Generalized Quantum Subspace Expansion

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(Received 29 July 2021; accepted 16 February 2022; published 6 July 2022)

One of the major challenges for erroneous quantum computers is undoubtedly the control over the effect of noise. Considering the rapid growth of available quantum resources that are not fully fault tolerant, it is crucial to develop practical hardware-friendly quantum error mitigation (QEM) techniques to suppress unwanted errors. Here, we propose a novel generalized quantum subspace expansion method which can handle stochastic, coherent, and algorithmic errors in quantum computers. By fully exploiting the substantially extended subspace, we can efficiently mitigate the noise present in the spectra of a given Hamiltonian, without relying on any information of noise. The performance of our method is discussed under two highly practical setups: the quantum subspaces are mainly spanned by powers of the noisy state ρ^m and a set of error-boosted states, respectively. We numerically demonstrate in both situations that we can suppress errors by orders of magnitude, and show that our protocol inherits the advantages of previous error-agnostic QEM techniques as well as overcoming their drawbacks.

DOI: 10.1103/PhysRevLett.129.020502

Introduction.—Control over computational errors is one of the central problems for the implementation of practical quantum computing algorithms using quantum devices subject to imperfections [1,2]. Towards the goal of achieving fully fault-tolerant computation based on logical operations, the number of required qubits was reduced, and their error rates were improved drastically in the recent years, although the realization of ultimate digital quantum computing is years ahead [3]. Therefore, it is important to ask whether we can establish information processing techniques which exploit the increasing quantum resource *without* performing fully functional error correction.

The quantum error mitigation (QEM) techniques perform postprocessing on measurement data (usually expectation values) to eliminate unwanted bias from computation results, in exchange for additional measurement costs [4–15]. One of the most prominent examples is the quasiprobability method [5,7]. Once the error profile of gate operations is given, stochastic operations are inserted to construct the inverse operations of each error map so that we can retrieve the computation result for the intended quantum operation. However, the characterization of the noise model, e.g., via the gate set tomography, is quite costly and easily deteriorated by noise drift.

Meanwhile, error-agnostic QEM methods which do not rely on prior knowledge on the error have been proposed: the quantum subspace expansion (QSE) method [16–19] and the virtual distillation (VD) method, which is also called the error suppression by derangement (ESD) method [20–23]. In the QSE method, we classically realize a variational subspace spanned by a set of quantum states $\{|\psi_i\rangle\}_i$ as $|\psi\rangle = \sum_i c_i|\psi_i\rangle$, which can be effectively generated via additional measurements and postprocessing. While the QSE method was initially proposed to compute excited states from a ground state realized on a quantum device, it also contributes to the mitigation of errors. By construction, the QSE method is well suited for mitigating coherent errors which may come from insufficient variational optimization, lack of quantum circuit representability, and etc. However, it cannot suppress stochastic errors efficiently, since in general we need a linear combination of exponentially many Pauli operators to construct a projector to the error-free subspace [4,16]. The VD/ESD method, on the other hand, is complementary in this sense. By applying entangling operations between M identical copies of noisy quantum states ρ, we can obtain the error-mitigated expectation value of an observable O as $\langle O\rangle_{\rm VD}^{(M)} = {\rm Tr}[O\rho_{\rm VD}^{(M)}]$ with $\rho_{\rm VD}^{(M)} = \rho^M/{\rm Tr}[\rho^M]$, whose fidelity with a dominant eigenvector of ρ exponentially approaches unity. Although this method can significantly compensate for stochastic errors, it is entirely vulnerable to coherent errors which distorts the dominant eigenvector.

In this work, we propose a unified framework of error-agnostic QEM techniques which we refer to as the generalized quantum subspace expansion (GSE) method. The central idea is to extend the notion of quantum subspaces to include general operators that are related to the target noisy quantum state, which allows us to distill the state into an error-mitigated eigenstate of the target Hamiltonian. We show that the GSE method, which provides a substantial generalization of the QSE method, inherits the advantages of previous error-agnostic QEM techniques as well as overcoming their drawbacks. This is demonstrated under two practical choices of the subspace. In the first example, the subspace consisting of powers of a noisy quantum state ρ^m achieves not only the exponential suppression of stochastic errors which is even more efficient than the VD/ESD method, but also efficiently mitigates coherent errors. In the second example, we span the subspace by nonequivalent quantum states corresponding to different noise levels. Unlike the commonly used error-extrapolation method, the GSE method with the subspace of error-controlled states is quite robust even when the control over noise level is imprecise, and hence highly beneficial to practical applications.

