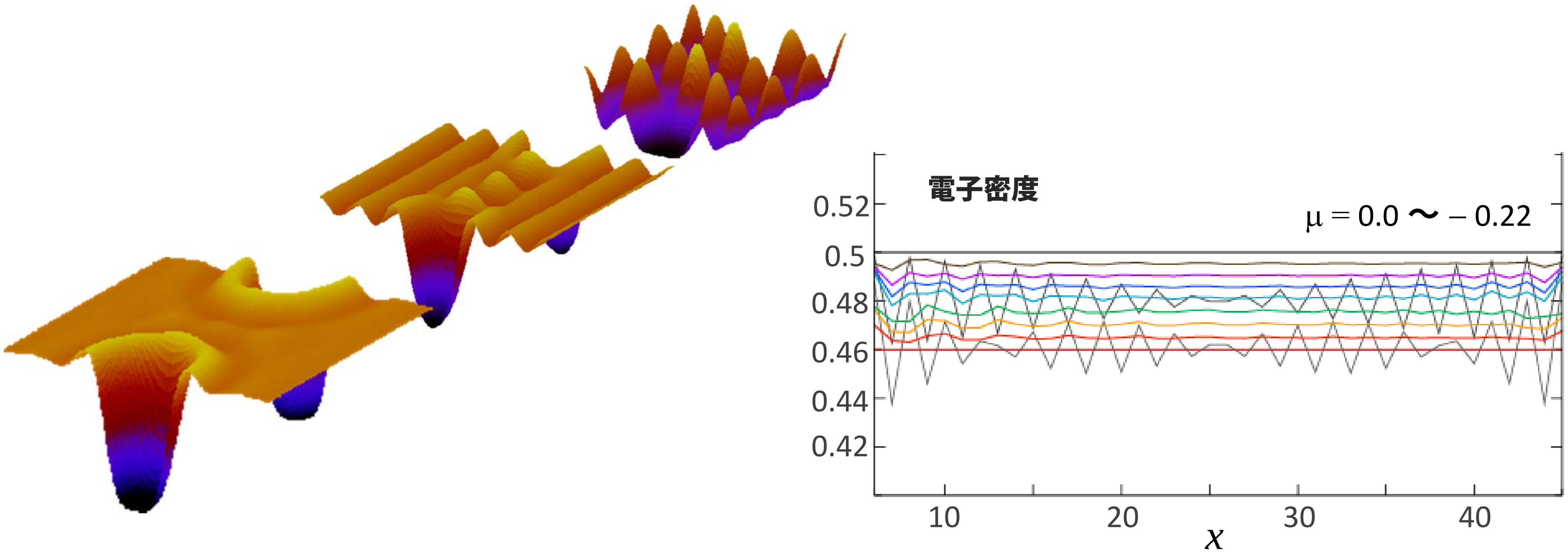
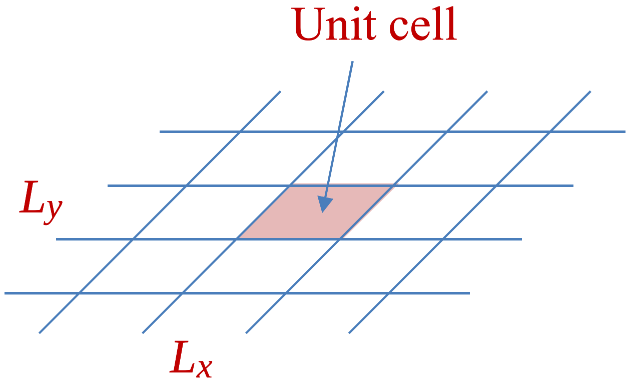
二次元量子系へのDMRG の応用と外場応答の計算

東北大学 理学研究科　柴田 尚和

- 量子二次元系への適用について
- トポロジカル・エンタングルメント・エントロピーの効果
- エネルギースケールの空間変調と外場応答
- カゴメ格子の多段磁化プラトー



Application of DMRG to 2D systems



Periodic boundary conditions
for both x and y directions

$k_y = 2\pi n/L_y = X_n / l^2$

Initial basis states

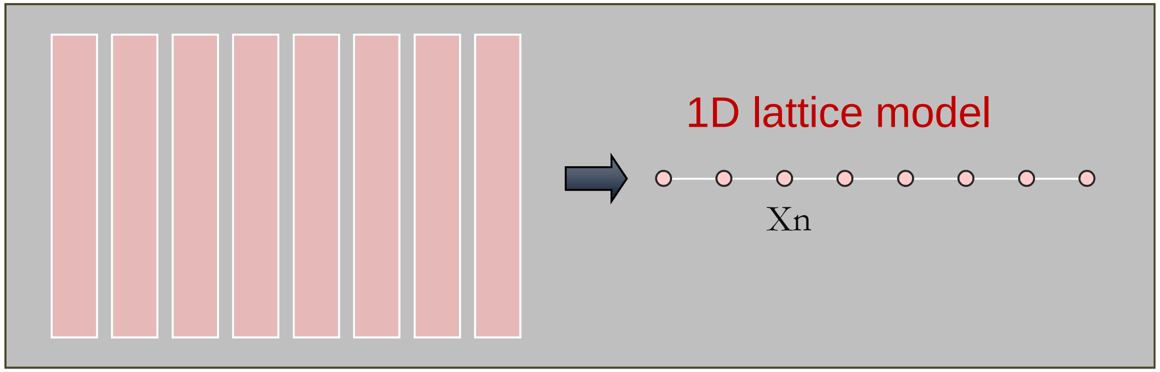
$$\varphi_{XN}(\mathbf{r}) = \exp\left[\, i\,\frac{X_n\, y}{l^2} - \frac{(x - X_n)^2}{2l^2}\right] H_N\!\left(\frac{x - X_n}{l}\right)$$

H_N : Hermite polynomials

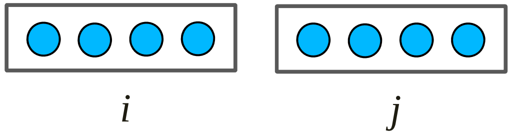
One particle states are uniquely
specified by X_n and N

X_n: guiding center
N : Landau level index

Mapping on to effective 1D lattice model



Density matrix renormalization



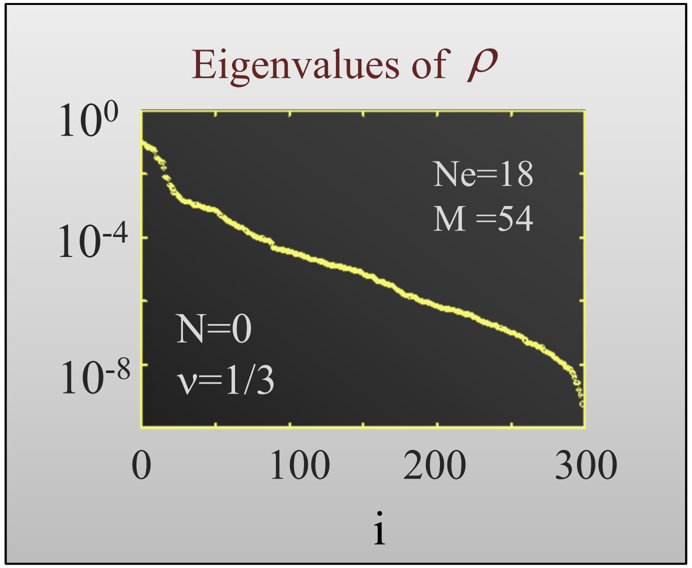
Ground state $|\Psi> = \Psi_{ij} \, |i>|j>$

Density matrix $\rho_{ii'} = \sum_j \Psi^{*}_{ij} \Psi_{i'j}$

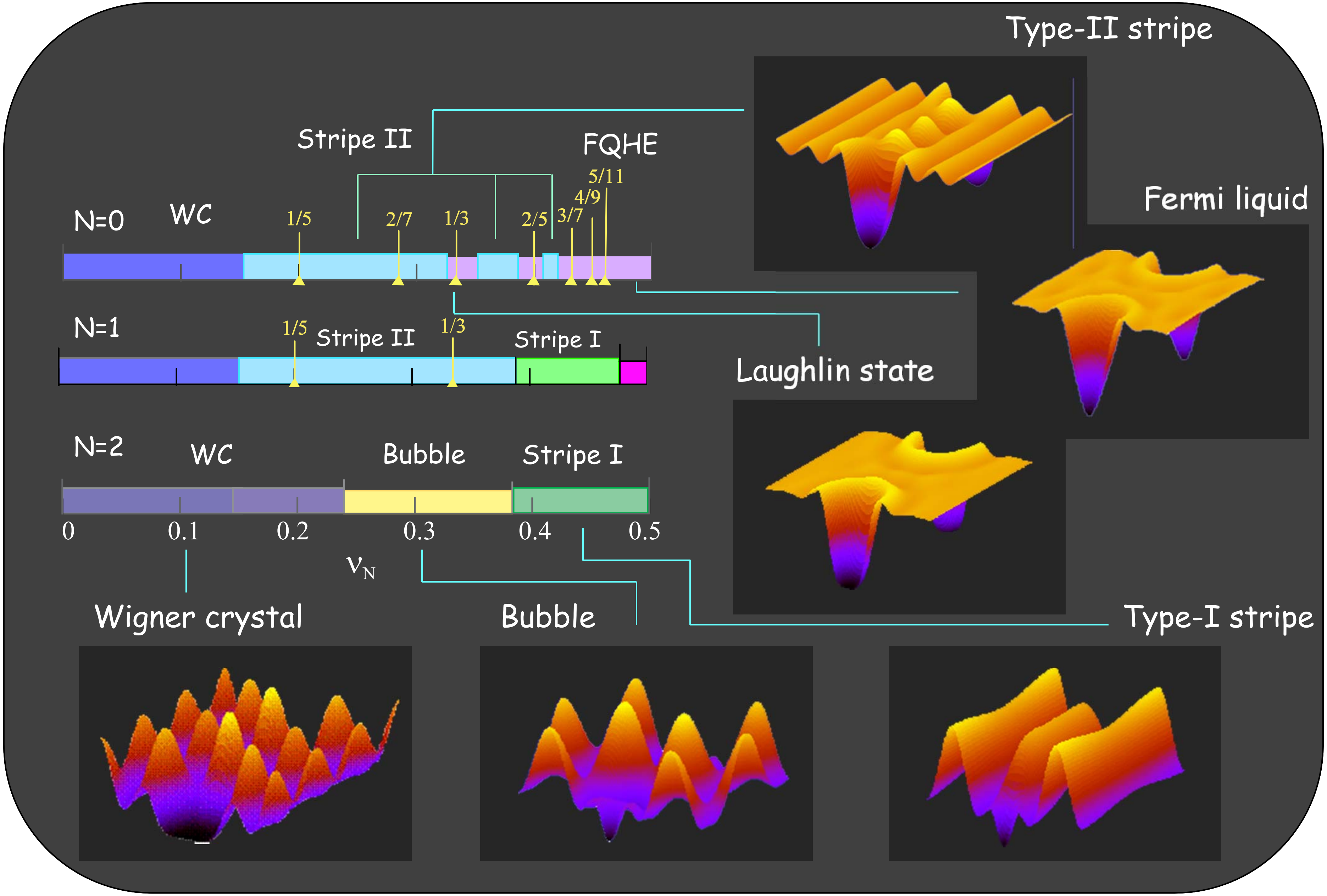
Norm $<\Psi|\Psi> = \mathrm{Tr}\, \rho$

Ground state energy (Ne=10)

