Non-uniform Deformations Applied to 1D Quantum Systems

Tomotoshi Nishino (Kobe University)
Toshiya Hikihara (Gumma University)
Andrej Gendiar (Slovak Academy of Sciences)
Hiroshi Ueda (Osaka Univ. / RIKEN)

Uniform .... infinite, or finite: examples

Open Boundary Condition $$\mathcal{H}^{(N)} = -t \sum_{j=1}^{N-1} (c_j^\dagger c_{j+1} + c_{j+1}^\dagger c_j)$$

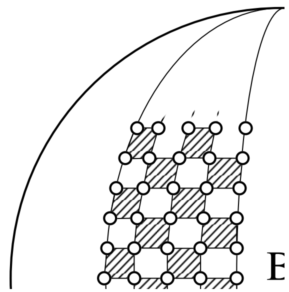
Periodic Boundary Condition $$\mathcal{H}^{(N)} \quad -t\,(c_N^\dagger c_1 + c_1^\dagger c_N)$$

Non-uniform: exp[λ j], cosh[λ j], random, etc., AND!

Sin^m Deformation

$$\mathcal{H}_{\rm sine}^{(N)} = -t \sum_{j=1}^{N-1} \left[\sin\left(\frac{j\pi}{N} \right) \right]^m (c_j^\dagger c_{j+1} + c_{j+1}^\dagger c_j)$$

The case m = 2, Sine-Square Deformation, is cool.



arXiv: 1012.0472, 1012.1472 / 1108.2973, 1104.1721, ...

Special thanks to the organizers.

Sincere thanks to my friends and all the participants.

Sincere thanks to the world.

We are on the way of long recovery.
No reactor is currently working in Japan.

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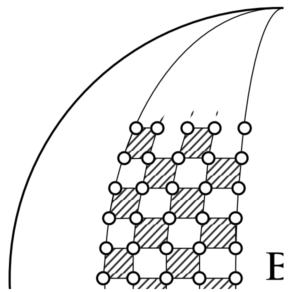


Why do we use the term Gauge?

H. Weyle introduced a gradual change of unit length, when he tried to unify Gravity and Electro Dynamics.

... one does not easily detect the change of the scale, as long as one stays within a small finite region.
(similar to the slow change in the metric.)

What is the 'slow variation/modulation' on the Lattice?

... we expect that the variation (almost) does not change the (ground or equilbrium) state, when the variation is sufficiently slow.

Set up a Question:

Is there an example where the ground state of an uniform Hamiltonian stays uniform even after the introduction of variation?

Probably yes. A very slow change in energy scale might not affect the physical (?) state so much.

Starting point: **Uniform 1D Hamiltonians**

$$\hat{H}_{\text{uniform}} = \sum_j \hat{h}_{i,i+1} = \hat{H}(\lambda = 0)$$

Local operators: $\hat{h}_{i,i+1} = J\,\hat{s}_i \cdot \hat{s}_j$

$$-t\,(\hat{c}^{\dagger}_{j+1}\hat{c}_j + h.c.)$$

$$-t\,(\hat{c}^{\dagger}_{j+1}\hat{c}_j + h.c.) + V\hat{n}_j n_{j+1}$$

Suppose that the ground state is uniform. (- - or commensulate)

... ferrro, AF, Fermi liquid, etc.

Deformed Hamiltonian

$$\hat{H}(\lambda) = \sum_j g_j(\lambda)\,\hat{h}_j$$

Deformation Function $g_j(\lambda)$

The non-zero real (or complex) function g varies very slowly from site to site. It contains a parameter λ .

$$g(\lambda = 1) = 1$$

The introduced ‘Deformation’ is NOT a perturbation.

Deformation

$$\hat{H}(\lambda) = \sum_j g_j(\lambda)\,\hat{h}_j$$

Only the local energy scale changes.

Perturbation

$$\hat{H}' = \sum_j \hat{h}_j + \sum_j \hat{V}_j$$

Energy scale does not change, but local operators are modified by perturbation V.

To connect these two cases is another issue....

(Key Wort: Position dependent mass in SUSY QM.)

Effect of deformation

$$\hat{H}(\lambda) = \sum_j g_j(\lambda)\,\hat{h}_j$$

Case 1: Gapped System

When there is finite excitation gap from the ground state, the correlation length is finite, and is inversely proportional to the gap.

$$\xi \sim 1/\Delta$$

If the deformation function varies far slower than the correlation length, it is natural to expect that the ground state is (relatively) unaffected.

Case 2: Finitely Correlated State / positive semidefinite operators

If the Hamiltonian is represented as a sum of (local) positive semi-definite operators, and if the ground-state energy is zero, the ground state is unchanged even when (the positive function) g changes randomly, and rapidly.

... there are analytic expressions for such cases:

matrix product states
finitely correlated states
etc.

Case 3: Critical Ground State

It is not hard to imagine that even a weak disturbance introduces non-negligible modulation to the critical state.

Question: Is there a way of deformation which does NOT introduce position dependence to the critical state?

Answer: **Yes, there are exponential, hyperbolic, sine-square deformations.**

Exponential Deformation

$$H^{\exp}(\lambda) = \sum_{j=-N}^{N} e^{j\lambda}\, h_{j,j+1}$$

Shift of the position, represented by S, causes magnification in energy scale.

$$\begin{aligned} S\,H^{\exp}(\lambda)\,S^{\dagger} &= \sum_{j=-\infty}^{\infty} e^{j\lambda}\,\left(S\,h_{j,j+1}\,S^{\dagger}\right) \qquad (2. \\ &= \sum_{j=-\infty}^{\infty} e^{j\lambda}\,h_{j+1,j+2} \\ &= \sum_{j=-\infty}^{\infty} e^{(j-1)\lambda}\,h_{j,j+1} = e^{-\lambda}\,H^{\exp}(\lambda) \end{aligned}$$

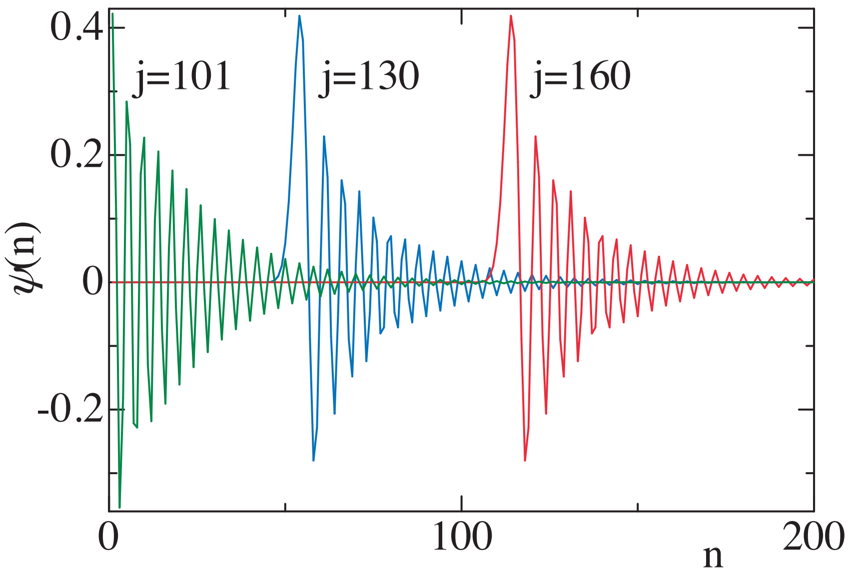
..... energy state. Thus we can say that if the zero-energy state is unique, it satisfies the translational invariance

$$S\,|\Phi\rangle = |\Phi\rangle\,. \qquad (2.10)$$

Exponential Deformation Example: free Fermions (at half-filling)

$$\mathcal{H}_\lambda = \sum_{n=1}^{N-1} e^{\lambda n}(c_{n+1}^\dagger c_n + c_n^\dagger c_{n+1})$$

The one-particle eigenstate is localized: ... the ground-state is not critical any more. As a result, the ground state stays to be uniform.



NRG successfully applied to the Kondo/Anderson impurity models, probably because of this locality and hierarch in the energy scale.

[1] K. Okunishi:J. Phys. Soc. Jpn. 76 (2007) 063001; cond-mat/0702581.
[2] K. Okunishi and T. Nishino: Phys. Rev. B 82 (2010) 144409; arXiv:1001.2594.

DMRG? iTEBD? applicable to the exp. deformation???

DMRG suffers from presence of the small energy scale under the exponential deformation, which prevents the numerical diagonalization of the super-block Hamiltonian. (NRG or Xiang's RG Scheme works better.)

Because of infinitesimal time evolution, direct application of iTEBD is not successful. Probably one has to shift the ground state MPS after each evolution, assuming the uniformity in the ground state.

