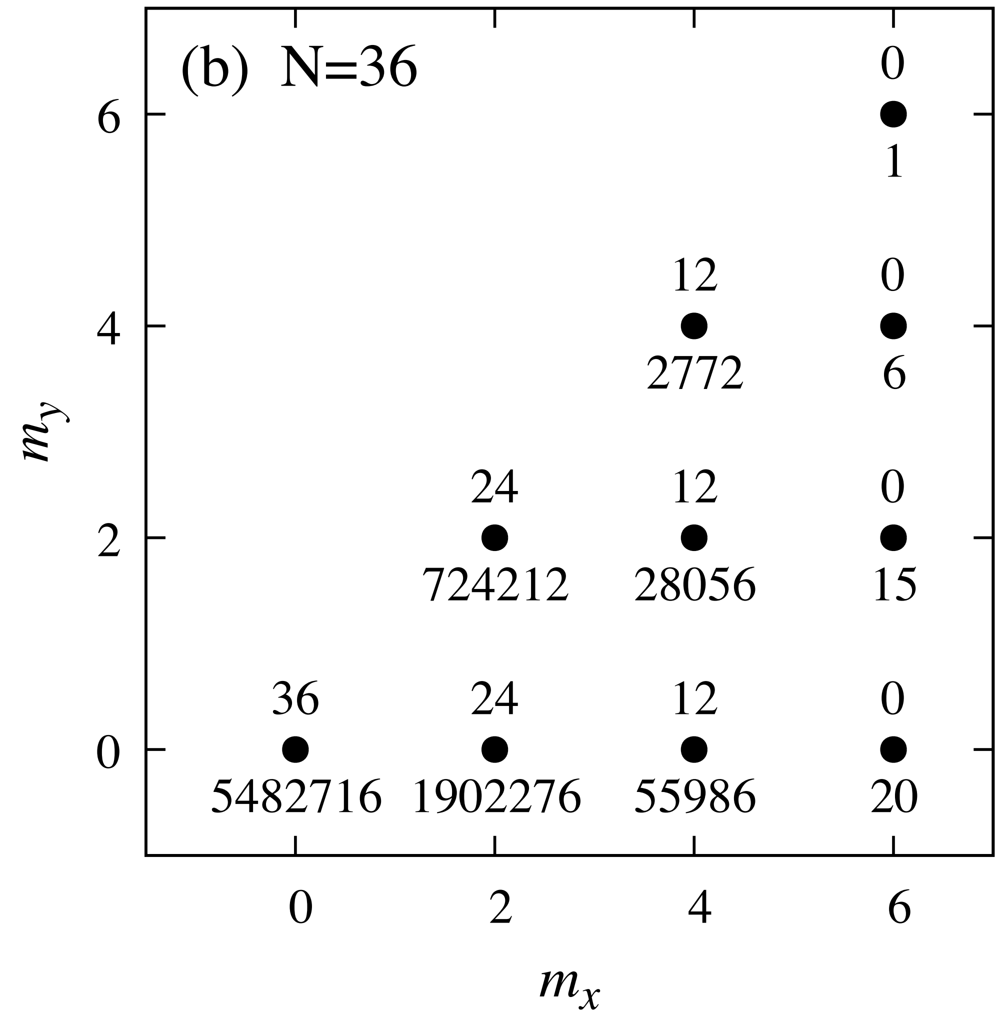
flux ≈ average arrow density

flux sectors