DMRG	m=100	-3.239340
	m=200	-3.239686
	m=300	-3.239981
	m=400	-3.239993
N=2 ν=1/2	Exact	-3.239995

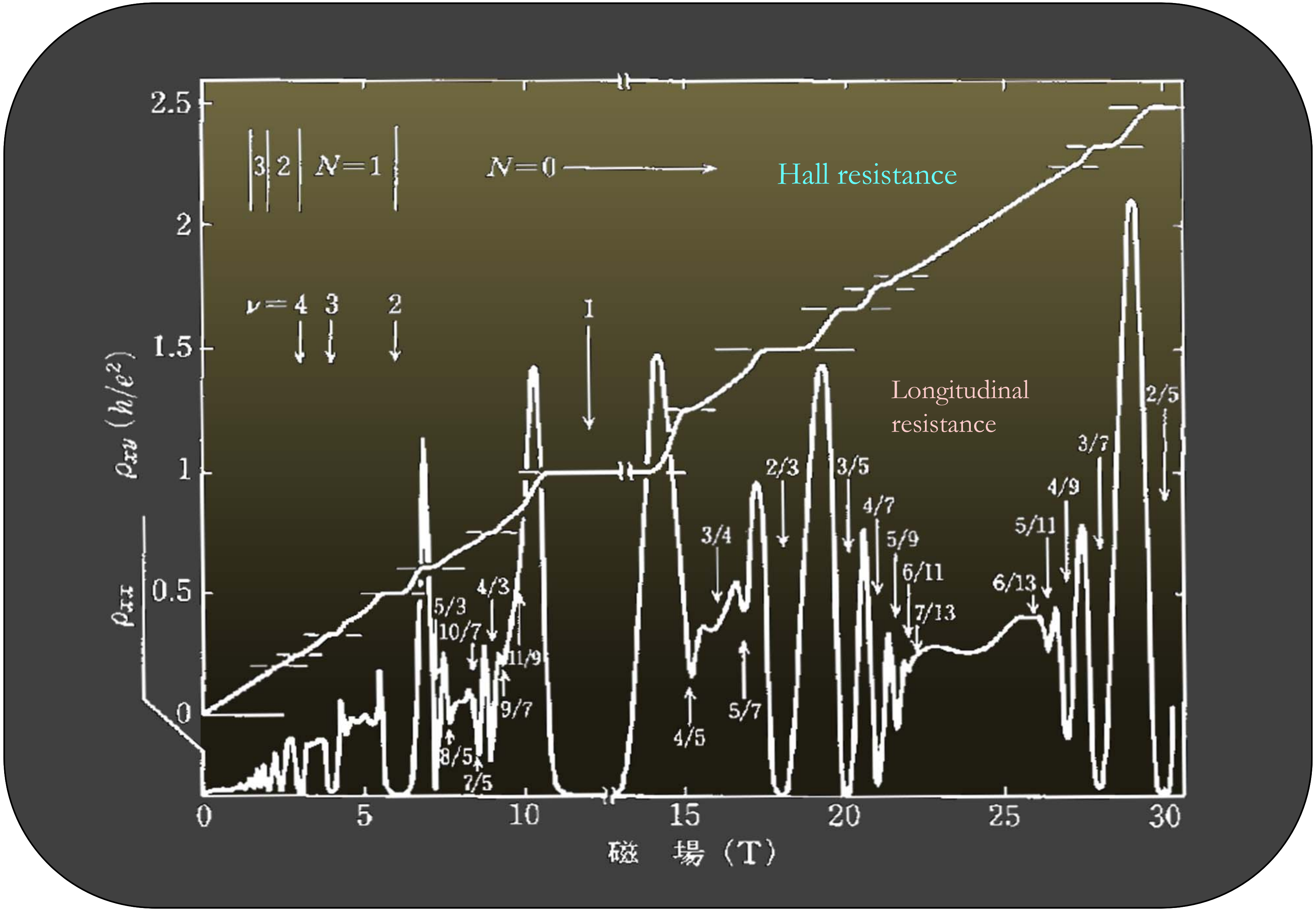


Ground state of quantum Hall systems



Fractional quantum Hall effect

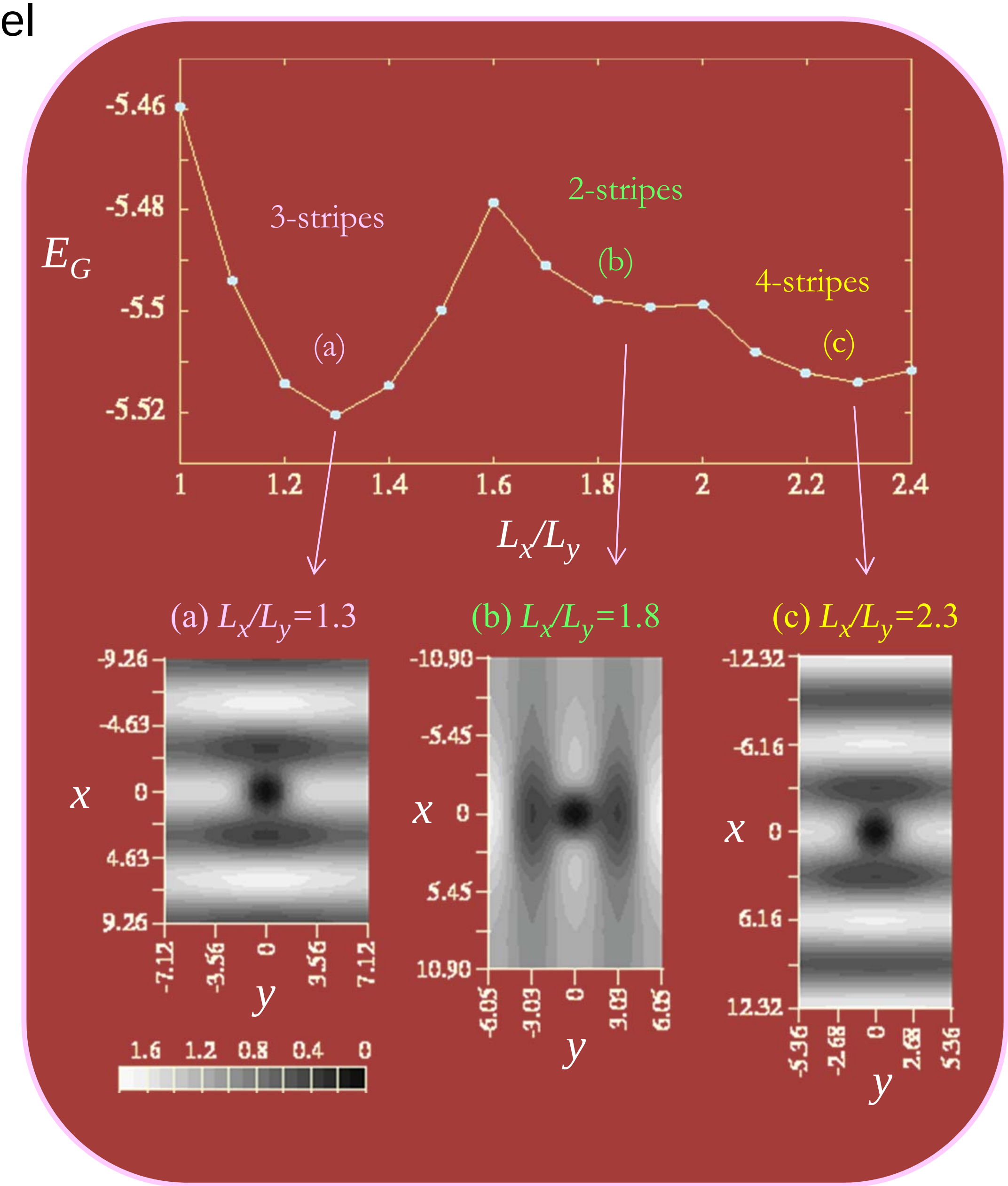
R. Willett *et al* (1987)



