Title: Monogamy of entanglement and improved mean-field ansatz for spin lattices

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Abstract: We consider rather general spin-1/2 lattices with large coordination numbers Z.
 Based on the monogamy of entanglement and other properties of the concurrence C,
 we derive rigorous bounds for the entanglement between neighboring spins,
 which show that C decreases for large Z. In addition, the concurrence C measures the deviation from mean-field behavior and can only vanish if the mean-field ansatz yields an exact ground state of the Hamiltonian. Motivated by these findings, we propose an improved mean-field ansatz by adding entanglement

Monogamy of entanglement and mean-field ansatz for spin lattices

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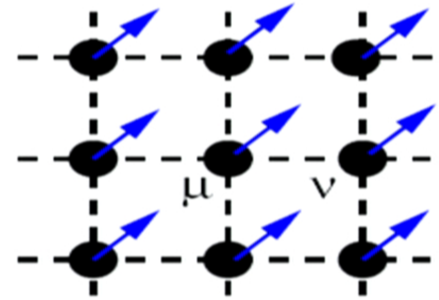
Spin Lattice



Regular lattice of 1/2-spins (qubits)
Pauli matrices $\hat{\boldsymbol{\sigma}}_\mu = (\hat{\sigma}^x_\mu, \hat{\sigma}^y_\mu, \hat{\sigma}^z_\mu)$
Coordination number Z (neighbours)

$$\hat{H} = \frac{1}{Z} \sum_{<\mu,\nu>} \hat{\boldsymbol{\sigma}}_\mu \cdot \boldsymbol{J} \cdot \hat{\boldsymbol{\sigma}}_\nu + \sum_\mu \boldsymbol{B} \cdot \hat{\boldsymbol{\sigma}}_\mu$$

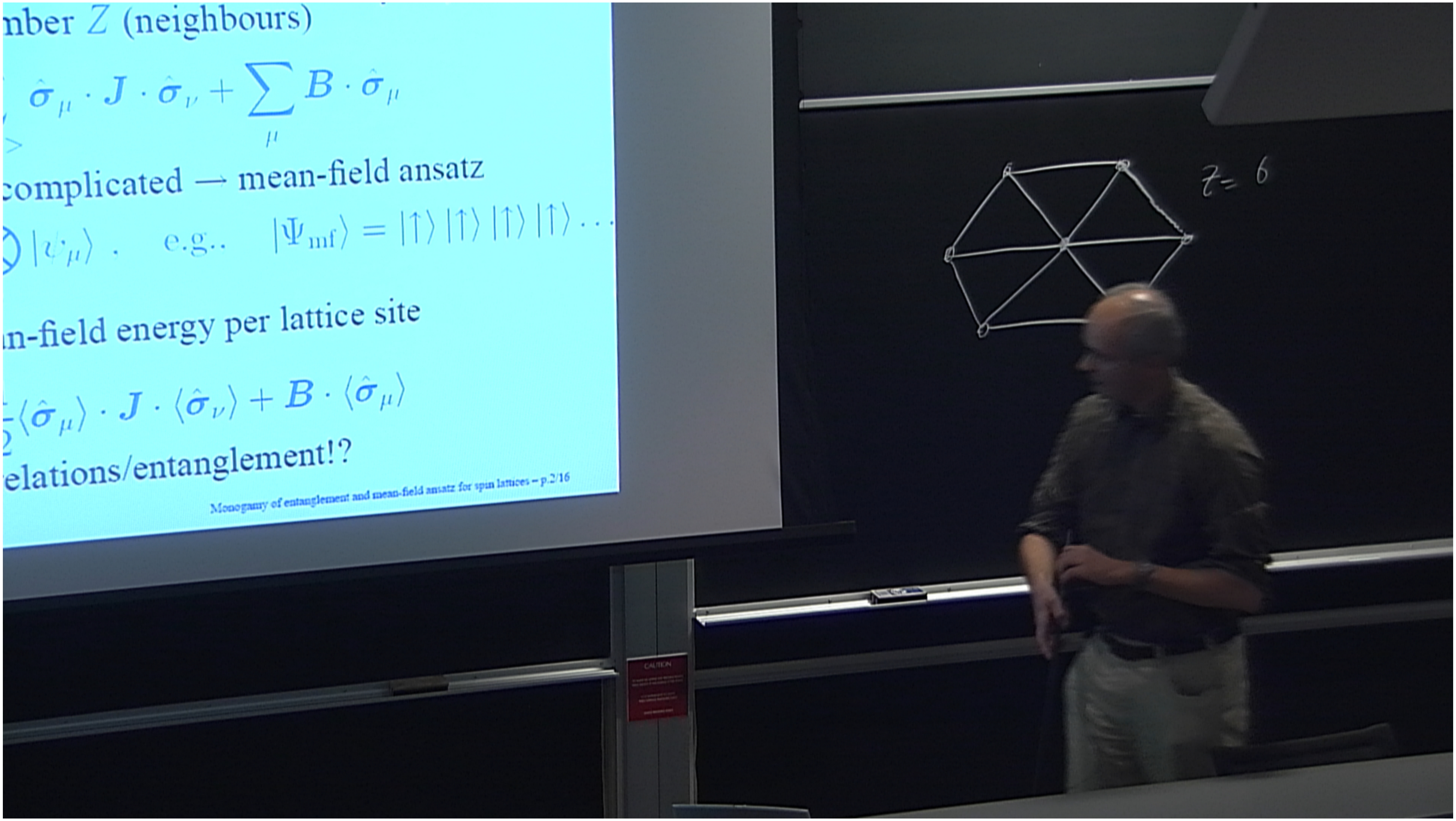
In general very complicated $\longrightarrow$ mean-field ansatz

$$|\Psi_{\mathrm{mf}}\rangle = \bigotimes_\mu |\psi_\mu\rangle \ , \quad \text{e.g.,} \quad |\Psi_{\mathrm{mf}}\rangle = |\uparrow\rangle\,|\uparrow\rangle\,|\uparrow\rangle\,|\uparrow\rangle \ldots$$

