Grand canonical analysis from ground state to finite temperature

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Collaborators

Naokazu Shibata (Tohoku Univ.)	Grand canonical
Satoshi Nishimoto (IFW, dresden)	2D-DMRG
Kenichi Asano (Osaka Univ)	finite T quantum sys.
Tota Nakamura (Shibaura Inst. Tech.) Takashi Nakamaniwa (previous M2)	classical sys.

Grand canonical analysis

Applications to Kagome antiferromagnet

Research interests

Our goal : reach the thermodynamic limit.

But, ... solving quantum many body problem is not that easy.

Numerical methods

N □ $O(10^2)$ ⟶ *bulk* □ $O(10^{23})$

Unbiased methods

exact diagonalization
Quantum Monte carlo
Density-matrix renormalization group

+ finite size scaling

Difficulties : 1. Finite size effect ～ size scaling often fails.
2. Boundary effect
3. Cluster shape , symmetry , aspect ratio

Outline or Summary

Grand canonical analysis : application of SSD

＊ quantum many body ground state

+ obtain precise magnetization curve/ μ - ρ curve.

+ see how/why it works.

"real space renormalization" particles localize as wave packets

no longer feel the system size/shape

＊ thermodynamic properties

+ excited energies also renomarlized properly !

+ dense low enegy DOS provide good low energy properties.

＊ classical Ising models.

+ partition functions (interacting sys) become an ensemble of localized free particles carrying varieties of energies.

Grand canonical analysis

Grand canonical analysis: how?

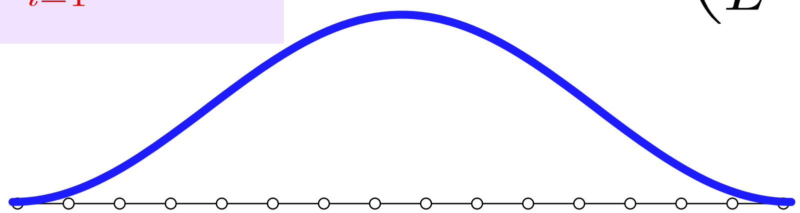
$$\mathcal{H} = \sum_{\langle i,j \rangle} h_l(i,j) + \sum_{i=1}^{N} u(i) - \mu \sum_{i=1}^{N} n_j$$

inter-site — onsite — **thermodynamic potential**

↓

$$\mathcal{H}_{\mathrm{deform}} = \sum_{\langle i,j \rangle} f\left(\frac{\boldsymbol{r}_i + \boldsymbol{r}_j}{2}\right) h_l(i,j) + \sum_{i=1}^{N} f(\boldsymbol{r}_i)\, u(i) - \mu \sum_{i=1}^{N} f(\boldsymbol{r}_i)\, n_j$$

$$f(\boldsymbol{r}_i) = \sin^2\left(\frac{\pi}{L}\left(i - \frac{1}{2}\right)\right)$$



"sine-squre-deformation"=SSD

Nishino, et al. proposed it as
one of the smooth boundary condition.

↓

Solve/diagonalize

↓

Translational symmetry is broken in general.

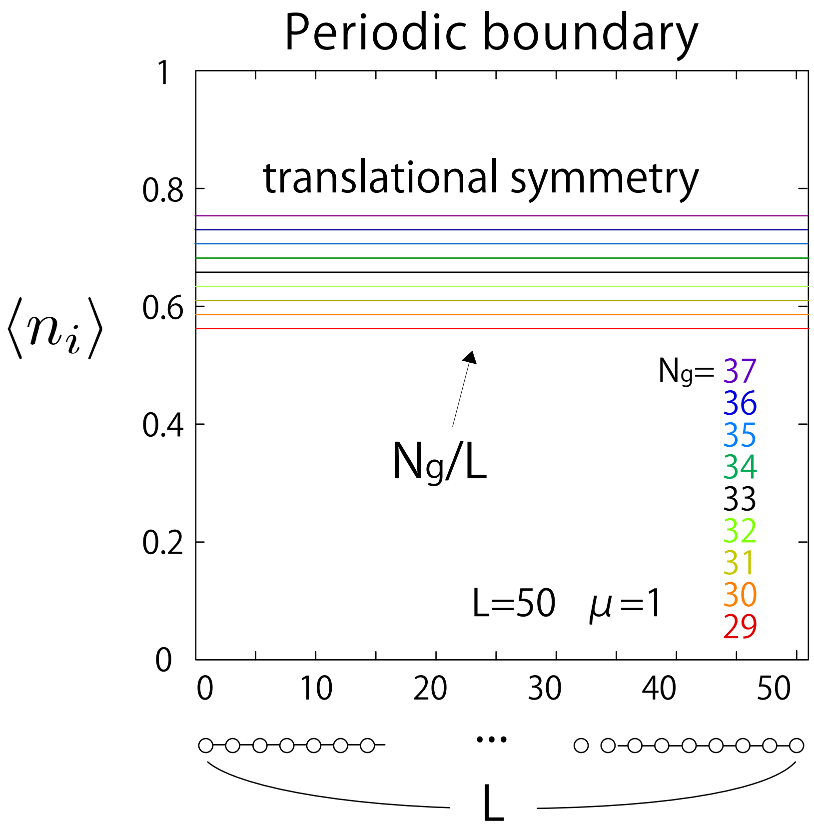
.... then what happens?

Grand canonical analysis

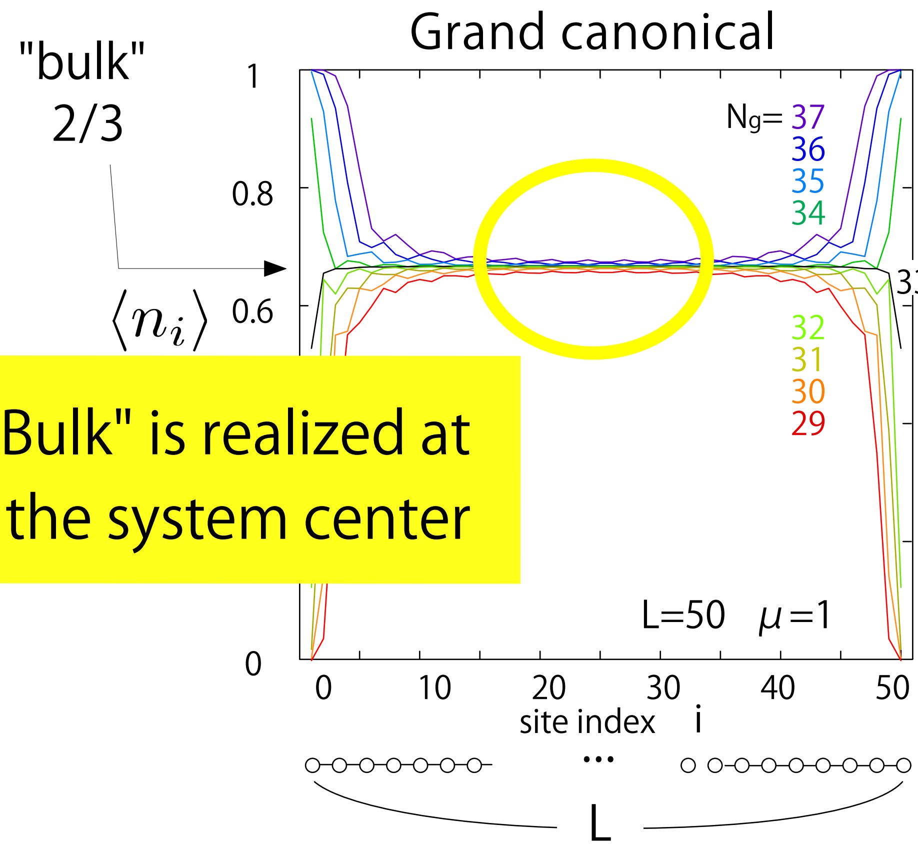
1D Free fermion: $\mathcal{H}_0 = -\sum_{j=1}^{L} (c_j^\dagger c_{j+1} + \mathrm{H.c.}) - \mu \sum_{j=1}^{L} n_j$

At μ=1, the exact particle density is $\langle n_i \rangle$ =2/3.

for L=50 Total particle number N_g =50×2/3 = 33.333....



deform



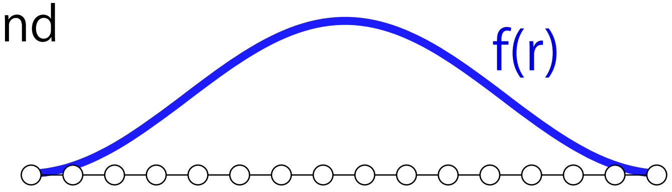
"Bulk" is realized at the system center

Grand canonical analysis

(1) **Deform the real space Hamiltonian by a smooth function f(r) on a finite size system**
Don't forget the thermodynamic potential !