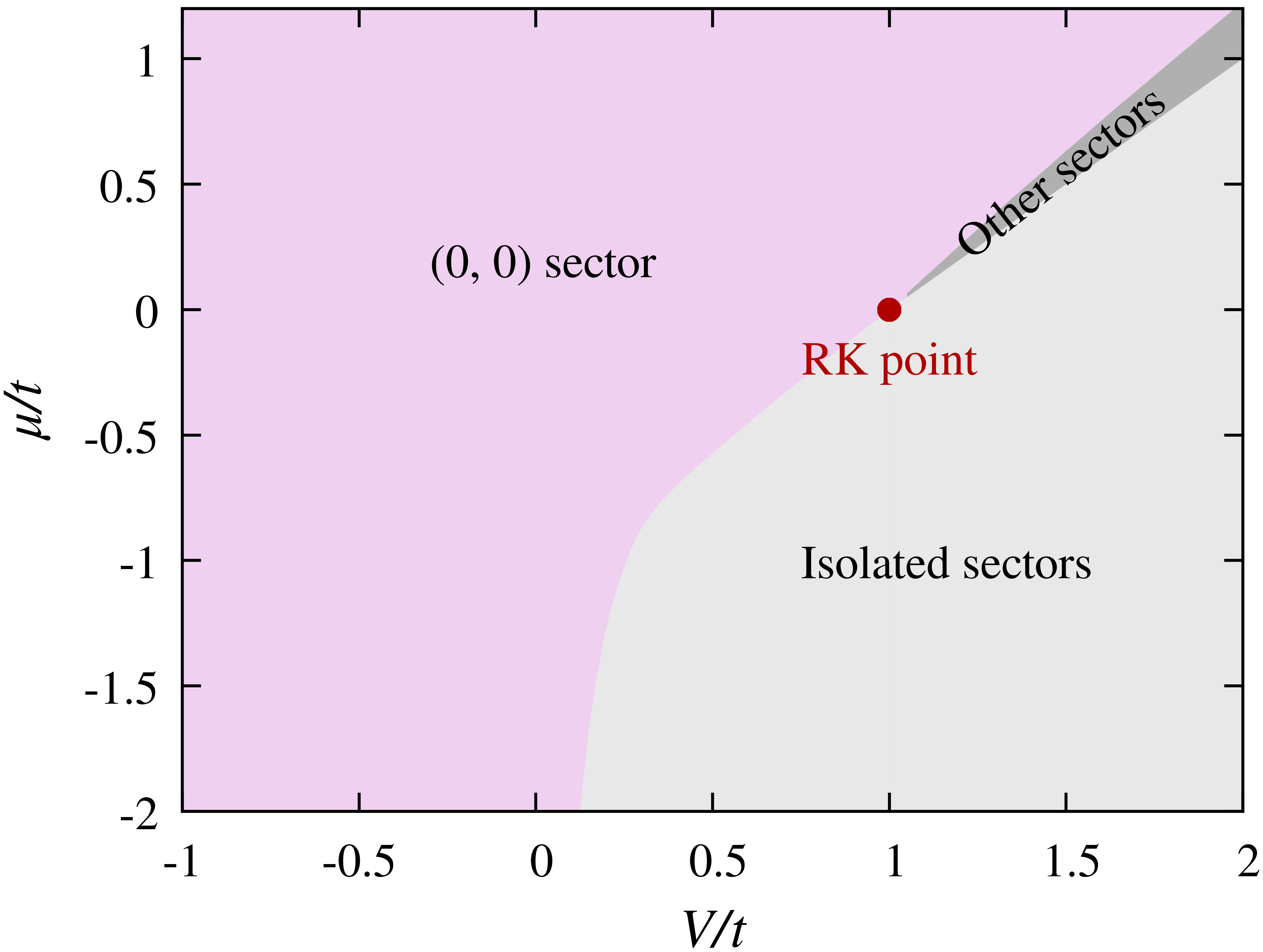
degeneracy of flux sectors for 32 spins



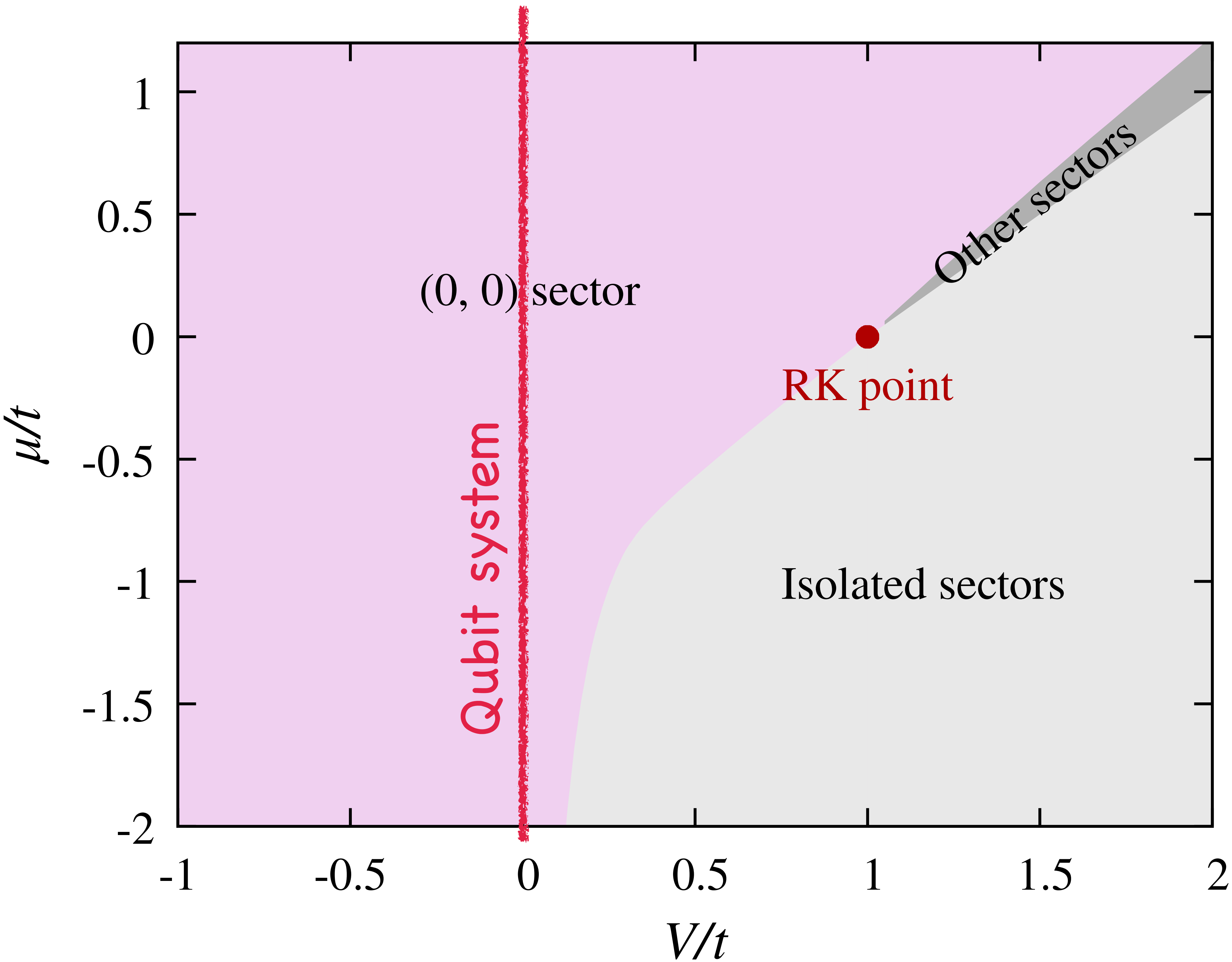
