Shadow Hamiltonian Simulation

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Abstract

We present shadow Hamiltonian simulation, a framework for simulating quantum dynamics using a compressed quantum state that we call the "shadow state". The amplitudes of this shadow state are proportional to the expectations of a set of operators of interest. The shadow state evolves according to its own Schrödinger equation, and under broad conditions can be simulated on a quantum computer.

We analyze a number of applications of this framework to quantum simulation problems. This includes simulating the dynamics of exponentially large systems of free fermions, or exponentially large systems of free bosons, the latter example recovering a recent algorithm for simulating exponentially many classical harmonic oscillators. Shadow Hamiltonian simulation can be extended to simulate expectations of more complex operators such as two-time correlators or Green's functions, and to study the evolution of operators themselves in the Heisenberg picture.

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1 Introduction

One of the most important applications of quantum computers is simulating the dynamics of quantum systems, often referred to as the Hamiltonian simulation problem. The standard presentation of this problem involves an initial quantum state $|\psi(0)\rangle$ that is easy to prepare on a quantum computer and a Hamiltonian H that describes the interactions in the system. The goal is to produce the state at a later time t>0, $|\psi(t)\rangle$, which satisfies the Schrödinger equation: $\frac{\mathrm{d}}{\mathrm{d}t}|\psi(t)\rangle=-\mathrm{i}H|\psi(t)\rangle$. A plethora of Hamiltonian simulation algorithms exist, with various complexities in terms of the relevant problem parameters, including the time t, the error ϵ to which the final state is prepared, and intrinsic properties of the Hamiltonian such as the magnitude of interaction strengths (cf. [Llo96, SOG+02, Aha03, BACS07, WBHS10, PQSV11, CW12, BCC+15, LC17, LC19, Cam19, ZS24]). Under reasonable assumptions, these complexities are logarithmic in the dimension of the Hilbert space, thus providing an exponential advantage over classical algorithms for this problem, which might require time polynomial in the dimension.

In applications of standard Hamiltonian simulation, once the final state $|\psi(t)\rangle$ has been prepared, one is often interested in obtaining some physical property, such as the expectation of a particular observable. One example is the ground state energy of the system, which can be obtained by measuring the expectation of H or by performing quantum eigenvalue estimation (cf. [SOG+02, ADLH05, DLT22, WFZ+23]). Another example could be the computation of an order parameter in a condensed matter system that can be obtained by measuring a two-body correlation function [Sac99, ZJL+20, MIQ+22]. Many of these properties can be extracted from a limited set of expectations, such as those of products of a few Pauli operators in qubit systems, or those of products of a few fermionic operators in fermionic systems, among others. While access to $|\psi(t)\rangle$ allows us to obtain the expectation of any observable on this state, for certain problems, it might suffice to prepare a different quantum state that does not encode all the information encoded by $|\psi(t)\rangle$, but instead only encodes information about certain properties. Doing so could result in significant computational savings; or, it could potentially let us use resources differently, for example, enabling the simulation of quantum systems of sizes that are significantly larger than those that can be studied with standard Hamiltonian simulation approaches.

Based on this observation, we introduce a framework to perform quantum simulation that we call "shadow Hamiltonian simulation". Rather than storing the entire time-dependent state in quantum memory during the quantum computation, we encode certain expectations in the amplitudes of a quantum state of smaller dimension, which we refer to as the "shadow state". We will see that, under a broad set of conditions, the shadow state evolves unitarily under its own Schrödinger equation, which captures the Heisenberg-picture dynamics of the observables. For many examples, this evolution can be simulated efficiently on a quantum computer. Furthermore, we will see that a shadow state is a projection of $|\psi(t)\rangle \otimes |\overline{\psi(t)}\rangle^1$ on a certain subspace specified by the operators whose expectations are encoded, hence creating a "shadow" of the state.

To provide an idea of what type of problems can be efficiently solved using the shadow Hamiltonian simulation approach, we apply it to free-fermion and free-boson systems, qubit systems, and other systems with a Lie algebraic structure that arises naturally within this context. In the first two cases, by encoding only the expectations of products of fermionic or bosonic operators of constant degree, we can leverage the exponential dimension of the shadow state to simulate systems of exponential size. These instances can be relevant for first-quantization simulations, where increasing the number of modes, corresponding to the number of points in a discretized grid, allow for better approximations

¹We use $|\overline{\psi}\rangle$ to denote the state whose amplitudes are complex conjugates of the amplitudes of $|\psi\rangle$ in the computational basis.

of the states [GSA+13, SBW+21]. They can also be relevant for simulating disordered quantum systems, where classical methods perform poorly. We can then use shadow states to compute, for example, energies associated with fermionic or bosonic modes at any time, including expectations of Hamiltonians that are interacting (i.e., they are not-free fermion or free-boson Hamiltonians), and other interesting quantities that would require exponential resources using standard Hamiltonian simulation methods. Moreover, using a classical–quantum correspondence, we are able to reproduce the results of Ref. [BBK+23] on simulating classical oscillators, which can alternatively be interpreted as an example of shadow Hamiltonian simulation using a classical–quantum correspondence.