μ , H	: External field
N_g , M_g	: total particle number, total S_z

given by hand



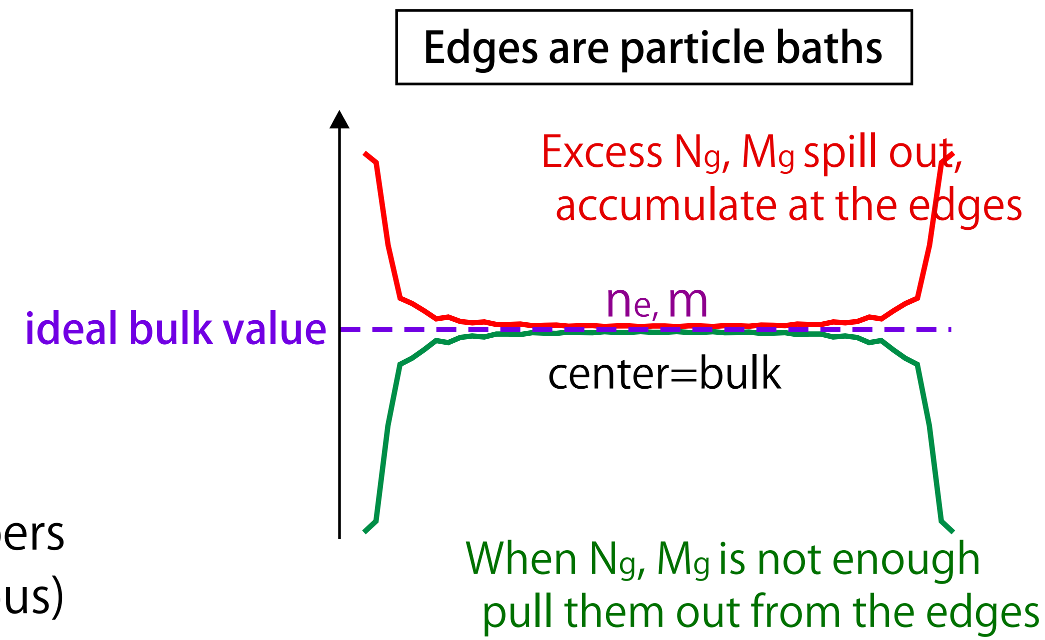
(2) **Solve the deformed Hamiltonian**
Any solver is OK !

(3) **Extract particle density n_e, magnetization m at the system center.**

$$n_e \neq N_g/N$$
$$m \neq M_g/N$$

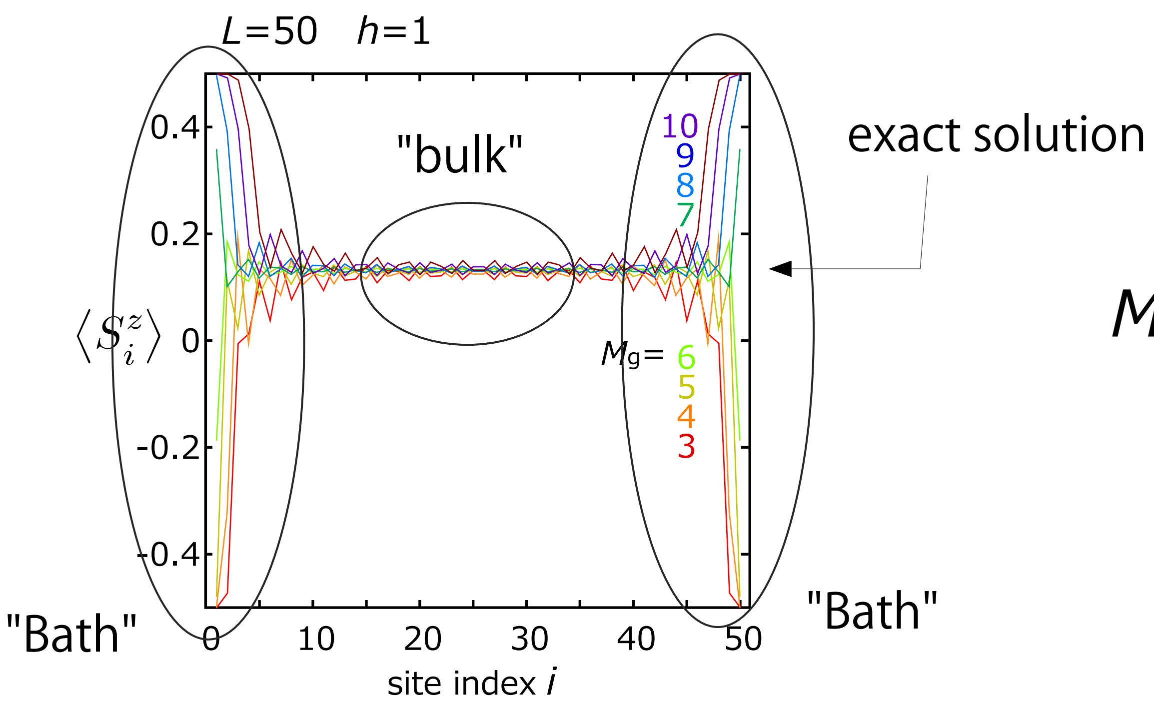
continuous functions of μ & H

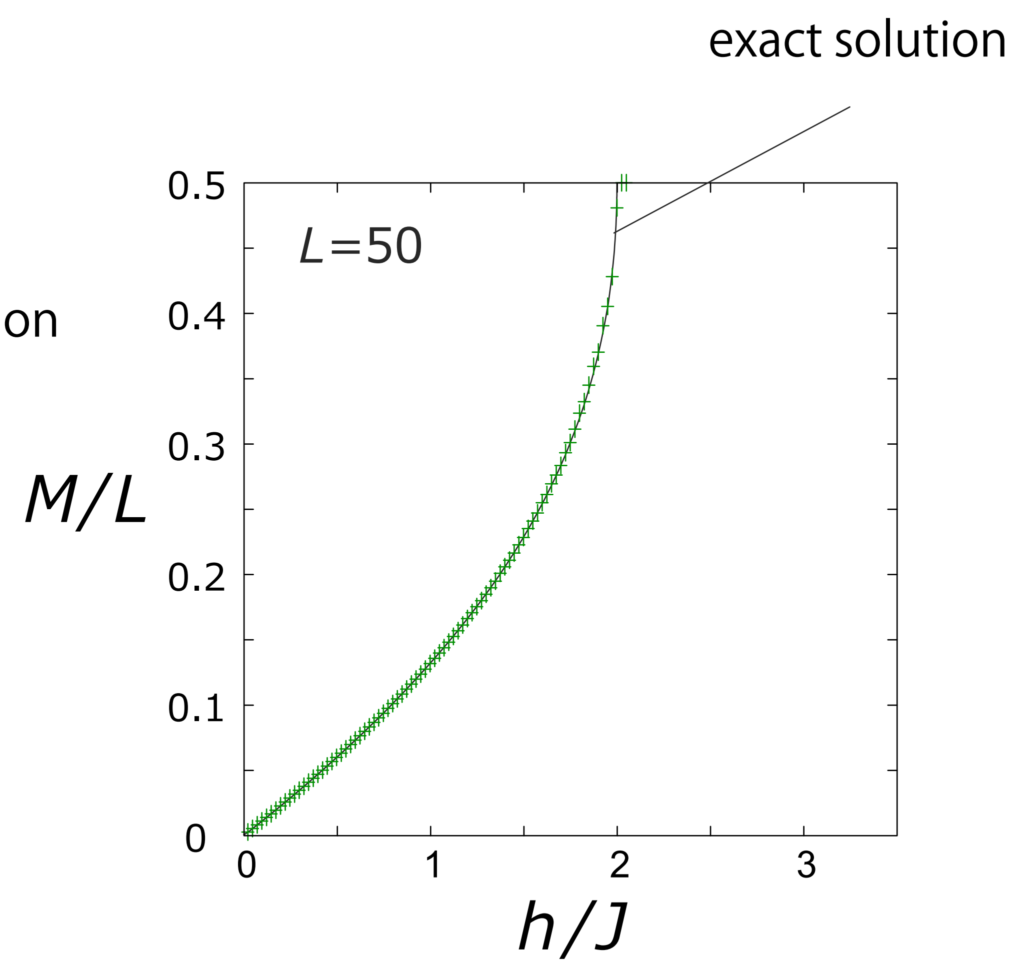
Rational numbers (discontinuous)