Variational mean-field energy per lattice site

$$\frac{\langle \hat{H} \rangle_{\mathrm{mf}}}{N} = \frac{1}{2} \langle \hat{\boldsymbol{\sigma}}_\mu \rangle \cdot \boldsymbol{J} \cdot \langle \hat{\boldsymbol{\sigma}}_\nu \rangle + \boldsymbol{B} \cdot \langle \hat{\boldsymbol{\sigma}}_\mu \rangle$$

Neglect of correlations/entanglement!?


nber Z (neighbours)
complicated → mean-field ansatz
e.g.
n-field energy per lattice site
elations/entanglement!?
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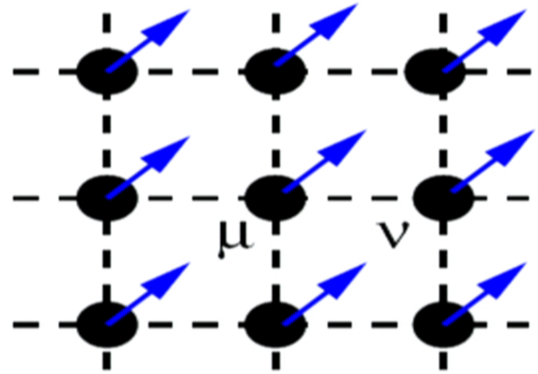
Z = 6

Correlations



Reduced density matrices
for lattice sites μ, ν etc.

$$\hat{\rho}_\mu = \mathrm{Tr}_{\not\mu}\{\hat{\rho}_{\mathrm{total}}\}$$
$$\hat{\rho}_{\mu\nu} = \mathrm{Tr}_{\not\mu\not\nu}\{\hat{\rho}_{\mathrm{total}}\}$$