Participants of this workshop

(a) have already solved this problem
(b) can easily find out the solution
(c) have no interest on this matter

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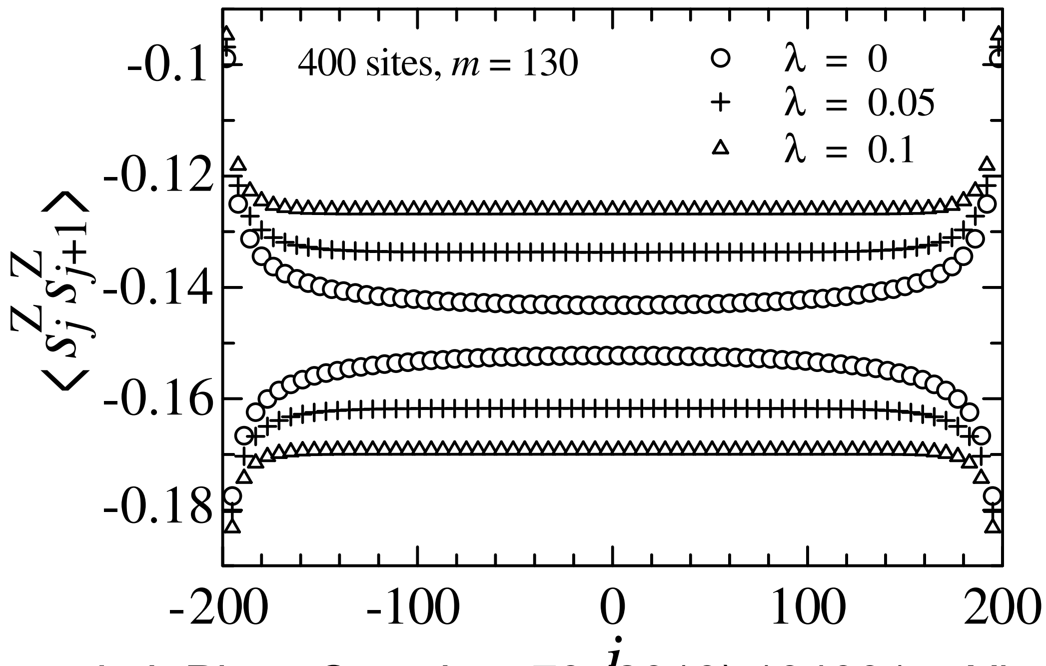
(c) have no interest on this matter
(d) prefer to climb up the mountains

Hyperbolic Deformation

$$H^{\cosh}(\lambda) = \frac{1}{2}\left[H^{\exp}(\lambda) + H^{\exp}(-\lambda)\right] = \sum_{j=-N}^{N} \cosh j\lambda \; h_{j,j+1} \,.$$

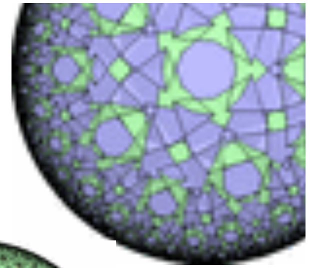
If one applies the deformation to the free fermion lattice, one would get similar off-critical state. (I have not calculated, since I'm more lazy than anyone.)

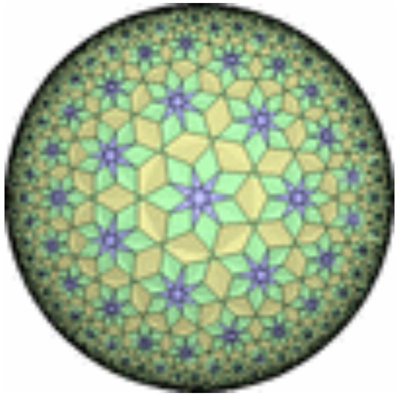
Example: S=1/2 Heisenberg Spin Chain (DMRG)

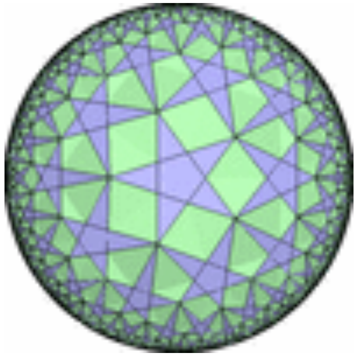


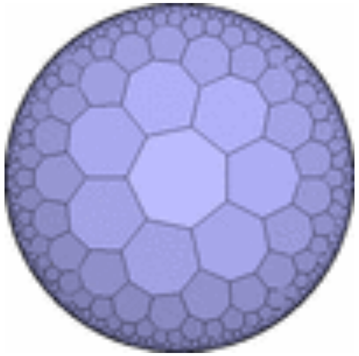
[3] H. Ueda et al: J. Phys. Soc. Jpn. 79 (2010) 104001;arXiv:1006.2652.
[4] H. Ueda et al: arXiv:1008.3458.

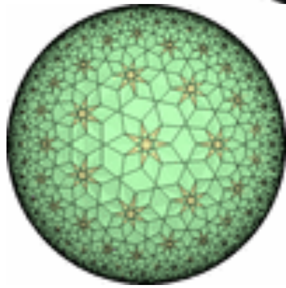
Classical Analogue: Ising Model on Hyperbolic Lattices

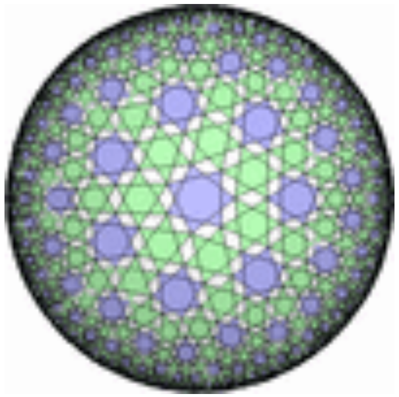




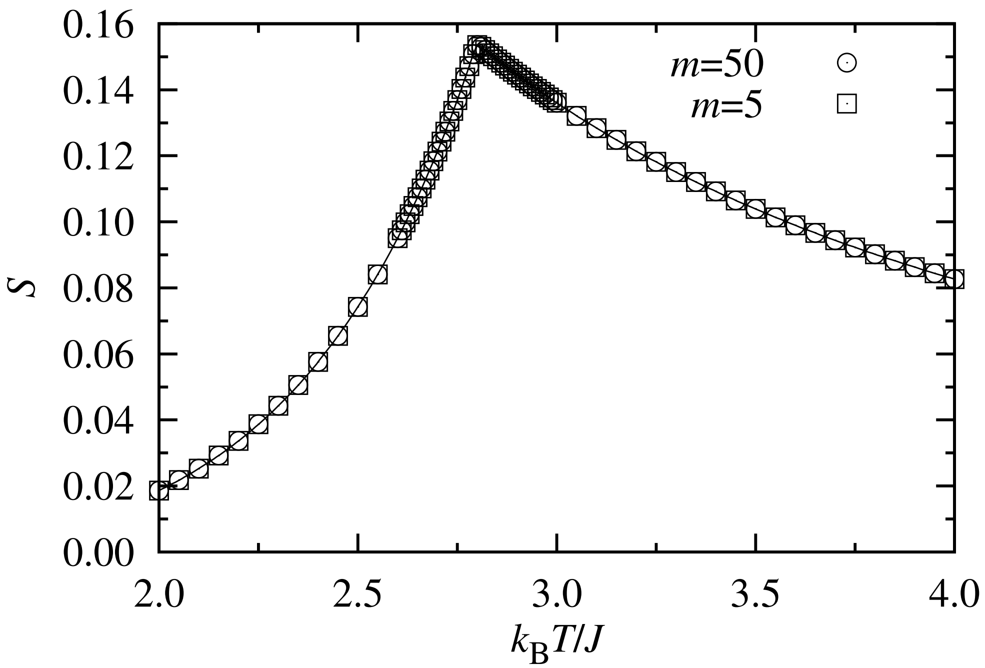








Entanglement Entropy of the 2D Hyperbolic Ising Model



No interest on Classical Subjects? For me, they are similar to Quantum ones ...

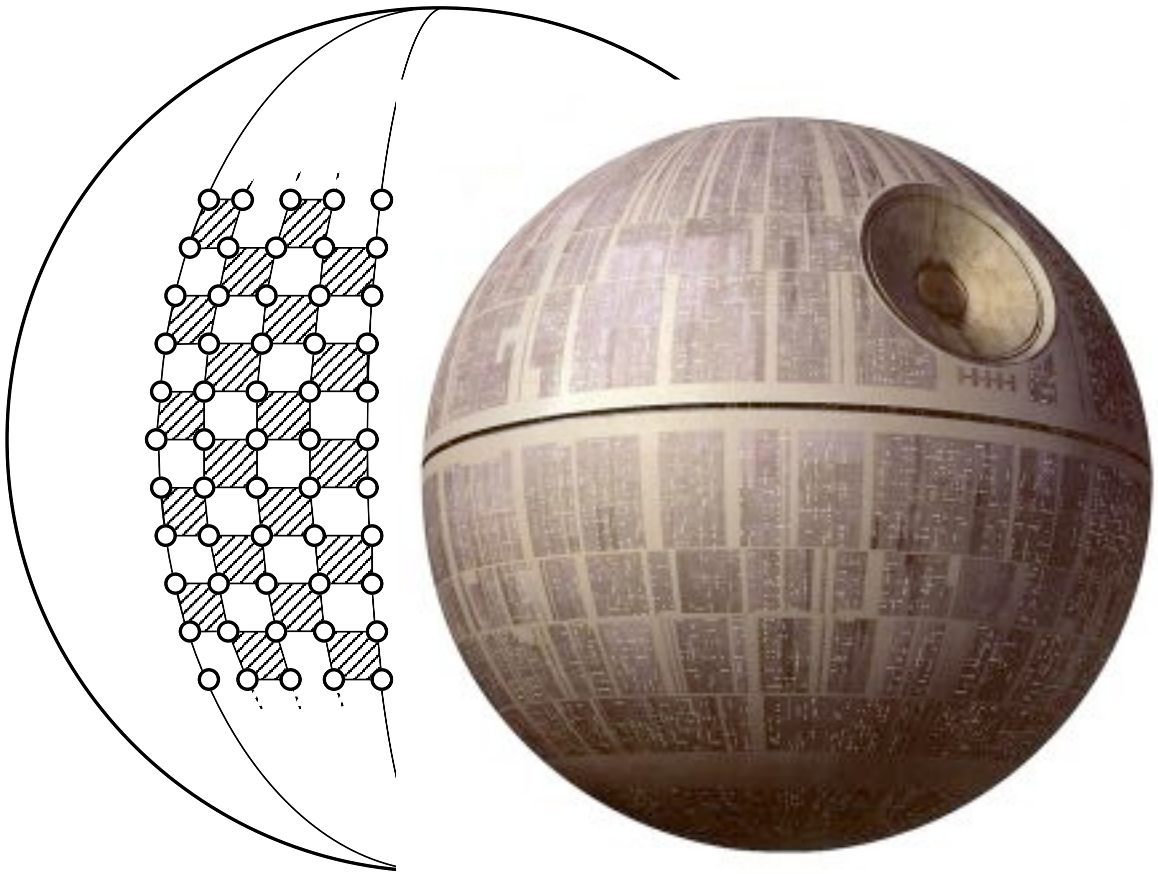
Matrix Product changes continuously at the transition point.

