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生成関数によるテンソルネットワークの和の計算方法

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WLT *et al.*, arXiv:2101.03935 (2021)

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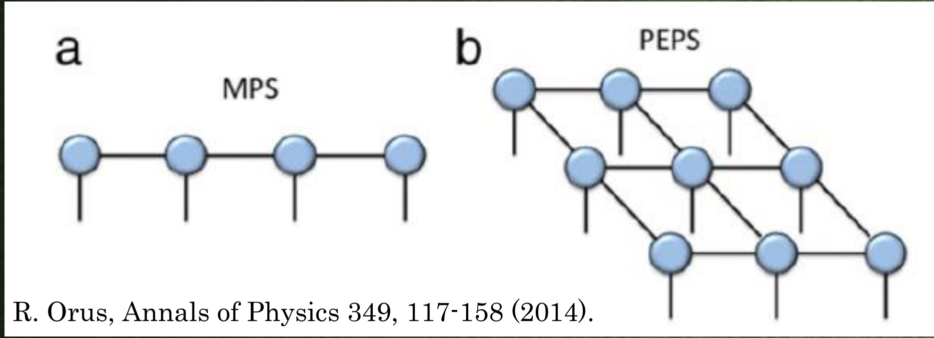
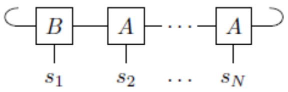
Tensor network:



R. Orus, Annals of Physics 349, 117-158 (2014).

One-particle excitation:

$$|\Phi_k(B)\rangle = \sum_{j=0}^{N-1} \mathrm{e}^{-ikj}\hat{T}^j$$



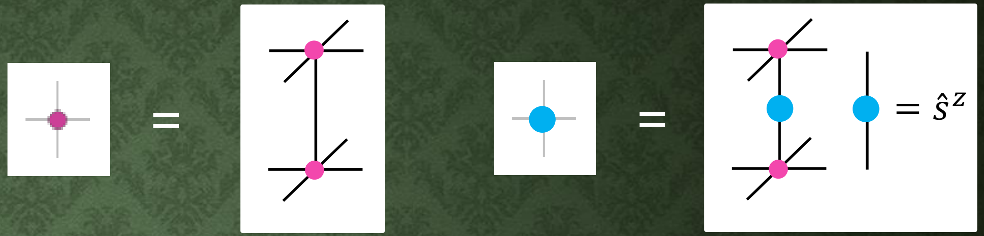
Static structural factor:

$$S^{\alpha,\beta}(k) = \frac{1}{N}\sum_{j,j'=1}^{N} e^{i\boldsymbol{k}\cdot(\boldsymbol{r}_j-\boldsymbol{r}_{j'})}\left\langle \hat{O}_j^{\alpha}\hat{O}_{j'}^{\beta}\right\rangle$$

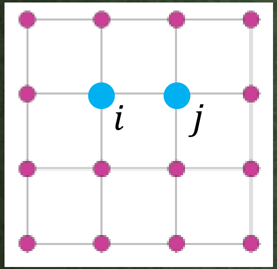
- Tensor network ansatz has become one of the reliable numerical approaches for quantum many-body systems.
- After obtaining the ground state ansatz, we need to calculate some physical observables or solve for low-energy excited states for further analysis.
- Within such evaluation, the summation of a series of tensor graphs is needed, which results in a large computational cost.

Spin static structural factor in 2D:

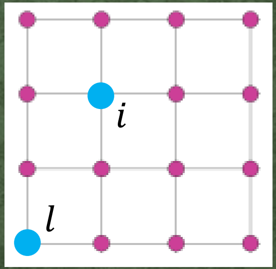
$$S^z(k) = \frac{1}{N}\sum_{j\neq j'}^{N} e^{i\boldsymbol{k}\cdot(\boldsymbol{r}_j-\boldsymbol{r}_{j'})}\langle \hat{s}_j^z \hat{s}_{j'}^z\rangle$$