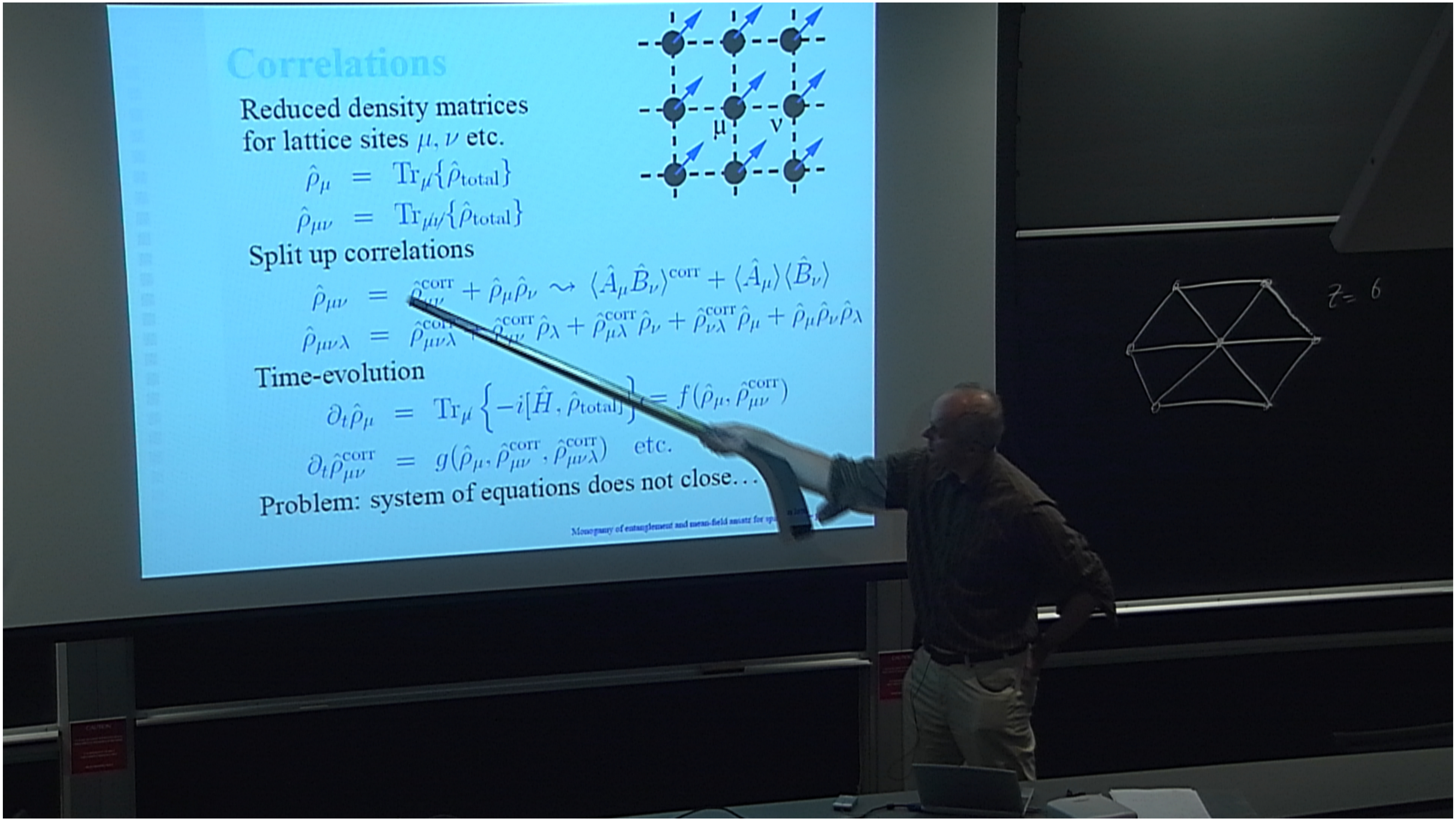
Split up correlations

$$\hat{\rho}_{\mu\nu} = \hat{\rho}^{\mathrm{corr}}_{\mu\nu} + \hat{\rho}_\mu\hat{\rho}_\nu \rightsquigarrow \langle\hat{A}_\mu\hat{B}_\nu\rangle^{\mathrm{corr}} + \langle\hat{A}_\mu\rangle\langle\hat{B}_\nu\rangle$$
$$\hat{\rho}_{\mu\nu\lambda} = \hat{\rho}^{\mathrm{corr}}_{\mu\nu\lambda} + \hat{\rho}^{\mathrm{corr}}_{\mu\nu}\hat{\rho}_\lambda + \hat{\rho}^{\mathrm{corr}}_{\mu\lambda}\hat{\rho}_\nu + \hat{\rho}^{\mathrm{corr}}_{\nu\lambda}\hat{\rho}_\mu + \hat{\rho}_\mu\hat{\rho}_\nu\hat{\rho}_\lambda$$

Time-evolution

$$\partial_t\hat{\rho}_\mu = \mathrm{Tr}_{\not\mu}\left\{-i[\hat{H},\hat{\rho}_{\mathrm{total}}]\right\} = f(\hat{\rho}_\mu, \hat{\rho}^{\mathrm{corr}}_{\mu\nu})$$
$$\partial_t\hat{\rho}^{\mathrm{corr}}_{\mu\nu} = g(\hat{\rho}_\mu, \hat{\rho}^{\mathrm{corr}}_{\mu\nu}, \hat{\rho}^{\mathrm{corr}}_{\mu\nu\lambda}) \quad \text{etc.}$$

Problem: system of equations does not close...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$\hat\rho_\mu = \mathrm{Tr}_{\mu'}\{\hat\rho_{\rm total}\}$
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Split up correlations
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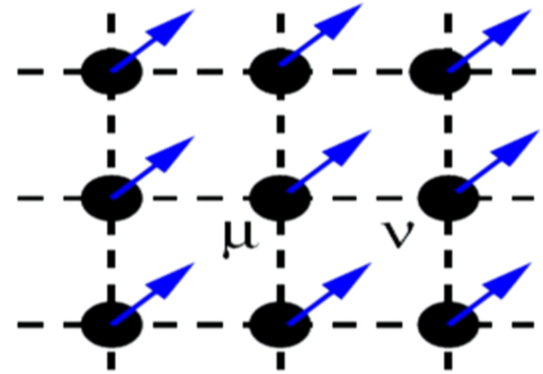
Problem: system of equations does not close…
μ
ν
z = 6

