Kernel-Function Based Quantum Algorithms for Finite Temperature Quantum Simulation

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Introduction

- Classical Kernel Polynomial Method (KPM):

$$f_{KPM}(x) = \int_{-1}^{1} \pi(1-y^2)^{\frac{1}{2}} K_N(x,y) f(y) dy;$$

$$K_N(x,y) = g_0\phi_0(x)\phi_0(y) + 2\sum_{n=1}^{N-1} g_n\phi_n(x)\phi_n(y)$$

- KPM achieves much success in classical simulation;
- However, to gain these moments $\{g_n\}_{n=0}^{N-1}$, the time complexity i s $O(ND)$, where D is the dimension of Hilbert space

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Success of KPM

- ✓ Calculation of the spectral density of Hermitian matrices;
- ✓ Static correlations at finite temperature;
- ✓ Dynamical correlations at finite temperature;
- ✓ Can be used as one component of other methods, like Monte Carlo simulations, Cluster Perturbation theory .....

Inspiration

The intrinsic relation between Chebyshev polynomials and cosine and sine functions,

$$T_n(x) = \cos[n \cdot \arccos(x)],\ \mathrm{U_n(x)} = \frac{\sin[(n+1)\arccos(x)]}{\sin[\arccos(x)]}$$

A new expansion method based on the Fourier Series:

1. For the density of states (Dos) only,

$$\rho(\epsilon) = c_0 + 2\sum_{n=1}^{N-1} c_n \cos(n\pi\epsilon)$$

2. For local observables $\hat{A}$

$$\alpha(\epsilon) = d_0 + 2\sum_{n=1}^{N-1} d_n \cos(n\pi\epsilon)$$

$$c_n = \frac{1}{D} Re\left[Tr\left(e^{-in\pi\hat{H}}\right)\right],\ d_n = \frac{1}{D} Re\left[Tr\left(\hat{A}e^{-in\pi\hat{H}}\right)\right]$$

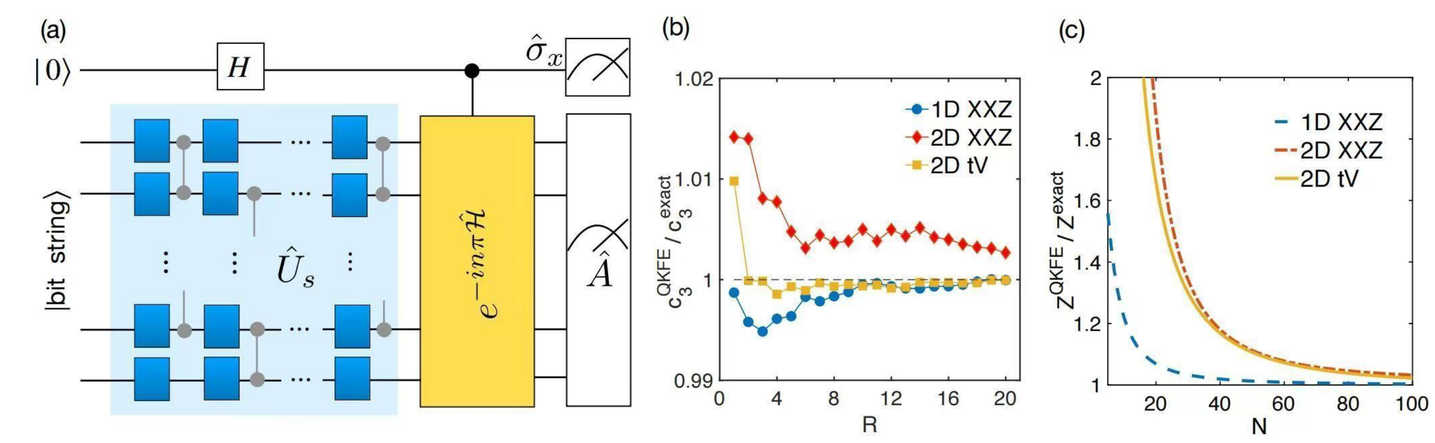
Models used

$$\hat{H}_{1D-XXZ} = \frac{1}{2}\sum_j \hat{\sigma}_j^x\hat{\sigma}_{j+1}^x + \hat{\sigma}_j^y\hat{\sigma}_{j+1}^y + \Delta\hat{\sigma}_j^z\hat{\sigma}_{j+1}^z\ (L=18);$$