Magnetization curve

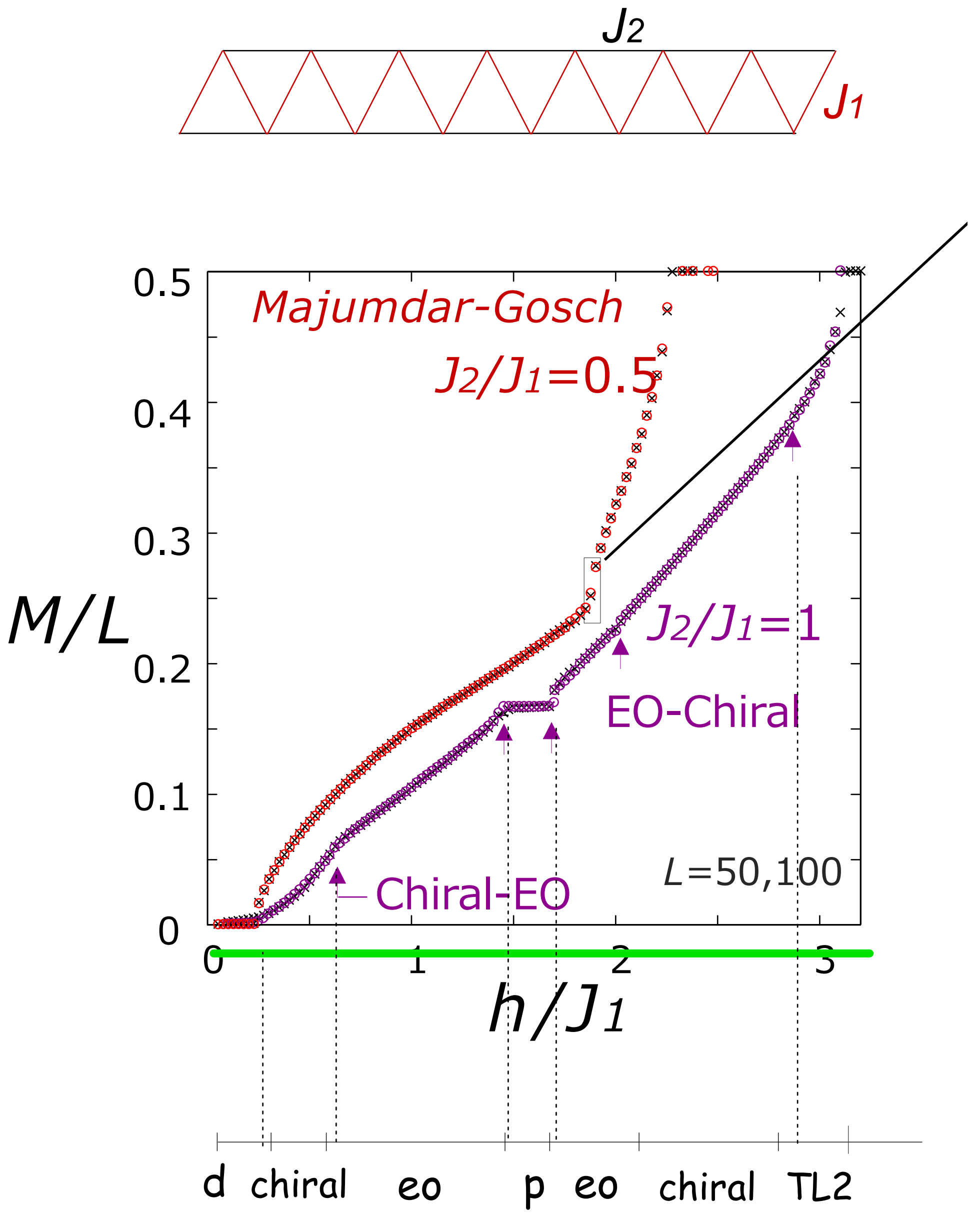
$$\mathcal{H} = \sum_{\langle i,j \rangle} S_i \cdot S_j - h \sum_{i=1}^{N} S_i^z,$$

