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Estimation of the local density of states on a quantum computer

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We report an efficient quantum algorithm for estimating the local density of states (LDOS) on a quantum computer. The LDOS describes the redistribution of energy levels of a quantum system under the influence of a perturbation. Sometimes known as the "strength function" from nuclear spectroscopy experiments, the shape of the LDOS is directly related to the survivial probability of unperturbed eigenstates, and has recently been related to the fidelity decay (or "Loschmidt echo") under imperfect motion reversal. For quantum systems that can be simulated efficiently on a quantum computer, the LDOS estimation algorithm enables an exponential speedup over direct classical computation.

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A major motivation for the physical realization of quantum information processing is the idea, intimated by Feynman, that the dynamics of a wide class of complex quantum systems may be simulated efficiently by these techniques [1]. For a quantum system with Hilbert space size N, an *efficient* simulation is one that requires only polylog(N) gates. This situation should be contrasted with direct simulation on a classical processor, which requires resources growing at least as N^2. However, complete measurement of the final state on a quantum processor requires $O(N^2)$ repetitions of the quantum simulation. Similarly, estimation of the eigenvalue spectrum of a quantum system admitting a polylog(N) circuit decomposition requires a phase-estimation circuit that grows as $O(N)$ [2]. For small N simulations it is still practical to read out the complete information about the system or final state [3]. However, for large N simulations there remains the important problem of devising efficient methods for the measurement of those characteristic properties of practical interest in the study of complex quantum systems. Recent work has shown that the stability under perturbation may be estimated efficiently on a quantum processor via simulation of imperfect motion reversal and subsequent direct measurement of the fidelity decay [4,5]. In this Rapid Communication we introduce an efficient quantum algorithm for estimating, to $1/\text{polylog}(N)$ accuracy, the local density of states (LDOS), a quantity of central interest in the description of both many-body and complex few-body systems. We also determine the class of physical problems for which the LDOS estimation algorithm provides an exponential speedup over known classical algorithms given this finite accuracy.

The LDOS describes the profile of an eigenstate of an unperturbed quantum system over the eigenbasis of perturbed version of the same quantum system. In the context of many-body systems the LDOS was introduced to describe the effect of strong two-particle interactions on the single particle (or single hole) eigenstates [6–10]. More recently, the LDOS has been studied to characterize the effect of imperfections (due to residual interactions between the qubits) in the operation of quantum computers [11,12]. This profile plays a fundamental role also in the analysis of system stability for few-body systems subject to a sudden perturbation [13], such as the onset of an external field, and has been studied extensively in the context of quantum chaos and dynamical localization [14,15]. Quite generally the LDOS is related to the survival probability of the unperturbed eigenstate [7,13,16], and there has been considerable recent effort to understand the conditions under which the LDOS width determines the rate of fidelity decay under imperfect motion reversal ("Loschmidt echo") [4,16–18].

A number of theoretical methods have been devised to characterize the LDOS for complex systems. These methods include banded random matrix models [6,19–21], models of a single level with constant couplings to a "picket-fence" spectrum [7,22], and perturbative techniques with partial summations over diagrams to infinite order [23]. Under inequivalent assumptions these approaches affirm a generic Breit-Wigner shape for the LDOS profile,

$$\eta^{\mathrm{BW}}(\phi) \propto \frac{\Gamma}{\phi^2 + \Gamma^2/4}. \tag{1}$$

However, the extent to which these methods correctly describe any real system is generally not clear [13,25], and therefore direct numerical analysis is usually necessary. It is worth stressing here that direct numerical computation of the LDOS requires the diagonalization of matrices of dimension N, and therefore demands resources that grow at least as N^2. Of course only coarse-grained information about the LDOS is of practical interest since one cannot even store the complete information efficiently for large enough systems. However, for generic systems there is no known numerical procedure that can circumvent the need to *manipulate* the $N \times N$ matrix in order to extract even coarse information about its LDOS. In this paper we report a quantum algorithm

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which enables estimation of the LDOS to $1/\mathrm{polylog}(N)$ accuracy with only $\mathrm{polylog}(N)$ resources.