The principles behind shadow Hamiltonian simulation can be generalized in a way that allows encoding the expectations of more complex operators, such as two-time correlators, in the amplitudes of a different quantum state. This is convenient for exploring other dynamical properties of the system, yet without requiring the preparation of the full system's state. Additionally, while shadow Hamiltonian simulation is mainly designed to track the time-dependent expectations of certain operators, it can be easily extended to track the evolution of these operators determined by Heisenberg's equations of motion, without making any reference to a system's state. This enables other efficient quantum computations, such as finding signatures of operator spreading (e.g., light cones) or scrambling [MRQ+21], for which classical algorithms can take exponential time.

Shadow Hamiltonian simulation relaxes the requirements of standard Hamiltonian simulation in the same way that shadow state tomography relaxes the requirements of full quantum state tomography [Aar18]. That is, in the traditional state tomography problem, we are given copies of an unknown state and need to learn a full classical description of the state, from which we can obtain the expectation of any observable. This task requires exponentially many (in the system size) copies of the unknown state in general. In contrast, in shadow tomography, the goal is to learn expectations of a limited set of observables on the state, a task that can be shown to be much easier than traditional state tomography. Nonetheless, both problems are different: while shadow tomography concerns the problem of learning some classical description of a quantum state, shadow Hamiltonian simulation is related to the problem of evolving expectations in time.

2 Formalism

2.1 Shadow states

Let $S = \{O_1, \ldots, O_M\}$ be a set of $M < \infty$ operators and suppose we are only interested in a set of expectations $\langle O_m \rangle$, for all $m \in [M] := \{1, \ldots, M\}$, with respect to a (potentially mixed) quantum state ρ . We would like to store a compressed version of ρ that does not necessarily allow us to reconstruct it, but does allow us to recover certain quantities that depend on the $\langle O_m \rangle$'s only. We call this the "shadow state" of ρ with respect to the set S and define it as follows.

Definition 1 (Shadow state). Let ρ be a quantum state and $S = \{O_1, \ldots, O_M\}$ be a set of operators. The shadow state of ρ with respect to S is the M-dimensional (pure) unit state

$$|\rho; S\rangle = \frac{1}{\sqrt{A}} \begin{pmatrix} \langle O_1 \rangle \\ \vdots \\ \langle O_M \rangle \end{pmatrix} = \frac{1}{\sqrt{A}} \sum_{m=1}^M \langle O_m \rangle |m\rangle,$$
 (1)

where $A = \sum_{m} \langle O_m \rangle^2$ and, for $m \in [M]$, $\langle O_m \rangle$ is the expectation of the operator O_m with respect to ρ . For finite-dimensional systems, $\langle O_m \rangle = \operatorname{tr}(\rho O_m)$.

In the definition, we implicitly assume that at least one expectation $\langle O_m \rangle$ is nonzero and that the expectations are bounded, or otherwise the definition of shadow state would be irrelevant. For a given set S, the same shadow state can correspond to infinitely many physical states ρ , which occurs when S is not a complete set of operators. In this case, $|\rho; S\rangle$ contains less information than ρ , in the sense that a classical description of ρ cannot be reconstructed from a classical description of $|\rho; S\rangle$ (whereas $|\rho; S\rangle$ is fully specified by ρ). Similarly, not every M-dimensional state corresponds to a valid system's state ρ , since shadow states contain certain structure determined by S. While $|\rho; S\rangle$ is a state of finite dimension M, we do not make any assumptions on the dimension of ρ . This allows us to consider infinite-dimensional systems as well, such as bosonic systems.

For example, when $S = \{1, X, Y, Z\}^{\otimes n}$ is the set of all 4^n products of Pauli operators acting on n qubits, and if $\rho = |\psi\rangle\langle\psi|$ is an n-qubit pure quantum state, then $|\rho; S\rangle$ will be a 2n-qubit state since $M = 4^n$. While the state $|\rho; S\rangle$ looks unfamiliar, we show in Section 4 that, up to a simple "Bell rotation", this is the state $|\psi\rangle\otimes|\overline{\psi}\rangle$ where $|\overline{\psi}\rangle$ is the complex conjugate of $|\psi\rangle$. For this choice of S, which spans the complete set of operators acting on \mathbb{C}^{2^n} , the shadow state contains all the information contained in $|\psi\rangle$. In fact, the shadow state is even more powerful than $|\psi\rangle$ in this case, in the sense that there are problems that can be solved with only one copy of $|\psi\rangle\otimes|\overline{\psi}\rangle$ while still needing exponentially many copies of $|\psi\rangle$ alone to solve (Theorem 8).