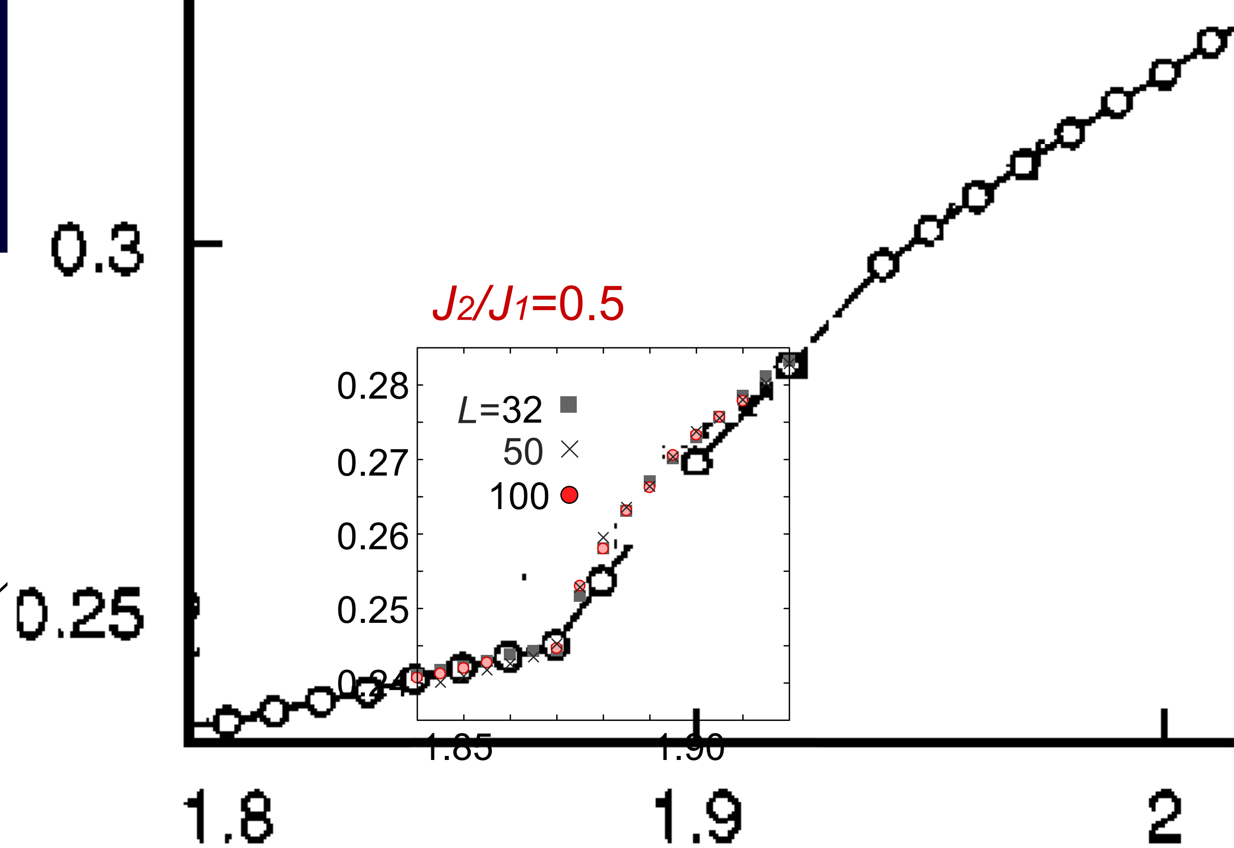


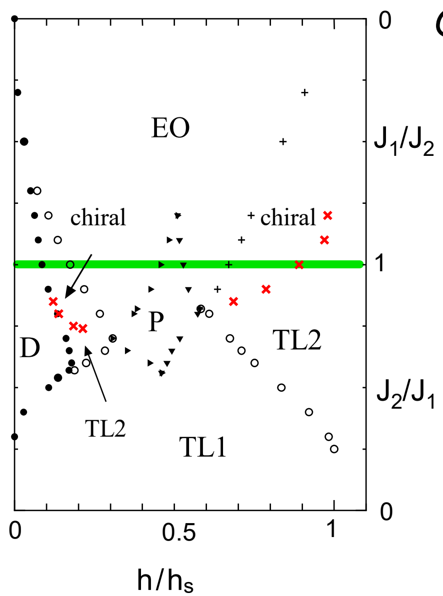


Accuracy 10^{-4}

Incommensurate states





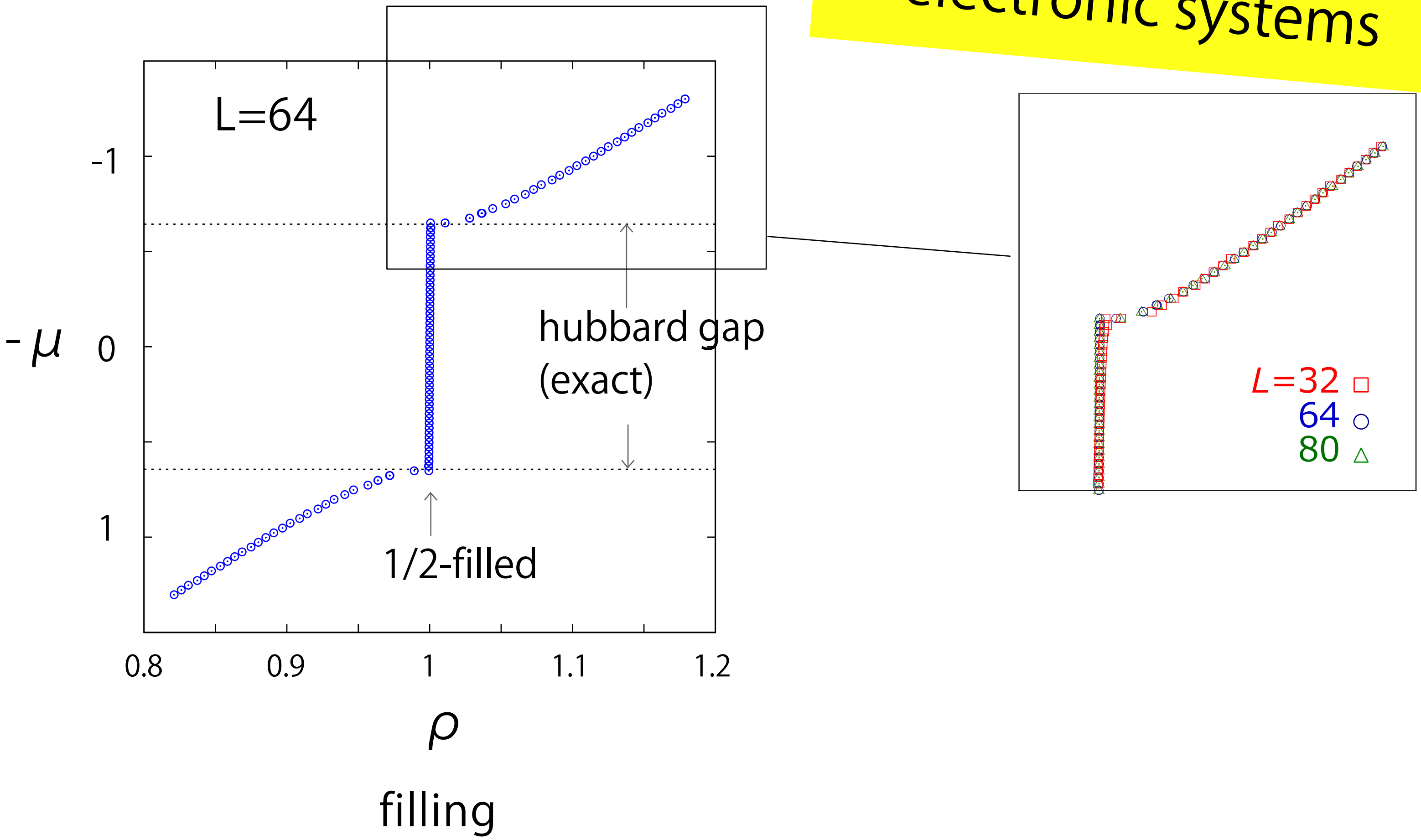


Okunishi (2008)
DMRG N<384

Particle density vs chemical potential

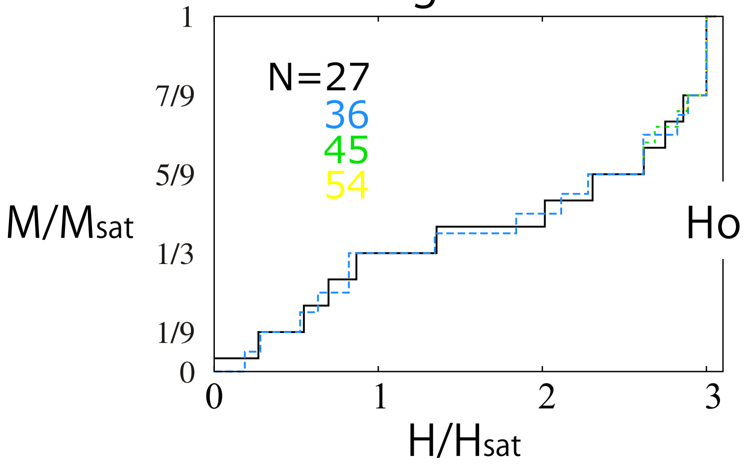
Hubbard chain

O(10 $^{-4}$)-accuracy even in electronic systems



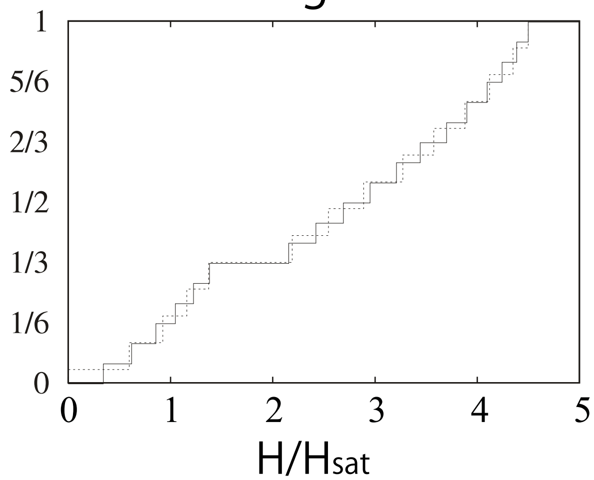
In 2D : How efficient is it ?

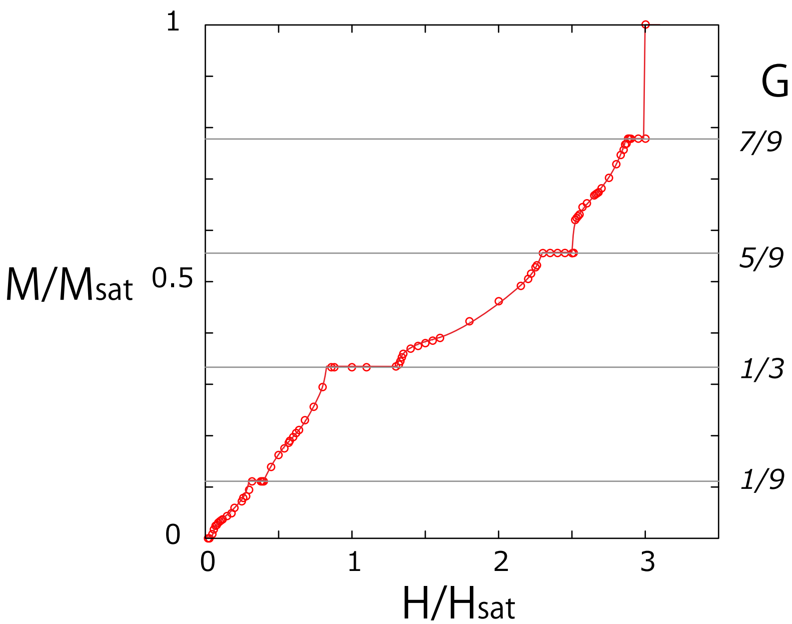
Kagome



Honecker,et.al.('03)