To specify the algorithm we represent the unperturbed quantum system by a unitary operator U, which may correspond either to a Floquet map, or to evolution under a time-independent Hamiltonian,

$$U = \exp(-iH_o\tau). \tag{2}$$

We represent the perturbed quantum system by the unitary operator $U(\sigma)$, which we express in the form

$$U(\sigma) = \exp(-i\delta V)U, \tag{3}$$

where δ is some dimensionless parameter and V is a Hermitian perturbation operator. The variable σ denotes an effective "perturbation strength" taking into account both the parameter δ and the size of the matrix elements of the perturbation,

$$\sigma^2 = \delta^2\,\overline{|\langle\phi_j|V|\phi_{j'}\rangle|^2}, \tag{4}$$

where the average is taken only over directly coupled eigenstates. Let $U|\phi_j\rangle = \exp(-i\phi_j)|\phi_j\rangle$, and $U(\sigma)|\phi_k(\sigma)\rangle = \exp(-i\phi_k(\sigma))|\phi_k(\sigma)\rangle$ denote the eigenphases and eigenstates of the unperturbed and perturbed systems, respectively. The LDOS for the jth eigenstate of U is then

$$\eta_j(\phi) = \sum_k P(\phi_k(\sigma)|\phi_j)\ \delta(\phi - [\phi_k(\sigma) - \phi_j]), \tag{5}$$

where δ is a Dirac delta function and where the transition probabilities,

$$P(\phi_k(\sigma)|\phi_j) = |\langle\phi_k(\sigma)|\phi_j\rangle|^2, \tag{6}$$

are the basic quantities of interest.

The coarse-grained distribution,

$$P(\Delta_l|\phi_j) = \sum_{\phi_k(\sigma)\in\Delta_l} P(\phi_k(\sigma)|\phi_j), \tag{7}$$

is a just the sum over the probabilities for those perturbed eigenphases $\phi_k(\sigma)$ lying within a band Δ_l. This band is centered about angle $2\pi l/M$, with width $\Delta = 2\pi/M$, and the integer l ranges from 0 to $M-1$. Similarly, an averaging over neighboring *unperturbed* eigenstates is often carried out to remove the effects of atypical states. The combination of both operations yields the probability distribution,

$$P(\Delta_l|\Delta_m) = N_m^{-1} \sum_{\phi_k(\sigma)\in\Delta_l} \sum_{\phi_j\in\Delta_m} P(\phi_k(\sigma)|\phi_j), \tag{8}$$

where the normalization constant N_m is just the number of unperturbed eigenphases in the angular range Δ_m. In practice one must choose M to be $O(\log_2(N))$ since otherwise the measured LDOS η would contain an exponential amount of information and therefore could not be processed efficiently.

We now describe the algorithm for estimating the LDOS on a quantum processor. The circuit for this algorithm is depicted in Fig. 1. The lower register implements the perturbed and unperturbed maps U and $U(\sigma)$, requiring $n_q = O(\log_2(N))$ qubits. The upper register holds the $m_q = \log_2(M)$ ancillary qubits which fix the precision of the

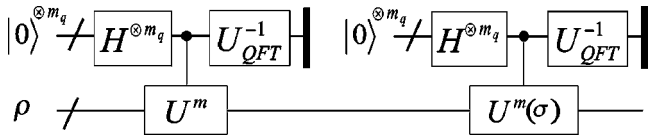

FIG. 1. Circuit diagram for measuring the local density of states, consisting of two successive phase-estimation circuits on different operators. The diagonal line denotes a bundle of qubits and the thick vertical bar denotes a projective measurement of the quantum state in the computational basis. The upper register contains $m_q = \log_2(M)$ qubits and the operations on the lower register are applied conditionally m times, where the integer $m \in [0, M-1]$ is determined from the binary representation of the computational basis states in the upper register.

phase-estimation algorithm. The upper register always starts out in the "ready" state $|0\rangle$. The appropriate choice of initial state ρ in the n_q register will depend on the context, as explained below. For the moment we assume the lower register is prepared in a pure state, $\rho = |\psi_o\rangle\langle\psi_o|$. The first step of the algorithm involves estimating the eigenphases of the unperturbed operator U. This takes the initial state through the sequence

$$\begin{aligned}
|0\rangle \otimes |\psi_o\rangle &\to \frac{1}{\sqrt{M}} \sum_{m=0}^{M-1} |m\rangle|\psi_o\rangle \\
&\to \frac{1}{\sqrt{M}} \sum_{m=0}^{M-1} |m\rangle (U)^m|\psi_o\rangle \\
&= \frac{1}{\sqrt{M}} \sum_{m=0}^{M-1} |m\rangle \sum_{j=0}^{N-1} c_j \exp(i\phi_j m)|\phi_j\rangle \\
&\to \sum_{j=0}^{N-1} c_j|m_j\rangle|\phi_j\rangle,
\end{aligned} \tag{9}$$