degeneracy of flux sectors for 72 spins



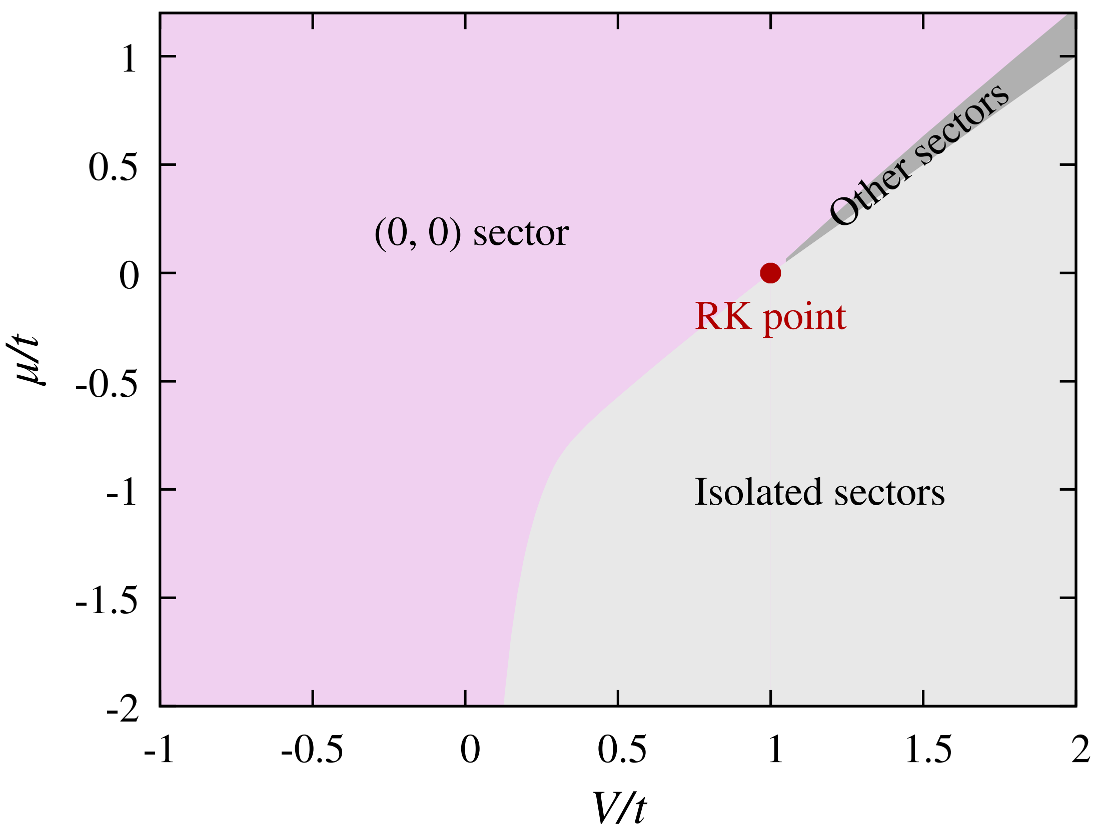