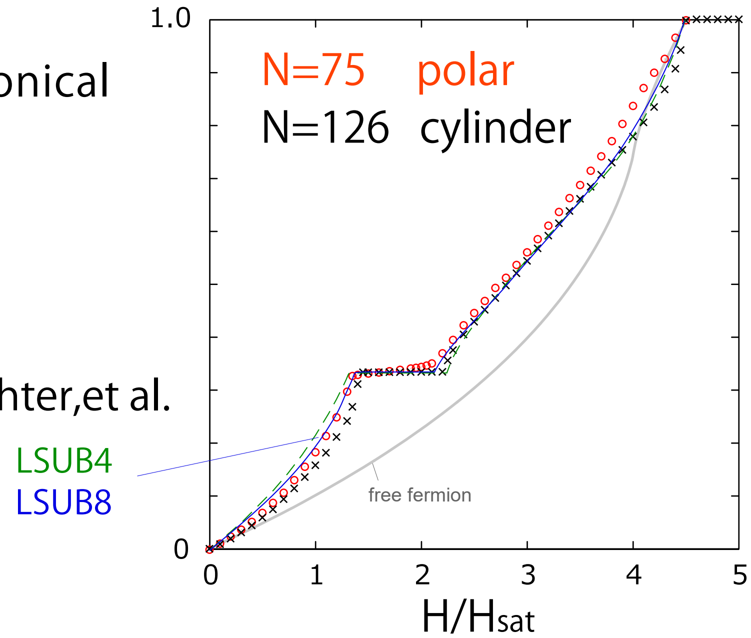
Triangle





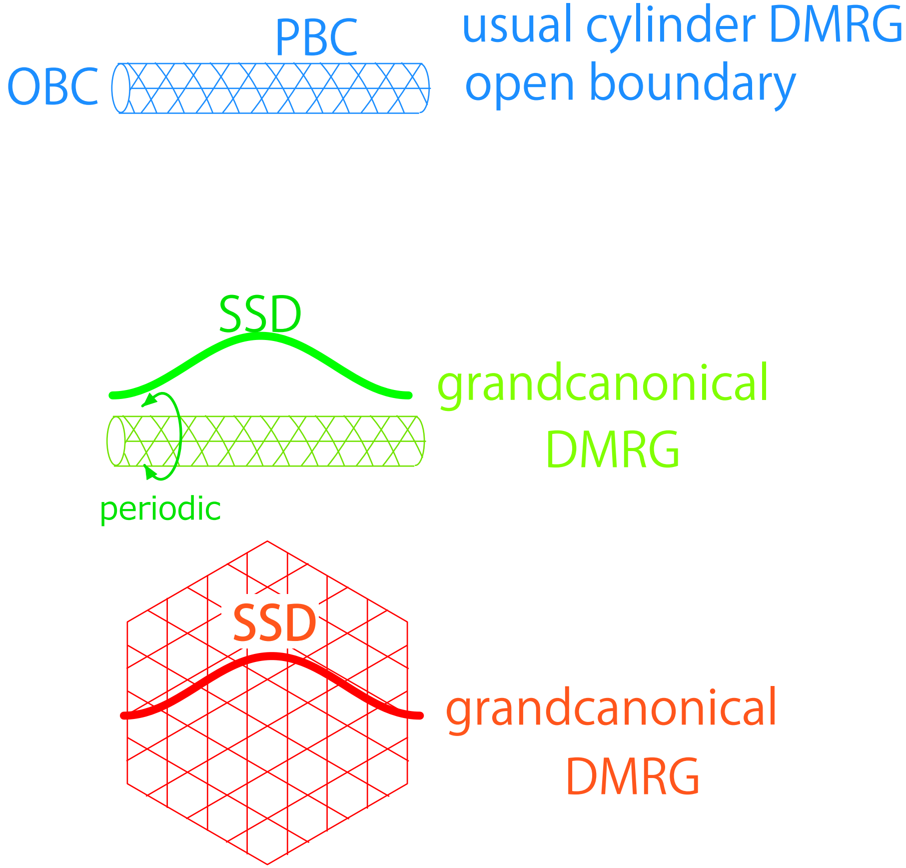
Grand canonical

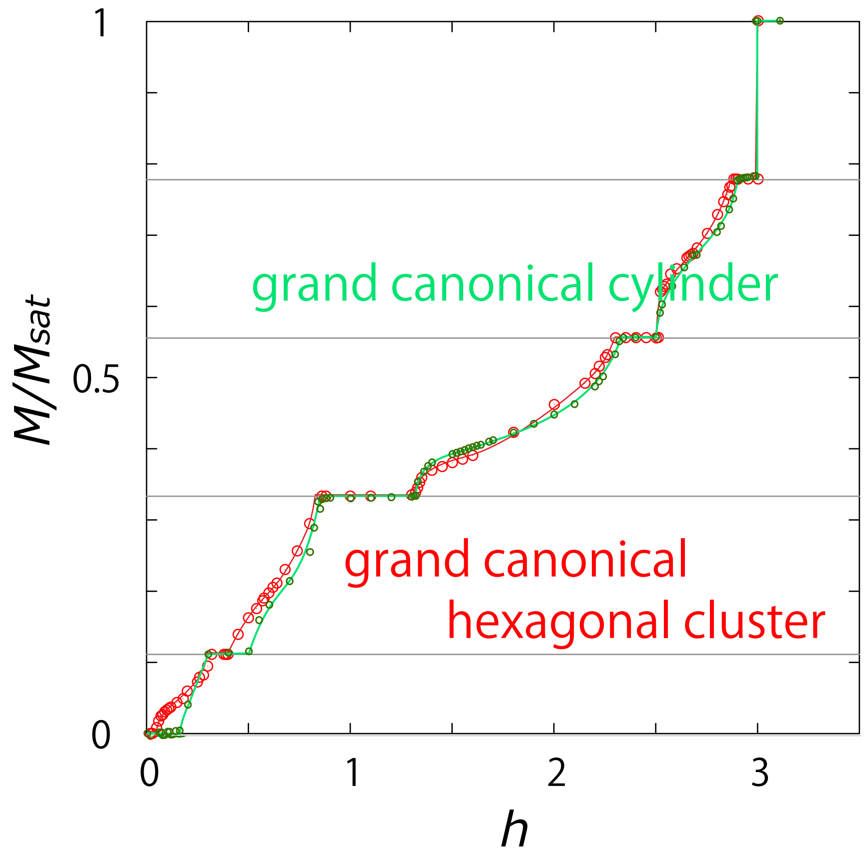
Richter,et al.



Kagome magnetization curve

$$\mathcal{H} = \sum_{\langle i,j \rangle} f\left(\frac{\boldsymbol{r}_i + \boldsymbol{r}_j}{2}\right) J\, S_i \cdot S_j - H \sum_{i=1}^{N} f(\boldsymbol{r}_i)\, S_i^Z$$

