Localized Virtual Purification

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Analog and digital quantum simulators can efficiently simulate quantum many-body systems that appear in natural phenomena. However, experimental limitations of near-term devices still make it challenging to perform the entire process of quantum simulation. The purification-based quantum simulation methods can alleviate the limitations in experiments such as the cooling temperature and noise from the environment, while this method has the drawback that it requires global entangled measurement with a prohibitively large number of measurements that scales exponentially with the system size. In this Letter, we propose that we can overcome these problems by restricting the entangled measurements to the vicinity of the local observables to be measured, when the locality of the system can be exploited. We provide theoretical guarantees that the global purification operation can be replaced with local operations under some conditions, in particular for the task of cooling and error mitigation. We furthermore give a numerical verification that the localized purification is valid even when conditions are not satisfied. Our method bridges the fundamental concept of locality with quantum simulators, and therefore is expected to open a path to unexplored quantum many-body phenomena.

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Introduction—Simulating quantum many-body systems is a fundamental issue for quantum information science [1], since it potentially has a significant impact on various fields [2] including condensed matter physics [3–5], statistical physics [6–9], quantum chemistry [10–12], and high-energy physics [13–15]. In particular, simulation of thermal equilibrium states, ground states, and nonequilibrium dynamics for quantum many-body Hamiltonians has attracted attention as a valuable application, since it is believed to be an exponentially difficult task on a classical computer. This has motivated the recent progress in quantum simulations using cold atoms in an optical lattice [16–20], nitrogen-vacancy centers in diamond [21], photonic devices [22], and superconducting qubits [23,24].

While it remains a challenge to perform all quantum tasks in the current quantum devices, it has been proposed that purification-based quantum simulation enables us to break the limitations in experiments. The key idea is to enhance the purity of a quantum state in a virtual way by utilizing the classical postprocessing, rather than directly realizing the purified quantum state. More specifically, one computes the expectation value $\langle \bullet \rangle_{\mathrm{FVP}} = \mathrm{Tr}[\rho_{\mathrm{FVP}}^{(n)} \bullet]$ corresponding to $\rho_{\mathrm{FVP}}^{(n)} = \rho^n / \mathrm{Tr}[\rho^n]$ [which is denoted as fully virtual purification (FVP) throughout this Letter] from an original quantum state ρ using n copies. It has been pointed out that, such an operation is capable of (i) simulating the canonical Gibbs state of temperature T/n using that of T [25], and (ii) suppressing the effect of noise in the context of quantum error mitigation [25–36]. However, these methods require multiple entangled measurement gates that act globally among multiple copies. This imposes a severe burden on the computation: nonlocal entangling gates among copies and an exponentially large number of measurements. It is crucial to seek whether we can alleviate the overhead of purification-based methods in a way that the accuracy of the simulation is maintained.

One promising direction is to utilize the geometrical locality of target models, which is present ubiquitously in condensed matter systems. In particular, the locality of interaction yields an upper bound on the velocity of information propagation: the Lieb-Robinson bound [37–40]. Recent works show that this powerful bound can be applied to yield various fundamental limits such as the finite correlation length of a gapped ground state [38–40] and approximation of time-evolution unitary in the interaction picture [41–43].

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Meanwhile, to our knowledge, there are very few frameworks of practical quantum algorithms other than Hamiltonian simulation [41–44] that incorporate the notion of geometrical locality. This implies that we are not fully harnessing the capacity of the quantum simulators for practical use.

In this Letter, we fill in these gaps by proposing the localized virtual purification (LVP) as a virtual purification on local subsets of qubits, and present theoretical guarantees and conditions that the method overcomes the problems in FVP when the locality of the system can be exploited. While the proposal itself was mentioned in the original paper as a task for cooling [25], our contribution is to clarify the conditions of the theoretical bounds and to show a practical advantage to an effect of noise among the entanglement measurement operations. While the output from the LVP generally deviates from that of the FVP due to a non-negligible correlation between purified and unpurified regions, we find that the deviation can be written as a generalized correlation function. In particular, this reduces to the two-point correlation function in some cases including cooling and error mitigation. Therefore, if we further assume the clustering property, i.e., the exponential decay of two-point correlation, we can derive two bounds that assure the accuracy of the LVP for these tasks. Finally, we verify our analytical results via numerical simulation, and also find that the LVP is capable of unifying the two tasks, namely the simulation of low-temperature Gibbs states from noisy high-temperature states.