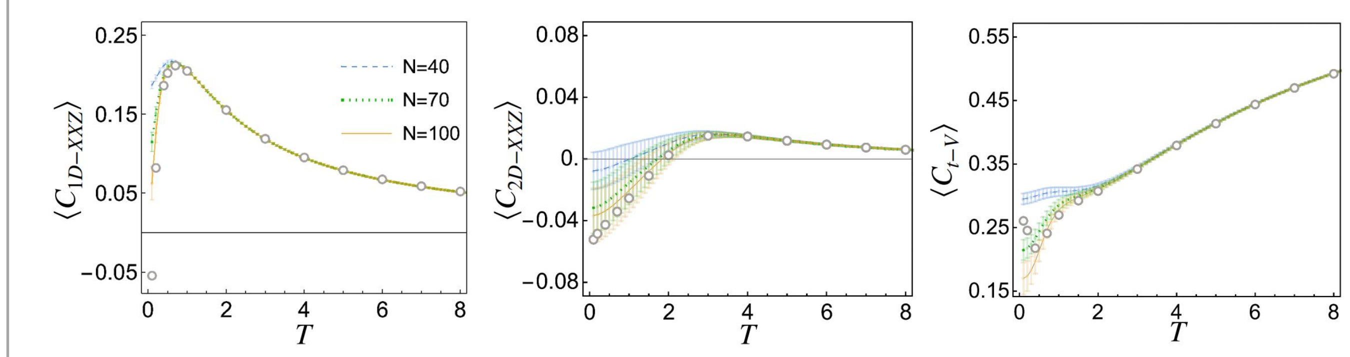
$$\hat{H}_{2D-XXZ} = \sum_{<i,j>} \hat{\sigma}_j^x\hat{\sigma}_{j+1}^x + \hat{\sigma}_j^y\hat{\sigma}_{j+1}^y + \Delta'\hat{\sigma}_j^z\hat{\sigma}_{j+1}^z\ (4\times4);$$

$$\hat{H}_{2D-tV} = -\sum_{<i,j>} \hat{c}_i^\dagger\hat{c}_j + \hat{c}_j^\dagger\hat{c}_i + \mathrm{V}\sum_{<i,j>} \hat{n}_i\hat{n}_j\ (4\times4);$$