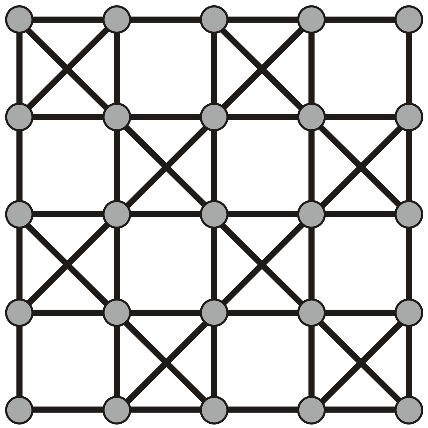


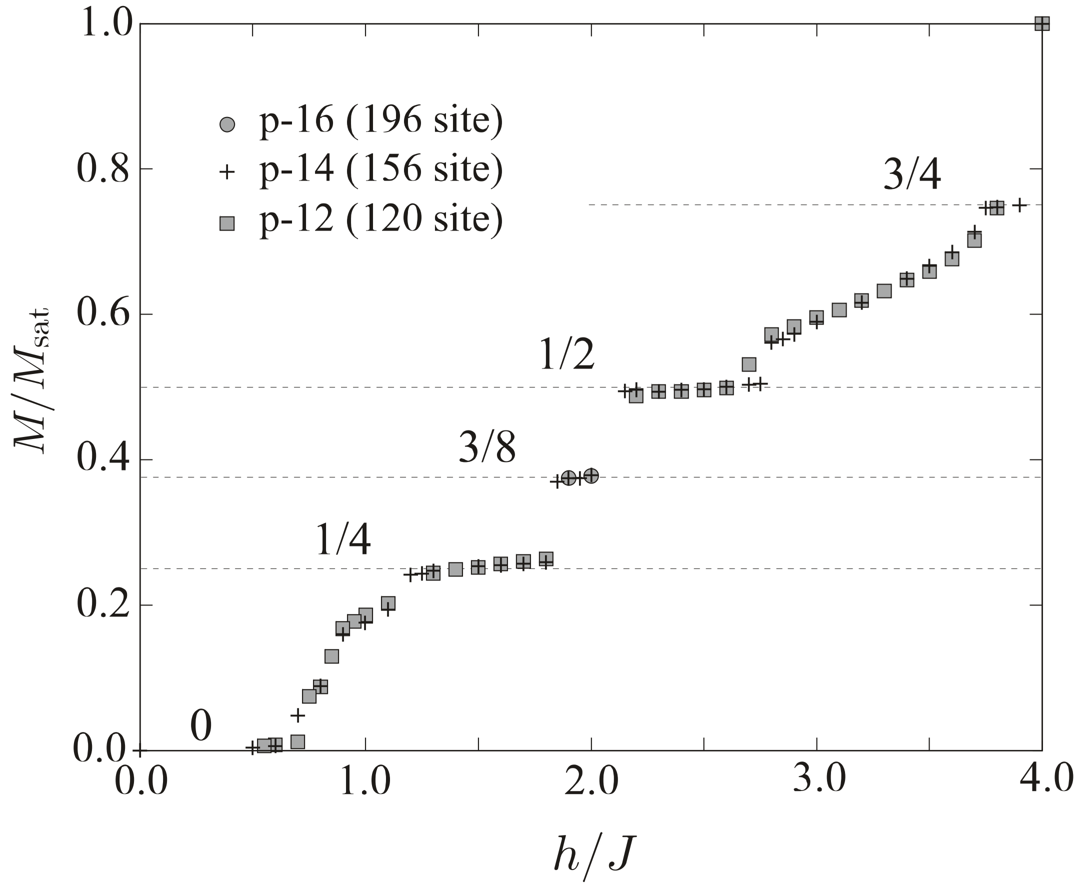


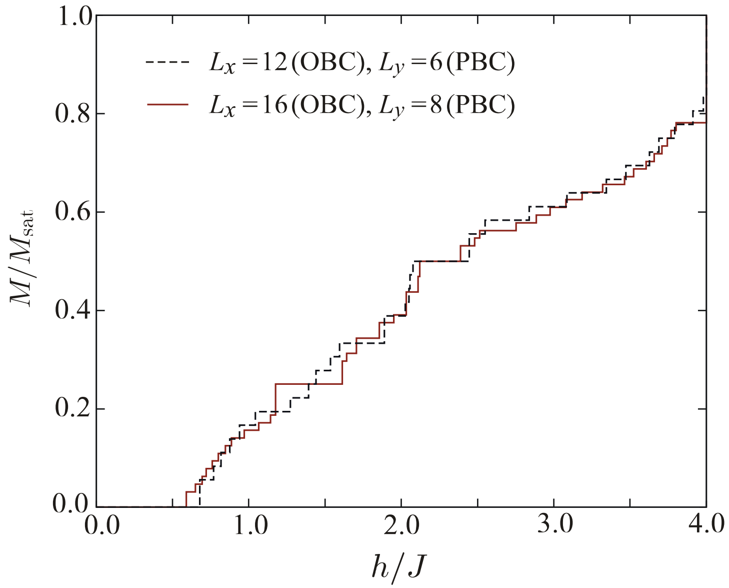
Bulk Sz is obtaind at the center of the cluster.
Precision = 10^{-3} in 2D

Checkerboard Heisenberg model

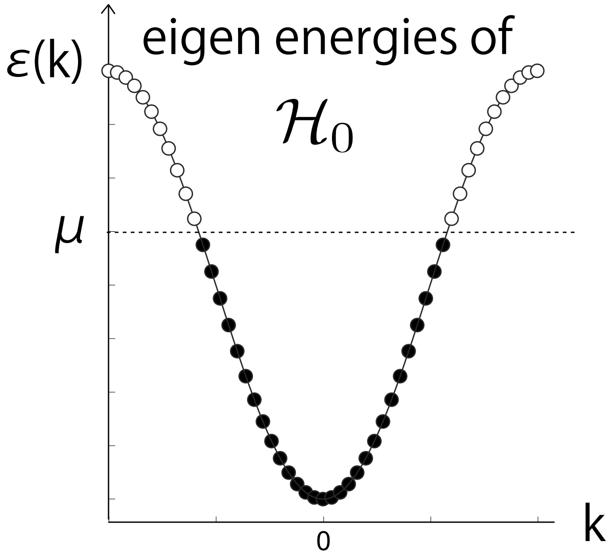
Morita-Shibata, PRB 94, 140404(R) (2016)

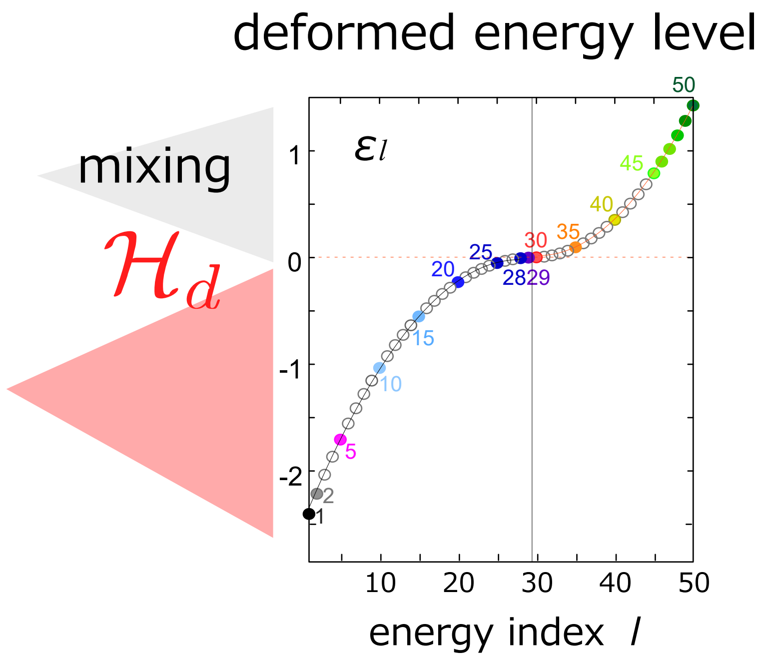






How SSD works　1D free fermion as examle





$$\mathcal{H}_0 = -\sum_{j=1}^{L} \left(c_j^\dagger c_{j+1} + \text{H.c.}\right) - \mu \sum_{j=1}^{L} n_j$$

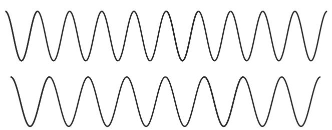
$$= \sum_k \epsilon(k)\, c_k^\dagger c_k,$$

$$\mathcal{H}_{\text{deform}} = -\sum_{j=1}^{L-1} f\left(j+\frac{1}{2}\right)\left(c_j^\dagger c_{j+1} + \text{H.c.}\right) - \mu \sum_{j=1}^{L} f(j)\, n_j$$

$$= \sum_k \epsilon(k)\, c_k^\dagger c_k - \sum_k \sum_n \hat{g}_n\, \epsilon\left(k + \frac{\delta n}{2}\right) c_{k+\delta n}^\dagger c_k$$