Setup—Let the Hamiltonian be defined on a d-dimensional hypercubic lattice with the periodic boundary condition that is represented as an undirected graph $G = (V, E)$, where the number of vertices $|V|$ is equivalent to the total number of sites (or qubits) N and the edges E denote the connectivity of each site. We assume that the interactions in the Hamiltonian are geometrically local: $H = \sum_X h_X$ satisfying $\max_{v \in V} \sum_{X: X \ni v} \|h_X\| \leq g$, where X is a subset of V and g is a positive constant independent of N. In the following, we will write each term of the Hamiltonian as h_{A_i} with a subset A_i denoting one vertex i on the support, as long as there is no confusion. We assume a spin-1/2 system that directly corresponds to qubits, while we expect that our theory can be naturally extended to higher-spin, fermionic, and bosonic systems, since the underlying mechanism of cluster property is commonly present. In fact, we numerically analyze two-dimensional fermionic systems in the Supplemental Material (SM) [45].

Localized virtual purification—We define the expectation values of LVP by

$$\langle \mathcal{O}^{(n)}_{\mathrm{LVP}} \rangle = \sum_i \frac{\mathrm{Tr}_{A_i+B_i}[(\rho_i^{(A_i+B_i)})^n o_{A_i}]}{\mathrm{Tr}_{A_i+B_i}[(\rho_i^{(A_i+B_i)})^n]}, \tag{1}$$

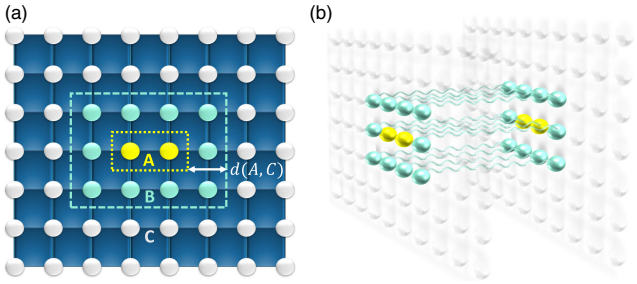

FIG. 1. Schematic description of our proposal, the localized virtual purification (LVP), assuming two-dimensional system with $n = 2$ copies of quantum state. (a) Dividing the entire lattice into three regions A, B, and C according to the local observable o_A and the distance $d(A, C) = 1$. The number of sites inside the regions A, B, and C are N_A, N_B and N_C, respectively, and the total number of sites is $N(= N_A + N_B + N_C)$. (b) The entangled measurement operation applied to regions A and B to perform the LVP.

where $\mathcal{O}$ is an observable that can be decomposed into a sum of local observables as $\mathcal{O} = \sum_i o_{A_i}$. Here, $\rho_i^{(A_i+B_i)} = \mathrm{Tr}_{C_i}[\rho]$ is the reduced density operator on regions A_i and B_i. To be more specific, we divide all sites into three regions [see Fig. 1(a)]: A_i is a region of the support of a local observable o_{A_i} and we perform the entangled measurement operations between n copies in the A_i and B_i regions, while we do not perform any operations on the region C_i. Without loss of generality, we may focus on an arbitrary single term o_{A_i} and therefore we omit the index i for simplicity. Note that the expectation values in Eq. (1) can be evaluated via LVP by operating an entangled measurement circuit on the region $A \cup B$ as shown in Fig. 1(b). This results in the measurement costs of $\mathrm{Tr}_{A+B}[(\rho^{(A+B)})^n]^{-2}$ [45], where measurement costs denote the increase of the variance for estimating the expectation values. The increase implies the greater number of measurements required.