where $c_j = \langle\phi_j|\psi_o\rangle$. The state m_j is the nearest m_q-bit binary approximation to the jth eigenphase of U,

$$\tilde{\phi}_j = 2\pi m_j/M \simeq \phi_j. \tag{10}$$

Upon strong measurement of the m_q register one obtains and records a single outcome m, and the state of n_q register must then be described by (viz., "collapsed to") the updated pure state,

$$|\psi(\Delta_m)\rangle = \sum_{\phi_j\in\Delta_m} \tilde{c}_j|\phi_j\rangle, \tag{11}$$

corresponding to the subspace of eigenstates with eigenphases in the band Δ_m of width $\Delta = 2\pi/M$ about the phase $2\pi m/M$. To keep normalization the coefficients have been rescaled as follows:

$$\tilde{c}_j = \frac{c_j}{(\sum_{\phi_j \in \Delta_m} |c_j|^2)^{1/2}}. \tag{12}$$

Next we reset the m_q qubit register to the ready state and run the phase-estimation algorithm on the operator $U(\sigma)$, producing the final state,

$$|\psi\rangle = \sum_{\phi_j \in \Delta_m} \tilde{c}_j \sum_{k=0}^{N-1} b(k|j)\ |m_k\rangle \otimes |\phi_k(\sigma)\rangle, \tag{13}$$

where $\tilde{\phi}_k(l) = 2\pi m_k / M$ is an m_q-bit approximation to $\phi_k(\sigma)$. The complex coefficients $b(k|j) = \langle \phi_j | \phi_k(\sigma) \rangle$ are the inner product of the perturbed and unperturbed eigenstates. Measurement of the m_q register now reveals an outcome l, associated with the eigenphases in the angular range $2\pi l/M \pm \Delta/2$. The outcome l occurs with probability,

$$P_{\psi_o}(l|m) = \sum_{\phi_k \in \Delta_l} \left| \sum_{\phi_j \in \Delta_m} \tilde{c}_j\ b(k|j) \right|^2, \tag{14}$$

which is conditional on the earlier outcome m and the choice of initial state.

We now specify how the initial state may be chosen to eliminate unwanted fluctuations arising from the variables $\tilde{c}_j$ in Eq. (14). Before describing the general solution we consider first a special case of particular interest: when a known eigenstate of U may be prepared efficiently. Such an initial state may be prepared (or well approximated) by an efficient circuit when U consists of some sufficiently simple integrable system (e.g., a noninteracting many-body system). In this case we have $\tilde{c}_j = \delta_{jk}$, and the final probability distribution Eq. (14) reduces exactly to the (coarse-grained) kernel Eq. (7),

$$P_{\phi_k}(l|m) \to P(\Delta_l|\phi_k). \tag{15}$$

When the eigenphase associated to the prepared eigenstate is known to sufficient accuracy (so that m is known), it is not even necessary to perform the first phase estimation routine. In the general case of a generic quantum system, it is sufficient to prepare the maximally mixed state as the initial state, in which case the final probability distribution reduces exactly to the (coarse-grained and averaged) probability kernel Eq. (8), i.e.,

$$P(l|m)_{\rho=\mathbf{1}/N} = \frac{1}{N_m} \sum_{\phi_k(\sigma) \in \Delta_l} \sum_{\phi_j \in \Delta_m} P(\phi_k(\sigma)|\phi_j). \tag{16}$$

This probability kernel contains all the information needed to compute the (coarse-grained and averaged) LDOS, $\eta_m(2\pi k/M) = \Sigma_l\ P(l|m)\,\delta_{k,(l-m)}$, completing our derivation.

The algorithm described above remains efficient provided that the quantum maps U and U_δ admit polylog(N) gate decompositions. Such decompositions have been identified both for many-body systems with local interactions and for a wide class of few-body quantized classical models. As mentioned earlier, for practical purpose M should be polylog(N) so the overall circuit of Fig. 1 is indeed efficient for such systems.