$$= \mathcal{H}_0 - \mathcal{H}_d$$

eigen states = plane waves



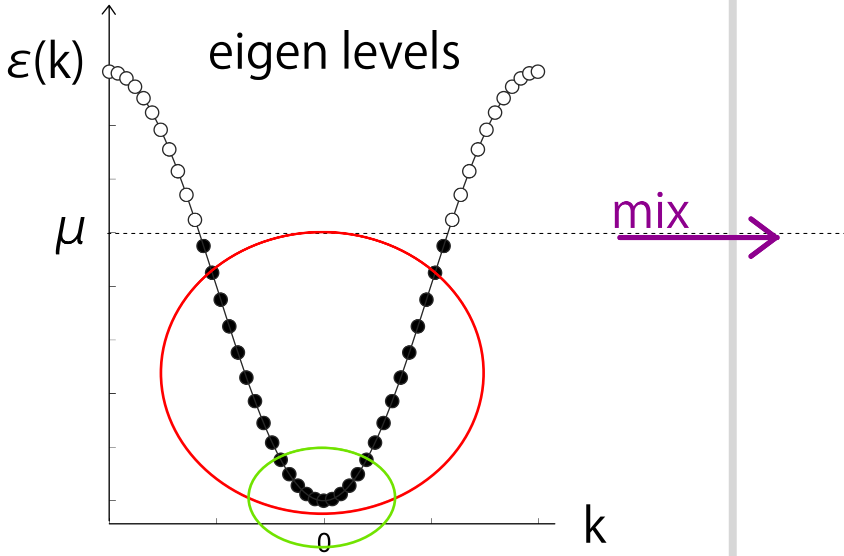
k : quantum number

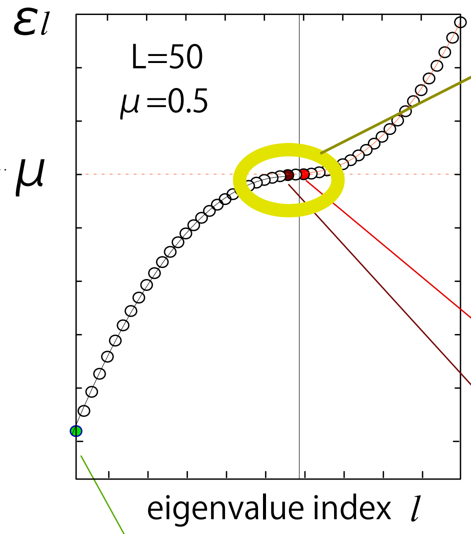
Maruyama-Katsura-Hikihara PRB 84,165132(2011)

How SSD works

Localized wave packets
insensitive to system size

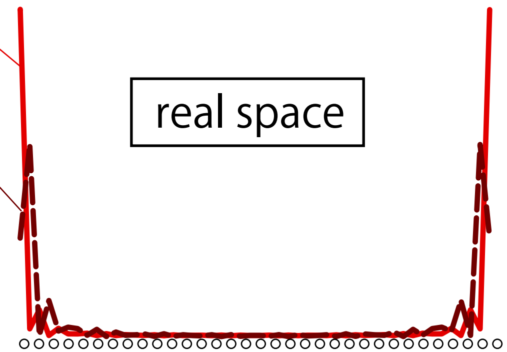
1D free fermion $\mathcal{H}_0$ → $\mathcal{H}_{\mathrm{SSD}} = \mathcal{H}_0 - \mathcal{H}_d$



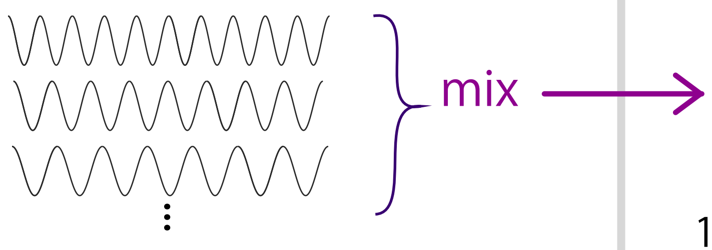


Dense low energy states near μ
fine-tune the particle # as buffer.

near μ
edge states are formed

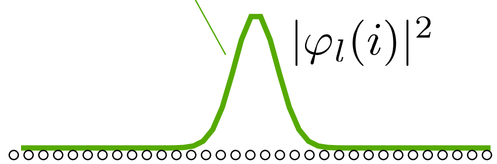


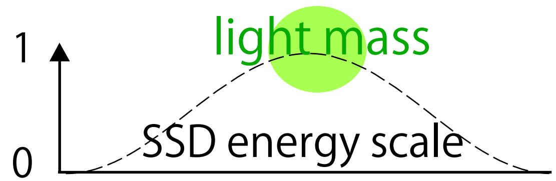
eigen states = plane waves

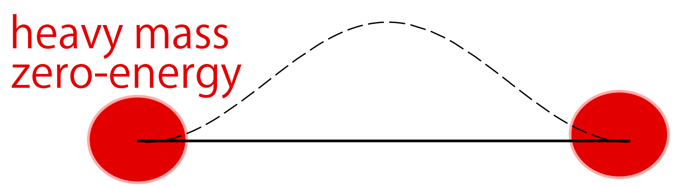


k : good quantum number

eigen states = wave packets



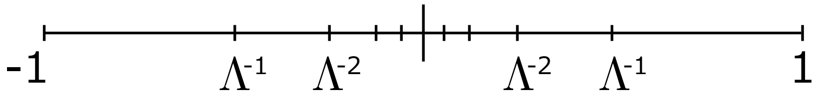




Wilson's Renormalization group

single impurity Kondo problem

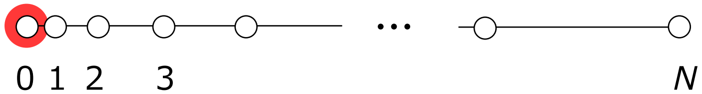
$$H_K = \int dk\, a_k^\dagger a_k - J A^\dagger \boldsymbol{\sigma} A\, \tau$$



logerithmic discretization

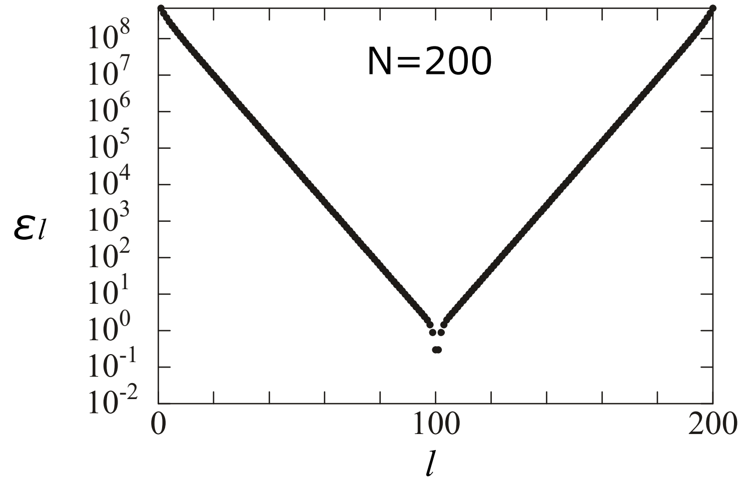
$$\mathcal{H}_K^N = \sum_{n=1}^{N} \Lambda^{-n/2} (f_{n-1}^\dagger f_n + \mathrm{H.c.}) - \tilde{J} f_0^\dagger \boldsymbol{\sigma} f_0 \boldsymbol{\tau}$$

impurity

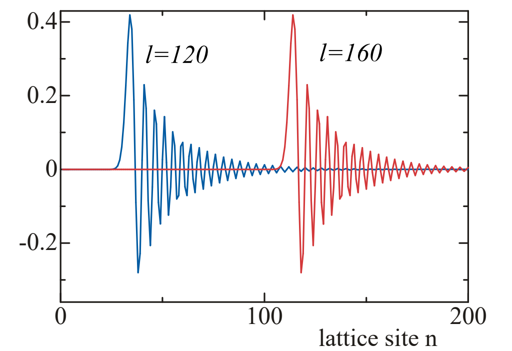


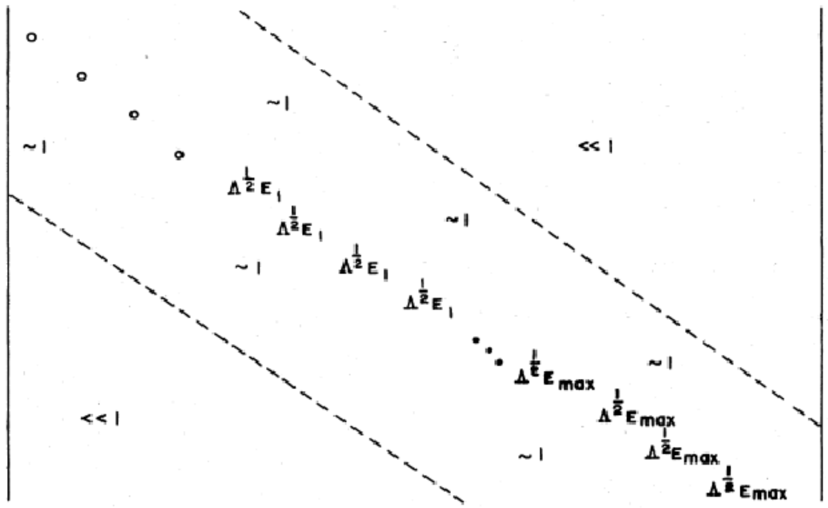
$$\mathcal{H}_K^{N+1} = \Lambda^{1/2} \mathcal{H}_K^N + f_N^\dagger f_{N+1} + \mathrm{H.c.} \quad =$$

scaling relation



Okunishi-Nishino





Deformed 1D free fermions

$$\mathcal{H}_0|\Psi_{\rm pbc}\rangle = \epsilon(k)|\Psi_{\rm pbc}\rangle$$

$$|\Psi_{\rm pbc}\rangle = \prod_{\epsilon_k \le 0} c_k^\dagger\,|0\rangle$$

k is a good quantum number.