In general, the estimation by the LVP is not equivalent to that of the FVP. Meanwhile, we find that we can understand the performance of LVP qualitatively by rewriting the difference of the expectation values $D^{(n)}(o_A) = \{(\mathrm{Tr}_{A+B}[(\rho^{(A+B)})^n o_A])/(\mathrm{Tr}_{A+B}[(\rho^{(A+B)})^n])\} - \{(\mathrm{Tr}[\rho^n o_A])/(\mathrm{Tr}[\rho^n])\}$ into the integration of the generalized correlation function as

$$D^{(n)}(o_A) = \int_0^1 d\lambda \int_0^1 d\tau \mathrm{Corr}^{\tau}_{\rho_\lambda}(X_n - Y_n, o_A), \tag{2}$$

where we have introduced a generalized correlation function $\mathrm{Corr}^{\tau}_{\rho}(O, O') = \mathrm{Tr}[\rho^{\tau} O \rho^{1-\tau} O'] - \mathrm{Tr}[\rho O]\mathrm{Tr}[\rho O']$. This is also referred to as the two-point quantum correlation function [68,69] or canonical correlation for thermal Gibbs states [70–72] in literature. We have also defined $\rho_\lambda = e^{H_\lambda}/\mathrm{Tr}[e^{H_\lambda}]$, $H_\lambda = Y_n + \lambda(X_n - Y_n)$, $Y_n = \log(\rho^n)$, and $X_n = \log[(\rho^{(A+B)})^n \otimes (\sigma_C)^n]$, where σ_C is an arbitrary

positive operator (see SM for derivation [45]). As we discuss in detail in the following, we find that the generalized correlation function reduces to the two-point correlation function for some cases, and thus it decays exponentially if the exponential clustering property holds.

Theoretical bounds for LVP—Now let us present our main results: the performance guarantees and their conditions for the LVP. We first discuss one of the most important cases, namely the cooling of thermal equilibrium states

$$\rho_\beta(H) = \frac{e^{-\beta H}}{\mathrm{Tr}[e^{-\beta H}]}, \tag{3}$$

where β is an inverse temperature. In this case, we can rewrite Eq. (2) as $D^{(n)}(o_A) = -n\beta \int_0^1 d\lambda \int_0^1 d\tau \mathrm{Corr}^{\tau}_{\rho_\lambda}(\Delta H, o_A)$ because simple relations $X_n = -n\beta(H + \Delta H)$ and $Y_n = -n\beta H$ hold for ΔH that is introduced to describe the deviation of the Hamiltonian from a Gibbs state $\rho_\beta(H^{(A+B)})$ tracing out the region C. Here, we assume that ΔH can be approximated by a local operator supported on the boundary of the region $A \cup B$ with exponentially small error, as shown in SM [45]. Note that although previous results have proved the above assumption based on a generalized linked-cluster expansion in order to evaluate $H + \Delta H$ [73–75], which is related to the Hamiltonian of mean force for strong coupling systems [76–79], a flaw in its proof was pointed out later [80]. While the proof is to be fixed, we reasonably expect that the locality of ΔH is valid in high-temperature regime, as proven in commuting Hamiltonians [81]. By noting that the support of o_A is separate from that of ΔH under this assumption, we prove the following theorem:

Theorem 1 (informal summary). Assuming the exponential clustering of the two-point correlation function [82–86], the deviation $|D^{(n)}(o_A)|$ is exponentially small in terms of $d(A, C)$:

$$|D^{(n)}(o_A)| = O(e^{-d(A,C)}). \tag{4}$$

The formal statement and its proof are shown in SM [45]. One of the most outstanding points of our LVP protocol applied to Gibbs states is the suppression of measurement costs: $\mathrm{Tr}_{A+B}[(\rho^{(A+B)})^n]^{-2} \simeq \exp[2n\beta(N_A + N_B)(f_{n\beta} - f_\beta)]$, where $f_\beta = -[(1)/((N_A + N_B)\beta)]\mathrm{Tr}[e^{-\beta H_{A+B}}]$ is a free energy density of the Hamiltonian $H^{(A+B)}$ at an inverse temperature β. This implies that the measurement costs of LVP are exponentially small regarding N_C compared with those of FVP [45]. Our LVP protocol for Gibbs states induces an exponentially small bias from FVP regarding $d(A, C)$, while it exponentially reduces the measurement costs. Whereas it seems that the above assumption regarding ΔH only holds for an extremely high-temperature region, as we later confirm in numerical simulations, this is expected to hold even for a low-temperature region [87].