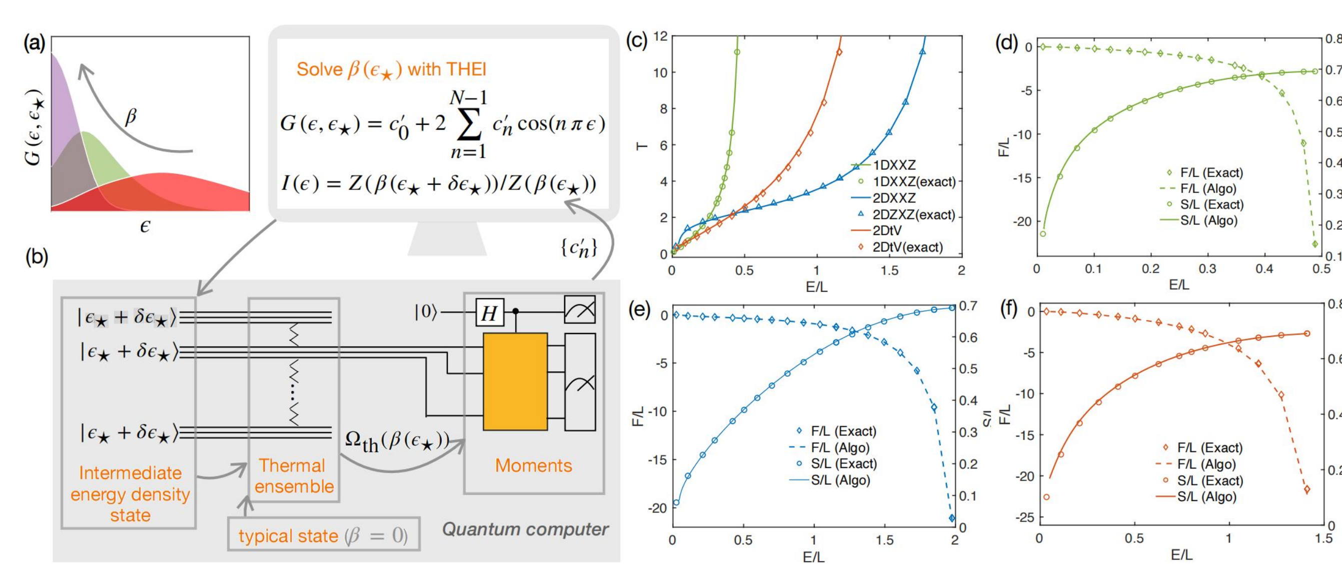
Moments As Results of quantum circuit outputs



Problems at low temperature regimes



The Thermal Ensemble Iteration subroutine



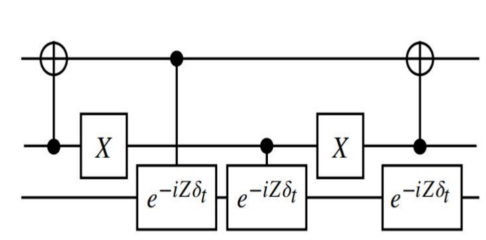
- ➢ Instead of $\rho(\epsilon)$, now the target function is

$$G(\epsilon,\epsilon_\star) = \frac{\rho(\epsilon)e^{-\beta(\epsilon_\star)\epsilon E_W}}{Z(\beta(\epsilon_\star))};$$

- ➢ The $\epsilon - independence$ condition of the function

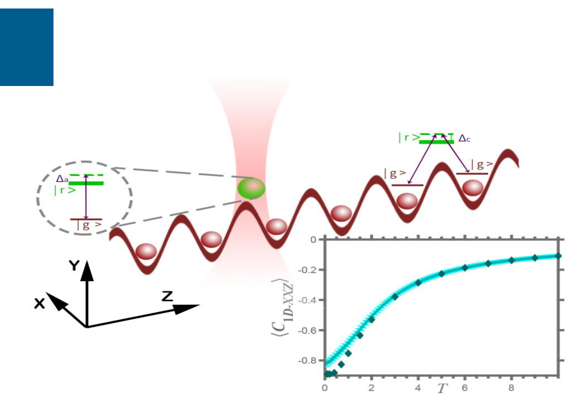
$$I(\epsilon) \stackrel{\text{def}}{=} \frac{G(\epsilon,\epsilon_\star)}{G(\epsilon,\epsilon_\star+\delta\epsilon_\star)} \times \frac{e^{\beta(\epsilon_\star)\epsilon E_W}}{e^{\beta(\epsilon+\delta\epsilon_\star)\epsilon E_W}}$$

Experimental Realization Protocols



Digital (Trotterization)

1D-XXZ model



Analog(atom-based simulation)

Summary

- ✓ Compared with KPM, our algorithms can achieve exponential advantages in terms of time and space cost;
- ✓ The THEI is efficient, once the target Hamiltonian's ground-state can be prepared by quantum circuits at polynomial cost;
- ✓ In terms of quantum digital and analog realizations, our plan is appealing to the NISQ era.

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