$$\mathcal{H}_{\rm SSD} = \mathcal{H}_0 - \mathcal{H}_d$$

mixing of k

$$\mathcal{H}_{\rm SSD}\,|\Phi_{\rm g}\rangle = \sum_{l=1}^{N_{\rm g}} \epsilon_l\,|\Phi_{\rm g}\rangle$$

$$|\Phi_{\rm g}\rangle = \prod_{l=1}^{N_{\rm g}}\left(\sum_k \psi_l^*(k)\,c_k^\dagger\right)|0\rangle = \prod_{l=1}^{N_{\rm g}}\left(\sum_{j=1}^{N} \varphi_l^*(j)\,c_j^\dagger\right)|0\rangle$$

$$\varphi_l(j) = \frac{1}{\sqrt{L}}\sum_k {\rm e}^{{\rm i}kj}\,\psi_l(k)$$

$$\begin{pmatrix} \ddots & \vdots & & & & 0 \\ \cdots & \epsilon(k_F-\delta) & -\frac{{\rm e}^{-{\rm i}\frac{\delta}{2}}}{2}\epsilon(k_F-\frac{\delta}{2}) & & & \\ & -\frac{{\rm e}^{{\rm i}\frac{\delta}{2}}}{2}\epsilon(k_F-\frac{\delta}{2}) & \epsilon(k_F) & -\frac{{\rm e}^{-{\rm i}\frac{\delta}{2}}}{2}\epsilon(k_F+\frac{\delta}{2}) & & \\ & & -\frac{{\rm e}^{{\rm i}\frac{\delta}{2}}}{2}\epsilon(k_F+\frac{\delta}{2}) & \epsilon(k_F+\delta) & -\frac{{\rm e}^{-{\rm i}\frac{\delta}{2}}}{2}\epsilon(k_F+\frac{3\delta}{2}) & \\ & & & -\frac{{\rm e}^{{\rm i}\frac{\delta}{2}}}{2}\epsilon(k_F+\frac{3\delta}{2}) & \epsilon(k_F+2\delta) & -\frac{{\rm e}^{-{\rm i}\frac{\delta}{2}}}{2}\epsilon(k_F+\frac{5\delta}{2}) \\ 0 & & & & -\frac{{\rm e}^{{\rm i}\frac{\delta}{2}}}{2}\epsilon(k_F+\frac{5\delta}{2}) & \ddots \end{pmatrix} \begin{pmatrix} \vdots \\ \psi_l(k_F-\delta) \\ \psi_l(k_F) \\ \psi_l(k_F+\delta) \\ \psi_l(k_F+2\delta) \\ \vdots \end{pmatrix} = \epsilon_l \begin{pmatrix} \vdots \\ \psi_l(k_F-\delta) \\ \psi_l(k_F) \\ \psi_l(k_F+\delta) \\ \psi_l(k_F+2\delta) \\ \vdots \end{pmatrix}$$

$$\hat{H}_{\rm SSD} \qquad \hat{\psi}_l$$

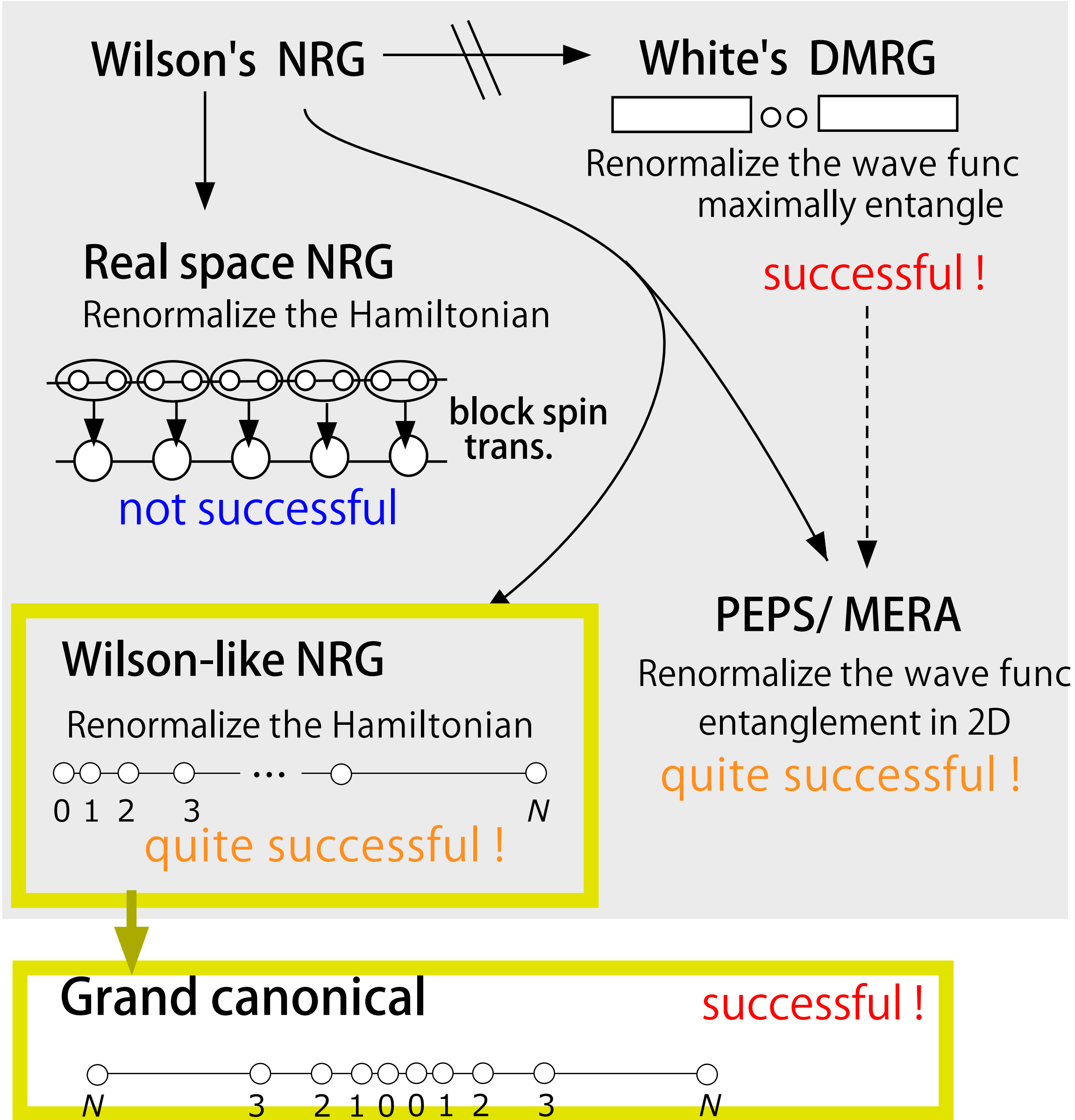
$$-\frac{{\rm e}^{{\rm i}\frac{\delta}{2}}}{2}\epsilon\left(k-\frac{\delta}{2}\right)\psi_l(k-\delta) - \frac{{\rm e}^{-{\rm i}\frac{\delta}{2}}}{2}\epsilon\left(k+\frac{\delta}{2}\right)\psi_l(k+\delta) = (\epsilon_l - \epsilon(k))\,\psi_l(k)$$

□0

1 : 1 : 1

edge states

c.f. Okunishi's work



Sorry, finite T projects are still on-going.
(unpublished)
Please wait for the publication.