Combination of Tensor Network States and Green’s function Monte Carlo

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We propose an approach to study the ground state of quantum many-body systems in which Tensor Network States (TNS), specifically Projected Entangled Pair States (PEPS), and Green’s function Monte Carlo (GFMC) are combined. PEPS, by design, encode the area law which governs the scaling of entanglement entropy in quantum systems with short range interactions but are hindered by the high computational complexity scaling with bond dimension. GFMC is a highly efficient method, but it usually suffers from the infamous negative sign problem which can be avoided by the fixed node approximation in which a guiding wave function is utilized to modify the sampling process. The trade-off for the absence of negative sign problem is the introduction of systematic error by guiding wave function. In this work, we combine these two methods, PEPS and GFMC, to take advantage of both of them. PEPS are very accurate variational wave functions, while at the same time, only contractions of single-layer tensor network are necessary in GFMC, which reduces the cost substantially and enable us to reach large bond dimension in PEPS. Moreover, energy obtained in GFMC is guaranteed to be variational and lower than the variational energy of the guiding PEPS wave function. Benchmark results of $J_1$-$J_2$ Heisenberg model on square lattice are provided.

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One of the most challenging tasks in condensed matter physics is to understand the many-body effect in strongly correlated quantum systems, in which numerous exotic phenomena emerge. These phenomena, including high-temperature superconductivity [1], fractional quantum Hall effect [2, 3] quantum spin liquid [4], are among the mostly studied but yet unsolved problems in condensed matter physics. Because exact solution for strongly correlated system is rare [5], most studies of these systems rely on numerical tools nowadays. Density Matrix Renormalization Group (DMRG) [6, 7] is one of the most successful methods in the study of strongly correlated systems. DMRG is extremely accurate for one-dimensional (1D) quantum systems [8, 9]. Shortly after the introduction of DMRG in 1992 [6], it was realized that the underlying wave functions are Matrix Product States (MPS) [10], which can be viewed as a generalization of the seminal AKLT state [11]. The concept of MPS can be traced back at least to 1968 [12]. It was found that MPS capture the entanglement structure of the ground state of 1D quantum systems and this results in the high accuracy of DMRG [13]. The adoption of concepts from the field of quantum information, entanglement for example, have inspired the development of the Tensor Network States (TNS) [14]. These advances provide us useful tools to both identify [15] and classify [16, 17] quantum phases.

When applying to two-dimensional (2D) systems, DMRG was found to suffer from the exponential growth of bond dimension with the width of system if we want to achieve the same accuracy [18]. Nevertheless, DMRG can still provide accurate results for systems on narrow cylinders with large enough bond dimension [19, 20]. A natural generalization of MPS to 2D, Projected Entangled Pair States (PEPS) [21], can solve the issue of the exponential growth of bond dimension in DMRG. It can be proved that the entanglement entropy in PEPS satisfies the area law [22] (with logarithm correction if a Fermi surface is present [23]) which is required to faithfully represent the ground state of 2D quantum systems [13]. PEPS and its generalizations have shown high accuracy in the study of strongly correlated 2D systems [24–30]. However, in contrast to $D^3$ scaling of complexity in MPS, the computational cost is as high as $D^{12}$ in PEPS. The heavily scaling of computational resource with bond dimension in PEPS hampers the reach to large bond dimension which is essential to resolve possible competing states in the low energy manifold of certain strongly correlated systems, e.g., the anti-ferromagnetic Heisenberg model on Kagome lattice [20, 31, 32, 33]

Quantum Monte Carlo (QMC) [31, 37] is a widely used methodology in the study of strongly correlated many-body systems. In QMC, physical quantities are evaluated stochastically [38]. In general, the computational complexity in QMC scales algebraically with system size which makes it an efficient approach. However, with few exception [31], the direct application of Monte Carlo method in many-body systems suffers from the infamous negative sign problem [39, 40], which causes the error of physical quantity to grow exponentially with system size and $\beta$, the inverse of temperature. One strategy to overcome the negative sign problem is to take advantage of the trade-off between variance and bias, which is the principle behind fixed node approximation in Green’s function Monte Carlo (GFMC) [31, 42] (also named as diffusion Monte Carlo (DMC) [43] in the literature), and constrained path approximation in auxiliary field quantum Monte Carlo [44]. In these methods, a guiding or trial wave function is employed to adjust the random walk process to get rid of the negative sign problem. But
the price to pay is the introduction of systematic error or bias in the result. In QMC calculation with fixed node, or constrained path approximation, the quality of guiding or trial wave function is the key and controls the accuracy. Empirically, different forms of guiding or trial wave functions can be chosen to give high accuracy for certain systems.