Today's Main (?) Subject: Spherical DeformationS

$$\mathcal{H}^{(N)}_{\rm sine} = -t \sum_{j=1}^{N-1} \left[\sin\left(\frac{j\pi}{N}\right)\right]^m (c_j^\dagger c_{j+1} + c_{j+1}^\dagger c_j)$$

arXiv: 1012.0472, 1012.1472

It is possible to extend the conjecture of uniformity to the cases where deformation function is given by cos(x). But this function could be zero or even negative. Thus, let us employ 2 [sin(x)]^2 = 1 – cos(x) as "the deformation function". The function is zero at the both end of the system x=0 and x=pi, and maximum at x=pi/2. Thus the function realizes so called the smooth boundary condition. We report that the ground state under the "Sine-Square Deformation"(SSD) is completely uniform.



Deformations for ‘Smooth Boundary’

Motivation:

if one is interested in the Bulk property,
how could the Boundary Effect be suppressed?

... here is an answer from a GIANT!

PHYSICAL REVIEW LETTERS

VOLUME 71 | 27 DECEMBER 1993 | NUMBER 26

Smooth Boundary Conditions for Quantum Lattice Systems

M. Vekić and S. R. White

Department of Physics, University of California, Irvine, California 92717

(Received 1 September 1993)

We introduce a new type of boundary conditions, *smooth boundary conditions*, for numerical studies of quantum lattice systems. In a number of circumstances, these boundary conditions have substantially smaller finite-size effects than periodic or open boundary conditions. They can be applied to nearly any short-ranged Hamiltonian system in any dimensionality and within almost any type of numerical approach.

PACS numbers: 02.70.−c, 05.30.Fk, 75.10.Jm

Before that, let us walk around the Bondary Effect.

Boundary Condition modifies the State

For example, look at water surface.

a glass of water

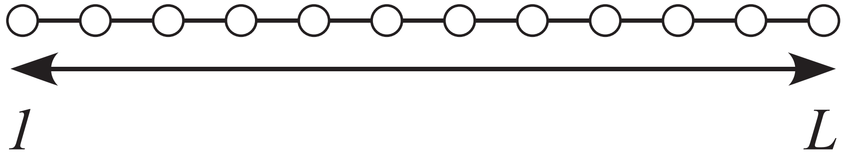
a `pacific' of water

I thought that this drawing magnifies the wave height, but actually a huge Tsunami attacked Japan many times, as that in last year.

drawing by active boundary

Free (spinless) Fermions in an OPEN chain (of N-site)

$$\mathcal{H}^{(N)} = -t \sum_{j=1}^{N-1} (c_j^\dagger c_{j+1} + c_{j+1}^\dagger c_j)$$

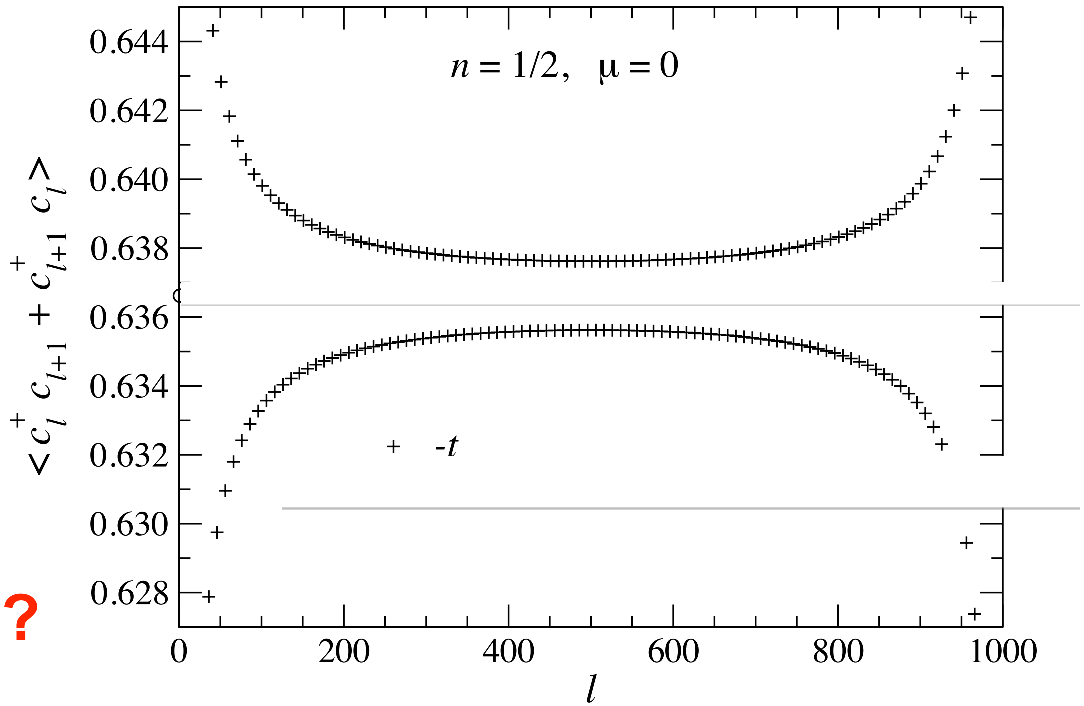


* For simplicity, we choose half-filling.
* Ground State is given by a Slater determinant.
* System is gapless. (... the gap is O(1/N).)

Boundary Effect:

Nearest Neighbor Correlation Function of the ground state is NOT uniform at all.

The value oscillates everywhere.



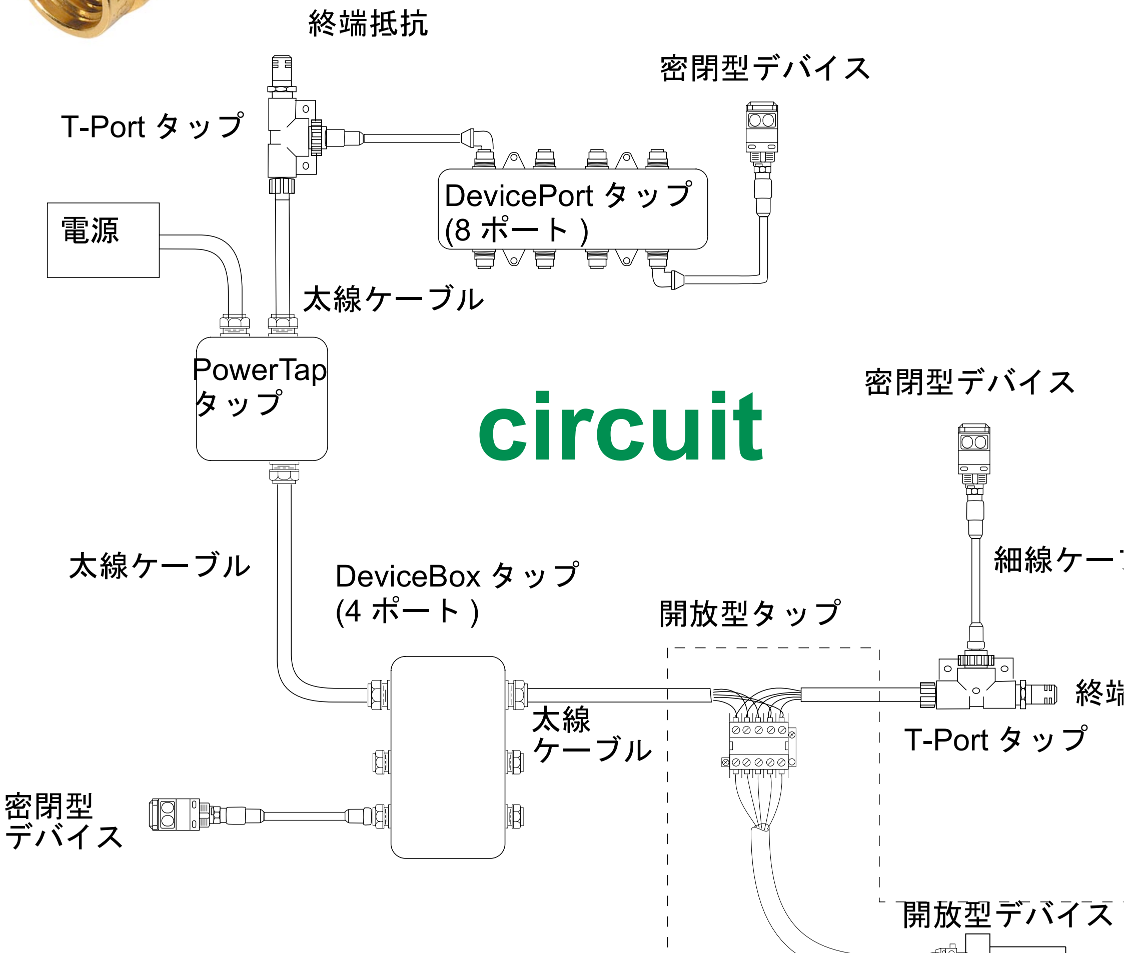
How to suppress the B.E.?