Framework of generalized quantum subspace expansion.—Suppose we obtain a noisy approximation ρ of some desired state, e.g., an eigenstate of a given Hamiltonian H using the variational quantum eigensolver (VQE) or its variants [24–33]. The GSE method uses the following ansatz in the extended subspace to represent an eigenstate

$$\rho_{\mathrm{EM}} = \frac{P^\dagger A P}{\mathrm{Tr}[P^\dagger A P]}, \tag{1}$$

where $P = \sum_i \alpha_i \sigma_i (\alpha_i \in \mathbb{C})$ is a general operator, σ_i is generally a non-Hermite operator, and A is a positive-semidefinite Hermite operator. In this Letter, we refer to σ_i as a base of the subspace. It is easy to check that ρ_{EM} is a positive-semidefinite Hermite operator whose trace is unity, which ensures that ρ_{EM} corresponds to a physical quantum state. Note that σ_i and A can be related to the noisy state ρ. For example, we can choose $\sigma_i = \rho$ and $A = \rho$; this highlights the crucial difference of the novel GSE method from the conventional QSE (see Supplemental Material for more details [34]) that it also includes general operators related to quantum states in the expanded subspace. To span the most general subspace, we can take a base as follows,

$$\sigma_i = \sum_k \beta_k^{(i)} \prod_{l=1}^{L_k} U_{lk}^{(i)} \rho_{lk}^{(i)} V_{lk}^{(i)}, \tag{2}$$

where $\beta_k^{(i)} \in \mathbb{C}$, $\rho_{lk}^{(i)}$ is a quantum state, $U_{lk}^{(i)}$ and $V_{lk}^{(i)}$ are operators that allow for an efficient measurement on quantum computers (e.g., local Pauli operators or unitary operators), and L_k denotes the number of quantum states. See Supplemental Material for more details [34].

To obtain the error-mitigated spectra of the Hamiltonian, we determine the coefficients $\vec{\alpha} = (\alpha_0, \alpha_1, \ldots)$ by solving the following generalized eigenvalue problem [34]:

$$\mathcal{H}\vec{\alpha} = E\mathcal{S}\vec{\alpha}, \tag{3}$$

where $\mathcal{H}_{ij} = \mathrm{Tr}[\sigma_i^\dagger A \sigma_j H]$ and $\mathcal{S}_{ij} = \mathrm{Tr}[\sigma_i^\dagger A \sigma_j]$ with E being the error-mitigated eigenenergy. The coefficients are normalized as $\vec{\alpha}^\dagger \mathcal{S} \vec{\alpha} = 1$ to satisfy $\mathrm{Tr}[\rho_{\mathrm{EM}}] = 1$. Note that $\mathcal{H}_{ij}$ and $\mathcal{S}_{ij}$ need to be efficiently computed on quantum computers. Once we find $\vec{\alpha}$ which suffices Eq. (3), we can compute the error-mitigated expectation value of any observable O as $\langle O \rangle = \sum_{ij} \alpha_i^* \alpha_j \mathrm{Tr}[\sigma_i^\dagger A \sigma_j O]$.

By implementing the generalized quantum subspaces spanned by Eq. (2), we can efficiently perform error-agnostic QEM. To illustrate the significance of our scheme, we will describe slightly more specific but highly practical two subclasses. Because of their features explained thereafter, we refer to the employed subspaces as the *power* subspace and *fault* subspace, respectively.