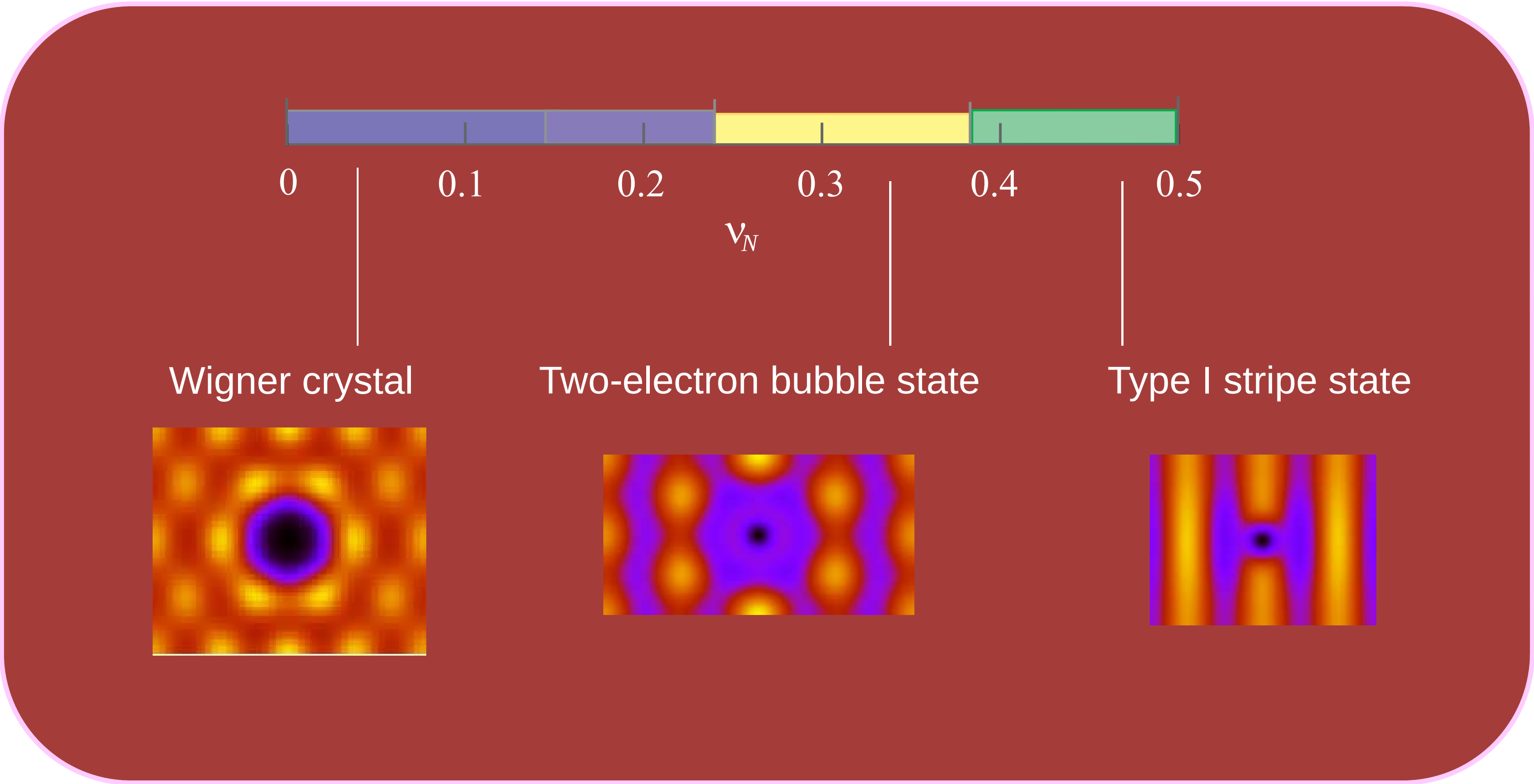
Stripe state

N=2 Landau level

$\nu=3/7$



Ground state of N=2 Landau level



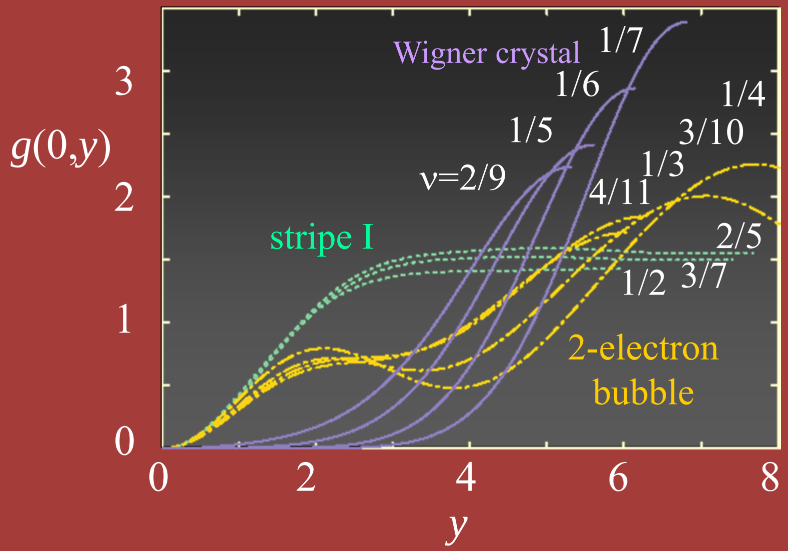
Wigner crystal

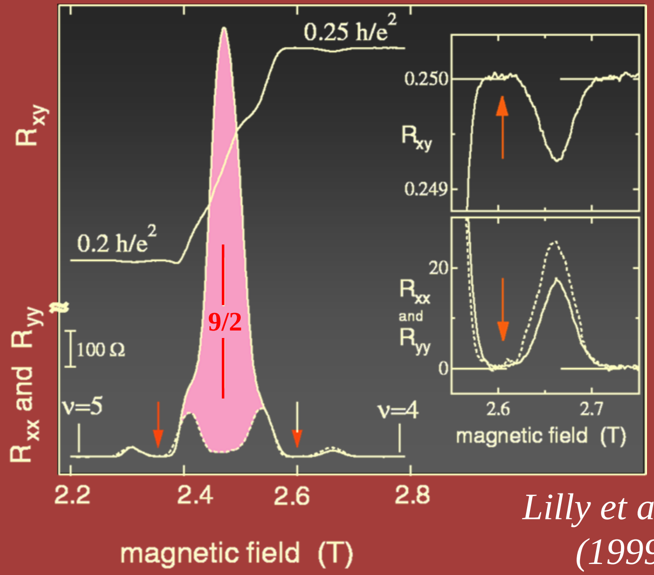
Two-electron bubble state

Type I stripe state

Shibata and Yoshioka: Phys. Rev. Lett. **86** 5755 (2001)

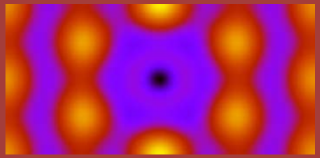
Stripe and bubble states



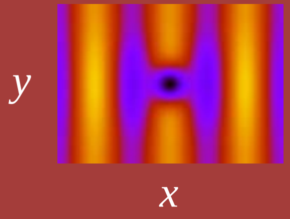


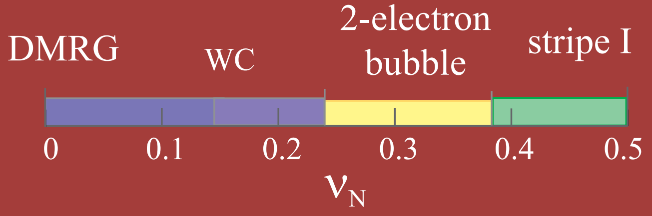
Lilly et al.
(1999)

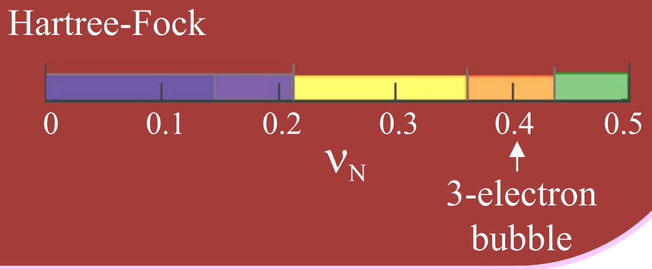
Two-electron bubble state



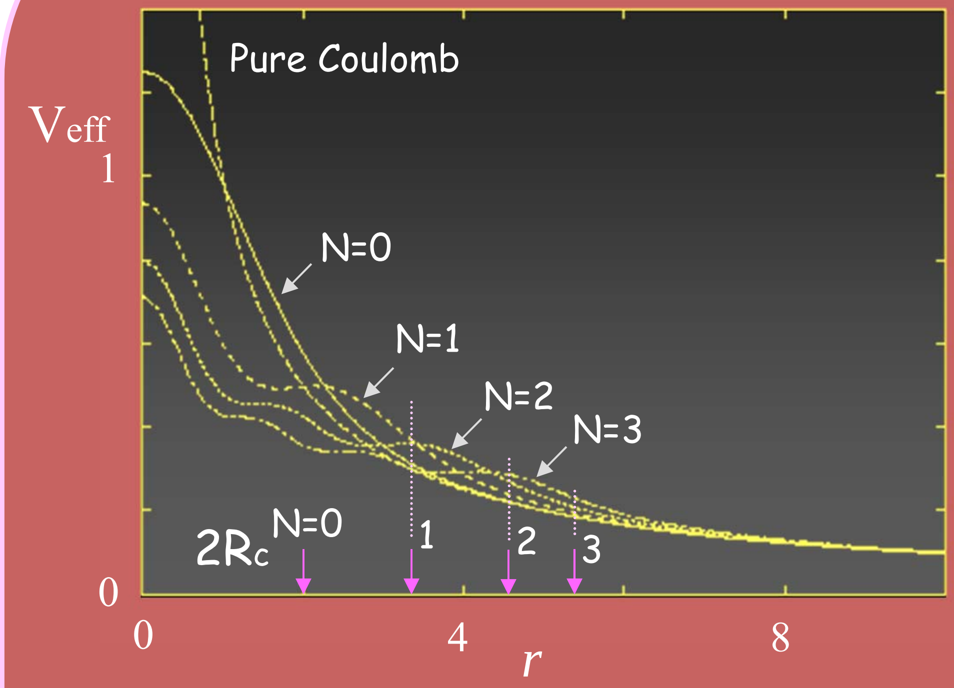
Type I stripe state



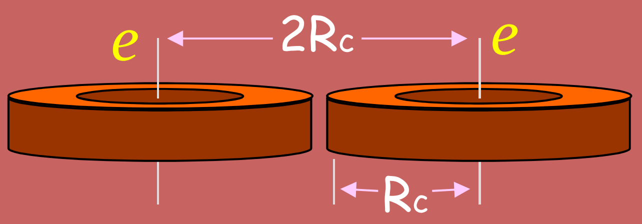




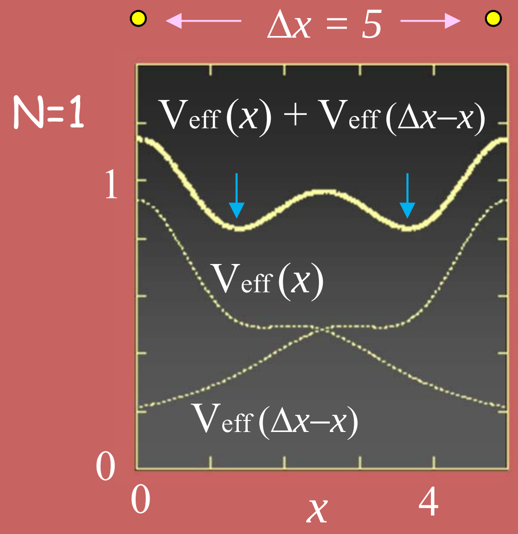
Effective interaction in higher Landau levels

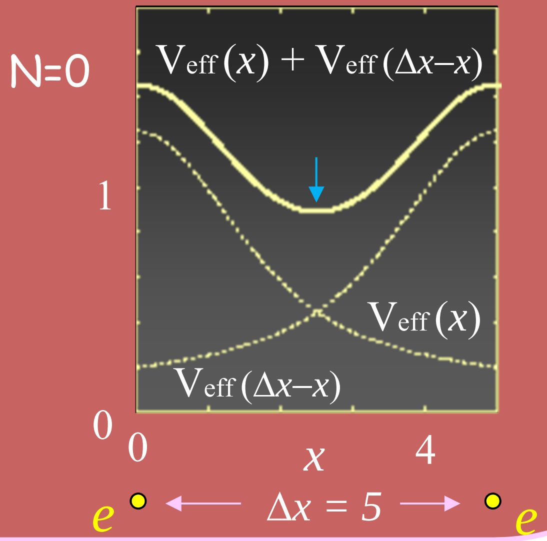


R_c : cyclotron radius



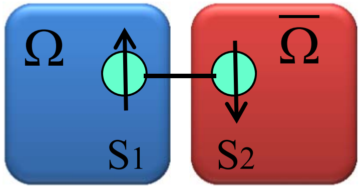
Potential energy generated by the two electrons separated by Δx





Entanglement entropy

S=1/2 2-Spin system



$S_1 = \uparrow$ or $\downarrow$

$S_2 = \uparrow$ or $\downarrow$

Wave function

$$|\Psi> = \sum_{S_1S_2} \Psi_{S_1S_2}\,|S_1>|S_2>$$

$$\Psi_{S1\,S2} : \begin{pmatrix} \Psi_{\uparrow\uparrow} & \Psi_{\uparrow\downarrow} \\ \Psi_{\downarrow\uparrow} & \Psi_{\downarrow\downarrow} \end{pmatrix} = \Psi$$