... the idea of Smooth B.C. is like the TERMINATOR.

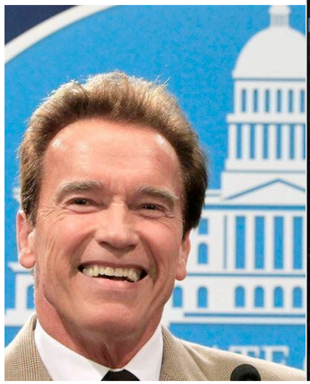
... which prevents reflections of signals at the boundary.

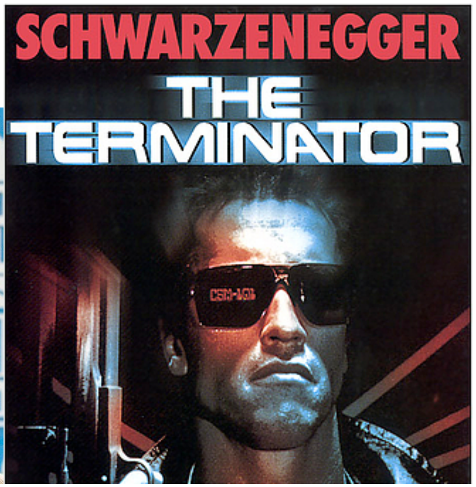
SCSI Terminator

A branched circuit needs many terminators.



circuit





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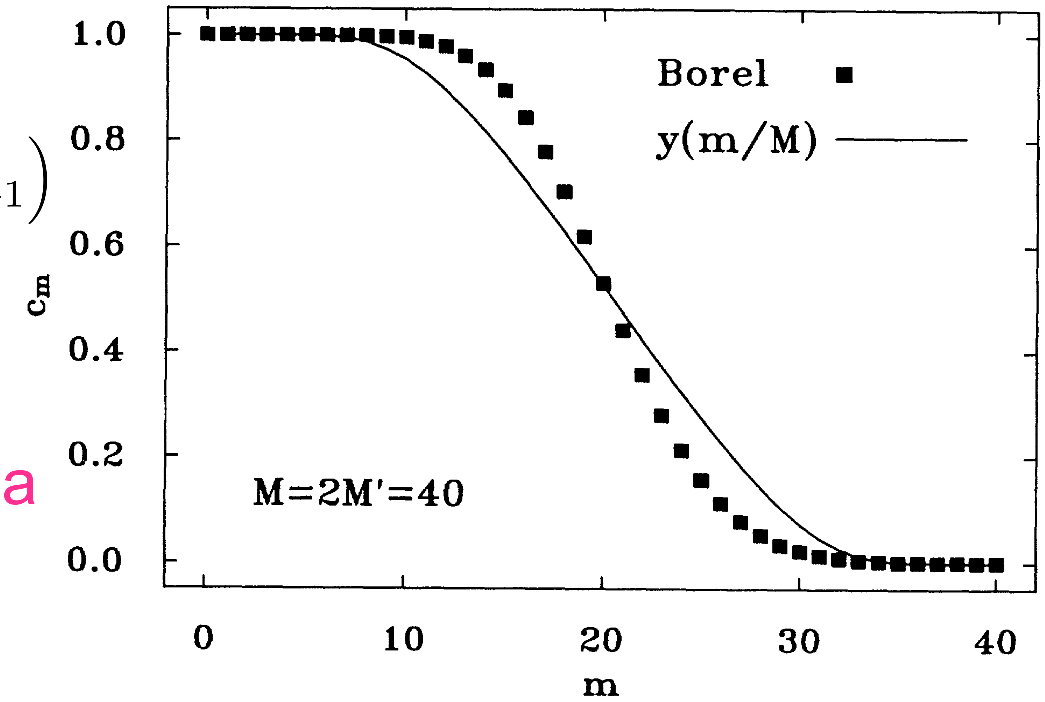
Vekic and White's setting:

$$H^{(N)}_{\text{smooth}} = \sum_{j=1}^{N-1} (-t_j) \left(c^\dagger_{j+1} c_j + c^\dagger_j c_{j+1} \right)$$



Smoothing function near the system boundary.

M: length of smoothing area

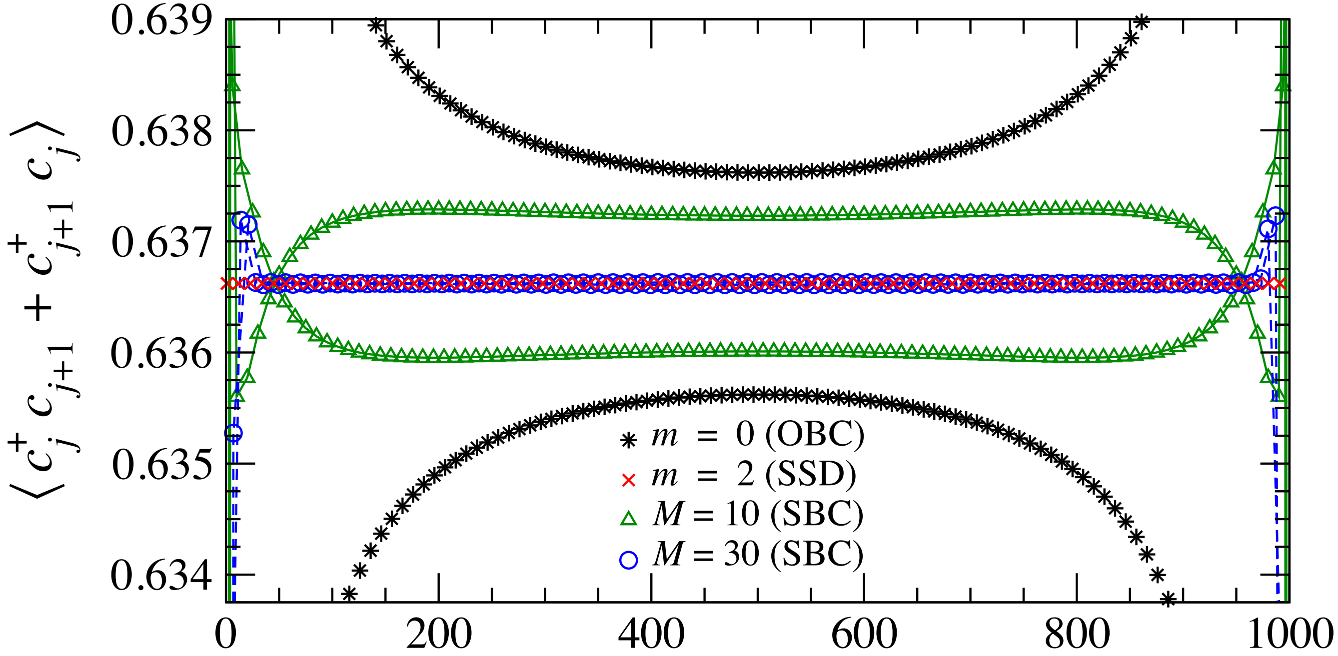
Boundary Effect:

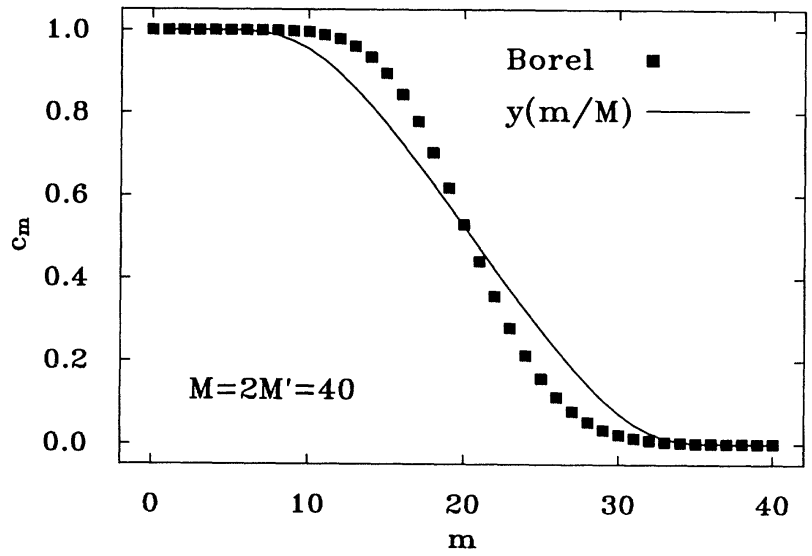
Black: OBC

Green: M=10

Blue: M=40

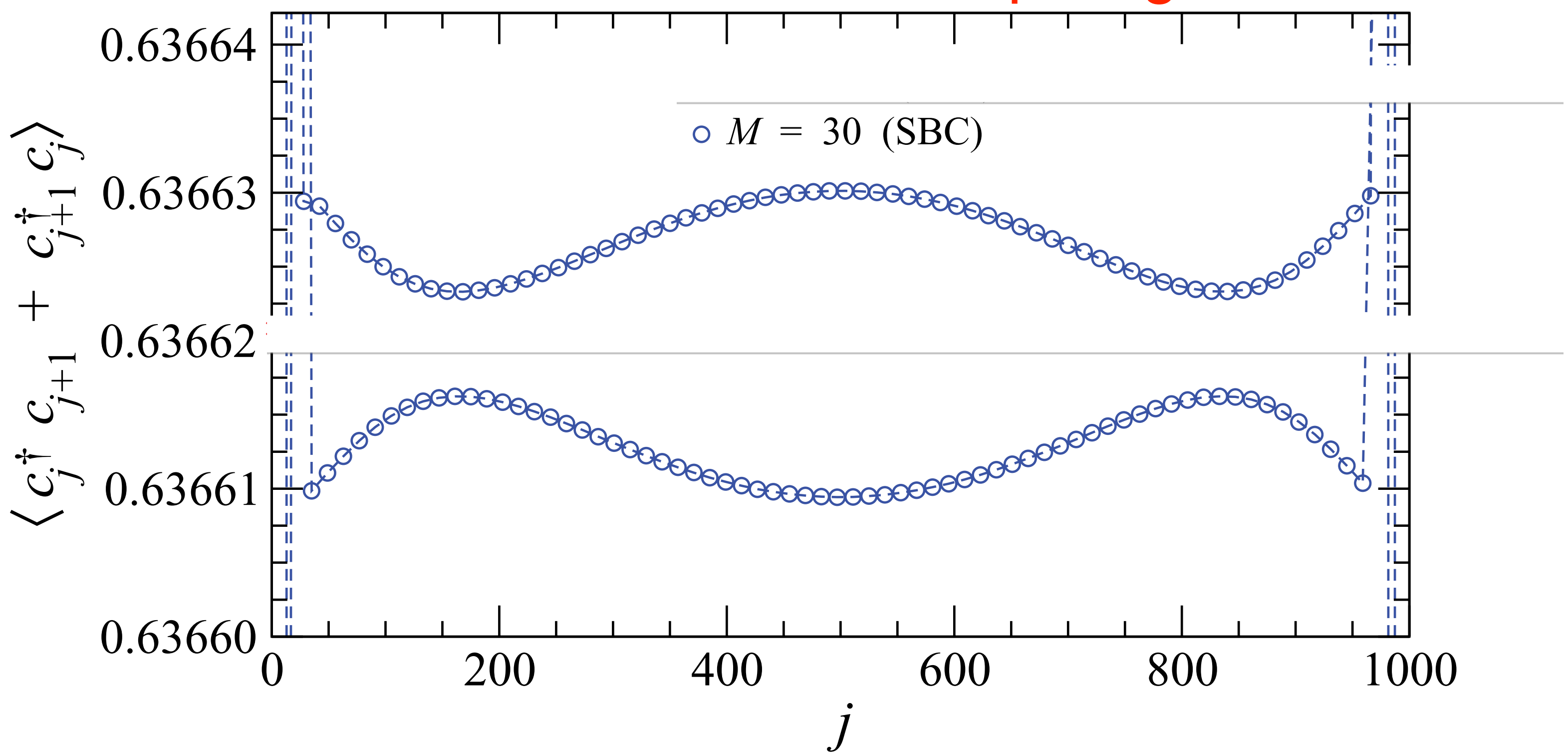
half-filling





Decrease the hopping parameter -t Smoothly to zero toward the boundary of the system.

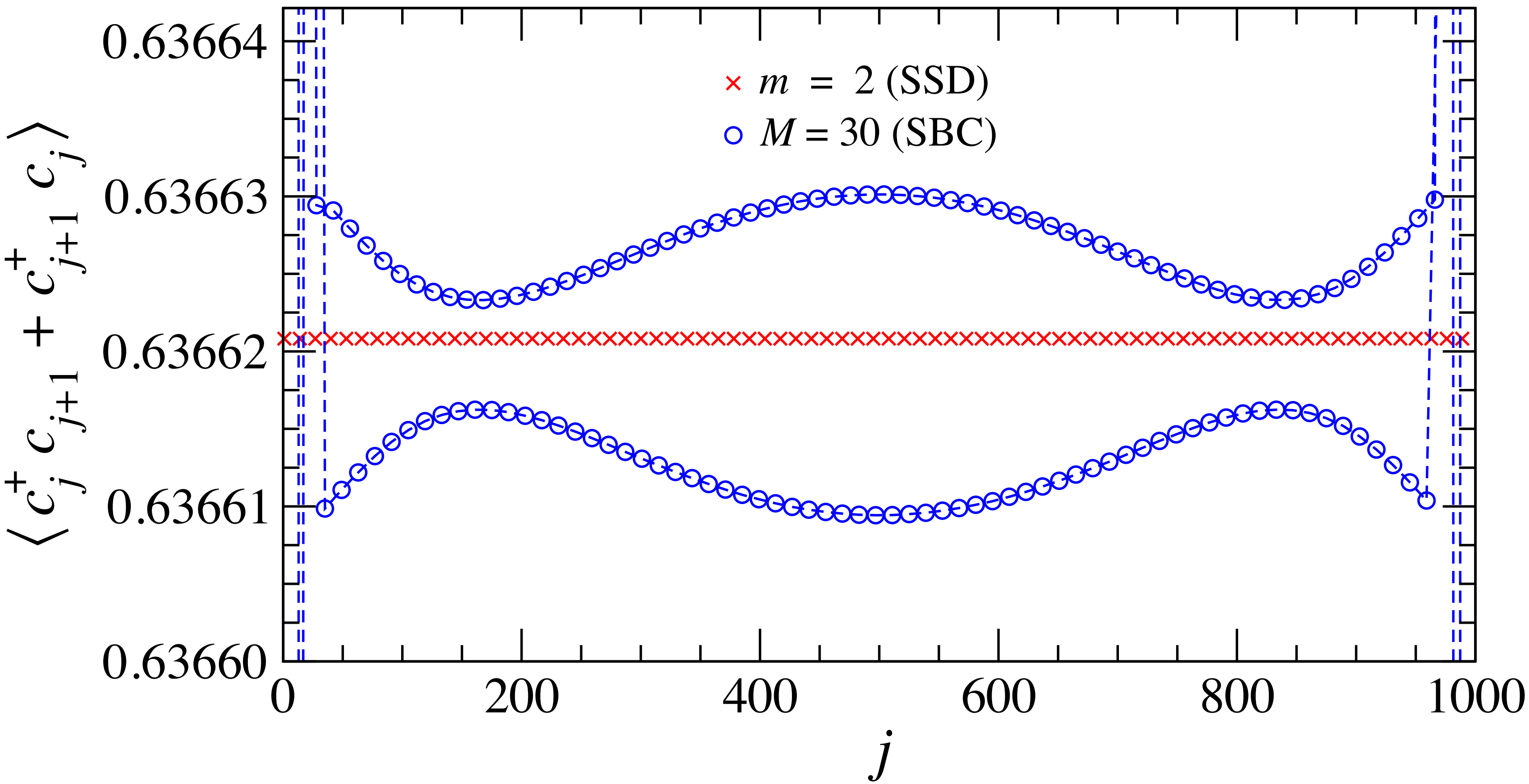
This modification works quite good.



... precisely speaking, weak boundary effect still exists.

Blue: M=40 (Smooth B.C.)

Red: (our result, see the next page)

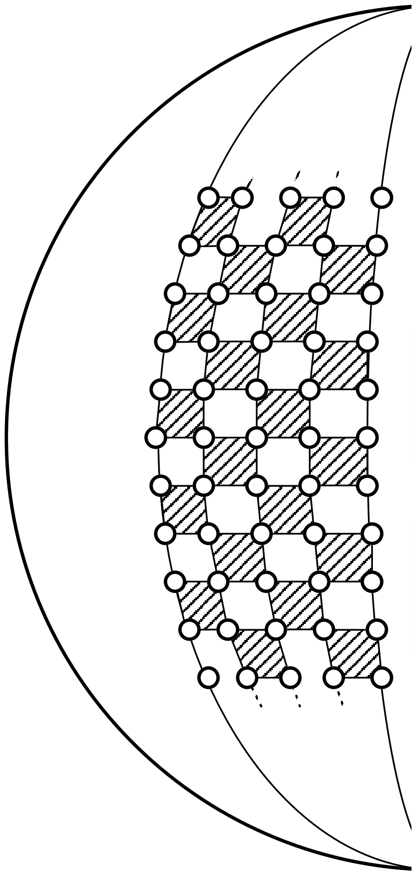


Then, what is the best Smoothing Function?