Power subspace.—Let us first restrict the bases of subspace to powers of noisy quantum states as $\sigma_i = \rho^i (i = 0, 1, \ldots, m)$ and set $A = I$:

$$\rho_{\mathrm{EM}} = \sum_{i,j=0}^{m} \alpha_i^* \alpha_j \rho^{i+j}. \tag{4}$$

This shows that the error-mitigated state ρ_{EM} is represented as the series expansion of the state ρ as $\rho_{\mathrm{EM}} = \sum_{n=0}^{2m} f_n \rho^n$, where $f_n = \sum_{i+j=n} \alpha_i^* \alpha_j$. Setting $m = 1$, for instance, leads to $\rho_{\mathrm{EM}} = f_0 I + f_1 \rho + f_2 \rho^2$, which clarifies that ρ_{EM} is represented as a polynomial of ρ [35].

It has been pointed out that higher order states themselves are extremely useful [20,21,36]. By effectively computing the expectation value of an observable corresponding to the state $\rho_{\mathrm{VD}}^{(M)} = \rho^M / \mathrm{Tr}[\rho^M]$ $(M = 2, 3, \ldots)$, we can exponentially suppress the contribution from the nondominant eigenstates of ρ (See Supplemental Material for details [34]). Our key insight is that the nondominant states will be suppressed even more efficiently by interfering them with each other. In fact, it is straightforward to see that the power subspace for $A = I$ completely includes $\rho_{\mathrm{VD}}^{(2m)}$, and therefore in the case of ground-state simulation we can always surpass the performance of the VD/ESD method when the dominant vector gives good approximation of the ground state [34].

To illustrate the expected gain by our approach, we numerically demonstrate our algorithm. Figure 1 shows the results for 6 lowest eigenstates of the one-dimensional transverse-field Ising (1D TFI) model, whose Hamiltonian

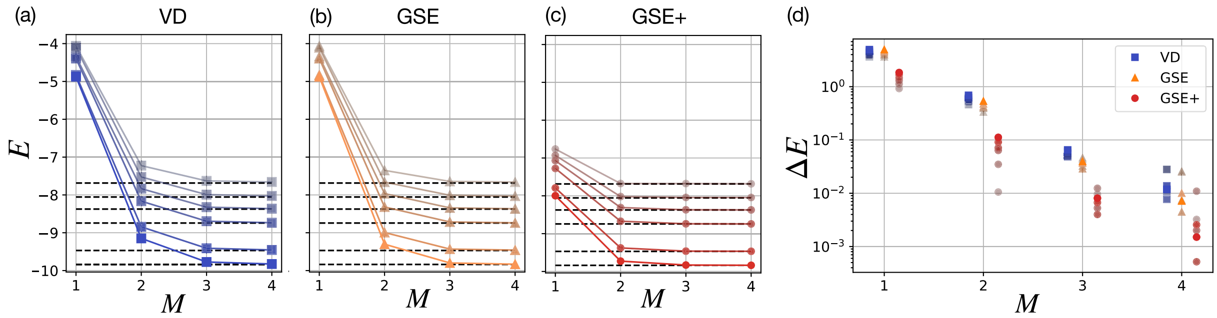

FIG. 1. Suppressing errors in 6 lowest eigenstate calculations of a one-dimensional transverse-field Ising model by interfering M copies of identical noisy quantum states. Eigenenergies computed by (a) the VD/ESD method, (b) GSE method based on the power subspace, and (c) GSE method with additional bases. For the power subspace, we take the bases as $\sigma_i = \rho^i$ $(i = 0, 1, \ldots, (M/2))$ and $A = I$ for even number of copies M, while we take $\sigma_i = \rho^i$ $(i = 0, 1, \ldots, [(M-1)/2])$ and $A = \rho$ for odd M's. In (c), we additionally include non-Hermite operators $\rho^m H$ $(m = 0, 1, \ldots, \lfloor M/2 \rfloor)$. (d) The log scale plot of the deviation ΔE from the exact eigenenergies. For each eigenstate level n, we generate the noisy state ρ by adding depolarizing error after each gate of a variational quantum circuit, whose parameters are optimized by the subspace-search VQE algorithm [24] to solve an 8-qubit system under $h = 1$. The depolarizing error rate p_{dep} is taken so that the expected number of total error in ρ is given as $N_{\mathrm{tot}} = N_{\mathrm{gate}} p_{\mathrm{dep}}$, where N_{gate} is the number of gates. For all data presented in this figure we set $N_{\mathrm{tot}} = 1.5$.