In this work, we combine PEPS and GFMC to take advantage of both of them. We take PEPS as guiding wave function in GFMC calculation. As we will discuss later, in our method, only contraction of single-layer tensor network is required, which highly reduces the computational complexity in the PEPS part. At the same time, PEPS are very accurate variational wave functions, with which systematic error can be reduced in GFMC.

**Models** – For concreteness, we take the $S = 1/2$ $J_1$-$J_2$ Heisenberg model on square lattice as an example to describe the method. The Hamiltonian is as follows:

$$H = J_1 \sum_{\langle i,j \rangle} S_i S_j + J_2 \sum_{\langle\langle i,j \rangle\rangle} S_i S_j$$

(1)

where $S_i$ is the spin operator on site $i$. $\langle i,j \rangle$ and $\langle\langle i,j \rangle\rangle$ represent nearest and next nearest neighboring interactions respectively. We consider anti-ferromagnetic interactions for both $J_1$ and $J_2$, and set $J_1$ as the energy unit. For simplicity, we study system on square lattice with open boundary conditions (OBC). The $J_1$-$J_2$ Heisenberg model is widely investigated in the exploration of the frustration effect in quantum systems \cite{53,54}. When $J_2$ is absent, the model can be solved with QMC without suffering from the negative sign problem \cite{53,54}. The ground state is known to have the long-range anti-ferromagnetic (AF) order, i.e., the Neel order. In the other limit when $J_1 = 0$, the system decouples into two independent square lattices and an infinitesimal $J_1$ can drive the ground state into the striped AF order. Between these two limits, the nature of the ground state is still under extensive debates \cite{55–62} in the vicinity of $J_2/J_1 = 0.5$ where the system is maximally frustrated in the sense that in the classical limit, the $J_1$-$J_2$ Ising model has macroscopic degenerate ground state. We will only show benchmark results of $J_1$-$J_2$ model on small lattice size where exact answer can be obtained, to demonstrate the effectiveness of our method, and leave the investigation of the ground state properties of $J_1$-$J_2$ model near $J_2/J_1 = 0.5$ for future study.

**Projected Entangled Pair States** – To construct a PEPS, we put a rank five tensor, $A_{l,d,r,u}^{\sigma}$ on each vertex of the square lattice (see Fig. 1(b)), where $\sigma$ is the physical degree of freedom with dimension $d$, while $l, d, r, u$ are the auxiliary degree of freedoms with dimension $D = 2^5$.

Contracting the auxiliary degree of freedoms gives the PEPS wave function

$$\psi = \sum_{\{\sigma\}} \text{Tr}(A^{[\sigma_0]}A^{[\sigma_1]} \cdots A^{[\sigma_{N-1}]})|\sigma_0, \sigma_1, \ldots, \sigma_{N-1}\rangle$$

(2)

To obtain the ground state of the $J_1 - J_2$ Heisenberg model in Eq(1), we apply the imaginary time projection operator $\exp(-\tau H)$ repeatedly to an initial PEPS till convergence. Same as in Trotter-Suzuku decomposition \cite{63}, we first divide the lattice into four groups of plaquettes in a way that the projection operators of each plaquette within a group are independent or commute with each other. In each group, a Projected Entangled Pair Operator (PEPO) (see Fig. 1(c)) for the projection operator within a single plaquette is constructed and are applied to the initial PEPS simultaneously. This procedure is carried out recurrently for the four groups (see FIG. 2: Energy versus step in the GFMC calculation for a $4 \times 4$, $J_2 = 0$ system with OBC. A PEPS with bond dimension $D = 4$ is used as the guiding function. The energy at step 0 is the variation energy of the $D = 4$ PEPS which is $-9.034333$. There is no sign problem in this case so GFMC should give numerical exact energy. The exact energy is $-9.189207$ as indicated by the blue dashed line, while the GFMC energy is $-9.189(1)$. The inset shows a zoom of the energy after equilibrium.