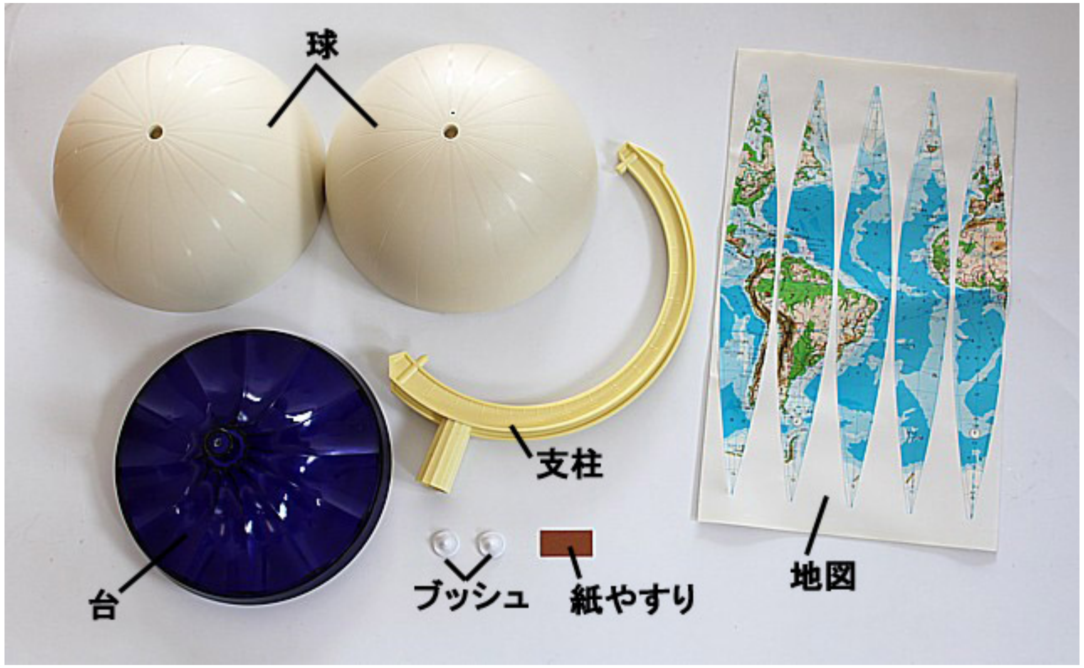
[5] A. Gendiar et al: Prog. Theor. Phys. 112 (2009) 953-967; arXiv:0810.0622.
[6] T. Hikihara, T. Nishino: Phys. Rev. E83 (2011) 060414; arXiv:1012.0472.
[7] H. Katsura: J. Phys. A: Math Theor 44 (2011) 252001; arXiv:1104.1721.
[8] I. Maruyama et al: Phys. Rev. B 84 (2011) 165132; arXiv:1108.2973.

Boundary effect appears because there are boundaries.

There is **no boundary** on the sphere.



Look at the **Globe** (not Google)



It is not possible to put **FLAT** paper on the sphere, if one speaks mathematically.

Look at the width of each peaces of paper. It is proportional to sin x, where 0 < x < ¥pi.

$$\mathcal{H}_{\rm sine}^{(N)} = -t \sum_{j=1}^{N-1} \left[\sin\left(\frac{j\pi}{N}\right) \right]^m (c_j^\dagger c_{j+1} + c_{j+1}^\dagger c_j)$$

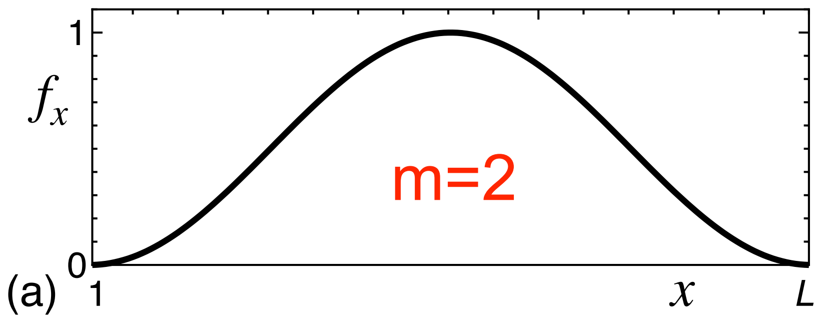
A. Gendiar puts a parameter “m” to the smoothing function.

Andrej Gendiar

Uniform Hamiltonian with Open Boundary Condition

$$\mathcal{H}^{(N)} = -t \sum_{j=1}^{N-1} (c_j^\dagger c_{j+1} + c_{j+1}^\dagger c_j)$$ **Before**

Sine Square Deformation



After

$$\mathcal{H}_{\text{sine}}^{(N)} = -t \sum_{j=1}^{N-1} \left[\sin\left(\frac{j\pi}{N} \right) \right]^m (c_j^\dagger c_{j+1} + c_{j+1}^\dagger c_j)$$

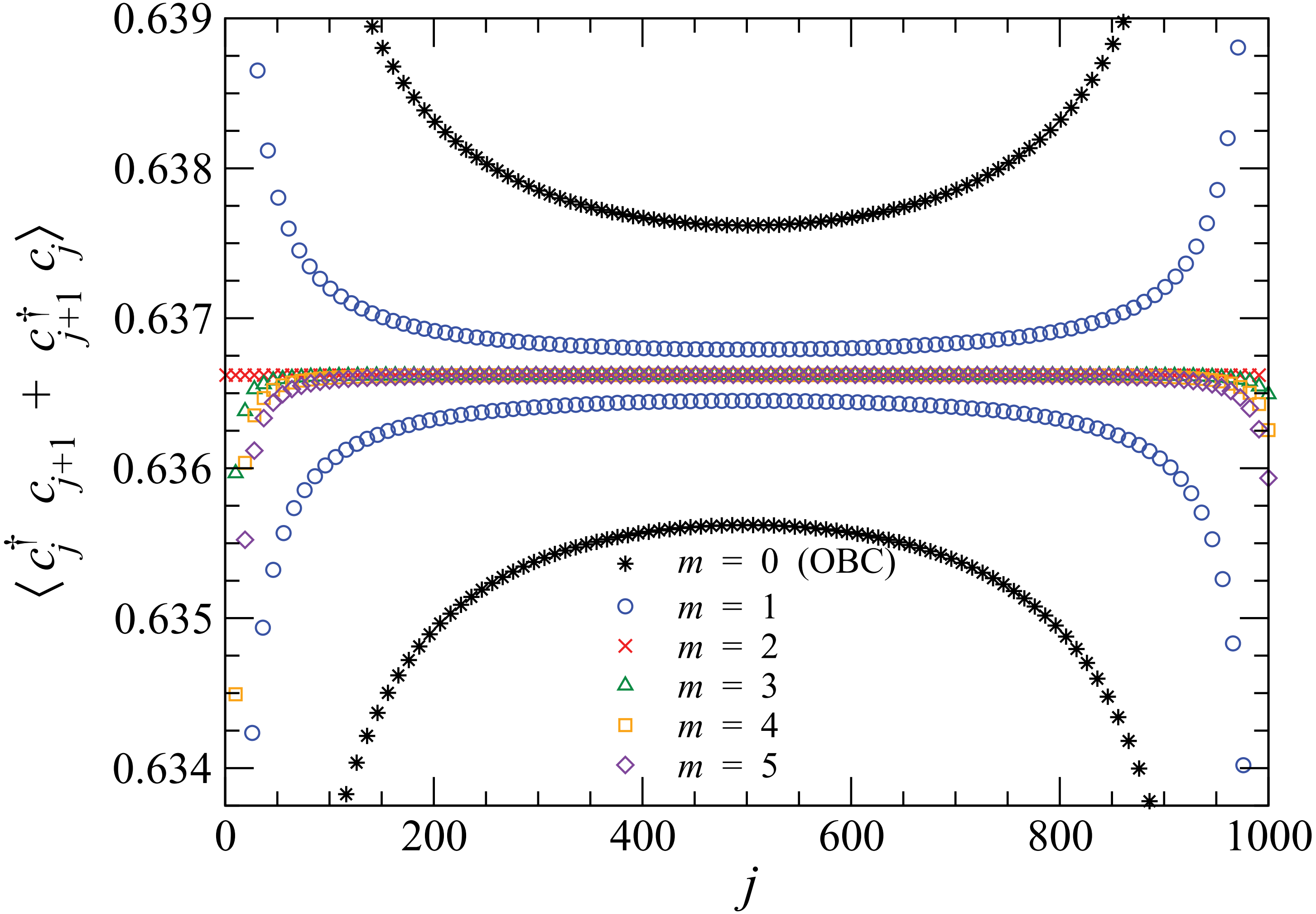
Note that the Hamiltonian is NOT uniform at all.