Correlations



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$$\partial_t \hat{\rho}_\mu = \mathrm{Tr}_{\not\mu}\left\{-i[\hat{H}, \hat{\rho}_{\mathrm{total}}]\right\} = f(\hat{\rho}_\mu, \hat{\rho}^{\mathrm{corr}}_{\mu\nu})$$
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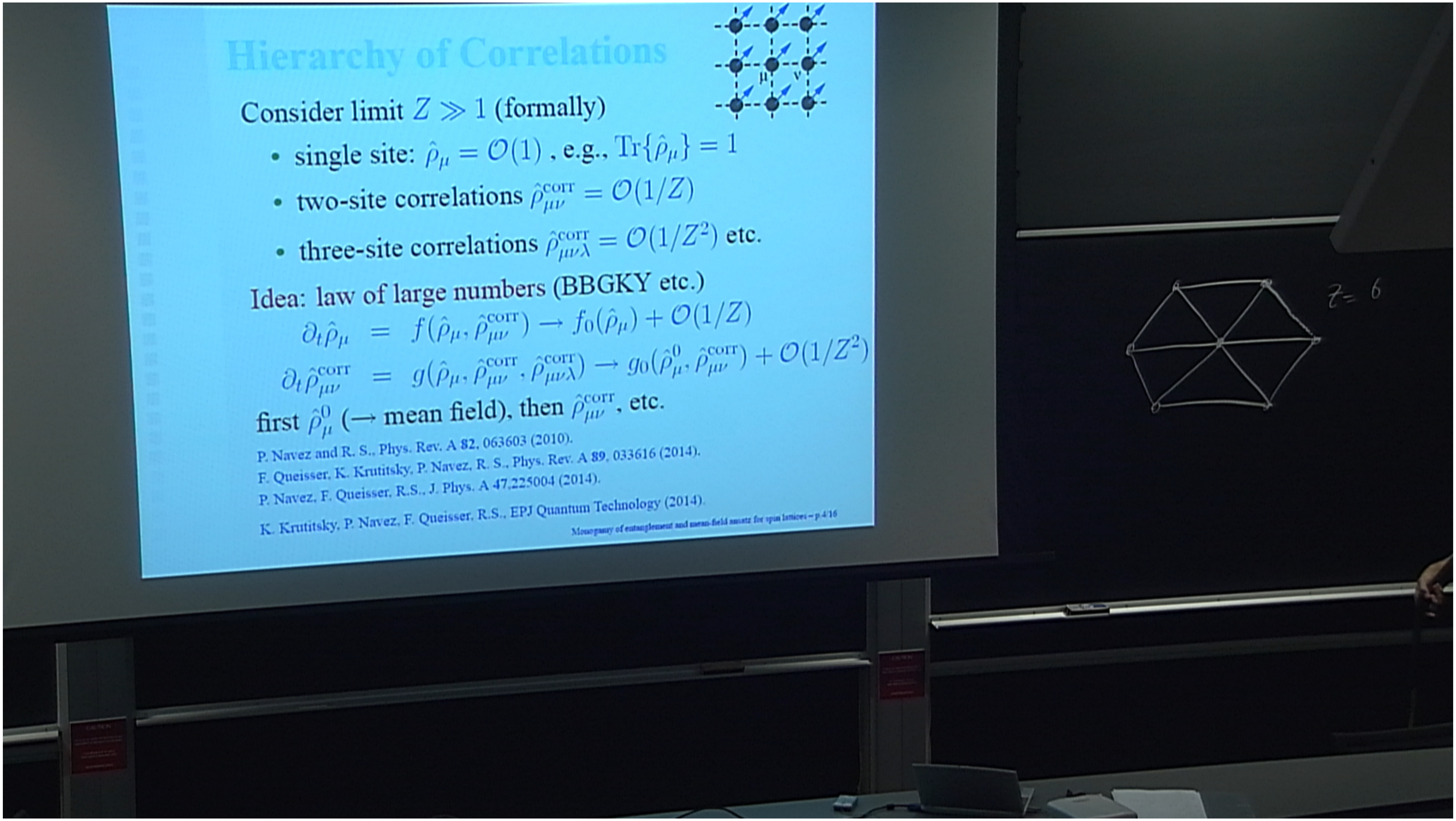
Hierarchy of Correlations
μ
ν
Consider limit $Z \gg 1$ (formally)
• single site: $\hat{\rho}_\mu = \mathcal{O}(1)$, e.g., $\mathrm{Tr}\{\hat{\rho}_\mu\} = 1$
• two-site correlations $\hat{\rho}^{\mathrm{corr}}_{\mu\nu} = \mathcal{O}(1/Z)$
• three-site correlations $\hat{\rho}^{\mathrm{corr}}_{\mu\nu\lambda} = \mathcal{O}(1/Z^2)$ etc.
Idea: law of large numbers (BBGKY etc.)
$\partial_t \hat{\rho}_\mu = f(\hat{\rho}_\mu, \hat{\rho}^{\mathrm{corr}}_{\mu\nu}) \to f_0(\hat{\rho}_\mu) + \mathcal{O}(1/Z)$
$\partial_t \hat{\rho}^{\mathrm{corr}}_{\mu\nu} = g(\hat{\rho}_\mu, \hat{\rho}^{\mathrm{corr}}_{\mu\nu}, \hat{\rho}^{\mathrm{corr}}_{\mu\nu\lambda}) \to g_0(\hat{\rho}^0_\mu, \hat{\rho}^{\mathrm{corr}}_{\mu\nu}) + \mathcal{O}(1/Z^2)$
first $\hat{\rho}^0_\mu$ (→ mean field), then $\hat{\rho}^{\mathrm{corr}}_{\mu\nu}$, etc.
P. Navez and R. S., Phys. Rev. A 82, 063603 (2010).
F. Queisser, K. Krutitsky, P. Navez, R. S., Phys. Rev. A 89, 033616 (2014).
P. Navez, F. Queisser, R.S., J. Phys. A 47,225004 (2014).
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Monogamy of entanglement and mean-field ansatz for spin lattices – p.4/16
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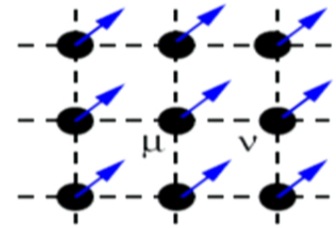

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Entanglement for Pure States

Consider two spins (qubits) μ and ν: not entangled iff

$$|\Psi_{\mu\nu}\rangle = |\psi_\mu\rangle\,|\psi_\nu\rangle \ , \text{ e.g., } |\uparrow\rangle_\mu \frac{|\uparrow\rangle_\nu + |\downarrow\rangle_\nu}{\sqrt{2}}$$

Maximum entanglement (Bell state)

$$|\Psi_{\mu\nu}\rangle = \frac{|\uparrow\rangle_\mu\,|\uparrow\rangle_\mu + |\downarrow\rangle_\nu\,|\downarrow\rangle_\nu}{\sqrt{2}} = |\text{Bell}\rangle_{\mu\nu}$$

General state with concurrence C with $0 \leq C \leq 1$

$$|\Psi_{\mu\nu}\rangle = \sqrt{1-C}\ |\psi_\mu\rangle\ |\psi_\nu\rangle + \sqrt{C}\,\hat{U}_\mu \hat{U}_\nu\,|\text{Bell}\rangle_{\mu\nu}$$

W.K. Wootters, Phys. Rev. Lett. **80**, 2245 (1998).

Note: qutrits or three qubits are more complicated

$$|\Psi_{\text{GHZ}}\rangle = \frac{|\uparrow\rangle\,|\uparrow\rangle\,|\uparrow\rangle + |\downarrow\rangle\,|\downarrow\rangle\,|\downarrow\rangle}{\sqrt{2}}$$