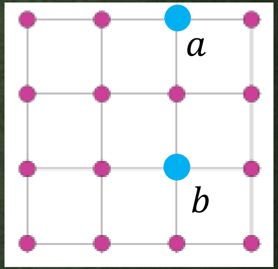
$$= \frac{1}{N} e^{i\boldsymbol{k}\cdot(\boldsymbol{r}_i-\boldsymbol{r}_j)}$$



$$+ \; e^{i\boldsymbol{k}\cdot(\boldsymbol{r}_i-\boldsymbol{r}_l)}$$



$$+ \; e^{i\boldsymbol{k}\cdot(\boldsymbol{r}_a-\boldsymbol{r}_b)}$$



$$+\cdots$$

$N(N-1)$ copies

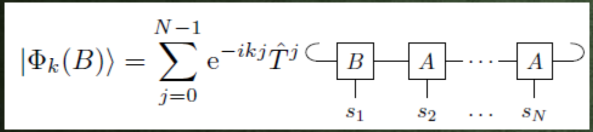
- Therefore, in the traditional way one needs to consider many distinct tensor graphs for the final summation.
- However, for a large system or large virtual bond dimension, calculation for single graph can be already cumbersome.

Generating function (GF):

- In field theory, this function is often constructed and by taking the derivative, one can obtain the target values.
- Here, we are going to borrow the same idea and apply it for the tensor network ansatz.

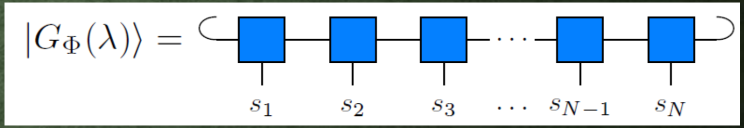
Taking 1D system as an example (with translational symmetry):

One-particle excitation:



$$\frac{\partial |G_\Phi(\lambda)}{\partial\lambda}|_{\lambda=0}$$

Corresponding GFs:

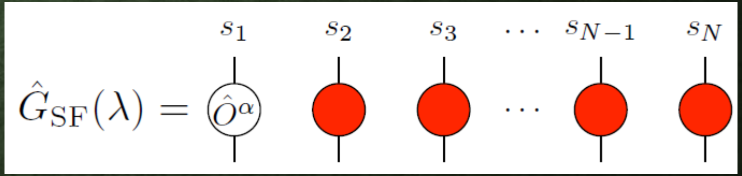


$$MPS_j(\lambda) = A + \lambda e^{-ikr_j} B$$

Static structural factor:

$$\left\langle \frac{\partial |\hat{G}_{SF}(\lambda)}{\partial\lambda}|_{\lambda=0} \right\rangle$$

$$S^{\alpha,\beta}(k) = \sum_{j=1}^{N} e^{i\boldsymbol{k}\cdot(\boldsymbol{r}_1-\boldsymbol{r}_j)} \left\langle \hat{O}_1^\alpha \hat{O}_j^\beta \right\rangle$$

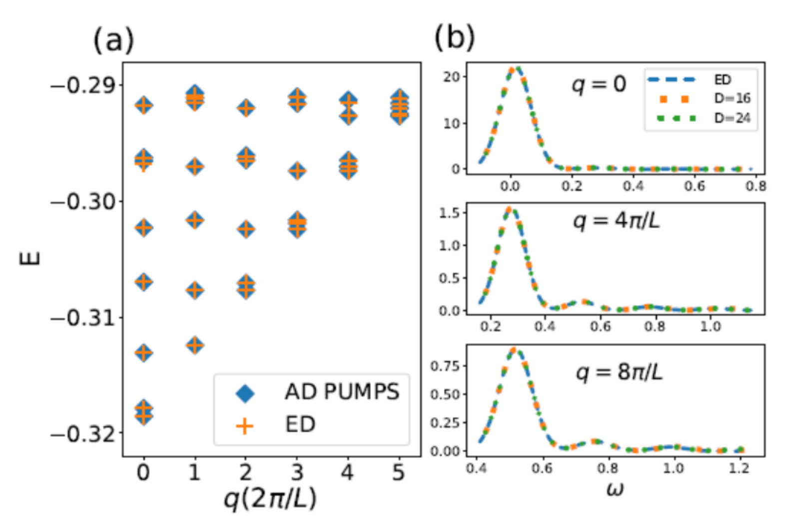


$$\hat{O}_j^\beta(\lambda) = I + \lambda e^{-ikr_j} \hat{O}^\beta$$

WLT *et al.*, arXiv:2101.03935 (2021)

- With generating functions, now we only need to calculate one or a few tensor graphs.
- Moreover, the derivatives can be evaluated using automatic differentiation(AD), which is often utilized in neural networks.