Many applications studied in this article, however, consider shadow states that contain less information than $|\psi\rangle$. As a simple illustrative example where this occurs, consider a one-qubit state and the set of Pauli operators $S = \{\mathbb{1}_2, X, Y\}$, where $\mathbb{1}_2$ is the 2×2 identity. Then, any state that is polarized along the Z direction, i.e., $\rho = \frac{1}{2}(\mathbb{1}_2 + \langle Z \rangle Z)$, satisfies $\langle X \rangle = \langle Y \rangle = 0$, and results in the same shadow state, prohibiting the recovery of the full state ρ from $|\rho; S\rangle$ in this example.

A different example is when S is the set of quadratic fermionic operators of the form $a_j^{\dagger}a_k$, where a_j^{\dagger} creates a fermion in the $j^{\rm th}$ mode and a_k annihilates a fermion in the $k^{\rm th}$ mode. In this case, $|\rho;S\rangle$ contains less information than ρ , which again follows from the fact that distinct fermionic states can give rise to exactly the same values for the expectations $\langle a_j^{\dagger}a_k\rangle$. In this example, however, the shadow state lets us encode exponentially many such expectations if we allow for M to be exponentially large. This enables the computation of certain properties of systems involving exponentially many fermionic modes, as we discuss in Section 3.1. Similar observations apply to bosonic systems.

One common task that can be solved with shadow states is the estimation of an arbitrary linear combination of the expectations $\langle O_m \rangle$, which reduces to an overlap estimation problem. Another common task is that of sampling from a distribution where probabilities are $\Pr(m) \propto |\langle O_m \rangle|^2$, which can be done by measuring the shadow state in the computational basis. These tasks are related to other problems, like estimating energies of a subset of modes in fermionic and bosonic systems of exponential size, which are discussed in Sections 3.1 and 3.2.

Having established the notion of shadow state, we proceed to discuss the problem of simulating quantum dynamics within this formalism.

2.2 Shadow Hamiltonian simulation

In standard Hamiltonian simulation, we are given a Hamiltonian H and the goal is to map the (possibly mixed) initial state of the system, $\rho(0)$, to the final state $\rho(t)$. The operation that implements this mapping is the evolution operator U(t) determined by H. In shadow Hamiltonian simulation, we are additionally given a set of operators S, and the goal is instead to map the initial shadow state $|\rho(0); S\rangle$ to the final shadow state $|\rho(t); S\rangle$. The challenge is to construct an efficient method that implements this mapping, which is different from U(t) in general.

For illustration, we return to the example of S being the set of all Pauli products acting on n qubits; the shadow state of a pure state $|\psi(t)\rangle$ is a simple Bell rotation of $|\psi(t)\rangle\otimes|\overline{\psi(t)}\rangle$. Despite the shadow state being more powerful than the original state in this example, the shadow Hamiltonian simulation problem is not much harder than standard Hamiltonian simulation. If we have an efficient quantum circuit to implement the unitary U(t) that maps a pure state $|\psi(0)\rangle$ to $|\psi(t)\rangle$, then we can also map $|\psi(0)\rangle\otimes|\overline{\psi(0)}\rangle$ to $|\psi(t)\rangle\otimes|\overline{\psi(t)}\rangle$ using the unitary $U(t)\otimes\overline{U(t)}$, where $\overline{U(t)}$ is the complex conjugate of U(t). Note that we can create an efficient circuit for $\overline{U(t)}$ by complex conjugating all the elementary gates appearing in the circuit that implements U(t). But, more generally, it is not always the case that $|\rho(0); S\rangle$ can be easily mapped to $|\rho(t); S\rangle$. Even worse, the vector $|\rho(0); S\rangle$ might not contain enough information to completely determine the vector $|\rho(t); S\rangle$ at a later time.

For it to be possible to obtain $|\rho(t); S\rangle$ from $|\rho(0); S\rangle$, even in principle, the expectations of the operators in S at time t should be a function of the initial expectations at time 0. This occurs when the Hamiltonian H leaves the space of operators spanned by S invariant, in the sense that the commutation relations between H and the operators in S yield a linear combination of operators in S only.

Definition 2 (Invariance property). Let H be a Hamiltonian and $S = \{O_1, \ldots, O_M\}$ be a set of operators. We say that H and S satisfy the invariance property if for all $m \in [M]$ we have

$$[H, O_m] = -\sum_{m'=1}^{M} h_{mm'} O_{m'} , \qquad (2)$$

where $h_{mm'}$ are coefficients. Let \mathbf{H}_S be the $M \times M$ matrix whose (m, m') entry is $h_{mm'}$. Then, we can write Eq. (2) as

$$[H, \vec{O}] = -\mathbf{H}_S \vec{O} , \qquad (3)$$

where $\vec{O} := (O_1, \dots, O_M)^T$ is a vector of operators.