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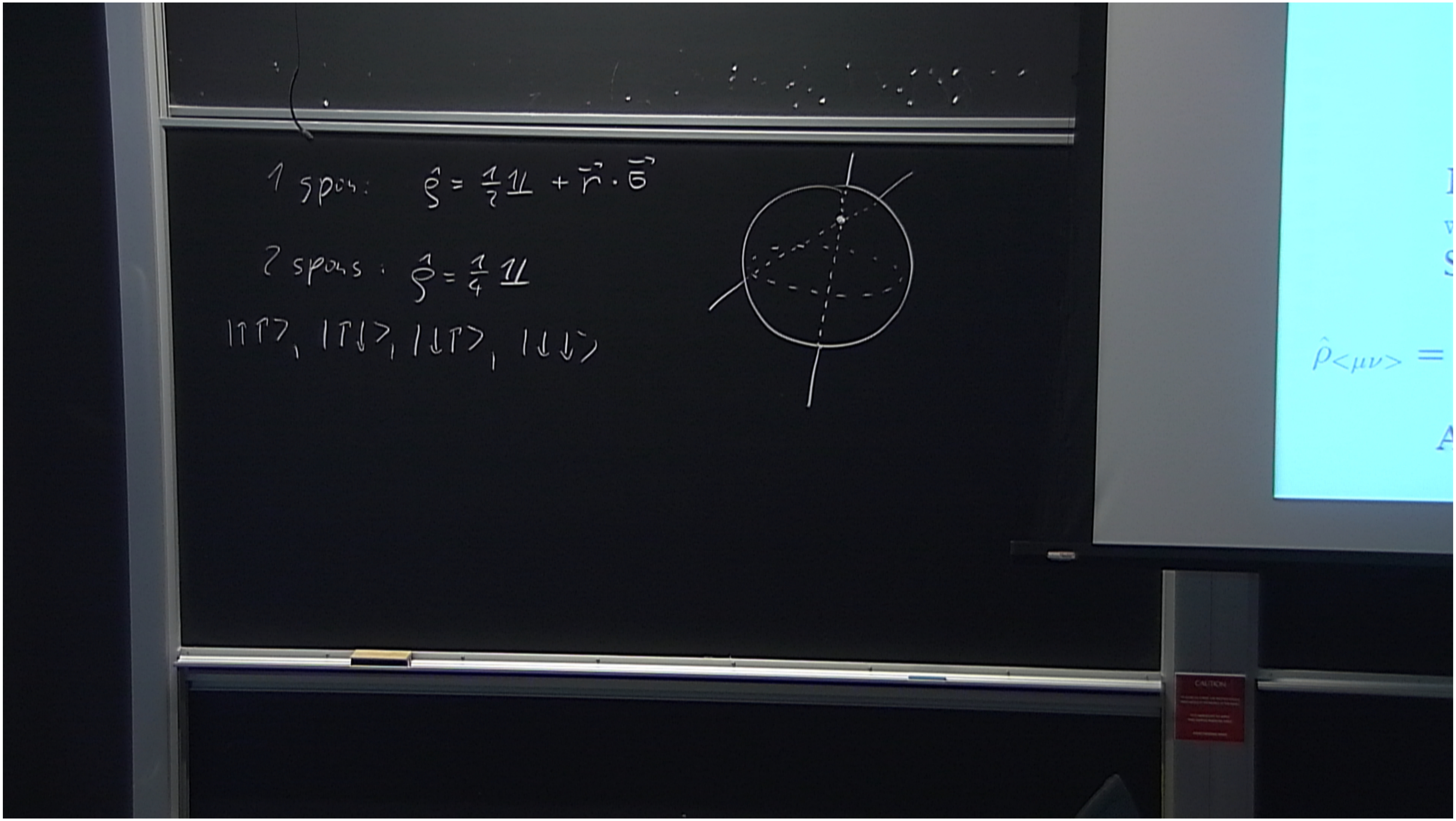

1 spin: ρ̂ = 1/2 𝟙 + r⃗ · σ⃗
2 spins: ρ̂ = 1/4 𝟙
|↑↑⟩, |↑↓⟩, |↓↑⟩, |↓↓⟩

Monogamy of Entanglement

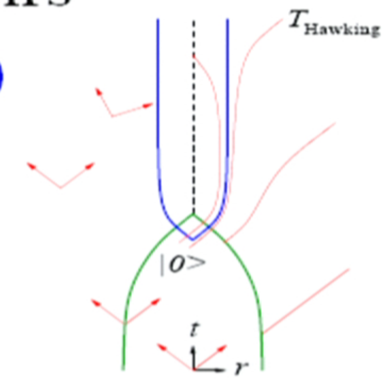
Upper bound for concurrence of qubit-pairs

$$\tau_1(\hat{\rho}_\mu) = 4\det(\hat{\rho}_\mu) \geq \sum_\nu C^2(\hat{\rho}_{<\mu\nu>})$$

with one-tangle $\tau_1(\hat{\rho}_\mu) \leq 1$

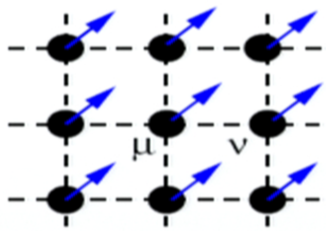
V. Coffman, J. Kundu, W.K. Wootters, Phys. Rev. A **61**, 052306 (2000);

T.J. Osborne, F. Verstraete, Phys. Rev. Lett. **96**, 220503 (2006).