1D critical Ising chain(L=24):



$$S^{\alpha}(k,\omega)=\sum_n |M_k^{\alpha}|^2\delta\left(\omega-E_n^k+E_0\right),$$
$$M_k^{\alpha}=\langle\Phi_k(B_n)|S_k^{\alpha}|\psi(A)\rangle,$$
$$S_k^{\alpha}=\frac{1}{\sqrt{N}}\sum_{j=1}^{N}e^{ikr_j}S_j^{\alpha}$$

- (a) low-energy spectrum by us and from exact diagonalization(ED).
- (b) spectrum weight(dynamical structural factor) with different bond dimension and ED

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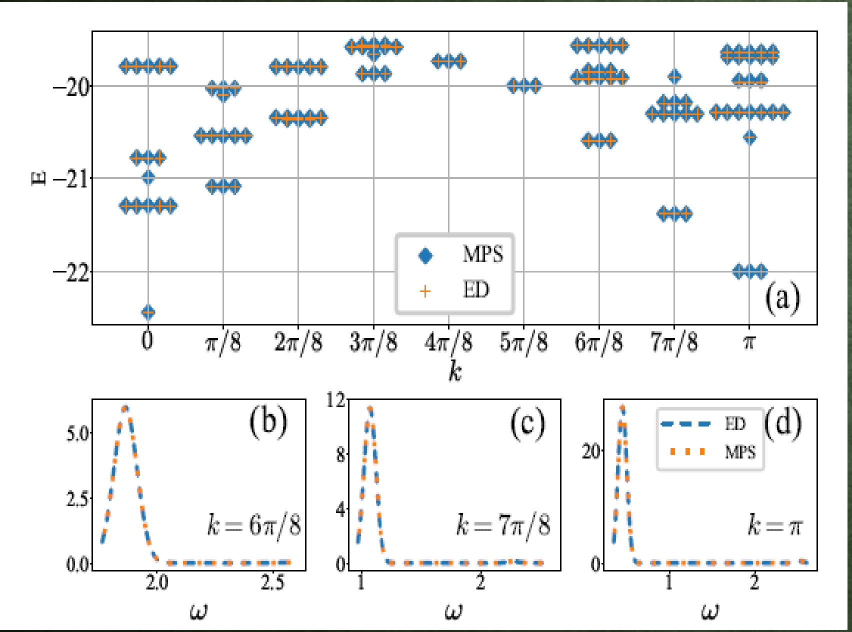
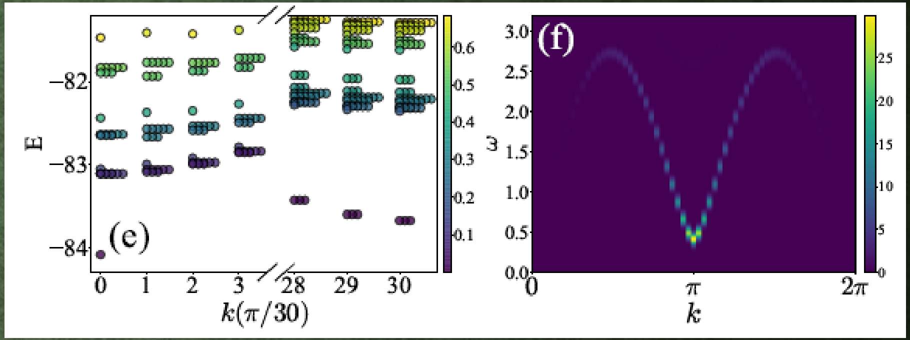
1D spin-1 Heisenberg model:

L=16:



L=60:



- Good benchmark accordance in smaller size with ED.
- Energy spectrum and dynamical structural factor can be obtained for larger system size.
- Haldane gap≈0.4105