The invariance property ensures that the shadow Hamiltonian simulation problem is solvable, but the map that takes $|\rho(0); S\rangle$ to $|\rho(t); S\rangle$ need not be simple in general. Our first result is that if the matrix \mathbf{H}_S is Hermitian, then the shadow state of the physical state $\rho(t)$ that evolves with H, evolves according to a Schrödinger equation but with the Hamiltonian \mathbf{H}_S .

Theorem 3. Let H be a Hamiltonian and $S = \{O_1, \ldots, O_M\}$ be a set of operators, such that H and S satisfy the invariance property. Let $\rho(t)$ be the state of the quantum system obtained by evolving $\rho(0)$ under H for time t. The shadow state $|\rho(t); S\rangle$ satisfies the differential equation:

$$\frac{\mathrm{d}}{\mathrm{d}t}|\rho(t);S\rangle = -\mathrm{i}\boldsymbol{H}_S|\rho(t);S\rangle. \tag{4}$$

Furthermore, if H_S is Hermitian, Eq. (4) is a Schrödinger equation.

Proof. Let $\rho(t) = U(t)\rho(0)U^{\dagger}(t) = \sum_{\ell} p_{\ell}|\psi_{\ell}(t)\rangle\langle\psi_{\ell}(t)|$, where the p_{ℓ} 's are probabilities. The amplitudes of $|\rho(t); S\rangle$ are proportional to $\langle O_m(t)\rangle = \sum_{\ell} p_{\ell}\langle\psi_{\ell}(t)|O_m|\psi_{\ell}(t)\rangle$, and Schrödinger's equation and the invariance property imply

$$\frac{\mathrm{d}}{\mathrm{d}t}\langle O_m(t)\rangle = \sum_{\ell} p_{\ell} \left(\frac{\mathrm{d}}{\mathrm{d}t} \langle \psi_{\ell}(t)| \right) O_m |\psi_{\ell}(t)\rangle + \langle \psi_{\ell}(t)| O_m \left(\frac{\mathrm{d}}{\mathrm{d}t} |\psi_{\ell}(t)\rangle \right)$$
 (5)

$$= i \sum_{\ell} p_{\ell} \langle \psi_{\ell}(t) | [H, O_m] | \psi_{\ell}(t) \rangle \tag{6}$$

$$=-\mathrm{i}\sum_{m'=1}^{M}h_{mm'}\langle O_{m'}(t)\rangle\;,\tag{7}$$

which is also Eq. (4).

Hence, we can perform shadow Hamiltonian simulation on a quantum computer if H_S is Hermitian and can be efficiently simulated. For finite-dimensional systems, this occurs when the operators in S are orthogonal.

Lemma 4. Let the system be finite-dimensional and the operators in S be orthogonal, satisfying $\operatorname{tr}(O_m^{\dagger}O_{m'}) = \lambda \delta_{mm'}$, for some $\lambda > 0$. Then \mathbf{H}_S is Hermitian.

Proof. Under the orthogonality condition, the entries of \mathbf{H}_S satisfy

$$h_{mm'} = -\frac{1}{\lambda} \operatorname{tr}(O_{m'}^{\dagger}[H, O_m]) = \underbrace{-\frac{1}{\lambda} \overline{\operatorname{tr}([O_m^{\dagger}, H] O_{m'})}}_{\text{(take Hermitian conjugate)}} = \underbrace{-\frac{1}{\lambda} \overline{\operatorname{tr}(O_m^{\dagger}[H, O_{m'}])}}_{\text{(cyclic property of trace)}} = \overline{h_{m'm}}.$$
 (8)

While orthogonality of the operators in S suffices for H_S to be Hermitian, this is not a necessary requirement in general. Indeed, Theorem 3 applies even if the operators in S are not linearly independent or even if $\rho(t)$ is infinite-dimensional. In Section 3.2, we discuss an example of a system of free bosons, or coupled quantum harmonic oscillators, where the underlying Hilbert space is infinite-dimensional. The Hamiltonian H is quadratic in b_j^{\dagger} and b_k , the creation and annihilation bosonic operators, respectively. For this specific example, Theorem 3 generalizes the result in Ref. [BBK⁺23], which considers a quantum algorithm for simulating classical harmonic oscillators, but for simulating quantum oscillators in this case.