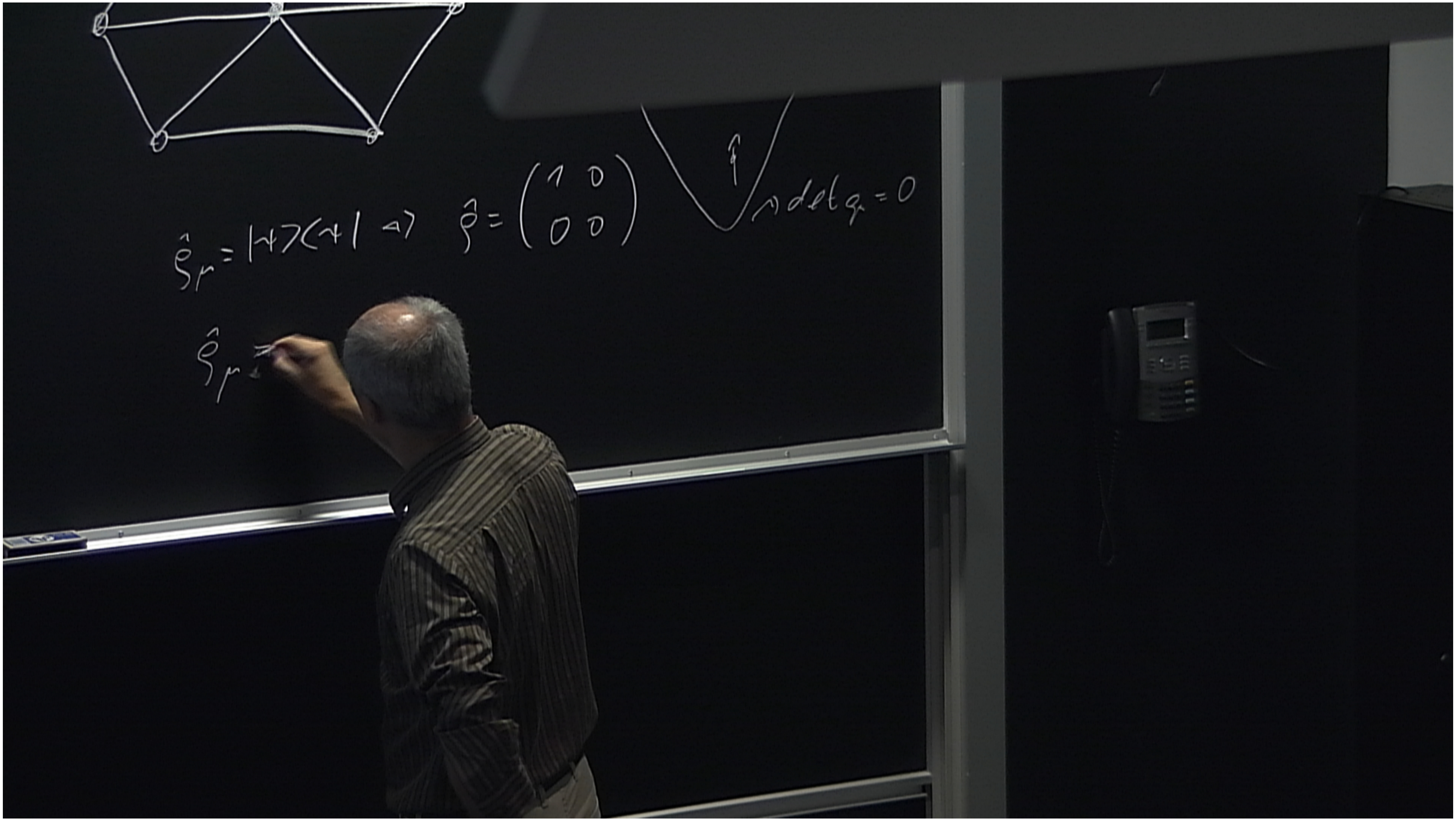
Lattice isotropy

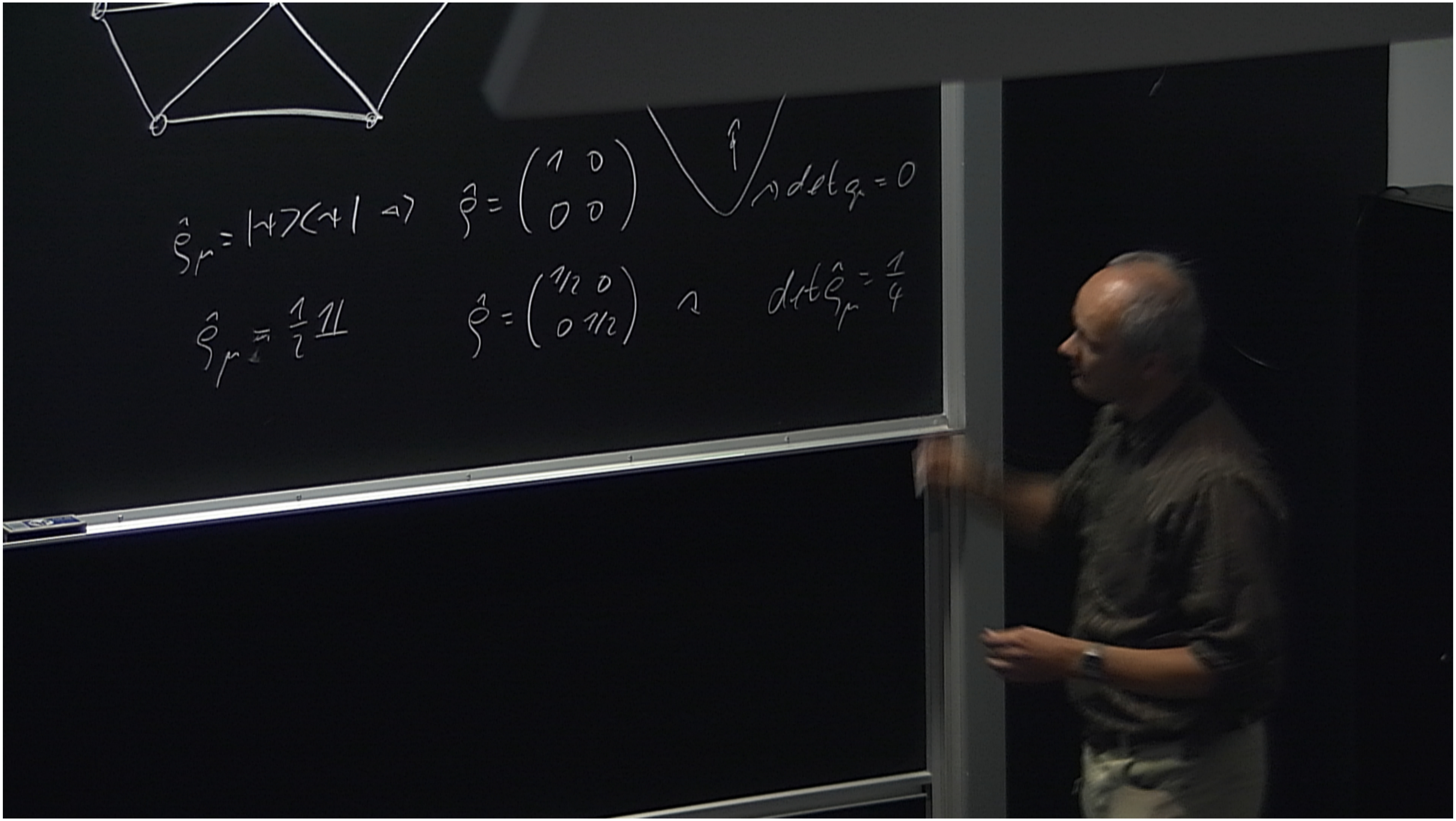
$$C(\hat{\rho}_{<\mu\nu>}) \leq \sqrt{\frac{\tau_1}{Z}} \leq \sqrt{\frac{1}{Z}}$$