is given as $H = -\sum_r Z_r Z_{r+1} + h \sum_r X_r$, where X_r and Z_r denote the x and z components of the Pauli matrix acting on the rth site and h is the amplitude of the transverse magnetic field. We set $h = 1$ in the following. It is clear from Fig. 1 that both the VD/ESD method and our GSE method yields exponential suppression of error with respect to the number of copies M. Moreover, the interference with nondominant states in ρ yields quicker convergence of the expectation value $\mathrm{Tr}[\rho_{\mathrm{EM}} H]$ towards the exact values; this is further boosted by including additional operators such as $\rho^m H$ to the bases, which is discriminated as the GSE+ method in the figures. While we observe a trade-off between the accuracy and estimation variance as shown in Fig. 2, the greater suppression in the GSE/GSE+ method gives us an advantage when the measurement resources are not too scarce. Such a gain in the performance is found not only in the energy, but also measures such as the fidelity and trace distance (See Supplemental Material for details [34]).

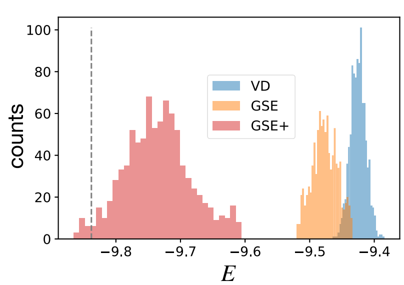

FIG. 2. Histograms of ground-state energy estimation by VD/ESD (blue), GSE method based on the power subspace (orange), and GSE+ method that includes the additional term ρH included in power-subspace bases (red) using $M = 2$ copies. Here, we take the number of total measurement shots to be 10^9. The gray dotted line indicates the exact ground state energy of the 1D TFI model with $N = 8$ qubits.

Now, let us further analyze the effect of the crucial obstacle for the previous exponential error suppression techniques—the coherent errors. It has been pointed out in Refs. [20,21,37] that the stochastic gate errors themselves may cause a deviation of the dominant vector, which is called the coherent mismatch. In addition, there are numerous other sources that give rise to the coherent errors, e.g., restrictions on the variational ansatz structure of quantum states due to experimental limitations. In this regard, we interestingly find that our method provides a significant improvement over previous methods, since the expressibility of quantum states can be enhanced effectively by the subspace.

Figure 3 shows the result for numerical simulations focused on the ground state to support our findings. While the accuracy of the raw noisy state and the conventional QSE method scales only linearly with respect to N_{tot}, both the VD/ESD and GSE methods using two copies of ρ provide quadratic suppression in the noisy regime. However, the difference of two methods is highlighted in the low-error regime, in which the accuracy of the VD/ESD method is bounded by the performance of the original VQE simulation. Namely, when the ideal quantum circuit is not powerful enough and involves algorithmic error, we cannot remedy the shortage by merely restoring the dominant vector. In sharp contrast, our method is capable of eliminating such unwanted errors.

It is important to remark that the required number of measurements for the GSE method scales quadratically with respect to the desired accuracy, just as in the usual quantum measurements (see Supplemental Material for details [34]). When the dominant vector of ρ gives a good approximation of the ground state, this is mainly accounted for by the sampling cost rooting from higher powers ρ^M.

Fault subspace.—Now we proceed to another practical subclass of the GSE framework that employs nonidentical