In general, the invariance property alone does not imply that \mathbf{H}_S is Hermitian. However, it is sometimes possible to take a particular linear combination of the O_m 's to fix this; that is, we can use the property $[H, \mathbf{A}\vec{O}] = -\mathbf{A}\mathbf{H}_S\vec{O}$ for an $M \times M$ matrix \mathbf{A} and take specific linear combinations of the O_m 's to obtain a Hermitian matrix. This provides some flexibility for shadow Hamiltonian simulation, and we will use this observation for simulating bosonic systems in Section 3.2. Also, note that Eq. (4) applies even if \mathbf{H}_S is not Hermitian. It might be possible to apply quantum algorithms for simulating differential equations to prepare the shadow states in this case, where the evolution is not unitary (cf. [Ber14, CLO21]). These analyses are outside the scope of this article.

Additionally, since quantum circuits can be interpreted as time evolution with a time-dependent Hamiltonian, our results can be extended to address this case. More precisely, let $G = G^L \dots G^1$ be a quantum circuit described as a sequence of gates G^j , $j \in [L]$. The analogous property to the invariance property in this case is

$$(G^{j})^{\dagger} O_{m} G^{j} = \sum_{m'} g^{j}_{mm'} O_{m'}, \tag{9}$$

for all $m \in [M]$ and $j \in [L]$, where $g_{mm'}^j \in \mathbb{C}$. These coefficients define an $M \times M$ matrix \mathbf{G}_S^j for each j. If these matrices are also unitary—the analogous condition to requiring \mathbf{H}_S be Hermitian—then we can simulate them and perform maps between the corresponding shadow states.

2.3 Beyond shadow Hamiltonian simulation

The basic idea underlying shadow Hamiltonian simulation can be generalized and applied to other related problems. We discuss two such problems in Sections 3.5 and 3.6. In one case we show how to encode the expectations of more complex operators, these being products of time-dependent operators, in the amplitudes of another quantum state. Each of these operators evolves according to the Heisenberg picture with their own Hamiltonians. This provides a more general result, in

which quantities like two-time correlators can be encoded. In another case, we show how to encode time-evolved operators in quantum states that can be simulated, without making reference to the state of the system. The approach here is similar to shadow Hamiltonian simulation, and by measuring the corresponding states we could obtain properties of the evolved operators, such as the size of their light cones as a function of time.

3 Applications

In this section, we first apply shadow Hamiltonian simulation to quantum systems obeying different statistics, and depict problems that can be solved efficiently using this formalism. Subsequently, we demonstrate how similar ideas can be applied to related problems: encoding two-time correlators or expectations of products of operators in a quantum state, and encoding a time-dependent operator, subject to Heisenberg's equations of motion, in a quantum state.

3.1 Free fermions

Free-fermion systems, which are modeled by quadratic fermionic Hamiltonians, appear ubiquitously in quantum chemistry and physics. Examples include spin models like the transverse-field Ising model [BM71], BCS superconductivity [Tak05], integer quantum Hall effect [Ton16], and other cases described by mean-field theories. For n fermionic modes, the number of degree-k fermionic operators is $\mathcal{O}(n^k)$, and in this case we could use shadow states to encode the expectations of operators acting on systems that are exponentially large, e.g., $n = 2^r$. These instances can arise in, for example, approaches based on first-quantization [GSA⁺13, SBW⁺21].

To map between shadow states, the first goal is to provide a method for shadow Hamiltonian simulation of these systems that is efficient, i.e., of complexity polynomial in r or polylog(n), and polynomial in the evolution time t. We will show this is possible for *free-fermion* systems under broad conditions. The Hamiltonian of a free-fermion system is

$$H = \sum_{j,k=1}^{n} \alpha_{jk} a_j^{\dagger} a_k + \beta_{jk} a_j a_k - \overline{\beta_{jk}} a_j^{\dagger} a_k^{\dagger} , \qquad (10)$$

where $a_j^{\dagger}(a_j)$ are fermionic creation (annihilation) operators satisfying anticommutation relations $\{a_j, a_k\} = \{a_j^{\dagger}, a_k^{\dagger}\} = 0$ and $\{a_j, a_k^{\dagger}\} = \delta_{jk}$. The coefficients $\alpha_{jk}, \beta_{jk} \in \mathbb{C}$ are "interaction strengths" and satisfy $\alpha_{kj} = \overline{\alpha_{jk}}$. To ease the exposition, we equivalently assume a presentation of H in terms of 2n Majorana operators, which are Hermitian and defined by

$$c_{2j-1} := a_j^{\dagger} + a_j , \quad c_{2j} := i(a_j^{\dagger} - a_j) , \quad j = 1, \dots, n .$$
 (11)

These satisfy the anticommutation relations

$$\{c_j, c_k\} = 2\delta_{jk} , \quad j, k = 1, \dots, 2n .$$
 (12)