Reduced density matrix

$$\rho_\Omega = \Psi^* \Psi^t$$

$$(\rho_\Omega)_{ii'} = \sum_j \Psi^*_{ij} \Psi_{i'j}$$

Entanglement entropy

$$S_\Omega = -Tr\,\rho_\Omega \ln \rho_\Omega$$

*S*1 is independent of *S*2

- Not correlated -

$$\frac{1}{\sqrt{2}}\underbrace{(|\uparrow\uparrow> + |\uparrow\downarrow>)}_{S_1S_2} \Rightarrow \Psi = \begin{pmatrix} \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \\ 0 & 0 \end{pmatrix}$$

$$= \frac{1}{\sqrt{2}}|\underset{S1}{\uparrow}> \otimes (|\underset{S2}{\uparrow}> + |\downarrow>)$$

$$\rho_\Omega = \overset{\Psi^*}{\begin{pmatrix} \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \\ 0 & 0 \end{pmatrix}} \overset{\Psi^t}{\begin{pmatrix} \frac{1}{\sqrt{2}} & 0 \\ \frac{1}{\sqrt{2}} & 0 \end{pmatrix}} = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}$$

$$S_\Omega = -\ln 1 = 0$$

disentangled

*S*1 depends on *S*2

- correlated -

$$\frac{1}{\sqrt{2}}(|\uparrow\downarrow> - |\downarrow\uparrow>) \Rightarrow \Psi = \begin{pmatrix} 0 & \frac{1}{\sqrt{2}} \\ -\frac{1}{\sqrt{2}} & 0 \end{pmatrix}$$

Singlet state

$$\rho_\Omega = \overset{\Psi^*}{\begin{pmatrix} 0 & \frac{1}{\sqrt{2}} \\ -\frac{1}{\sqrt{2}} & 0 \end{pmatrix}} \overset{\Psi^t}{\begin{pmatrix} 0 & -\frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} & 0 \end{pmatrix}} = \begin{pmatrix} \frac{1}{2} & 0 \\ 0 & \frac{1}{2} \end{pmatrix}$$

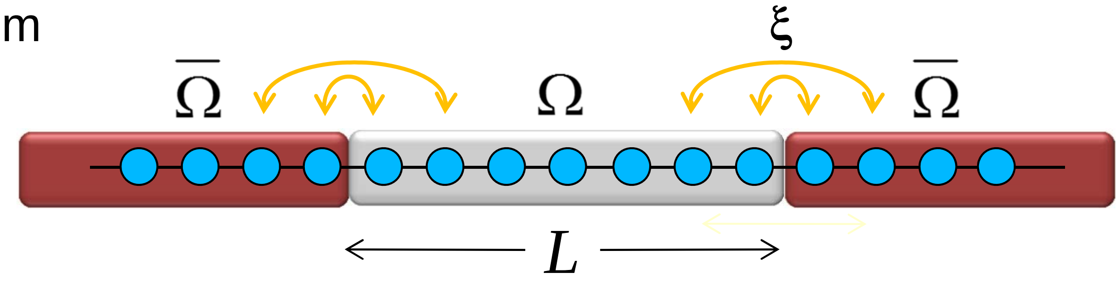
$$S_\Omega = 2\left(\frac{1}{2}\ln 2\right) = \ln 2$$

entangled

Scaling of entanglement entropy

$$S_{\Omega(L)} = -Tr\,\rho_{\Omega(L)} \ln \rho_{\Omega(L)}$$

1D system



Short range correlation :

$$S_{\Omega(L)} \approx const.$$

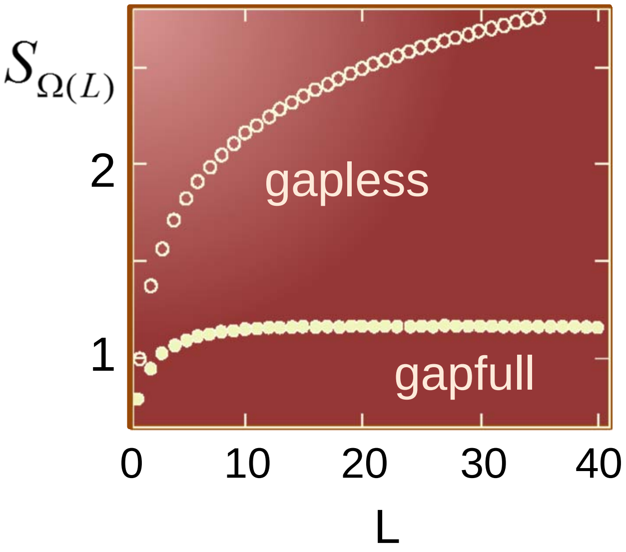
(L >> **correlation length** ξ)

Power law correlation : (1D critical system)

$$S_{\Omega(L)} \approx \frac{c}{3} \ln L + s_0$$

$$L \rightarrow \infty$$

1D-XXZ model



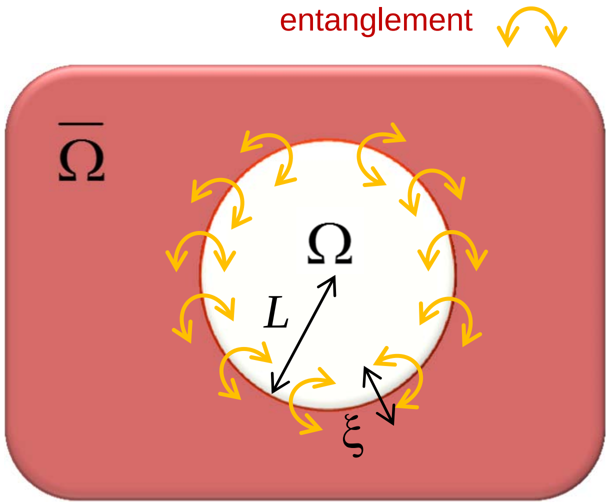
Scaling of entanglement entropy

Short range correlation $(L >> \xi)$

D-dimensional system

Area law $S_{\Omega(L)} \propto L^{D-1}$

L^{D-1} : boundary size (length)



Topological order in 2D

$$S_{\Omega(L)} = \underbrace{\alpha L}_{\text{Boundary term}} - \underbrace{\ln D}_{\text{Topological term}}$$