Fluxes in ground state



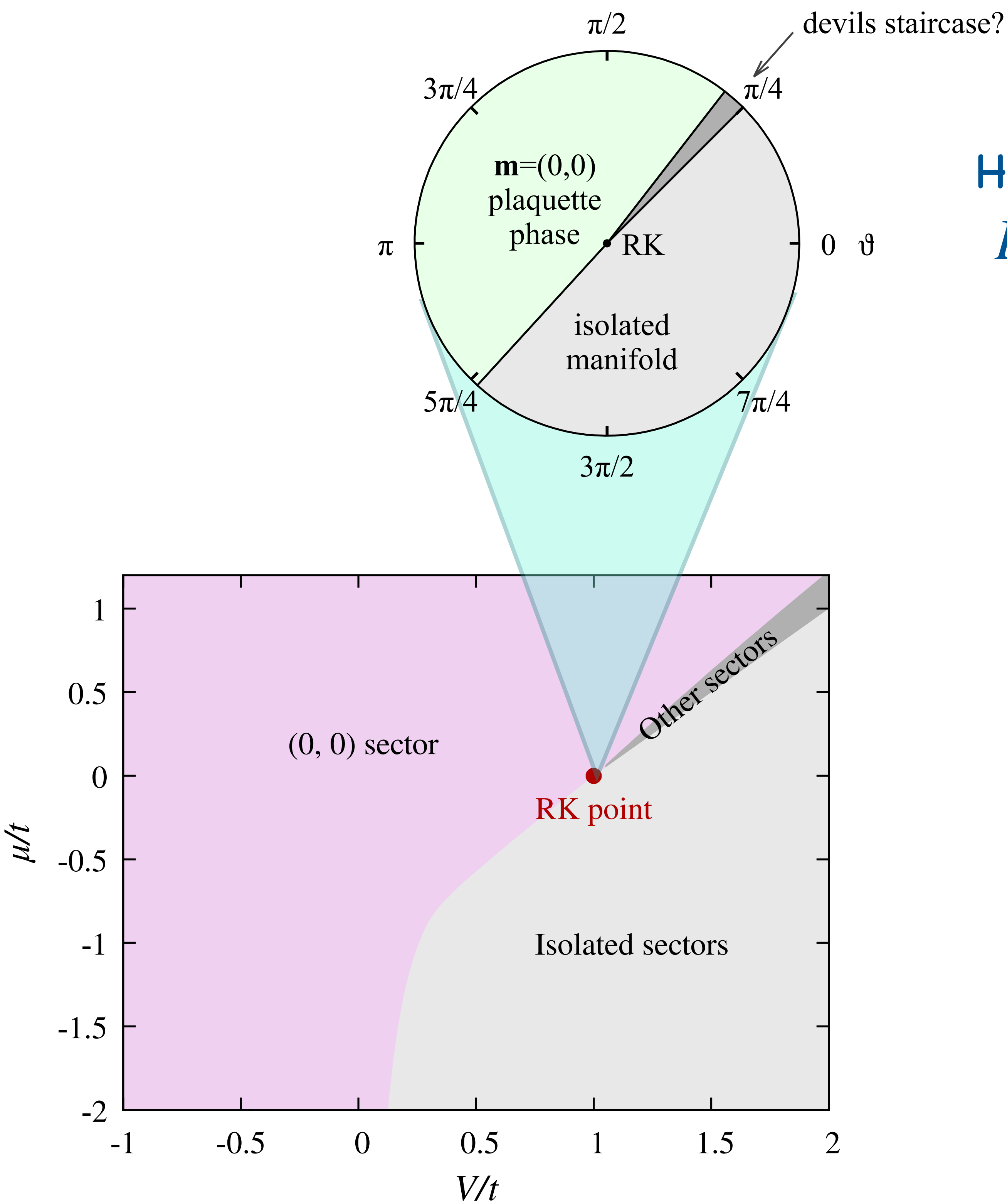
Fluxes in ground state