Next, we discuss another interesting application of the LVP: error mitigation. Here, we first provide a theoretical bound when ρ is pure, and then present results when the noise is present.

When the target state is pure, the deviation $|D^{(n)}(o_A)|$ can be written as a simpler form of the two-point correlation function: $D_0^{(n)}(o_A) = \mathrm{Tr}_{A+C}[(\rho^{(A+C)} - \rho^{(A)} \otimes \rho^{(C)}) o_A \otimes (\rho^{(C)})^{n-1}/\mathrm{Tr}[(\rho^{(C)})^n]]$ [45]. Here, $D_0^{(n)}(o_A)$ denotes the deviation $D^{(n)}(o_A)$ for a pure state ρ_0, and $\rho^{(A)}$ and $\rho^{(C)}$ denote the reduced density operator of the region A and C. Regarding the deviation $D^{(n)}(o_A)$ for pure states and noisy states under global depolarizing noise channel, we prove the following theorem.

Theorem 2. If the ground state is unique with a finite energy gap between the first excited states, the deviation for a noiseless pure state ρ_0 can be rewritten as

$$|D_0^{(n)}(o_A)| \le c\|o_A\| \frac{\|(\rho^{(C)})^{n-1}\|}{\mathrm{Tr}[(\rho^{(C)})^n]} \exp\left(-\frac{d(A, C)}{\xi}\right), \tag{5}$$

where c and ξ are constants independent of N. In particular, if the system of interest is a one-dimensional system, the term $\|(\rho^{(C)})^{n-1}\|/\mathrm{Tr}[(\rho^{(C)})^n]$ can be bounded by a constant independent of $d(A, C)$ for any n, which leads to $|D_0^{(n)}(o_A)| \le c'\|o_A\| \exp(-d(A, C)/\xi) = O(e^{-d(A,C)})$, where c' is a constant independent of N. Furthermore, the deviation for the noisy ground state under the global depolarizing noise can be bounded as $|D^{(n=2)}(o_A)| \le |D_0^{(n=2)}(o_A)| + |\delta_1| + |\delta_2|$, and $\delta_1 = O(e^{-N})$ and $\delta_2 = O(e^{-(N_A+N_B)})$. The global depolarizing noise channel is defined by $\mathcal{D}[\rho] = (1 - p)\rho + p(\mathbb{I}/2^N)$, where p $(0 \le p \le 1)$ is the error rate.

Proof. The nontrivial part of this theorem has been done by explicitly showing the expression of Eq. (2) and rewriting Eq. (2) as the two-point correlation function for pure state cases. The proof can be done by applying the exponential clustering property [90], which is derived from Lieb-Robinson bounds using the Fourier transformation [38–40]: $|\mathrm{Tr}[\rho^{(A+C)} M_A \otimes M_C] - \mathrm{Tr}[\rho^{(A)} M_A]\mathrm{Tr}[\rho^{(C)} M_C]| \le c\|M_A\|\|M_C\| \exp(-d(A, C)/\xi)$. When we choose $M_A = o_A$ and $M_C = (\rho^{(C)})^{n-1}/\mathrm{Tr}[(\rho^{(C)})^n]$, the correlation function is equivalent to $D_0^{(n)}(o_A)$. For one-dimensional systems, the area law of entanglement entropy $S(\rho_C) := -\mathrm{Tr}[\rho^{(C)} \log \rho^{(C)}]$ holds; $S(\rho^{(C)}) \le \text{const.}$, as shown in Ref. [95]. This implies that the term $\|(\rho^{(C)})^{n-1}\|/\mathrm{Tr}[(\rho^{(C)})^n]$ can be bounded by a constant value independent of $d(A, C)$ for any n [45], which leads to $|D_0^{(n)}(o_A)| = O(e^{-d(A,C)})$. For the case of the noisy ground state under the global depolarizing noise channel [96], the derivation of the inequality and the explicit forms of δ_1 and δ_2 are shown in SM [45]. ∎