Non-trivial universal correction

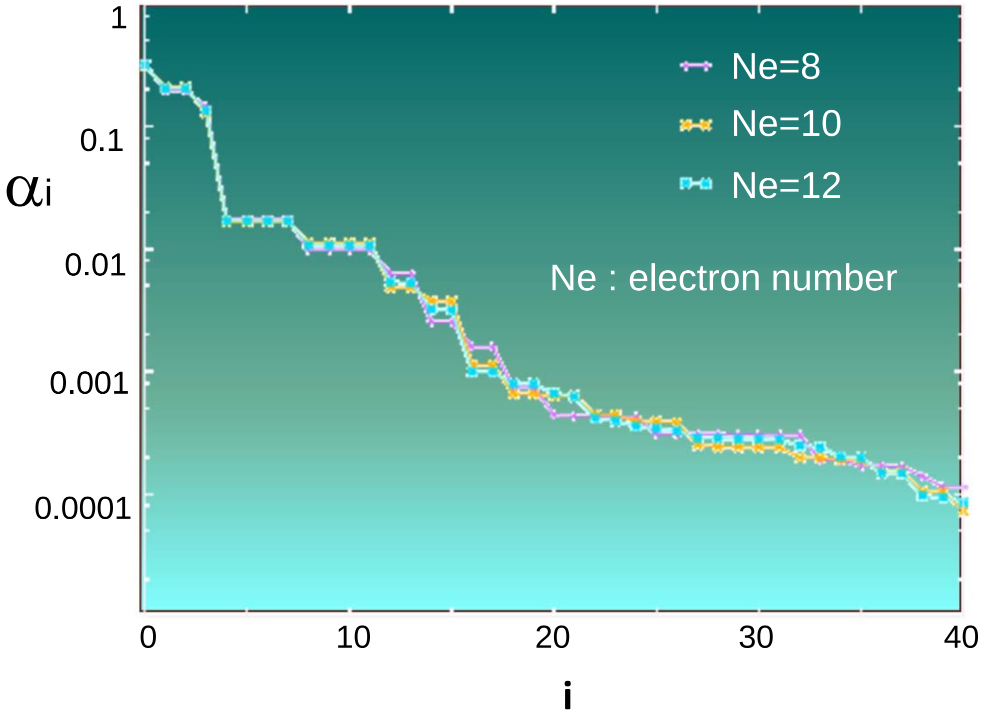
Fractional quantum Hall state

$\nu = 1/m$ Laughlin state : $D = m^{1/2}$

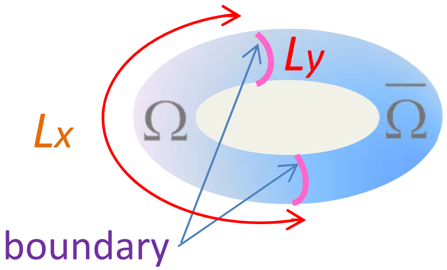
Density matrix eigenvalues α_i

Torus geometry

Fractional quantum Hall state $\nu = 1/3$



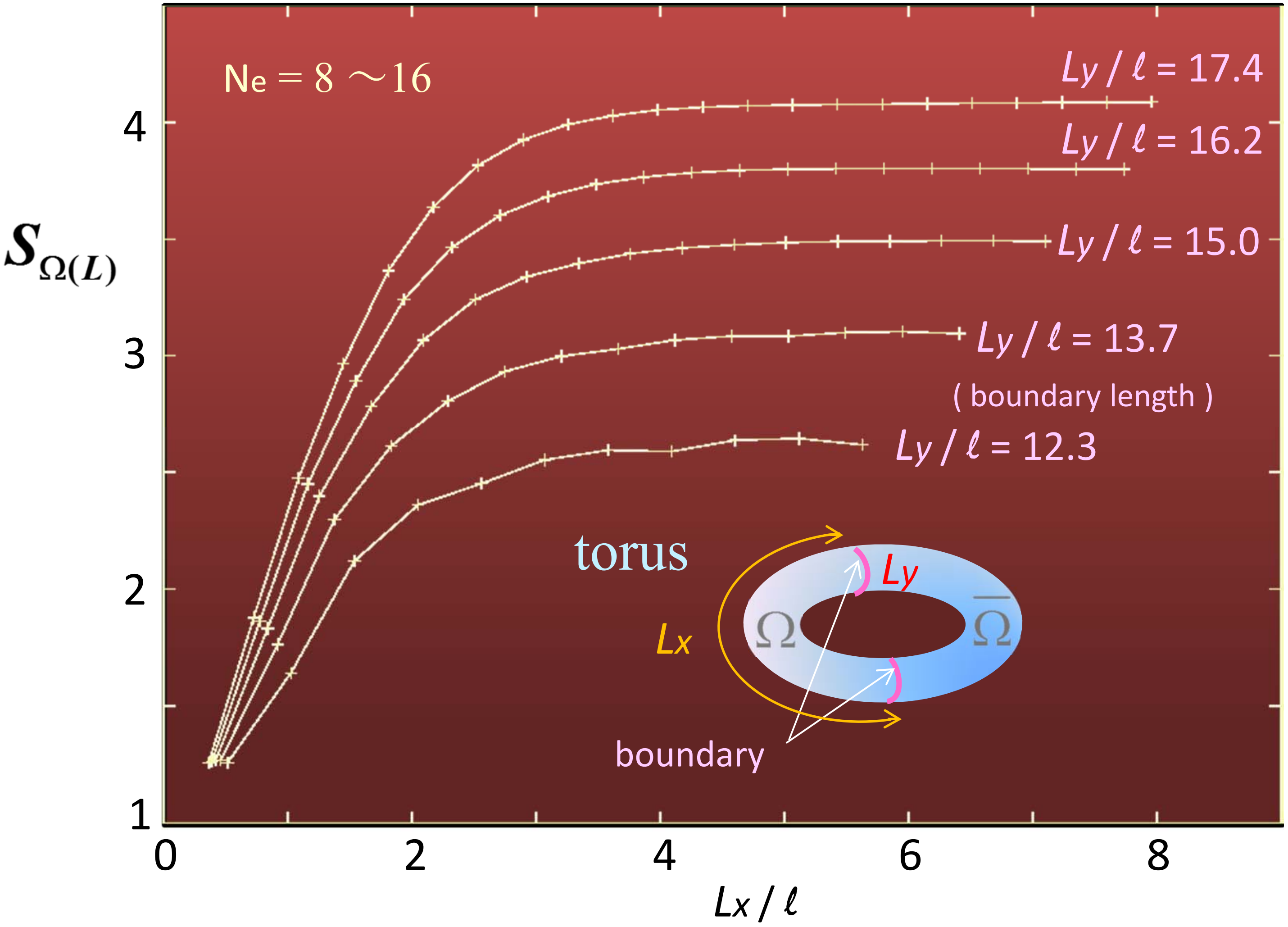
torus



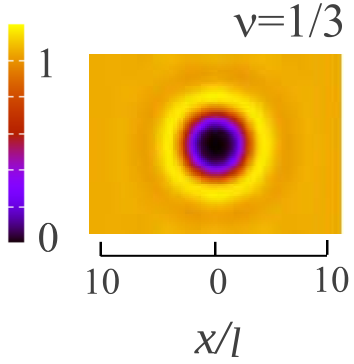
Entanglement entropy

Torus geometry

Fractional quantum Hall state $\nu = 1/3$



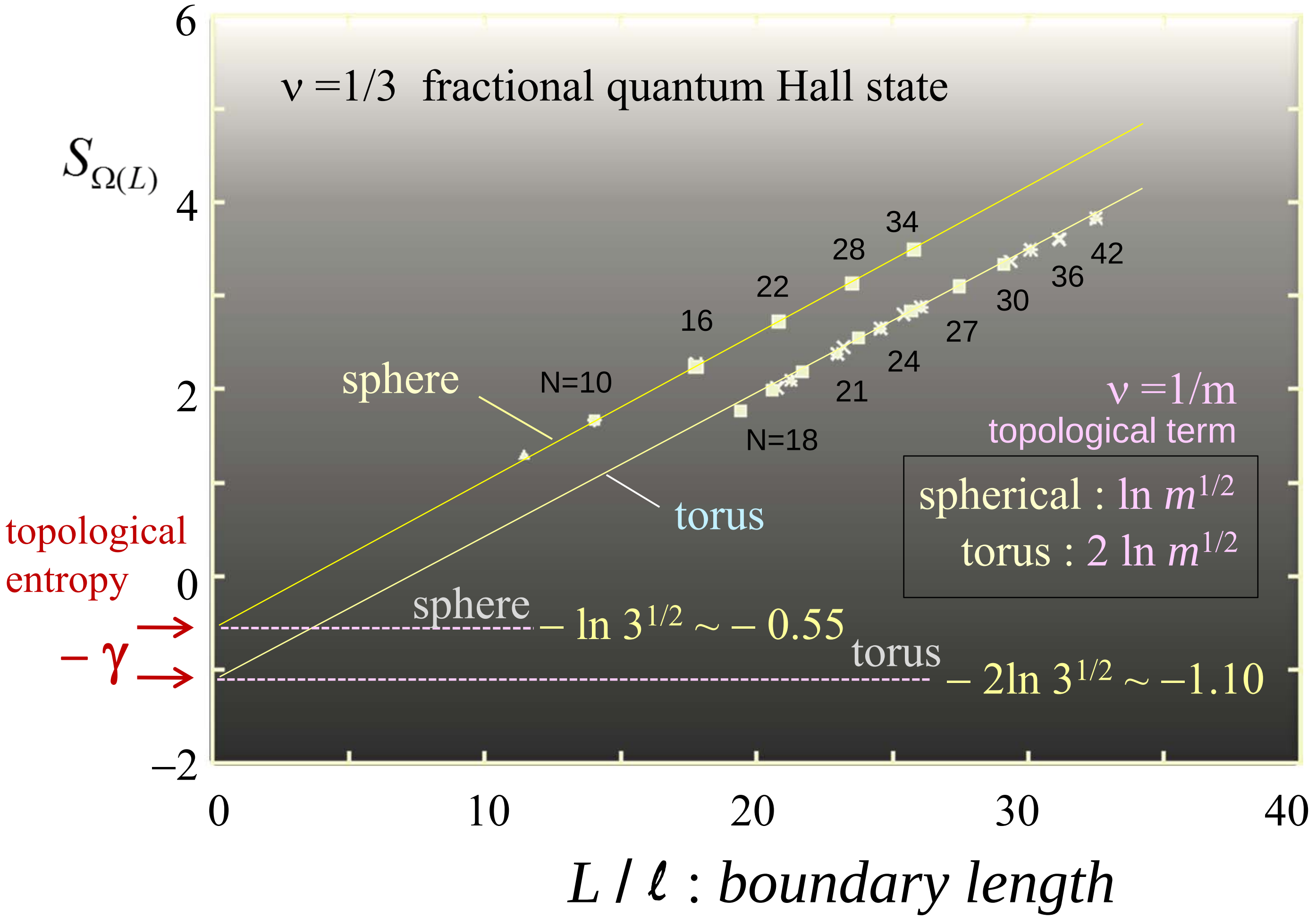
Pair correlation functions



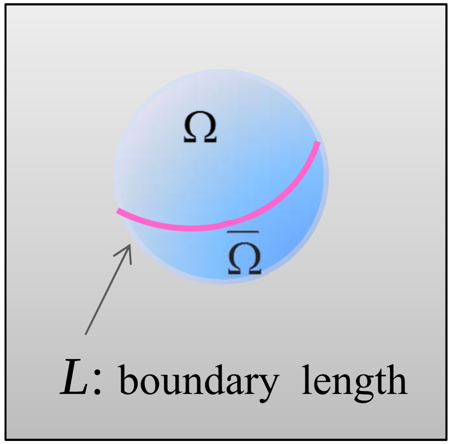
Entanglement entropy

Entanglement entropy $S_{\Omega(L)} = \underline{\alpha L} - \underline{\gamma}$

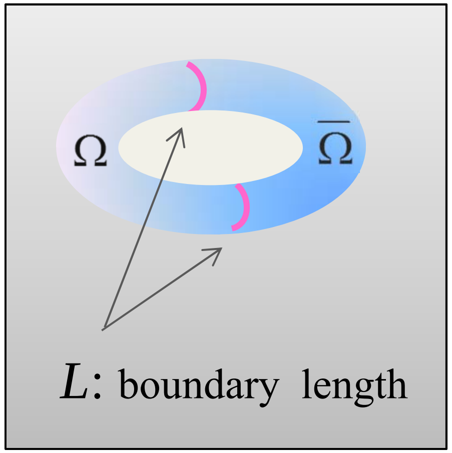
boundary term topological term



sphere



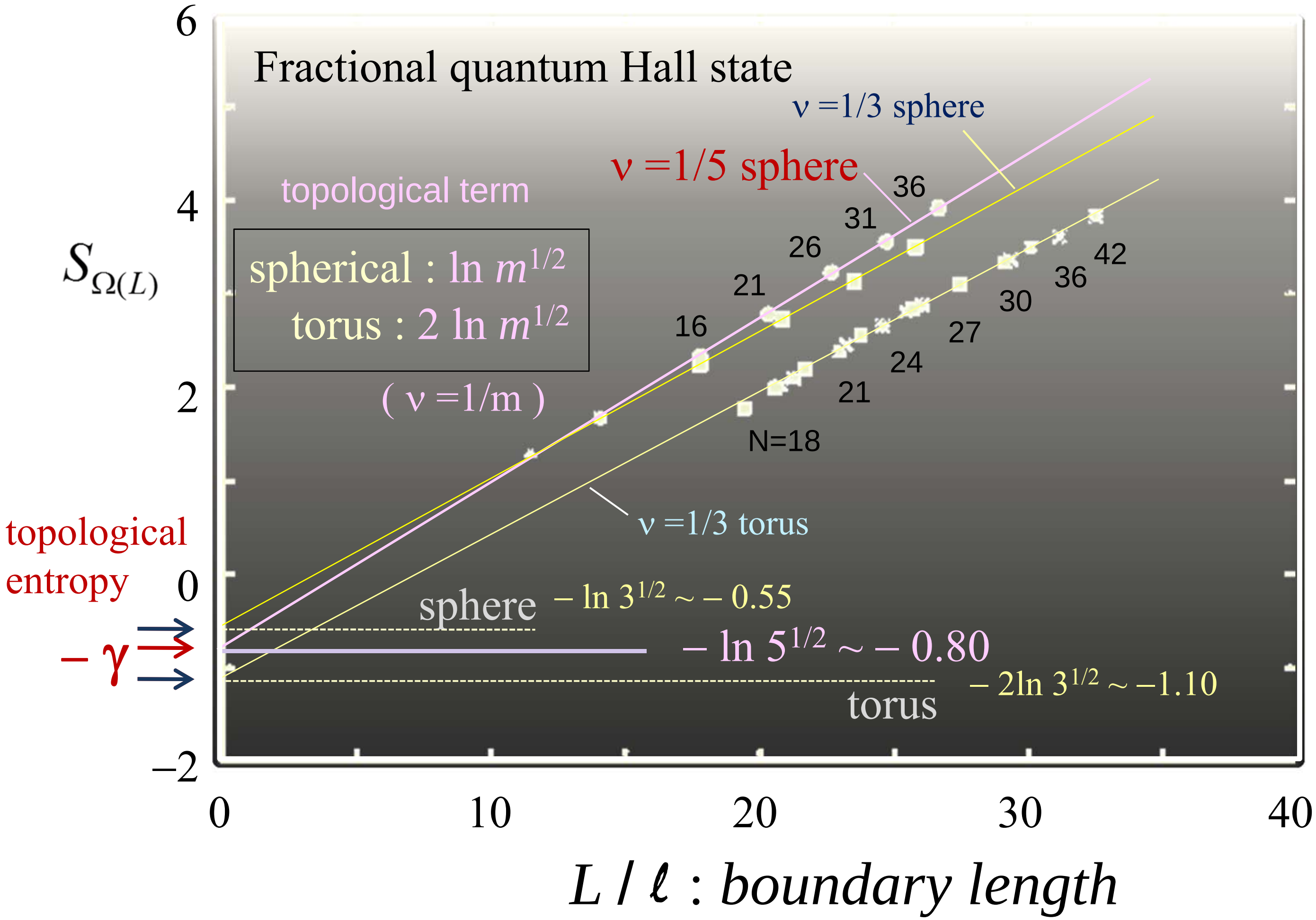
torus



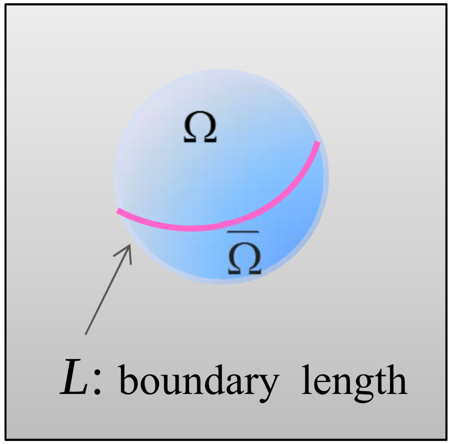
Entanglement entropy

Entanglement entropy $S_{\Omega(L)} = \underline{\alpha L} - \underline{\gamma}$

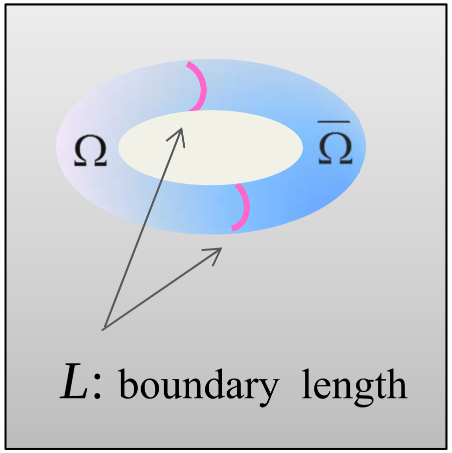
boundary term topological term



sphere

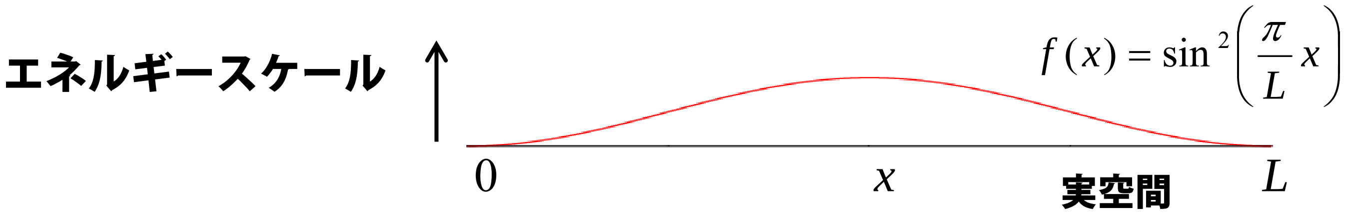


torus

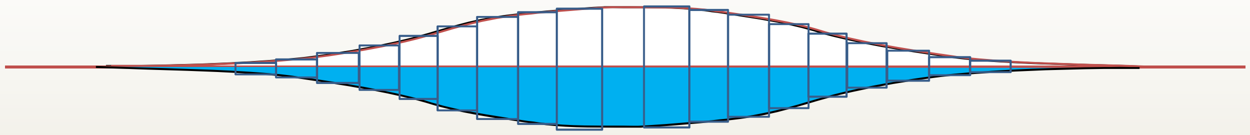


エネルギースケールの空間変調

$f(x)=\sin^2\left(\frac{\pi}{L}x\right)$ の形で変形させる



エネルギーの原点を化学ポテンシャルの位置に合わせることで

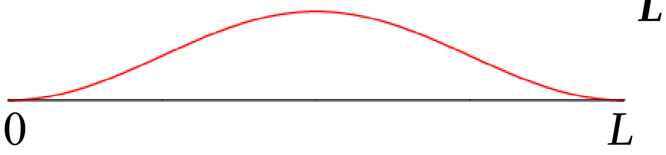