Is the ground state uniform? **Yes!**

Numerical Result at Half-filling

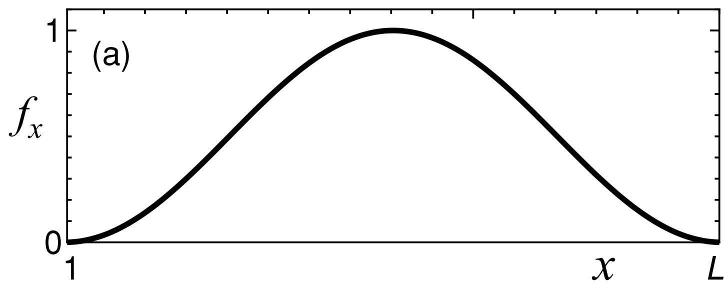
$$\mathcal{H}_{\text{sine}}^{(N)} = -t \sum_{j=1}^{N-1} \left[\sin\left(\frac{j\pi}{N} \right) \right]^m (c_j^\dagger c_{j+1} + c_{j+1}^\dagger c_j)$$

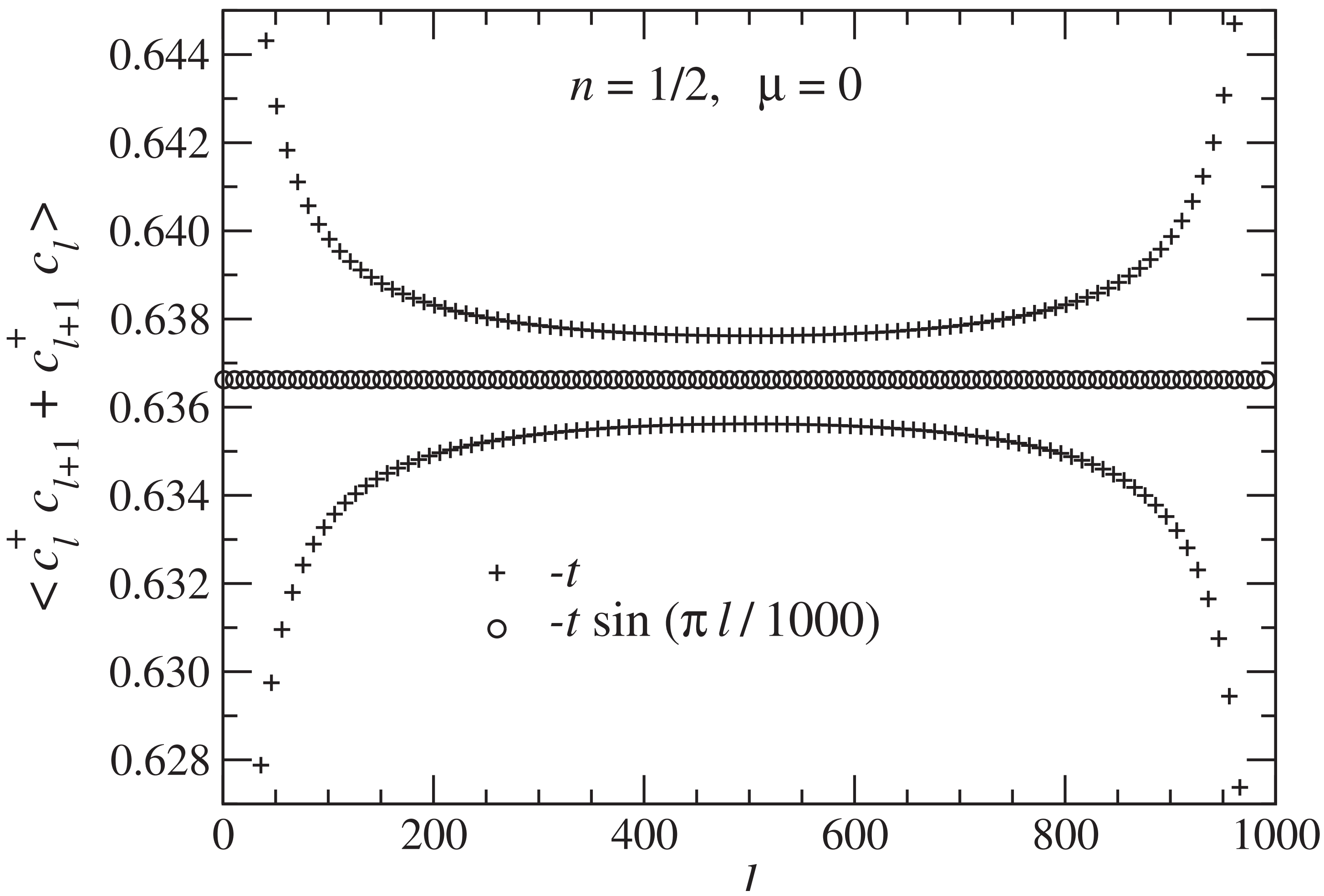
bond correlation function of G.S. at half-filling



m=2 is super!

$$\hat{H}_{\mathrm{S}} = -t \sum_{\ell=1}^{N-1} \sin^2 \frac{\ell\pi}{N} \left(\hat{c}_\ell^\dagger \hat{c}_{\ell+1} + \hat{c}_{\ell+1}^\dagger \hat{c}_\ell \right)$$





a mistake: $$\mathcal{H}_{\rm sine}^{(N)} = -t \sum_{j=1}^{N-1} \left[\sin\left(\frac{j\pi}{N} \right) \right]^m (c_j^\dagger c_{j+1} + c_{j+1}^\dagger c_j)$$

Progress of Theoretical Physics, Vol. 122, No. 4, October 2009

Spherical Deformation for One-Dimensional Quantum Systems

Andrej Gendiar,[1,2] Roman Krcmar[1] and Tomotoshi Nishino[2,3]

Errata

Spherical Deformation for One-Dimensional Quantum Systems

Andrej Gendiar, Roman Krcmar and Tomotoshi Nishino

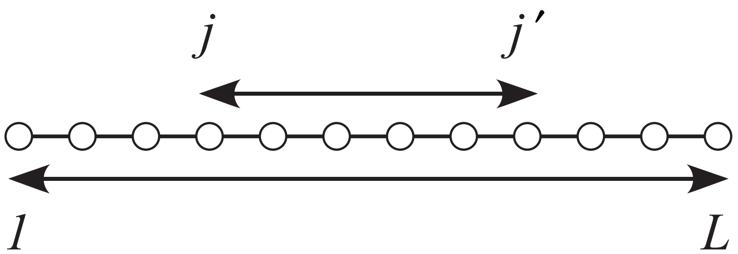
Prog. Theor. Phys. **122** (2009), 953.

(Received December 10, 2009; Revised December 23, 2009)

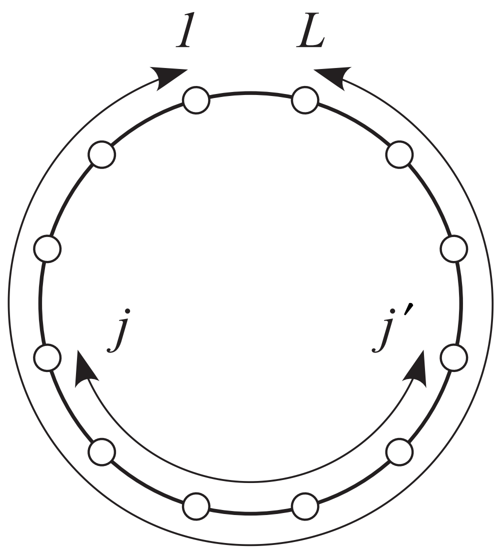
When m=2, the effect of Boundary is missing!!!

$$\mathcal{H}_{\text{sine}}^{(N)} = -t \sum_{j=1}^{N-1} \left[\sin\left(\frac{j\pi}{N}\right)\right]^m (c_j^\dagger c_{j+1} + c_{j+1}^\dagger c_j)$$

Looking at the ground state wave function (GSWF) of the above Hamiltonian at half-filling, it is the same as the GSWF of the system with Periodic Boundary Condition.



$\rightarrow$



Periodic

$$\mathcal{H}^{(N)} = -t \sum_{j=1}^{N-1} (c_j^\dagger c_{j+1} + c_{j+1}^\dagger c_j) - t\,(c_N^\dagger c_1 + c_1^\dagger c_N)$$

Mathematical Proof by Katsura

J. Phys. A: Math. Theor. 44 (2011) 252001

Exact ground state of the sine-square deformed XY spin chain

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Department of Physics, Gakushuin University, Mejiro, Toshima-ku, Tokyo 171-8588, Japan

E-mail: `hosho.katsura@gakushuin.ac.jp`,

Abstract. We study the sine-square deformed quantum XY chain with open boundary conditions, in which the interaction strength at the position x in the chain of length L is proportional to the function $f_x = \sin^2[\frac{\pi}{L}(x - \frac{1}{2})]$. The model can be mapped onto a free spinless fermion model with site-dependent hopping amplitudes and on-site potentials via the Jordan-Wigner transformation. Although the single-particle eigenstates of this system cannot be obtained in closed form, it is shown that the many-body ground state is identical to that of the uniform XY chain with periodic boundary conditions. This proves a conjecture of Hikihara and Nishino [Hikihara T and Nishino T 2011 *Phys. Rev. B* **83** 060414(R)] based on numerical evidence.