What are the other sectors?



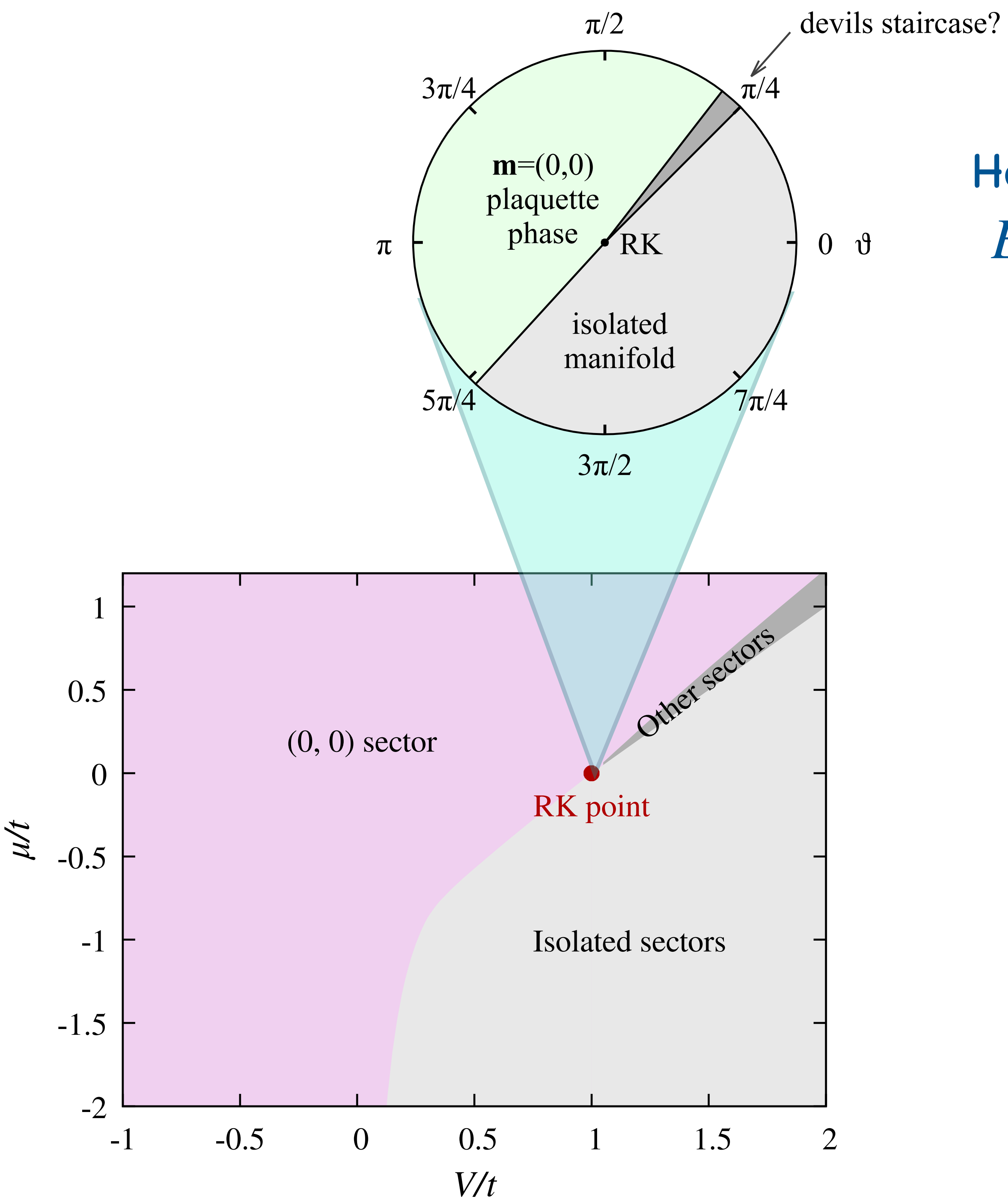
What are the other sectors?