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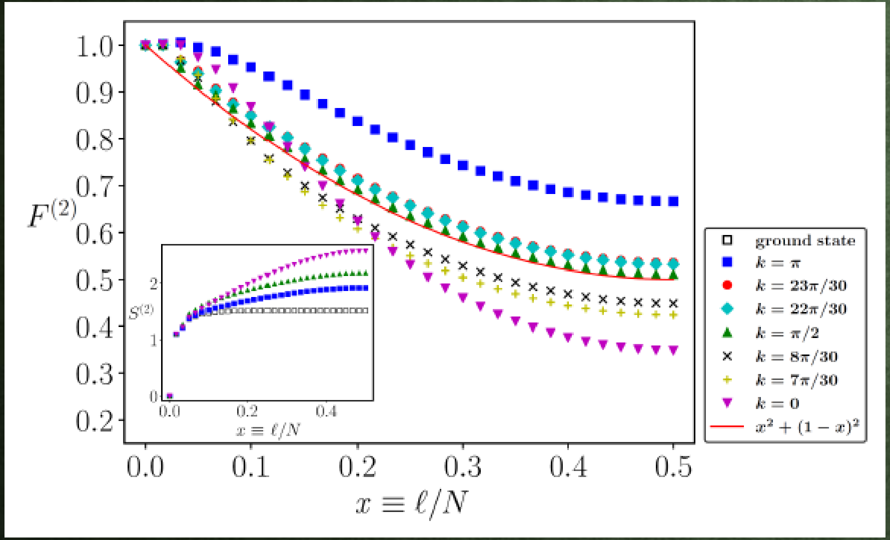
1D spin-1 Heisenberg model:

Entanglement entropy:



$$\rho_l^n = Tr_{\bar{l}}|\psi><\psi| \text{ or } Tr_{\bar{l}}|\Phi><\Phi|$$

$$S^{(n)} = \frac{1}{1-n} log Tr_l \rho_l^n$$

$$F^{(n)} = \frac{Tr\rho_\Phi^n}{Tr\rho_\psi^n}$$

$|\psi>$: Ground state

$|\Phi>$: Excited state

- Red line indicates the theoretical prediction that accords with our result for $k = \pi/2$.
- Traditionally this character is hard to calculate with TN due to a large summation of complex TN graphs.

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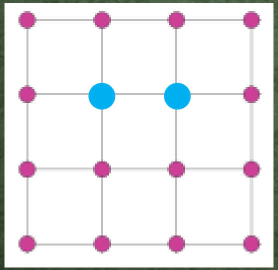
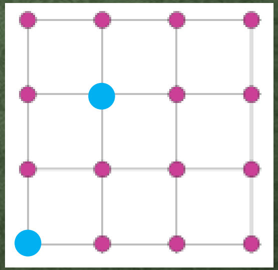
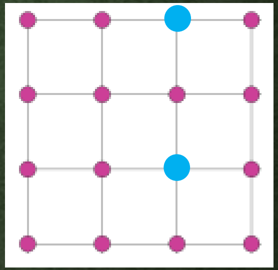
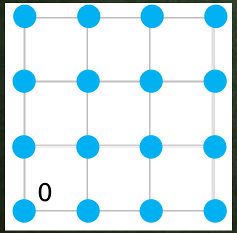
Future goals:

- Although we only demonstrate translationally invariant 1D systems, the idea of generating function can be in principle extended to other scenarios such as in two dimension.
- Moreover, even when we try to calculate the ground state energy for some long-range interactive model, generating function can be also applied.

$$H = \sum_{ij} S_i^z S_j^z$$

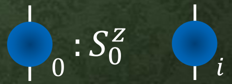
$< H >=$  $+$  $+$  $+\cdots$

N(N-1)/2 terms

$G(H) =$ 

+ other terms with different reference point

Only N terms!!



$: S_0^z$ $\quad : I + \lambda S_i^z$

$$< H >= \frac{1}{2} \frac{\partial G(H)}{\partial \lambda} |_{\lambda=0}$$

- It might be useful for complex models of quantum chemistry

SUMMARY

- We borrow the idea of generating function originating from field theory and apply it to the tensor network ansatz.
- Our results indicated that this is an useful approach and reduces the obstacle while performing TN summation.
- Possible extension includes its application in 2D systems, and we may also utilize the generating function for long-range interactive models.