バンド占有率は空間的に一様にできる

A. Gendiar, R. Krcmar, and T. Nishino, Prog. Theor. Phys. **122**, 953 (2009); **123**, 393 (2010).

スケール変換 $f(x)=\sin^2\left(\frac{\pi}{L}x\right)$

$$\Delta k/2=\frac{\pi}{L}$$



$$\Delta k=\frac{2\pi}{L}$$

$$\begin{aligned}f(x)&=\sin^2(\Delta kx/2)\\&=\frac{1}{2}\{1-\cos(\Delta kx)\}\\&=\frac{1}{2}-\frac{1}{4}\{\exp(i\Delta kx)+\exp(-i\Delta kx)\}\end{aligned}$$

$$H_{Original}=\sum_k(\varepsilon_k-\mu)c_k^+c_k$$

$$\begin{aligned}H_{Deform}=&\sum_k\frac{1}{2}(\varepsilon_k-\mu)\,c_k^+c_k\\&-\sum_k\frac{1}{4}(\varepsilon_{k+\frac{\Delta k}{2}}-\mu)\,c_{k+\Delta k}^+c_k\\&-\sum_k\frac{1}{4}(\varepsilon_{k+\frac{\Delta k}{2}}-\mu)\,c_k^+c_{k+\Delta k}\end{aligned}$$

$$H_{Deform}=\begin{bmatrix}1&-0.4&&&&&&&&-0.4\\-0.4&0.7&-0.3&&&&&&&\\&-0.3&0.3&0&&&&&&\\&&0&-0.3&0.3&&&&&\\&&&0.3&-0.7&0.4&&&&\\&&&&0.4&-1&0.4&&&\\&&&&&0.4&-0.7&0.3&&\\&&&&&&0.3&-0.3&0&\\&&&&&&&0&0.3&-0.3\\-0.4&&&&&&&&-0.3&0.7\end{bmatrix}$$

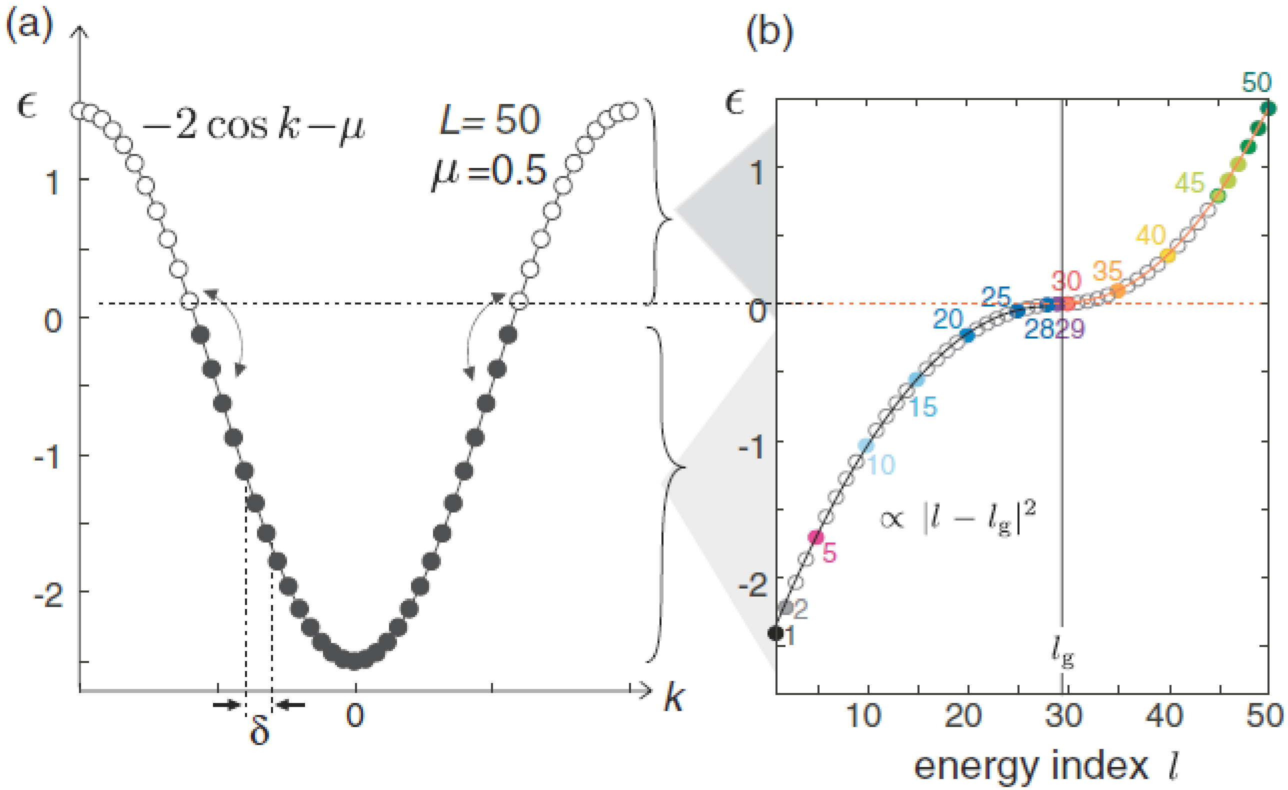
正のエネルギーと
負のエネルギーの状態が分離

多体の基底状態は並進対称な系の基底状態と完全に一致

T. Hikihara and T. Nishino, Phys. Rev. B **83**, 060414(R) (2011)
H. Katsura, J. Phys. A **44**, 252001 (2011)

エネルギースペクトル

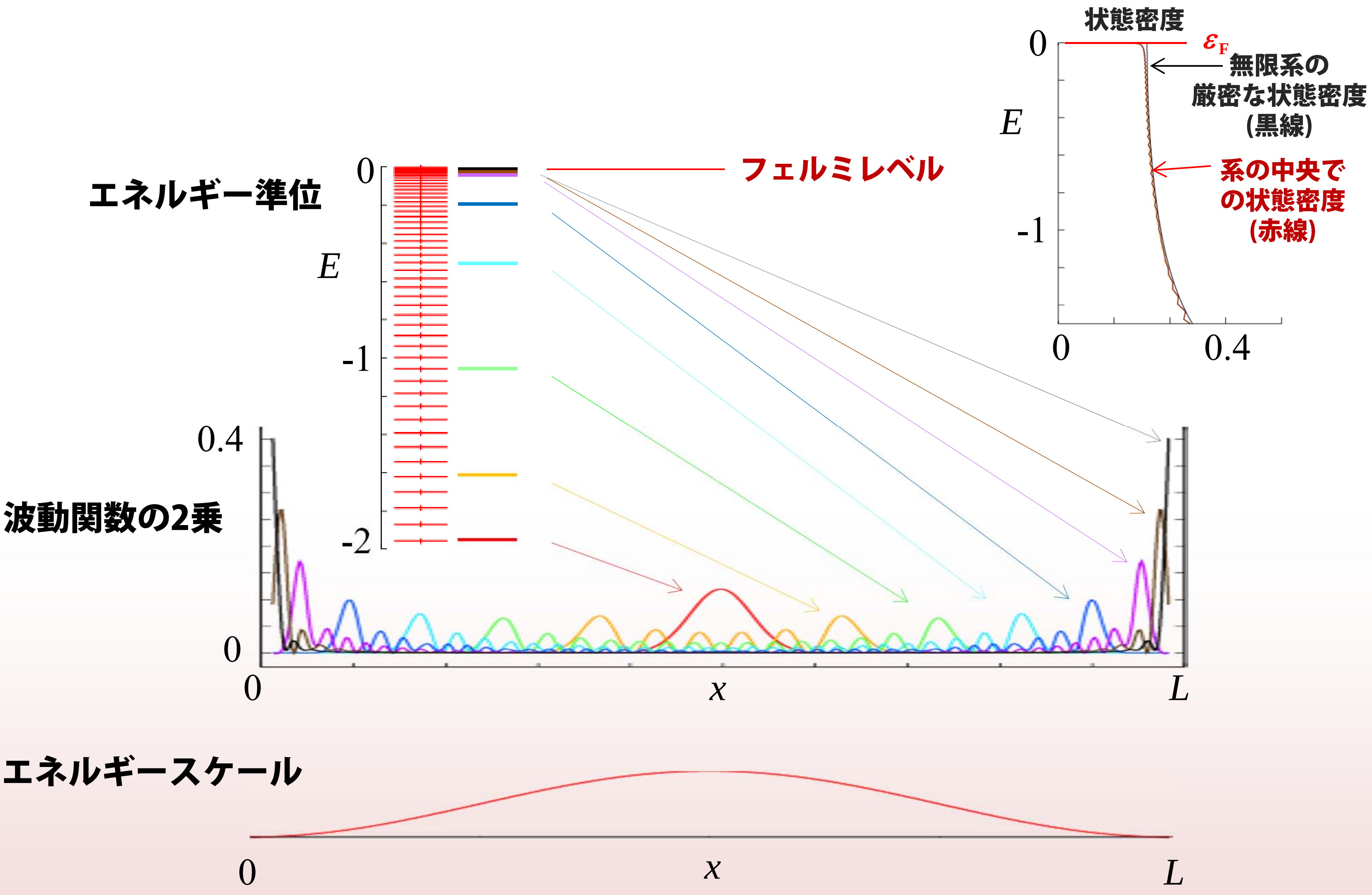
OBC **SSD**



Shibata and Hotta: Phys. Rev. B **84** 115116 (2011)