Hence, Eq. (10) becomes

$$H = \sum_{j,k=1}^{2n} \gamma_{jk} c_j c_k , \qquad (13)$$

where the interaction strengths $\gamma_{jk} \in \mathbb{C}$ define a $2n \times 2n$ Hermitian matrix Γ .² Majorana operators are orthogonal and are mapped to products of Pauli operators acting on n qubits using the Jordan-Wigner transform [JW28]. Furthermore, it is known that quadratic fermionic operators are closed

²Without loss of generality, we can assume Γ to be purely imaginary.

under taking commutators.³ More precisely, the relevant commutation relations are given by

$$[c_j c_k, c_l] = 2\delta_{lk} c_j - 2\delta_{lj} c_k, \tag{14}$$

which follow from Eq. (12). This implies that H and the set S of degree-k fermionic operators satisfy the invariance property in Definition 2 for any $k \geq 1$. Thus, we may choose our operator set S to be given by monomials of Majorana or creation and annihilation operators; examples are $S = \{c_j\}_{1 \leq j \leq 2n}$, $S = \{c_jc_k\}_{1 \leq j < k < l < m \leq 2n}$, $S = \{a_j^{\dagger}a_k, a_ja_k, a_j^{\dagger}a_k^{\dagger}\}_{1 \leq j \leq n, 1 \leq k \leq n}$, or, when H is fermion number-conserving, $S = \{a_j^{\dagger}a_k\}_{1 \leq j \leq n, 1 \leq k \leq n}$. In the other limit, we could consider all possible products of fermionic operators (up to degree-2n), but this case is not too interesting as it is equivalent to standard Hamiltonian simulation that provides access to the full state $|\psi(t)\rangle$; see Section 4. All these sets satisfy the invariance property; however, for H_S to be Hermitian, some specific linear combinations of these operators might be necessary to make them orthogonal.

As an illustrative example, we choose $S = \{c_j c_k\}_{1 \le j \le k \le 2n}$, and note that the $c_j c_k$'s are readily orthogonal. The amplitudes of the shadow state $|\rho(t); S\rangle$ are proportional to the expectations $\langle c_i c_k(t) \rangle = \operatorname{tr}(\rho(t) c_i c_k)$, which in this case coincide with the entries of the so-called 1-RDM (reduced density matrix) of the evolved system's state $\rho(t)$ [RBM18]. To prepare the shadow state at time t from that at time 0, we would like to simulate the Hamiltonian H_S in Eq. (4) efficiently. We can do this with standard Hamiltonian simulation methods when H_S is sparse and when we have efficient access to its nonzero entries. That is, in the sparse-access model, given a row index of H_S , we can efficiently locate and compute the nonzero entries for that row (cf. [BC12, BCK15, CKS17]). Since H_S is obtained from the commutation relations between H and S, Eq. (14) implies that a sufficient property for having efficient sparse access to H_S is having efficient sparse access to the matrix Γ . This occurs when the graph underlying the interactions in Eq. (13) is of bounded degree d, and holds even if the number of fermionic modes, and hence the dimension of H_S , is exponentially large (poly(n)). For this example, the dimension of H_S is $M = \mathcal{O}(n^2)$, its sparsity is $d' \leq 2d$ (at most 2d quadratic operators in H do not commute with a given $c_j c_k$, and the commutator $[c_j c_k, c_l c_m]$ between two quadratic operators is another quadratic operator or zero), and its largest entry in magnitude satisfies $\|H_S\|_{\max} \leq 2 \max_{jk} |\gamma_{jk}| = 2\|\Gamma\|_{\max}$. A query to H_S can be constructed with $\mathcal{O}(d)$ queries to Γ : any row of H_S is labeled by some (j,k) corresponding to an operator in S, and all of the neighbors of j and k in the graph can be learned with at most 2d queries to Γ . Hence, H_S can be simulated efficiently under these assumptions, with complexity polylog(n) and polynomial in $t\|\Gamma\|_{\max}$, using known Hamiltonian simulation approaches.

For shadow Hamiltonian simulation to be efficient, we also need a procedure that prepares the initial shadow state $|\rho(0); S\rangle$ efficiently. This is not always possible, but for many interesting states that can be expressed succinctly, efficient quantum circuits might be constructed. One example is the preparation of the shadow state corresponding to the bare vacuum $\rho(0) = \rho = |\text{vac}\rangle\langle\text{vac}|$. The bare vacuum is the pure state containing no fermions, so it is destroyed by all annihilation operators: $a_j|\text{vac}\rangle = 0$ for all $j \in [n]$. In this state, the expectations of quadratic Majorana operators are

$$\langle c_j c_k \rangle = \begin{cases} i & (j, k) = (2l - 1, 2l) \text{ for } l \in [n], \\ 0 & \text{otherwise.} \end{cases}$$
 (15)

The corresponding shadow state with respect to S is (up to a global phase)

$$|\rho;S\rangle = \frac{1}{\sqrt{n}} \sum_{l=1}^{n} |2l-1,2l\rangle . \tag{16}$$

³Quadratic fermionic operators span the Lie algebra $\mathfrak{so}(2n)$; see Section 3.4.