Numerical simulations—Next, we present the results of numerical simulation to justify our expectation that the LVP is widely valid, even when the conditions for theoretical

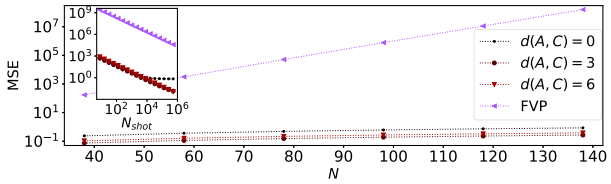

FIG. 2. MSE χ_{LVP} and χ_{FVP} against the number of qubits N for various $d(A,C)$ at a temperature $\beta = 1.0$ and $N_{\mathrm{shot}} = 2^{14}$. Inset: MSE against N_{shot} for various $d(A,C)$ with $N = 138$.

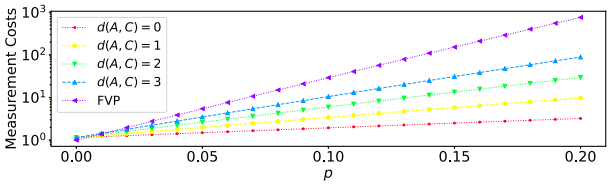

FIG. 3. Measurement costs to perform error mitigation by FVP and LVP for a ground state of H_{TFI} in Eq. (6) with $\lambda = 2$. Here, we take $n = 2$ copies of noisy ground state for $N = 12$ qubits under local depolarizing noise of error rate p.

guarantees do not hold such as the cases of a low-temperature region or gapless (critical) systems [45]. For numerical simulations, we consider the transverse-field Ising (TFI) Hamiltonian on one-dimensional periodic lattice as

$$H_{\mathrm{TFI}} = -\sum_{i=1}^{N} Z_i Z_{i+1} - \lambda \sum_{i=1}^{N} X_i, \tag{6}$$

where X_i and Z_i denote the Pauli-X and Z operators acting on the ith site, and λ is the amplitude of the transverse magnetic field.

First, we evaluate the performance of the LVP in the context of cooling. As a metric of the performance of LVP, we introduce the mean square error (MSE) χ [97] of the energy of the low-temperature state $\rho_{n\beta}(H_{\mathrm{TFI}})$ that is estimated using the high-temperature state $\rho_{\beta}(H_{\mathrm{TFI}})$. The MSE χ is composed of two contributions, namely the variance obtained by N_{shot} and the bias from the true value, and also the square root MSE can be understood as the estimation precision under N_{shot} measurements.

Figure 2 shows the MSE χ_{LVP} and χ_{FVP} against the number of qubits N for various $d(A,C)$. We find that our LVP protocol only requires the number of measurements proportional to N, while the original FVP suffers the exponential number of measurements. We can also see that $\chi_{\mathrm{FVP}}, \chi_{\mathrm{LVP}} \propto (N_{\mathrm{shot}})^{-1}$ widely holds, which implies that the contribution from the bias is negligible unless N_{shot} is taken to be a significantly large number.

Second, we verify the performance of the LVP in the context of error mitigation. Concretely, we prepare the ground state of H_{TFI} in Eq. (6) at $\lambda = 2$ (noncritical) so that two-point correlation functions as well as Eq. (5) decay exponentially. We consider the single-qubit local depolarizing noise, often employed to explain the experimental results [98], which is defined by $\mathcal{E}^{(k)}[\rho] = (1-p)\rho + (p/3)(X_k\rho X_k + Y_k\rho Y_k + Z_k\rho Z_k)$ for the kth qubit, where p is the error rate.