![Figure 1: PEPS and the optimization process](image)

(a) shows a PEPS on a square lattice, where there is a local tensor on each vertex. (b) is the local tensor. The wave function is obtained by contracting all the auxiliary indexes. (c) shows PEPO for a plaquette. (d) the application of a PEPO to PEPS in a plaquette. (e) the bond dimension of PEPS is increased after the application of a PEPO. (f) the bond dimension is truncated back to the original value as in (a).
The guiding wave function is a $D = 4$ PEPS with variational energy $-16.763(4)$ (the energy at step 0). GFMC energy is $-16.965(1)$ and exact energy (the blue dashed line) for this system is $-17.24733$.

Fig. 1 (d)). Because the bond dimension increases after the application of PEPO [61] (see Fig. 1 (e)), we need to truncate it back to the original value $D$ to make the calculation under-control (see Fig. 1 (f)). This is done in a variational fashion [63], where a PEPS with bond dimension $D$ is optimized to have the largest overlap with the PEPS after the application of PEPO. The whole procedure is a realization of the cluster update approach [66] which is a generalization of simple update [20]. To consider the effect of tensors outside the plaque (the environment) when performing the truncation, we need to adjust the form of PEPS in Eq. (1) by including a vector $A$ on each bond of the lattice [20]. The accuracy of the converged PEPS is controlled directly by the bond dimension $D$. The most time-consuming part of this approach is the calculation of physical quantities after the PEPS are optimized, which requires contraction of double-layer tensor networks with bond-dimension $D^2$. As we will discuss later, when combining PEPS with GFMC, we only need to calculate single-layer tensor networks with bond-dimension $D$, which reduces the complexity substantially. We notice the existence of single-layer like algorithm in the literature [67]. In more sophisticated full update scheme of PEPS, the contraction of double-layer tensor network is also needed in the optimization process [27] [68].

Green’s function Monte Carlo – In Green’s function Monte Carlo [69], the ground state of a system is also obtained by imaginary time projection $|\psi_g\rangle \propto \lim_{\beta \to \infty} \exp(-\beta H)|\psi_0\rangle$. The projection length, $\beta$, is then divided into small slices with $\beta = M \tau$ and $\tau$ a small number. In GFMC, we take the first order expansion of the exponential function: $\exp(-\tau H) \propto C-H$ with $C$ a positive real number large enough to ensure all the diagonal elements of $H$ are positive. Then the ground state can formally be written as $|\psi_g\rangle \propto \lim_{\beta \to \infty} K^0|\psi_0\rangle$ with $K = C-H$. Mixed estimate is employed in GFMC to calculate the ground state energy as $E = \langle \psi_g | H | \psi_G \rangle / \langle \psi_g | \psi_G \rangle$, which gives the exact ground state energy if $|\psi_g\rangle$ is the true ground state of $H$. Here we introduce a guiding wave function $\psi_G$ whose effect will be discussed later. We use $S$ to denote spin configuration of the whole system, i.e., $S = (s_1^z, s_2^z, ..., s_N^z)$, which is also walker in the sampling process. We define the kernel as $K(S', S) = \psi_G^*(S')K(S', S)/\psi_G^*(S)$ with $K(S', S) = \langle S' | K | S \rangle$ and $\psi_G(S) = \langle S | \psi_G \rangle$. Then the ground state energy from mixed estimate is

$$E = \frac{\langle \psi_g | H | \psi_G \rangle}{\langle \psi_g | \psi_G \rangle} = \frac{\sum_{\{S\}} E_{loc}(S) \psi_G(S) \psi_g^*(S)}{\sum_{\{S\}} \psi_G(S) \psi_g^*(S)}$$

(3)

where the local energy is defined as $E_{loc}(S) = \langle S | H | S \rangle$. By introducing $f^*(S) = \psi_G^*(S) \psi_g(S)$, we have

$$E = \frac{\sum_{\{S\}} E_{loc}(S)f(S)}{\sum_{\{S\}} f(S)}$$

(4)

So we can view $f(S)$ as probability density and take advantage of Monte Carlo techniques, metropolis for example, to evaluate the summation in Eq. (4). It is easy to show $f^*(S) = \sum \tilde{K}(S, S_M)\tilde{K}(S_M, S_{M-1})...\tilde{K}(S_2, S_1)\psi_0(S_1)\psi_G^*(S_1)$ where the summation is over $\{S_1, S_2, ..., S_M\}$.