This state has a simple form, i.e., it is an equal superposition over basis states and can be prepared on a quantum computer in time $\mathcal{O}(\log(n))$ using elementary gates. It is equivalent to the shadow state corresponding to the completely filled state, which is the state with one fermion in every mode. This is implied by the fact that operators in S change sign under a particle-hole transformation that maps $a_j^{\dagger} \mapsto a_j^{\dagger}$ and $a_j \mapsto a_j^{\dagger}$ [Zir21]. More generally, for this choice of $S = \{c_j c_k\}_{1 \leq j < k \leq n}$, the shadow state of any ρ is invariant under the particle-hole transformation (up to a global sign). This property can be useful to identify other shadow states that can also be prepared efficiently. Indeed, other examples of shadow states that can be prepared efficiently are those corresponding to fermionic product states $\prod_{i \in I} a_i^{\dagger} | \text{vac} \rangle$ that contain one or no fermions in each mode $j \in [n]$, where $I \subseteq [n]$ is a subset of modes. These shadow states can be obtained from Eq. (16) by simply changing some signs of the amplitudes, which can be done efficiently if we have access to an oracle that specifies Iefficiently. The shadow states of more general fermionic Gaussian states (Slater determinants) $|\phi\rangle$ could be prepared, for example, by means of Thouless's theorem [BR86], which asserts that $|\phi\rangle$ can be obtained as $e^{-i\tilde{H}}\prod_{j\in I}a_j^\dagger|\mathrm{vac}\rangle$. Here, \tilde{H} is a free-fermion and number-conserving Hamiltonian. If \dot{H} can be accessed efficiently as explained above, then the Hamiltonian \dot{H}_S required for mapping corresponding shadow states can also be implemented efficiently. In general, there will be other shadow states that can be prepared efficiently, and which do not necessarily correspond to fermionic Gaussian states.

Given the shadow state of an exponentially large fermionic system, there are various quantities of interest which can be extracted from the shadow state. As an example, consider the problem of estimating the energy $\langle H_J \rangle$ corresponding to a subset $J \subseteq [2n]$ of Majorana modes, where $H_J := \sum_{j \in J, k \in J} \gamma_{jk} c_j c_k$. This problem can be reduced to an overlap estimation problem, since

$$\langle H_J \rangle = G\sqrt{A}\langle \psi_J | \rho; S \rangle ,$$
 (17)

where $|\psi_J\rangle := \frac{1}{G} \sum_{j \in J, k \in J} \gamma_{jk} |j, k\rangle$ is a unit quantum state that encodes the interaction strengths γ_{jk} corresponding to J, and $G = [\sum_{j \in J, k \in J} \gamma_{jk}^2]^{1/2}$ is a normalization constant. The constant A is also for normalization, i.e., $|\rho; S\rangle = \sum_{jk} \langle c_j c_k \rangle |j, k\rangle / \sqrt{A}$. The overlap $\langle \psi_J | \rho; S \rangle$ can be obtained within additive precision ϵ using Heisenberg-limited methods, which require the unitary that prepares $|\rho; S\rangle$ and its inverse $\mathcal{O}(1/\epsilon)$ times [KOS07]. For instances where the set J is extensive so that |J| is proportional to n, and when the matrix Γ of interaction strengths is sparse and bounded, then $G = \mathcal{O}(\sqrt{n} \|\Gamma\|_{\text{max}})$. Also, $A \leq n$ in general, since this is maximized for fermionic Gaussian states, including the bare vacuum specified by Eq. (15). Computing the (intensive) property $\langle H_J \rangle / (n \|\Gamma\|_{\text{max}})$ is then a problem that can be solved efficiently, given access to shadow states with respect to the set S of quadratic fermionic operators.

More generally, we can consider shadow states that encode the expectations of degree-k fermionic operators, k > 2, and with them compute linear combinations of these expectations. This would allow us to estimate energies of interacting fermionic systems. For example, a standard problem in fermionic simulations involves preparing a fermionic Gaussian state and then computing properties of an interacting fermionic Hamiltonian that involves quartic fermionic operators. The fermionic Gaussian state can be prepared through an evolution of a simple state with a free-fermion Hamiltonian. Using shadow Hamiltonian simulation, we can prepare the shadow state of this Gaussian state efficiently using the techniques above, even if we allow for encoding expectations of quartic operators (see also Section 3.5). Estimating the energy of the interacting system also reduces to an overlap estimation problem that uses this shadow state.