Hotta and Shibata: Phys. Rev. B **86** 041108(R) (2012)

エネルギースペクトルと波動関数



状態密度

ε_F

無限系の厳密な状態密度（黒線）

系の中央での状態密度（赤線）

エネルギー準位

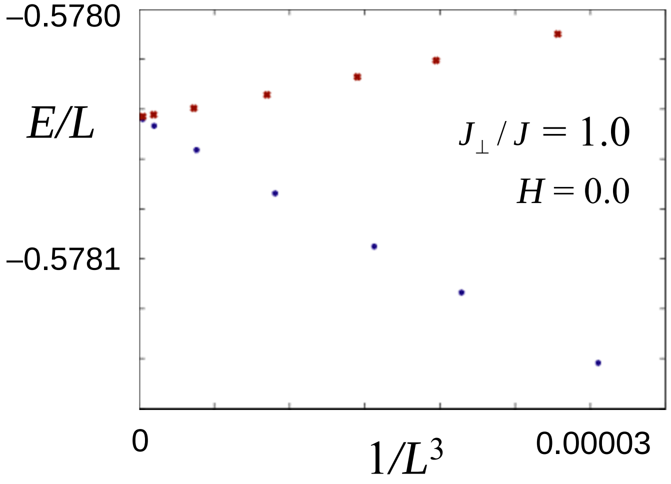
フェルミレベル

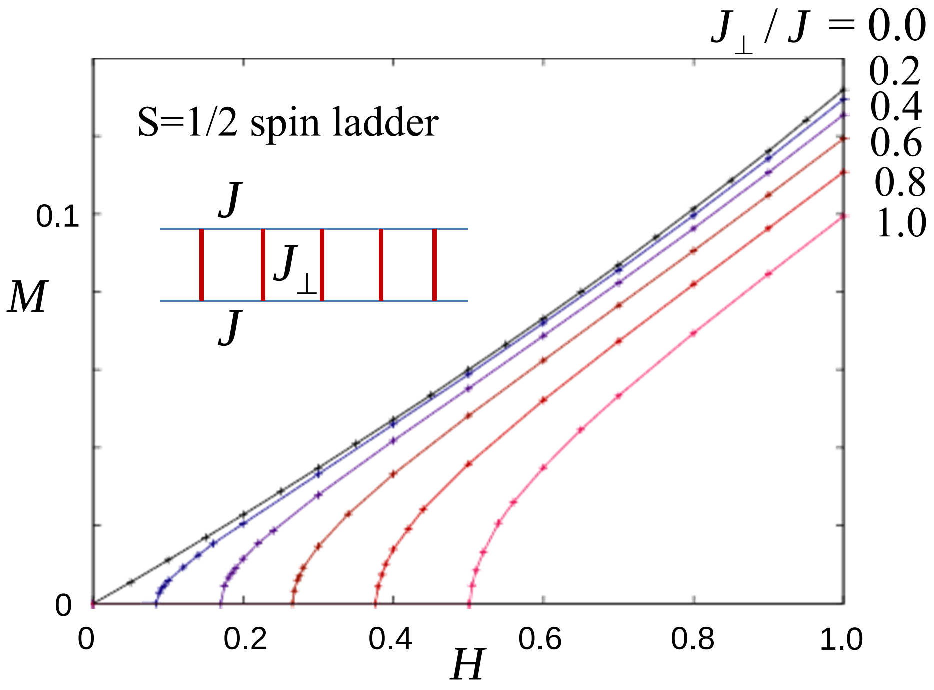
波動関数の2乗

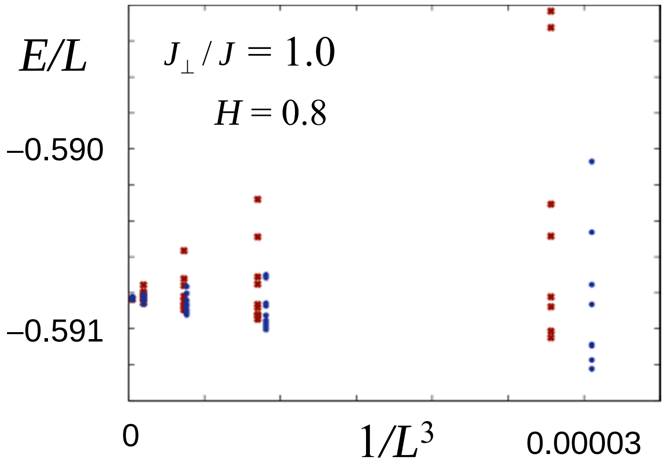
エネルギースケール

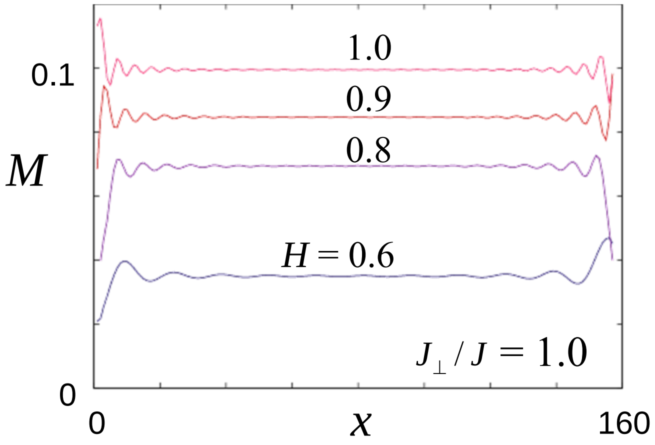
外場応答とサイズスケーリング

S=1/2 Heisenberg spin ladder

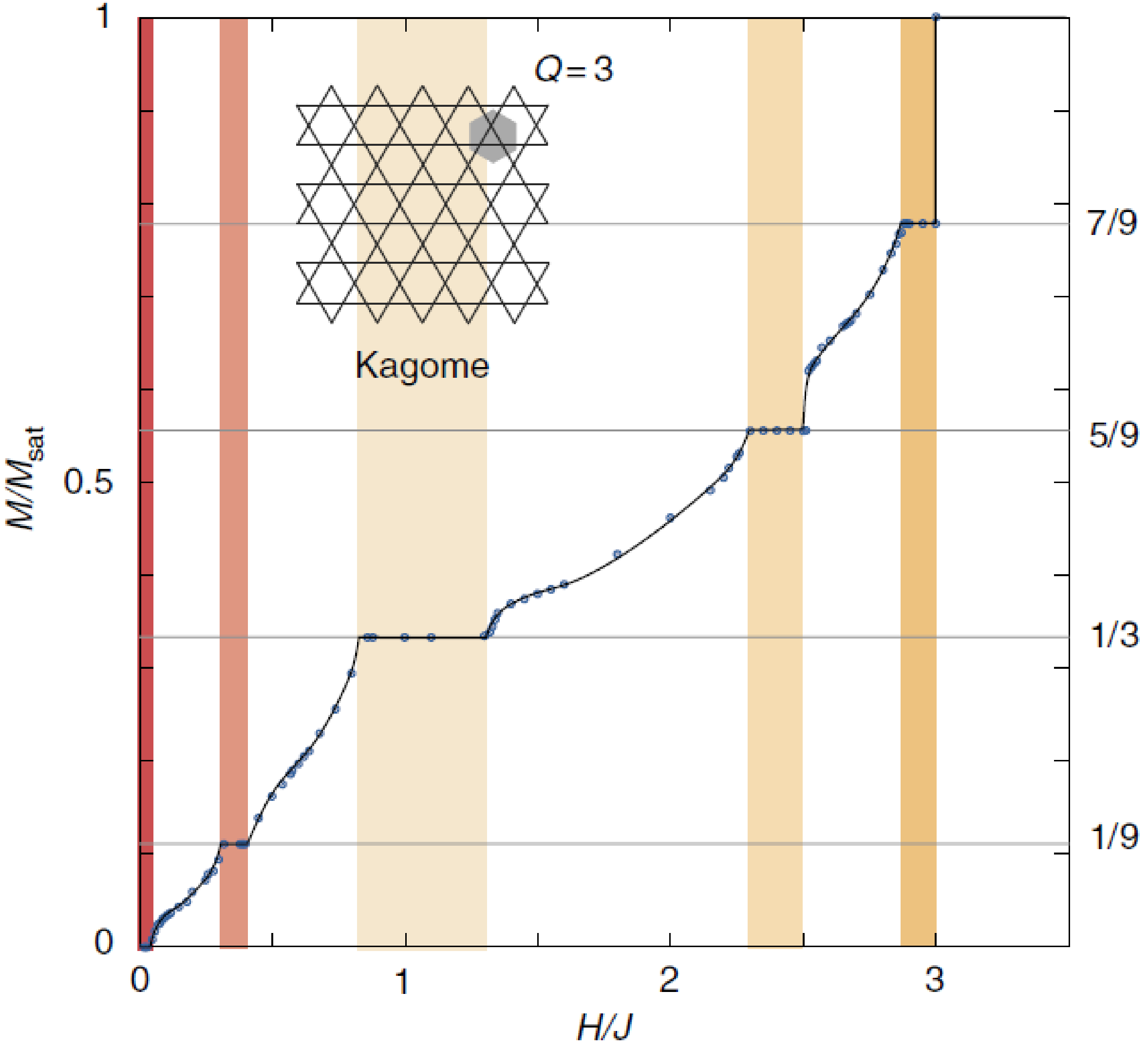






