Exponential tensor renormalization group

From the microscopic aspect, the understanding of novel quantum states and statistic properties of quantum manybody systems is of significant importance in condensed matter physics. In particular, due to the relation to high-T superconductivity, quantum Hall effect, and topological quantum spin liquid states, 2D quantum matter and related materials are of great research interest.

Efficient and accurate simulations of quantum manybody systems are crucial to better understand these correlated electronic models and related materials. In particular, accurate calculations of thermal quantities such as specific heat, magnetization, and susceptibility, allow direct comparisons between theoretical predictions and experimental data, which is of key importance in understanding 2D quantum materials. Quantum Monte Carlo (QMC) and renormalization group (RG) are two prevailing approaches to simulate quantum lattice systems. However, suffering from the notorious minus-sign problem, unbiased QMC is desperately inefficient to sample frustrated spin systems and fermion systems away from half-filling. On the other hand, free from sign problem, the deterministic RG methods so far mainly focus on the ground-state properties, i. e., zero-temperature physics. It is thus of both theoretical and experimental importance to extend it to finite-T calculations of 2D quantum systems.

Recently, PhD student Binbin Chen (first author), undergraduate student Lei Chen (co-first author), and Associate Professor Wei Li (corresponding author) from the School of Physics of Beihang University, together with their collaborators from Brookhaven National Laboratory (USA), achieved this goal by developing a thermal tensor network method – exponential
tensor renormalization group (XTRG), which has been published in the prestigious physics journal *Phys. Rev. X*\(^{[1]}\).

Compared to the prevailing methods, XTRG benefits significantly in both efficiency and precision, and can be used to simulate both 1D and 2D systems. The main idea of the traditional linear tensor RG (LTRG) and XTRG is shown in Fig 1. As shown in Fig 1(a), the linear evolution scheme in inverse temperature \(\beta\) is as follows: starting with the density operator at a high temperature, one evolves the density operator by a small imaginary time (inverse temperature) in each iteration, successively cooling the system down to a specific temperature. It can be seen clearly in Fig 1(a) that the “cooling” speed is getting really slow when approaching the low-T regime.

![Diagram](image)

**Fig 1.** (a) Linear tensor renormalization group (LTRG) and (b) exponential tensor renormalization group (XTRG)

Recently, it has been realized that in conformal field theory (CFT) at finite temperature\(^{[2, 3]}\), the entanglement entropies of the thermal states in 1+1D critical systems scale logarithmically with inverse temperature \(\beta\). This indicates that the entanglement entropy of
the system actually changes significantly only when inverse temperature changes by a factor (say, $\beta$ to $2\beta$). This means, instead of linear evolution, by exponential evolution, one can cool down the system as fast as possible, i.e., exponentially, towards the low-temperature regime. This is still affordable, for the computational cost scales only polynomially with the number of iterations considering the logarithmic entanglement entropy. In the meantime, since the iteration steps have been significantly reduced, XTRG can more accurately simulate the low-temperature properties, also beyond traditional LTRG framework.

The basic idea of XTRG is also shown in Fig 2, where we start from the density operator (trivial identity matrix) at high temperature, then double the inverse temperature $\beta$ by squaring the density operator until reaching the specified temperature.

![Diagram](image)

**Fig 2.** Exponential tensor renormalization group (XTRG)

The results of applying XTRG to the simulations of 2D quantum lattice models are shown in Fig 3 and Fig 4, including Heisenberg XXZ model on square lattice (cf. Fig 3), and triangular
lattice Heisenberg model (cf. Fig 4).

Fig 3. Finite-temperature phase transition in Heisenberg XXZ square lattice: (a-b) the entanglement landscape $S_E$ versus bond index and temperature $T$; (c) entanglement entropy (left) as well as specific heat (right) versus $T$; (d) binder ratio $U_4$ versus $T$.

We showed that XTRG can be used to simulate 2D models efficiently. As shown in Fig 3, the thermal data of 2D square lattice XXZ Heisenberg model (axial anisotropy $\Delta = 5$) are presented. It includes the finite-temperature entanglement entropies, specific heat curves, and the binder ratio $U_4$. To make a long story short, we observed that the entanglement entropies peak at around the exact transition point $T_c = 0.56^{[4]}$ [Fig 3(a-c)]. Binder ratio can provide a very accurate estimate of critical point by pinpointing the intersection $T$ of the curves of various sizes, from which we obtained the phase transition temperature $T = 0.554$, which
constitutes a very accurate estimate of $T_c$ (relative error $\sim 1\%$). Based on these simulations, we believe that XTRG can be used to efficiently and accurately simulate the finite temperature properties of quantum lattice models, including the 2D systems with a finite-T phase transition.

Fig 4. Finite-temperature phase diagram of triangular lattice Heisenberg model (from left to right): high-temperature paramagnetic (spin gas) regime, anomalous liquid regime, and low-temperature stripe solid regime.

Beyond the bipartite square lattice, XTRG can also be applied to investigating the intriguing frustrated magnets. In Fig 4, we present some data on the triangular lattice Heisenberg (TLH) model. Since Anderson’s famous conjecture on resonating valence bond (RVB) state in the frustrated TLH was proposed\cite{5}, it has been intriguing scientists. Earlier studies have already noticed thermodynamics anomaly, which shows no signature of spin ordering of TLH, even at low temperatures. Here, we simulated the thermal properties of TLH on cylindrical
geometry of width $W = 4$, as a first exploration of the interesting system.

In Fig 4, we plotted the spin structure factors $S(q)$ and the corresponding phase diagram consisting of (from left to right) the high-temperature paramagnetic regime, intermediate-temperature anomalous “liquid” regime, where the 120-degree order and stripe order strongly compete, and the low-temperature stripe ordered “solid” due to special geometry constraint of the system. By using XTRG, the “cooling” of the system can be vividly seen by inspecting the spin structure factors and bond energy textures in Fig 4, from which one can clearly recognize the three different temperature regimes mentioned above.

Besides the frustrated magnets, there are still many interesting problems to be further explored, including the interacting fermionic system, and finite-temperature dynamics, etc., where we believe XTRG can play an important role.

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References