Hellman-Feynmann theorem:

$$E(\mathbf{m}) = \mu\langle \mathsf{RK}_{\mathbf{m}} | \hat{N}_{II} | \mathsf{RK}_{\mathbf{m}} \rangle + V \langle \mathsf{RK}_{\mathbf{m}} | \hat{N}_{V} | \mathsf{RK}_{\mathbf{m}} \rangle$$

What are the other sectors?



Hellman-Feynmann theorem:

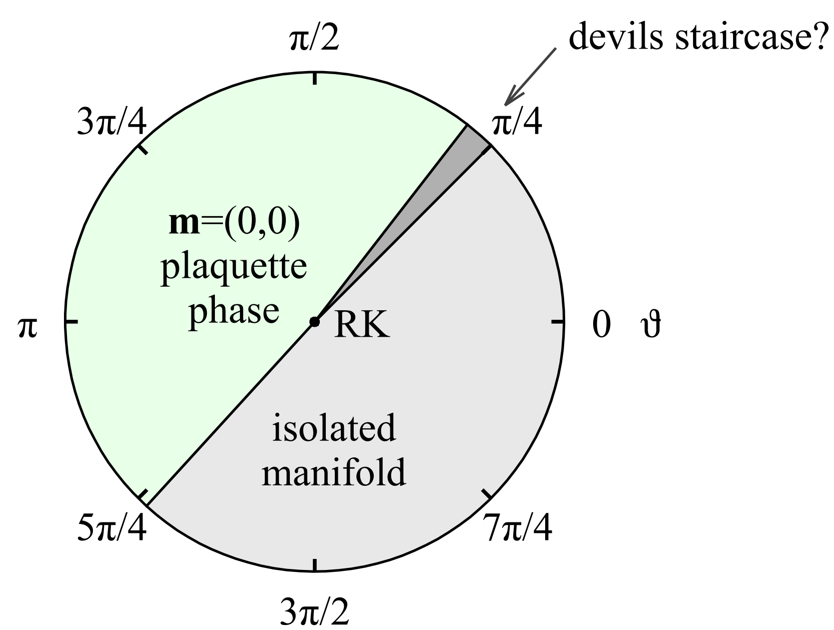
$$E(\mathbf{m}) = \mu\langle \mathsf{RK}_\mathbf{m} | \hat{N}_{\mathrm{II}} | \mathsf{RK}_\mathbf{m}\rangle + V\langle \mathsf{RK}_\mathbf{m} | \hat{N}_V | \mathsf{RK}_\mathbf{m}\rangle$$