We now turn to the question of how many times K the algorithm must be repeated to arrive at interesting physical conclusions about the final probability distribution. This issue arises because the final probability distribution is not measured directly on the quantum processor; rather, it governs the relative frequency of outcomes obtained in each repetition of the algorithm. Indeed, it is by repeating the algorithm illustrated in Fig. 1 and accumulating joint statistics of the l and m outputs that one can estimate the parent distribution $P(l|m)$. The accuracy of this estimation depends on the number of times K the distribution is sampled. In order to bound K it is convenient to cast the physical problems related to the LDOS in terms of hypothesis testing. We consider the important case of testing which of two candidates distributions η_1 or η_2 best describes the LDOS of a given system and a given perturbation. For example, one might be testing whether the Lorentzian has one of two candidate widths, or whether the profile is Gaussian or Lorentzian. Only when $K \leqslant$ polylog(N) will the overall computation remain efficient. This problem is resolved in general by the Chernoff bound [24]. A random variable is distributed according to either $P_1(x)$ or $P_2(x)$, and we wish to determine which distribution is the right one. Then, the probability P_e that we make an incorrect inference decreases exponentially with the number of times K the variable was sampled: $P_e \leqslant \lambda^K$. Here, $0 \leqslant \lambda \leqslant 1$ is a measure of similarity between distributions defined as

$$\lambda = \min_{0 \leqslant \alpha \leqslant 1} \sum_x P_1(x)^\alpha P_2(x)^{(1-\alpha)}; \tag{17}$$

in particular, λ is bounded above by the fidelity between P_1 and P_2. Thus a constant error probability ϵ requires a sample of size $K = \ln(\epsilon)/\ln(\lambda)$. Therefore, as long as the concerned distributions are at a polylog(N) distance, i.e., $1-\lambda \geqslant 1/\text{polylog}(N)$, they can be distinguished efficiently. We note that the test can be inconclusive when both hypotheses are equally likely to describe the underlying physics.

Efficient application of the LDOS algorithm under these restrictions may be illustrated explicitly by working through a problem of practical interest from the recent literature. We consider the problem of testing whether the Breit-Wigner (BW) profile Eq. (1) applies when a given quantized classically chaotic model is subjected to a perturbation of interest. From the Bohigas-Giannoni-Schmit conjecture [26] and studies of (banded) random matrix models [6,19–21], it is generally expected that for fully chaotic models with generic perturbations Eq. (1) applies with

$$\Gamma(\sigma) = 2\pi\sigma^2\rho_E, \tag{18}$$

provided that the effective perturbation strength lies in the range

$$1 \ll \sigma\rho_E \ll \sqrt{b}, \tag{19}$$

where b is the bandwidth of the perturbation in the ordered eigenbasis of U and ρ_E is the level density. It should be stressed that Γ may be estimated *a priori* if the perturbation is known [4,19,20]. Deviations from this hypothesis can arise for a wide variety of reasons (i.e., integrable or mixed clas-

sical dynamics in the unperturbed or perturbed system, nongeneric properties of the perturbation, hidden symmetries, etc.) and therefore analysis of the LDOS remains an active area of numerical study for both dynamical models [14,25] and real systems [8].

The lower bound of Eq. (19) is determined from the breakdown of perturbation theory and leads to a width Γ that decreases linearly with N. Since the circuit can only efficiently resolve the LDOS with accuracy $1/\mathrm{polylog}(N)$, the BW profile with width $\Gamma = O(N^{-1})$ may not be verified efficiently near this lower bound. However, near the upper bound of Eq. (19) the validity of the BW profile may be tested efficiently. In the case of fully chaotic models one has $b = N/2$ and the upper bound for Γ is therefore $O(1)$. Hence the validity of Eq. (1) provides a hypothesis which may be tested efficiently for any perturbation such that $1/\mathrm{polylog}(N) \ll \Gamma(\sigma) \ll O(1)$. Within this range one can also determine whether the chaotic model manifests dynamical localization, since localized systems fail to exhibit certain necessary random matrix properties, such as eigenvalue repulsion, and initially nearby eigenstates of the unperturbed model will not remain concentrated in the same eigenphase region of the perturbed model.

In summary we have reported an algorithm for efficiently estimating the LDOS of a quantum system subject to perturbation. There is wide range of contexts in which important coarse features of the LDOS, such as the width, may be estimated with only $\mathrm{polylog}(N)$ resources. We have described in detail the important problem of testing the Breit-Wigner hypothesis as one example for which the LDOS estimation algorithm gives an effective exponential speedup over classical computation.

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