Figure 3 shows the measurement costs to perform the LVP for the noisy ground state of the Hamiltonian H_{TFI} in Eq. (6) at $\lambda = 2$ (noncritical). We can see that the growth of the measurement costs for LVP is significantly slower than that of FVP. For example, the measurement costs of FVP for $p = 0.15$ in Fig. 3 are more than 100 while those of LVP are around 10, and thus we have a cost reduction by a factor of 10. Note that there is a trade-off between the bias and measurement cost regarding $d(A,C)$ [99].

Finally, we consider a unification of these two protocols: cooling and error mitigation. Namely, we consider a situation that any Gibbs state cannot be prepared perfectly. In order to describe the imperfection, we assume that the input state is a Gibbs state subject to the local depolarizing noise channel on all qubits. Figure 4 shows the expectation values of H_{TFI} in Eq. (6) for Gibbs states with local depolarizing noise. We see that the purification-based approaches are capable of performing both cooling and error mitigation simultaneously, and also that the deviation between LVP and FVP decreases exponentially with $d(A,C)$ while the measurement costs are also suppressed significantly.

Discussion and conclusion—In this Letter, we have introduced the localized virtual purification (LVP) that incorporates and utilizes the property of geometrical locality to enhance the utility of purification-based quantum simulation. We have given theoretical guarantees that the LVP significantly alleviates the severe measurement overhead of the FVP when the two-point correlation function decays exponentially. This includes the cooling of the Gibbs states of local Hamiltonians (Theorem 1) and error mitigation of ground state simulation in gapped systems (Theorem 2). We have also verified our findings via numerical simulation, and also shown that the LVP is capable of unifying both tasks.

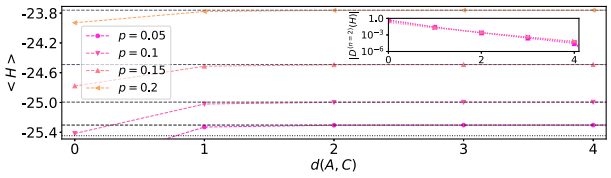

FIG. 4. Unifying cooling and error mitigation to simulate $\langle H_{\mathrm{TFI}} \rangle$ for $\lambda = 2$. The LVP and FVP is performed for $n = 2$ copies of noisy Gibbs state at $\beta = 1$ for $N = 12$ qubits. Horizontal dashed and dotted lines indicate the results from the FVP with and without noise, respectively. Inset: total deviation of the expectation values $D^{(n=2)}(H)$, where we define $|D^{(n)}(H)|$ by $|D^{(n)}(H)| = |\langle H \rangle^{(n)}_{\mathrm{LVP}} - \langle H \rangle^{(n)}_{\mathrm{FVP}}|$, between FVP and LVP against $d(A,C)$.

We comment that an additional advantage of our LVP protocol is to alleviate the noise effect among the entangled measurement operations. A previous study [100] has shown that the measurement costs of FVP increase exponentially with the number of qubits due to errors in the entangled measurement circuit. Using our LVP method, the measurement costs do not exponentially increase because the controlled derangement circuit is operated only in a local region. This is true not only for error mitigation but also for cooling achieved from FVP.

The LVP for the high-temperature regions of Gibbs states in Eq. (3) is one of the most effective cases of our protocol for practical quantum advantages. For many practical cases, calculating thermodynamic properties for large system sizes of two- or higher-dimensional quantum systems is a challenging task on classical computers even with tensor network methods such as projected entangled-pair states [101]. On the other hand, there exists an efficient quantum algorithm for preparing thermal states [102], under the assumption of the exponential clustering of two-point correlation functions and approximating quantum Markov property, using quantum belief propagation [102–105]. That situation completely matches that of our LVP protocol and therefore LVP works on a practical situation using quantum computers.

Last but not least, we comment on other promising applications of the LVP: the detection of topological orders [106,107], the measurement of a characterized quantity of quantum chaos [108], and an entanglement measure for mixed states [109]. These quantities are well-known as fundamental concepts in condensed matter physics and quantum information and must be measured efficiently on quantum computers. By applying our protocol, it may be possible to not only detect such physical quantities but also to incorporate error mitigation or cooling simultaneously. We believe that these are important issues for future research.

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