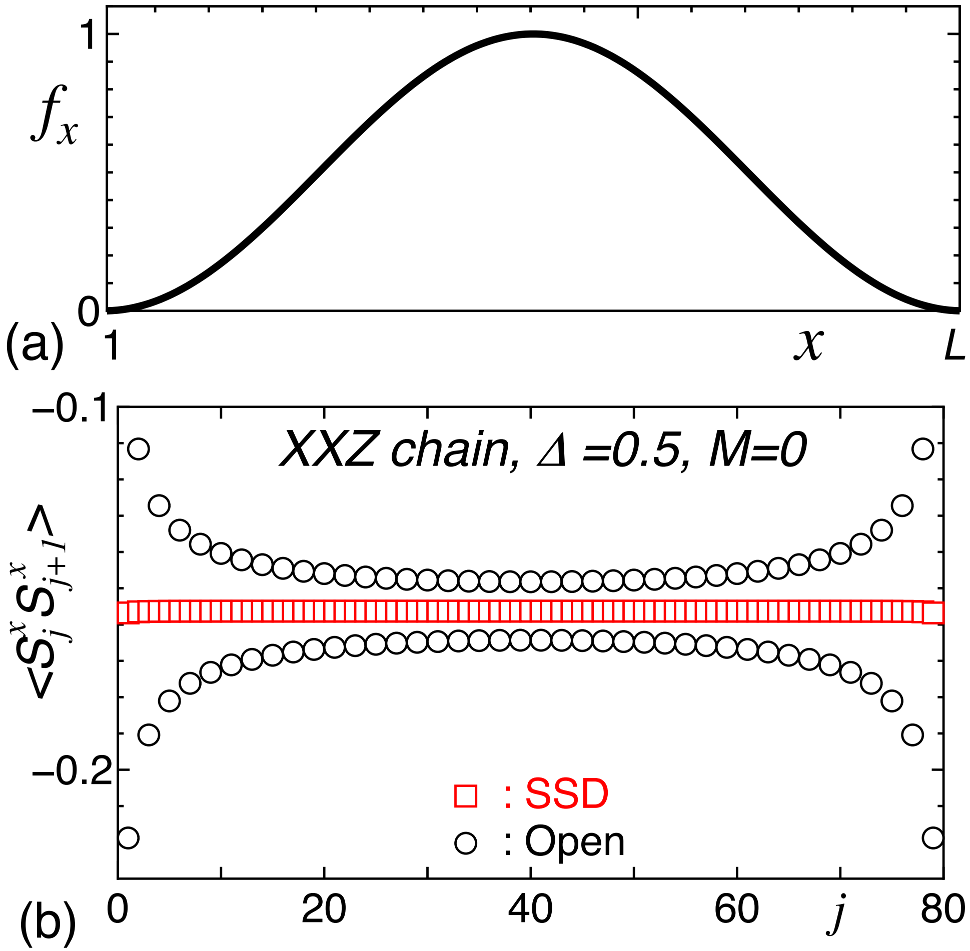
$$\hat{H}_{\mathrm{S}} = -t \sum_{\ell=1}^{N-1} \sin^2 \frac{\ell\pi}{N} \left(\hat{c}_\ell^\dagger \hat{c}_{\ell+1} + \hat{c}_{\ell+1}^\dagger \hat{c}_\ell \right)$$

Correlated case:

$$f_x = \sin^2\left[\frac{\pi}{L}\left(x - \frac{1}{2}\right)\right]$$

Heisenberg Spin Chain

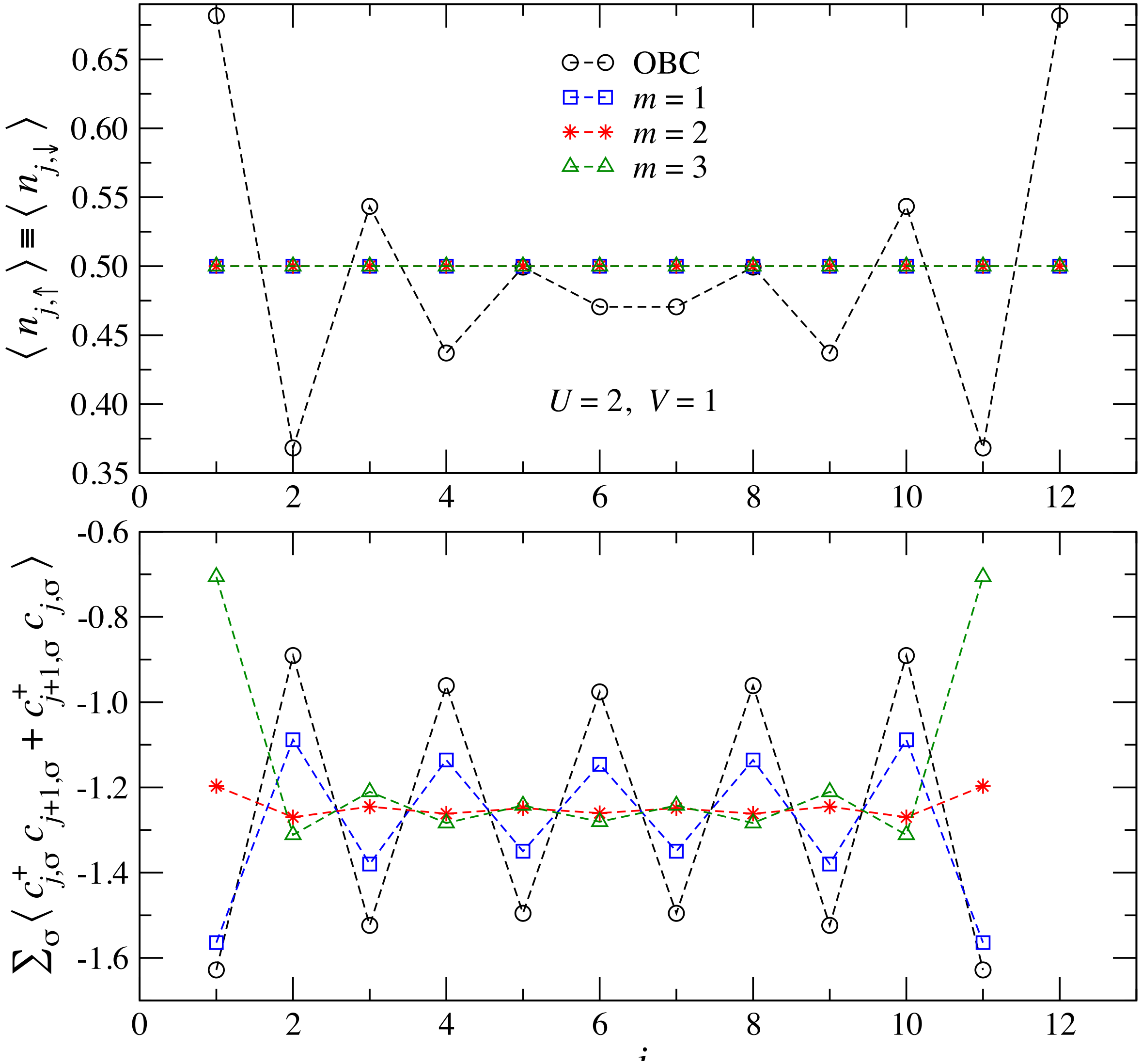
$$\mathcal{H}_{\mathrm{XXZ}} = J\sum_{j=1}^{L-1} f_{j+\frac{1}{2}}\left(S_j^x S_{j+1}^x + S_j^y S_{j+1}^y + \Delta S_j^z S_{j+1}^z\right)$$



Correlated case:

Extended Hubbard Model

$$
\begin{aligned}
h_{j,j+1} = & -\ t \sum_{\sigma=\uparrow,\downarrow} \left(c^\dagger_{j\sigma} c_{j+1\sigma} + c^\dagger_{j+1\sigma} c_{j\sigma} \right) \\
& + \frac{U}{2} \left[\left(n_{j\uparrow} - \tfrac{1}{2} \right) \left(n_{j\downarrow} - \tfrac{1}{2} \right) \right. \\
& \qquad \left. + \left(n_{j+1\uparrow} - \tfrac{1}{2} \right) \left(n_{j+1\downarrow} - \tfrac{1}{2} \right) \right] \qquad (\\
& + \ V \left(n_{j\uparrow} + n_{j\downarrow} - 1 \right) \left(n_{j+1\uparrow} + n_{j+1\downarrow} - 1 \right)
\end{aligned}
$$



Sin^m Deformation

$$\mathcal{H}_{\text{sine}}^{(N)} = -t \sum_{j=1}^{N-1} \left[\sin\left(\frac{j\pi}{N} \right) \right]^m (c_j^\dagger c_{j+1} + c_{j+1}^\dagger c_j)$$

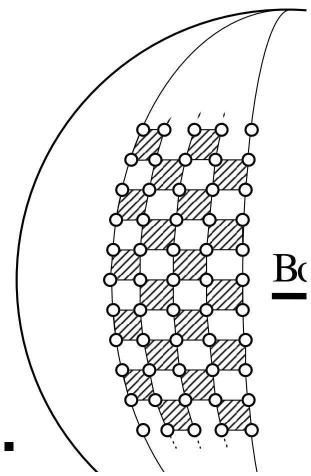
* How to apply TEBD? (DMRG is straight forward.)

* How does MPS look like?

* Generalization to Complex deformation functions? Matrix valued deformations?

* Higher Dimensional Generalization?

* ...



arXiv: 1012.0472, 1012.1472 / 1108.2973, 1104.1721, ...

Non-uniform Deformations Applied to 1D Quantum Systems

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Uniform .... infinite, or finite: examples

Open Boundary Condition $$\mathcal{H}^{(N)} = -t \sum_{j=1}^{N-1} (c_j^\dagger c_{j+1} + c_{j+1}^\dagger c_j)$$

Periodic Boundary Condition $$\mathcal{H}^{(N)} \quad -t\,(c_N^\dagger c_1 + c_1^\dagger c_N)$$

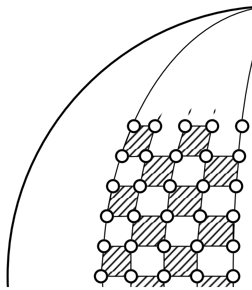
Non-uniform: exp[cj], cosh[cj], random, etc., AND!

Sin^m Deformation

$$\mathcal{H}^{(N)}_{\rm sine} = -t \sum_{j=1}^{N-1} \left[\sin\left(\frac{j\pi}{N}\right)\right]^m (c_j^\dagger c_{j+1} + c_{j+1}^\dagger c_j)$$

The case m = 2, Sine-Square Deformation, is cool.

arXiv: 1012.0472, 1012.1472 / 1108.2973, 1104.1721, ...



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