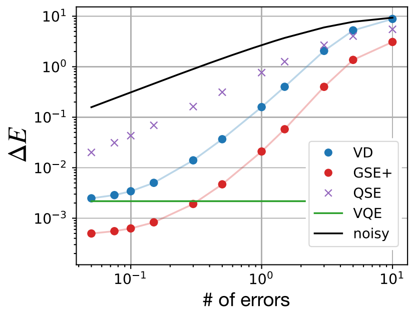

FIG. 3. Relationship of the expected number of errors $N_{\rm tot}$ and the ground-state energy deviation ΔE. Blue filled circles and red filled circles denote the data from the VD/ESD and GSE+ methods using $M = 2$ copies of identical noisy quantum states, respectively. Note that GSE+ denotes the GSE method with the additional term ρH included in the bases of subspace $\{\sigma_i\}$. The purple crosses indicate the ordinary QSE method which corresponds to choosing $A = \rho$ and $\sigma_i \in \{I, H\}$. The black and green lines indicate results from the raw noisy quantum state and error-free optimized circuit, respectively. While the accuracy by the VD/ESD result is bounded by the insufficient expressibility of the variational quantum circuit, the GSE method can reach beyond this limit by further exploring the subspace.

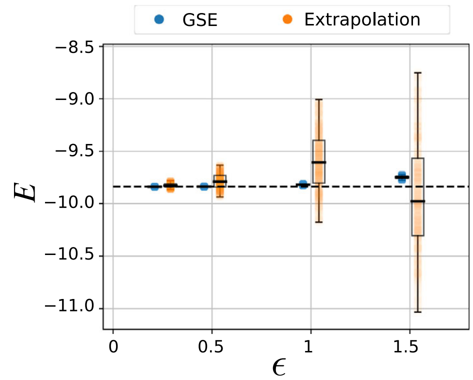

FIG. 4. Influence of fluctuation in the stretch factor λ_i. The blue and orange points denote the results from the GSE method using fault subspace and the extrapolation method for the VD/ESD calculation using $M = 2$ copies, respectively. It can be clearly observed that the extrapolation method under uncertain noise control yields both systematic deviation and increased variance. For each error unit ϵ, we generate 500 sets of noisy quantum states $\rho(\hat{\lambda}_i\epsilon)$ where $\hat{\lambda}_i = \lambda_i + \mathcal{N}(0, \lambda_i\epsilon\sigma^2)$ for $\lambda_i \in \{1, 2, 3\}$ and $\sigma = 0.1$. We assume that each Pauli term is estimated without any shot noise.

quantum states to span the quantum subspace. Here, the error-agnostic QEM is realized by utilizing quantum states from different noise levels, and hence the subspace is referred to as the fault subspace; we take $\sigma_i = \rho(\lambda_i\epsilon)$ where ϵ is the unit of the controlled error (e.g., infidelity per gate) and $\lambda_i \geq 1$ determines the actual error level. For instance, we consider an error-mitigated state as follows:

$$\rho_{\rm EM} = \sum_{ij} \alpha_i^* \alpha_j \rho(\lambda_i\epsilon)\rho(\lambda_j\epsilon), \tag{5}$$

where we have set $A = I$ and $\sigma_i = \rho(\lambda_i\epsilon)$. We may also extend the fault subspace to include high orders $\rho^m(\lambda_i\epsilon)(m \geq 2)$ or operators $U_l^{(i)}$ and $V_l^{(i)}$.

The concept of the fault subspace is closely related to the celebrated error-extrapolation method [5,6]. In the error-extrapolation method, one estimates the zero-noise limit of the expectation value of a given observable O based on results at $n+1$ noise levels $\langle O(\lambda_i\epsilon)\rangle = {\rm Tr}[\rho(\lambda_i\epsilon)O]$. The estimated computation result is given as $O^* = \sum_{i=0}^n \beta_i \langle O(\lambda_i\epsilon)\rangle + \mathcal{O}(\epsilon^{n+1})$, where $\beta_i \in \mathbb{R}$, $\sum_{i=0}^n \beta_i = 1$ and $\sum_{i=0}^n \beta_i \lambda_i^k = 0$ for $k = 1, 2, \ldots, n$ (see Supplemental Material for details [34]). This implies that the error-extrapolation method constructs an effective density matrix as $\rho_{\rm ex} = \sum_{i=0}^n \beta_i \rho(\lambda_i\epsilon)$.

Because of its simplicity and practicality, the extrapolation method has been investigated widely both theoretically and experimentally. However, the extrapolation is based on a highly nontrivial assumption that the noise level can be accurately controlled (e.g., by extending the gate execution duration). Moreover, since the extrapolation is a purely mathematical operation that does not take any physical constraint into account, it may produce unphysical results even if the measurement is done perfectly, e.g., $\rho_{\rm ex}$ can be an unphysical state whose eigenvalues can be negative.