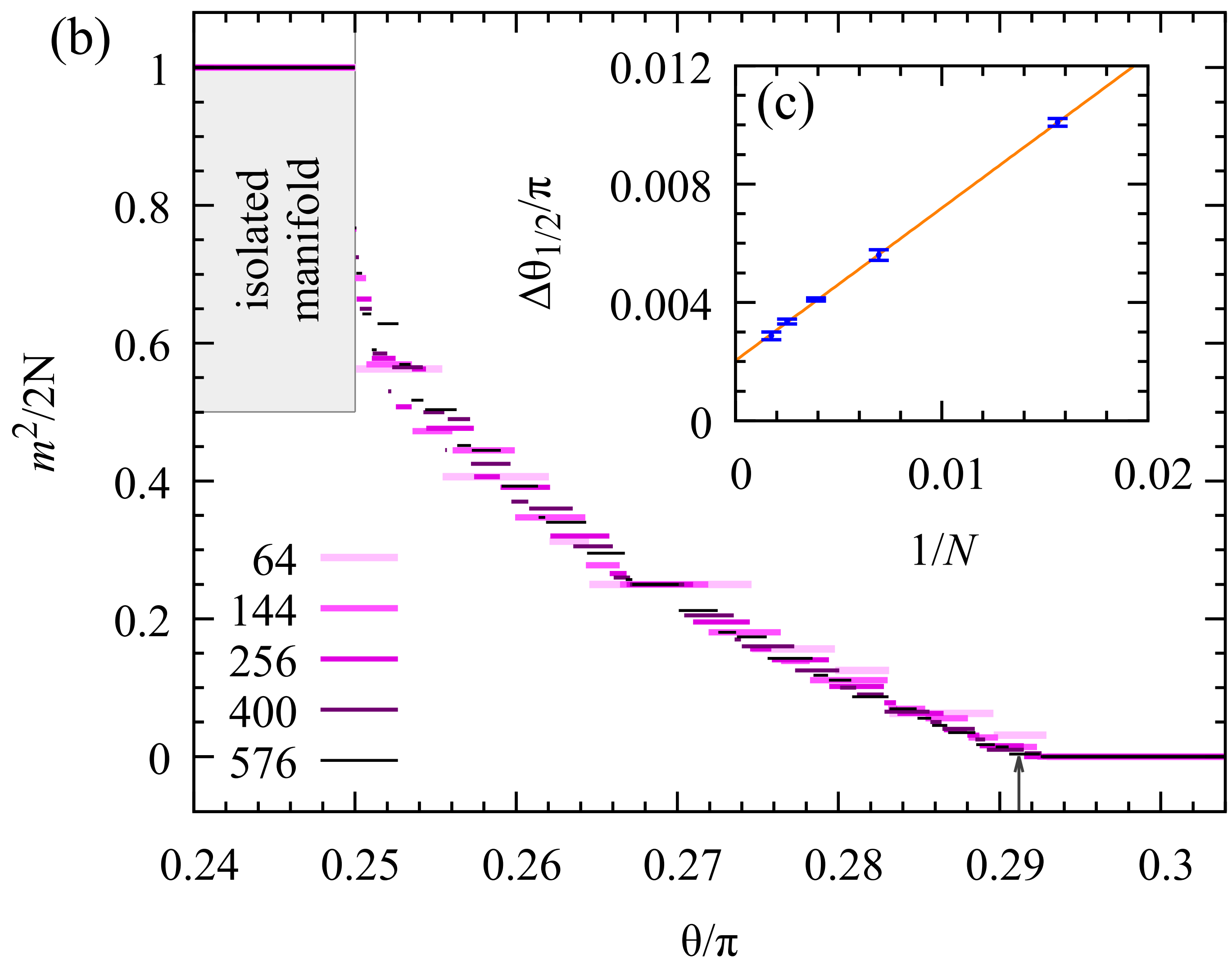
Monte Carlo sampling of the $\langle \mathsf{RK}_\mathbf{m} | \hat{N}_{\mathrm{II}} | \mathsf{RK}_\mathbf{m}\rangle$ and $\langle \mathsf{RK}_\mathbf{m} | \hat{N}_V | \mathsf{RK}_\mathbf{m}\rangle$ in the Rokshar-Kivelson wave function.

Devils staircase?

Hellman-Feynmann theorem:

$$E(\mathbf{m}) = \mu\langle \mathrm{RK}_\mathbf{m} | \hat{N}_{\mathrm{II}} | \mathrm{RK}_\mathbf{m}\rangle + V\langle \mathrm{RK}_\mathbf{m} | \hat{N}_V | \mathrm{RK}_\mathbf{m}\rangle$$





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A. Vishwanath, L. Balents, and T. Senthil, PRB **69**, 224416 (2004);
T. Schlittler, T. Barthel, G. Misguich, J. Vidal, and R. Mosseri, Phys. Rev. Lett. **115**, 217202 (2015)

Conclusions

- New platforms appear (quantum simulators) that make your dreams come true.
- Exotic phases appear - devils staircase
- Is it time to revisit LiV_2O_4?