The procedure of GFMC can be summarized as follows. At the first step, we sample $S_1$ according to $\psi_0(S_1)\psi_G^*(S_1)$, and set the weight of each walker to 1. This gives us an ensemble of walkers $\{S_1, \omega_1^1 = 1\}$. We usually choose $\psi_0 = \psi_G$ and sample $\{S_1\}$ with probability $|\psi_G(S_1)|^2$. Then each walker $\{S_1, \omega_1^1\}$ is propagated to $\{S_2, \omega_2^1\}$ with probability $p(S_2^1) = \tilde{K}(S_2^1, S_1^1)/\beta_{2,1}^1$, where the normalization factor is $\beta_{2,1}^1 = \sum_{S_2} \tilde{K}(S_2^1, S_1^1)$. After a new walker is chosen, we update the weight of it by multiplying the normalization factor as $\omega_2^1 = \beta_{2,1}^1 \omega_1^1$. This process is repeated and we can start the measurement of energy after equilibrium is reached.

When the off-diagonal elements of the $H$ are all non-positive, the ground state of $H$ can be chosen to be
non-negative according to the Perron–Frobenius theorem. Under this circumstance, \( f(S) \) is non-negative if we choose an arbitrary non-negative guiding wave function because it is easily to prove the kernel \( K(S',S) \) is non-negative. Then we can view \( f(S) \) as probability density without suffering from the negative sign problem.

For Hamiltonian whose off-diagonal elements are not all negative, e.g., when the system is frustrated, we can’t ensure the non-negativeness of \( f(S) \) and the negative sign problem emerges. Applying the fixed node approximation \([73]\) can solve this issue. With fixed node approximation, we actually study an effective Hamiltonian \( H_{\text{eff}} \) instead of the original Hamiltonian \( H \). The off-diagonal of \( H_{\text{eff}} \) is defined as \( \langle S'|H_{\text{eff}}|S \rangle = \langle S'|H|S \rangle \) if \( \psi_G(S') H(S',S)/\psi_G(S) < 0 \) and it is 0 if \( \psi_G(S') H(S',S)/\psi_G(S) \geq 0 \), which means the off-diagonal elements causing the sign problem are discarded in \( H_{\text{eff}} \). The diagonal part is defined as \( \langle S|H_{\text{eff}}|S \rangle = \langle S|H|S \rangle + \langle S|V_{\text{sf}}|S \rangle \) with \( \langle S|V_{\text{sf}}|S \rangle = \sum_{S'} \langle S|H|S' \rangle \psi_G(S')/\psi_G(S) \) where the summation is over all neighboring configurations \( S' \) of \( S \) for which \( \psi_G(S') H(S',S)/\psi_G(S) > 0 \). The effect of \( V_{\text{sf}} \) is a repulsion suppressing the wave function close to the node which is essential for the energy to be variational \([73]\). The off-diagonal elements of \( H_{\text{eff}} \) are now all non-positive by definition which allows to obtain the ground state of it with GFMC without suffering from negative sign problem. It can be proven that the ground state energy of the effective Hamiltonian, \( E_{\text{eff}} \) is no less than the ground state energy of the original Hamiltonian \( H \), which guarantees GFMC is variational \([73]\). Moreover, it can be proved that \( E_{\text{eff}} \leq \langle \psi_G |H| \psi_G \rangle / \langle \psi_G | \psi_G \rangle \) which ensures GFMC gives a more accurate energy than the variational energy of \( \psi_G \) \([73]\). In practice, a fixed number of walkers are carried in the projection process \([74]\) and a reconfiguration process is performed periodically \([74]\) to reduce the fluctuation among walkers.