The GSE method using the fault subspace can solve the above problems. First, the results obtained from the GSE method correspond to a physical density matrix. Second, the GSE method using the fault subspace does not rely on the accurate knowledge of noise levels. This is because the GSE method simply aims to construct a truncated Hilbert space so that the lowest eigenstate is included. It suffices to employ bases that are not identical to each other, while the choice of error levels may affect the practical efficiency.

As a demonstration, we numerically investigate the ground state of 1D TFI model assuming that the control over the noise level is imperfect (see Supplemental Material for simulation of excited states [34]). Here, we consider three noise levels $\rho_i = \rho(\hat{\lambda}_i\epsilon)$, where $\hat{\lambda}_i = \lambda_i + \mathcal{N}(0, \lambda_i\epsilon\sigma^2)$ for $\lambda_i \in \{1, 2, 3\}$ and variance σ^2. The energy at the zero-noise limit is estimated by the Richardson extrapolation for each set of data $\hat{\mathcal{D}} = \{(\lambda_i, {\rm Tr}[H\rho^2(\hat{\lambda}_i\epsilon)]/{\rm Tr}[\rho^2(\hat{\lambda}_i\epsilon)]\}$. (See Supplemental Material for details [34]). The extrapolated value fluctuates due to the random realization of $\hat{\lambda}_i$, which does not affect the GSE method almost at all. We highlight this contrast in Fig. 4. Because of the stability, the GSE method is suitable for experiments on quantum devices.

Summary and outlook.—We have proposed a generalized quantum subspace expansion which unifies the advantages of previously reported error-agnostic methods and furthermore overcomes their drawbacks. As a practical demonstration, we have first discussed to include powers of the noisy quantum state ρ^m in the base of the subspace. This does not only provide the exponential suppression of stochastic error, which is even more efficient than the VD/ESD method, but it also eliminates the coherent errors of the dominant vector. In the second strategy, we have presented a method that spans the subspace using quantum states with various noise levels. Unlike the commonly used error-extrapolation technique, the GSE method exhibits robust performance even when the control over noise level is imprecise.

There are several future directions. First, an efficient combination of the proposed scheme and other QEM methods is worth exploring. For example, we can combine the quasiprobability method with the proposed method to suppress the bias of error-mitigated expectation values due to finite characterization errors. We also expect that exploiting symmetry of the system in the subspace [17,36] will also improve the computational accuracy. Second, our method is not restricted to near-term quantum computing, but may help improve computational accuracy even in the fault-tolerant quantum computing regimes, when problems of interest involve calculation of eigenspectra. Namely, we may apply the proposed method to mitigate the effect of errors due to decoding of logical qubits or insufficient number of T gates without any characterization. This is in contrast with the previous works based on the quasiprobability method [38–41]. The study of suitable subspace in our GSE framework is also important in future works.

We thank fruitful discussions with Zhenyu Cai, Bálint Koczor, and Kosuke Mitarai. This work was supported by the Leading Initiative for Excellent Young Researchers MEXT Japan and JST presto (Grant No. JPMJPR1919) Japan. This Letter was partly based on results obtained from a project, JPNP16007, commissioned by the New Energy and Industrial Technology Development Organization (NEDO), Japan. This work is supported by PRESTO, JST, Grants No. JPMJPR1916, No. JPMJPR2114, No. JPMJPR2119; ERATO, JST, Grant No. JPMJER1601; CREST, JST, Grant No. JPMJCR1771; MEXT Q-LEAP Grants No. JPMXS0120319794 and No. JPMXS0118068682. This work also was supported by JST [Moonshot R&D] [Grant No. JPMJMS2061]. This work was supported by JST COI-NEXT program (JPMJPF2014). Part of numerical calculations were performed using Qulacs [42] and QuTiP [43].

Note added.—Recently, Ref. [44] appeared as a preprint, which considers a method similar to the power subspace corresponding to Eq. (4).

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