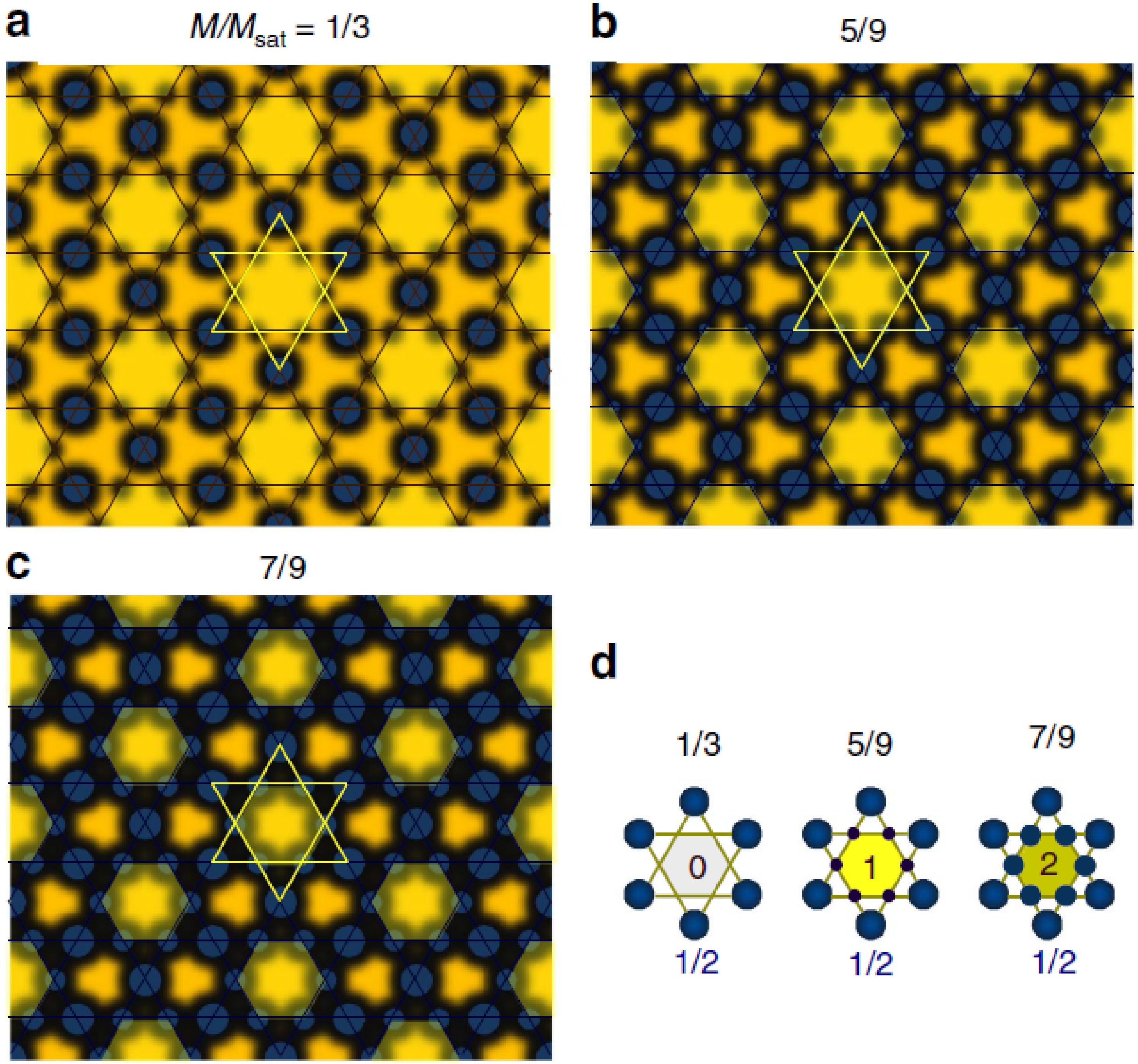


カゴメ格子の磁化曲線

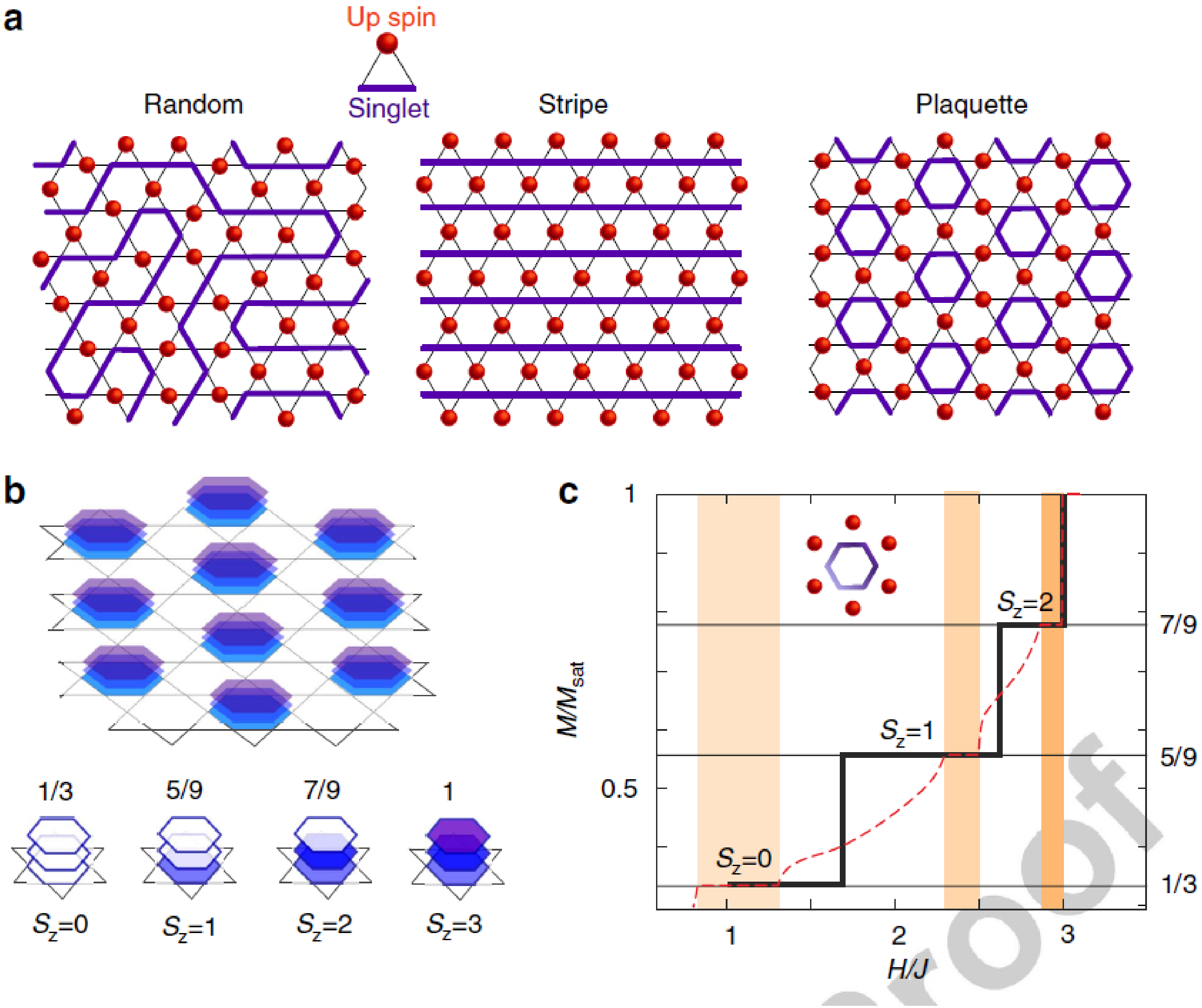


Nishimoto, Shibata and Hotta: Nature Communications **4** 2287 (2013)

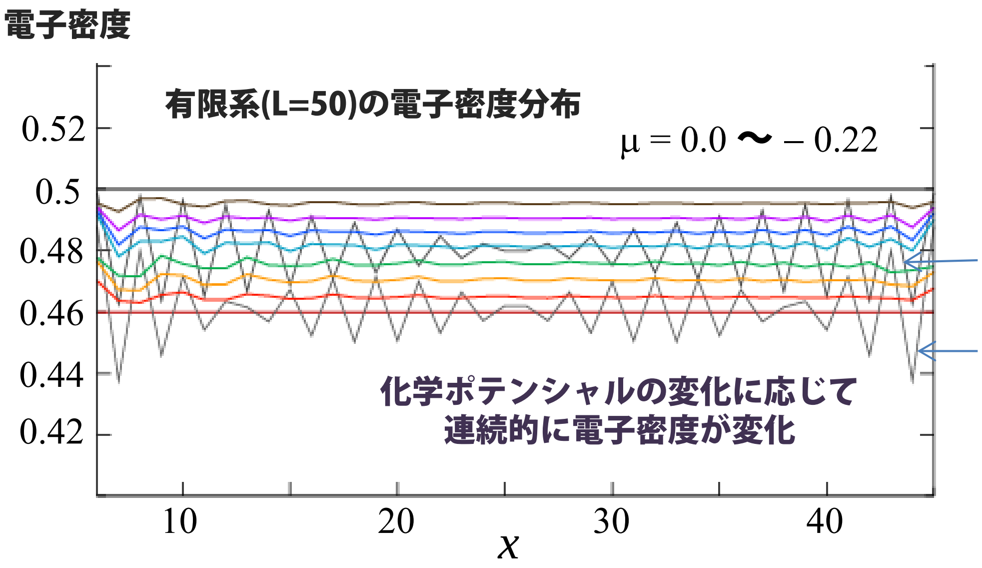
磁化プラトー内のスピン構造



カゴメ格子の磁化プラトー



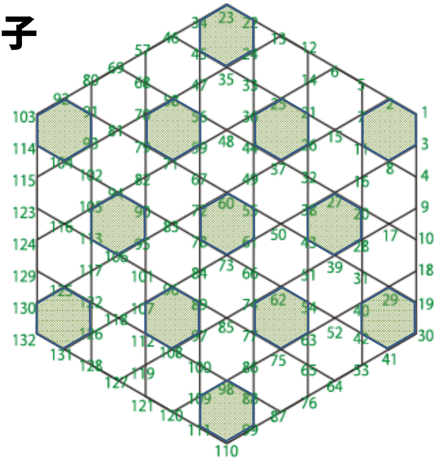
外場応答を有限系で計算

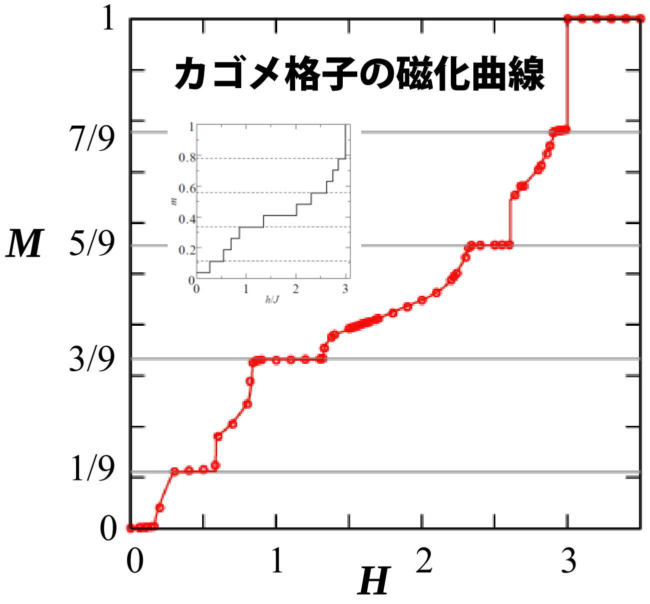


通常の境界条件
Ne=49

通常の境界条件
Ne=48

カゴメ格子





境界条件の影響を効果的に消去

無限系の応答を再現