We can see that \( \psi_G \) serves as an important function in the GFMC sampling process when there is no sign problem. When the sign problem is present, \( \psi_G \) is also used to control the sign problem. So the quality of \( \psi_G \) controls both the accuracy and efficiency of GFMC. PEPS are known to be accurate wave function for 2D systems, which makes them good candidates for \( \psi_G \). In GFMC, we only need to calculate the overlap between \( \psi_G \) and walker which is a direct product state or a PEPS with \( D = 1 \). The overlap between PEPS with bond dimension \( D \) and direct product state is a tensor network also with bond dimension \( D \), while in the calculation the physical quantities of PEPS, contraction of double-layer tensor network with bond dimension \( D^2 \) is needed. Although it is known that the rigorous contraction of tensor network in two dimension is fundamentally difficult \([75]\), many effective approximate algorithms exist \([65,76,83]\) in the literature.

This work is not the first time TNS and GFMC are combined. Many attempts have been made in the past to either optimize tensor network states \([84–88]\) with Monte Carlo techniques, or to take MPS as guiding \([89]\) or trial wave function \([90]\) to control the negative sign problem. The advance in our work is that we take true 2D TNS, PEPS, as guiding wave function in GFMC, which can reduce the cost of PEPS substantially and at the same time improve the accuracy over PEPS.

Results – It is known that the Heisenberg model without \( J_2 \) term is sign problem free \([69,72]\). By a rotation of the spin along z-axis on one sub-lattice, sign of the coupling for \( x \) and \( y \) components is flipped, and the off-diagonal elements of \( H \) in Eq. (1) are all negative. This is the so-called Marshall sign in the ground state of Heisenberg model \([91]\) on bipartite lattices. It is worth mentioning that one of the most accurate estimation of the staggered magnetization of Heisenberg model was obtained by GFMC-like method in the valence bond basis \([92]\).

In Fig. 2 we show results for \( J_2 = 0 \) on a \( 4 \times 4 \) lattice with open boundary conditions. We first obtain a \( D = 4 \) PEPS with cluster update, which gives \( E_{\text{PEPS}} = -9.034333 \). We then carry out a GFMC calculation with this PEPS as guiding wave function. As we can see from Fig. 2 the final converged energy \((−9.189(1)) \) match the exact energy \((-9.189207)\) within error bar, which is reasonable because there is no negative sign problem here.

We then move to the more challenging \( J_2 \neq 0 \) case, where the negative sign problem emerges and we need to employ the fixed node approximation. In Fig. 3 we show the GFMC results for a system on \( 6 \times 6 \) lattice with OBC and \( J_2 = 0.5 \), which represents the most difficulty region of the \( J_1-J_2 \) Heisenberg model. A PEPS with \( D = 4 \) from cluster update is taken as guiding wave function in GFMC. The variational energy for the \( D = 4 \) PEPS is \(-16.763(4) \) while the energy from GFMC is \(-16.965(1) \). This means the error to exact energy \((-17.24733) \) is reduced nearly a half with GFMC in this case. In Fig. 4 we show the comparison of converged GFMC energy and the energy of the corresponding PEPS guiding wave function for a range of bond dimensions. We can see for all the \( D \) values, the GFMC energies are lower than PEPS energy and the errors are reduced by about 40%.

Summary and perspectives – In conclusion, we proposed a new approach to study the ground state properties of quantum many-body systems in which TNS and GFMC are combined to take advantage of both of them. Benchmark results for \( J_1-J_2 \) Heisenberg model on square lattice were provided to demonstrate the effectiveness of this method. One benefit to combine PEPS and GFMC is that only contraction of single-layer tensor network is needed which reduces the computational complexity substantially and enable the reach of large bond dimension in PEPS, if the optimization process doesn’t involve contraction of double-layer tensor network. Nevertheless, after obtaining the optimized PEPS with full update, we can further improve the energy by taking it as guiding wave function, though the bottleneck is the optimization of PEPS itself in full update. The energy obtained...
function in GFMC is guaranteed to be variational and lower than the PEPS guiding wave function. Our method can be improved in many aspects. With the stochastic reconfiguration technique [8], the bias from guiding wave function can be reduced. We can generalize single PEPS guiding function to a linear combination of PEPS [9] which can give lower variational energy. Generalization to fermionic systems is straightforward [45, 46]. We only calculated ground state energy in this work, but excitation gaps can be calculated easily by enforcing symmetry in PEPS. Quantities other than energy can be calculated with the forward propagation technique [72] without increasing of computational complexity. Tensor Network States other than PEPS [95–97] can also be adopted as guiding wave function. We believe that this new approach will provide us an accurate and efficient tool in the study of strongly correlated many-body systems in the future.

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