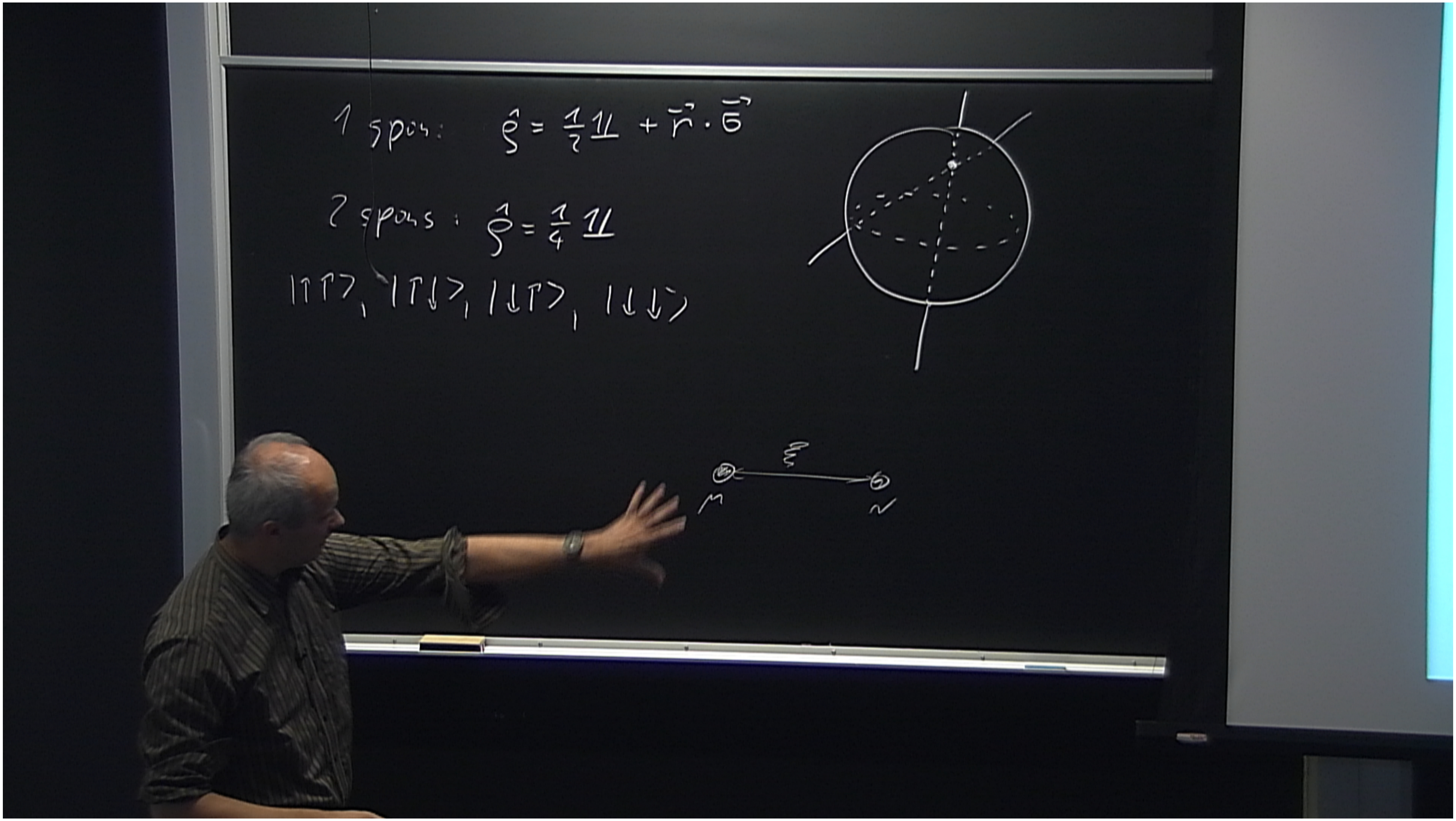


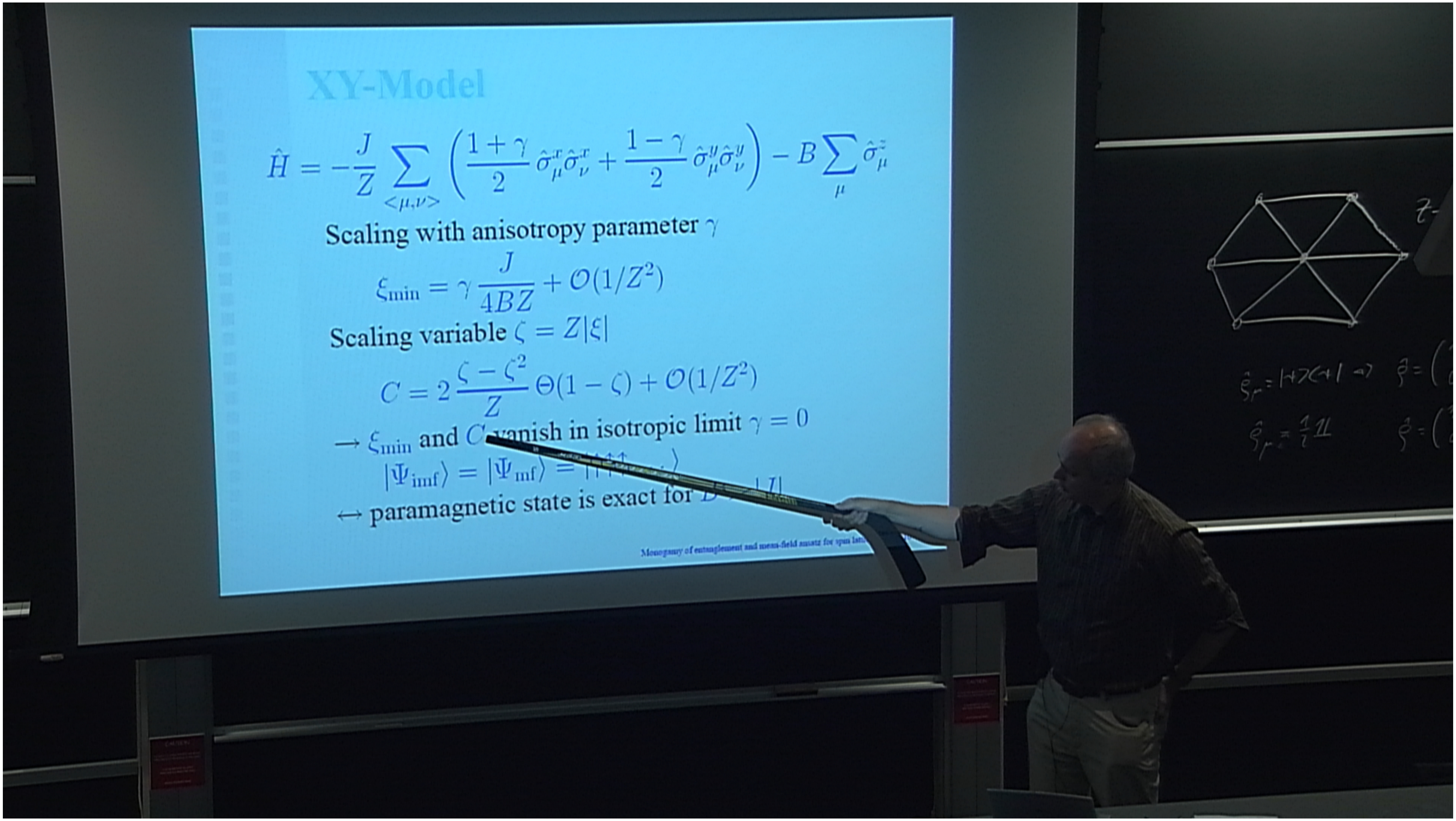
Entanglement decreases for large Z

Expectation: mean-field ansatz becomes better

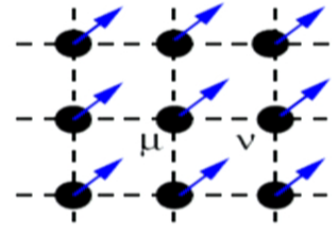



$\hat{\rho}_\mu = |+\rangle\langle+| \rightarrow \hat{\rho} = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} \rightarrow \det \rho_\mu = 0$
$\hat{\rho}_\mu = \frac{1}{2}\mathbb{1} \quad \hat{\rho} = \begin{pmatrix} 1/2 & 0 \\ 0 & 1/2 \end{pmatrix} \rightarrow \det \hat{\rho}_\mu = \frac{1}{4}$


1 spin: ρ = ½ 𝟙 + r⃗ · σ⃗
2 spins: ρ = ¼ 𝟙
|↑↑>, |↑↓>, |↓↑>, |↓↓>


XY-Model
$\hat{H} = -\frac{J}{Z} \sum_{<\mu,\nu>} \left(\frac{1+\gamma}{2} \hat{\sigma}^x_\mu \hat{\sigma}^x_\nu + \frac{1-\gamma}{2} \hat{\sigma}^y_\mu \hat{\sigma}^y_\nu \right) - B \sum_\mu \hat{\sigma}^z_\mu$
Scaling with anisotropy parameter γ
$\xi_{\min} = \gamma \frac{J}{4BZ} + \mathcal{O}(1/Z^2)$
Scaling variable $\zeta = Z|\xi|$
$C = 2\frac{\zeta - \zeta^2}{Z} \Theta(1-\zeta) + \mathcal{O}(1/Z^2)$
$\rightarrow \xi_{\min}$ and C vanish in isotropic limit $\gamma = 0$
$\leftrightarrow$ paramagnetic state is exact for

Conclusions & Outlook



Nearest-neighbour interactions only:

$$\frac{\langle\hat{H}\rangle_{\mathrm{mf}}}{N} - \frac{\langle\hat{H}\rangle_{\mathrm{exact}}}{N} \leq (||\boldsymbol{J}|| + 2||\boldsymbol{B}||)\sqrt{C} + \mathcal{O}(C)$$

Concurrence C measures deviation from mean field

- $C = 0 \leftrightarrow$ mean field yields exact ground state
- monogamy: $Z \gg 1 \rightarrow C \leq 1/\sqrt{Z} \ll 1$
- unique mean-field ground state: $C = \mathcal{O}(Z^{-2/3})$
- improved mean-field ansatz: $C = \mathcal{O}(1/Z)$
  (note: not rigorously proven)

Outlook: bi-partite $\longrightarrow$ tri-partite entanglement. . .

A. Osterloh, R.S., arXiv:1406.0311