3.1.1 Comparison to first-quantization

First-quantization methods enable the simulation of exponentially many fermionic modes as well [SBW⁺21]. Consider a free-fermion Hamiltonian whose terms are number-conserving, i.e., it is a linear combination of $a_j^{\dagger}a_k$ only. In the subspace of a single fermion, the Hilbert space dimension is n, and H can be represented as an $n \times n$ matrix. Simulating this Hamiltonian in that subspace can be done efficiently if we have efficient sparse access to this matrix. This simulation approach will produce a quantum state that corresponds to the single-fermion evolved state. This state can be used to compute properties of the 1-RDM at any time; note that the entries of the 1-RDM for any fermionic state, including those without a well-defined number of fermions and non-Gaussian states, can be faithfully reproduced and evolved by free-fermion Hamiltonians simply by working in the single-fermion subspace. First-quantization methods can be used to simulate two or more fermions, which would require increasing the number of registers and the dimension accordingly, to compute properties of the 2-RDM and so on.

First-quantization and shadow Hamiltonian simulation coincide in the special case where the Hamiltonian is free-fermion and number preserving, and the system contains only a single fermion. In this case, the shadow state is equivalent to $|\psi\rangle|\overline{\psi}\rangle$, where $|\psi\rangle$ is the first-quantized wavefunction.

However, there are important differences between the two techniques. First of all, the two approaches depart from one another when there are many fermions in the system. Secondly, shadow Hamiltonian simulation can deal with free-fermion Hamiltonians that are *not* number preserving, and it can also encode the expectations of non-number-preserving operators such as $a_i a_j$ and $a_i^{\dagger} a_j^{\dagger}$ in the corresponding shadow states, using a proper choice for S. On the other hand, first quantization can simulate interacting fermionic Hamiltonians, as long as they are number-preserving; shadow Hamiltonian simulation breaks down in this case, since the invariance property is not satisfied.

3.2 Free bosons

Free-boson systems are also prevalent in physics, being able to describe physical phenomena such as superfluidity [Bog47], quantum optics [SZ97], and more. Free-boson systems can also be understood as a collection of coupled quantum harmonic oscillators, which are quantum particles evolving under the influence of quadratic potentials. Like in the prior example, we are interested in simulating exponentially large systems efficiently, in time polylog(n) and poly(t).

A free-boson system is described by a quadratic Hamiltonian of the form

$$H = \sum_{j,k=1}^{n} \alpha_{jk} b_j^{\dagger} b_k + \beta_{jk} b_j b_k + \overline{\beta_{jk}} b_j^{\dagger} b_k^{\dagger} , \qquad (18)$$

where b_j^{\dagger} (b_j) are the bosonic creation (annihilation) operators satisfying the canonical commutation relations $[b_j, b_k^{\dagger}] = \delta_{jk}$, $[b_j^{\dagger}, b_k^{\dagger}] = [b_j, b_k] = 0$. The coefficients $\alpha_{jk} \in \mathbb{C}$ and $\beta_{jk} \in \mathbb{C}$ are "interaction strengths" that satisfy $\alpha_{jk} = \overline{\alpha_{kj}}$. In contrast to the free-fermion case, the Hilbert space dimension is now infinite. We equivalently assume a presentation of H in terms of 2n operators associated with position and momentum operators, which are Hermitian and defined via

$$Q_j \propto \frac{1}{\sqrt{2}} (b_j^{\dagger} + b_j) , \ P_j \propto \frac{i}{\sqrt{2}} (b_j^{\dagger} - b_j) , \quad j = 1, \dots, n .$$
 (19)

(The constants of proportionality can depend on j.) Hence, Eq. (18) becomes quadratic in the Q_j 's and P_j 's. If we let $\vec{Y} := (P_1, P_2, \dots, Q_1, Q_2, \dots)^T$ be the vector of 2n operators, we can write

 $H = \frac{1}{2}\vec{Y}^T\Gamma\vec{Y}$, where Γ is a $2n \times 2n$ Hermitian matrix of interaction strengths γ_{jk} , and we can assume these to be real, i.e., $\Gamma = \overline{\Gamma}$.

It is well known that quadratic bosonic operators are closed under commutation.⁴ More precisely, the commutation relations between generalized coordinates can be compactly expressed as $[Y_j, Y_k] = i\Omega_{jk}$, for $j, k \in [2n]$. Here, Ω_{jk} is the entry of the symplectic matrix $\mathbf{\Omega} = \begin{pmatrix} \mathbf{0} & -\mathbb{1}_n \\ \mathbb{1}_n & \mathbf{0} \end{pmatrix}$, where $\mathbb{1}_n$ is the $n \times n$ identity. This implies

$$[Y_j Y_k, Y_l] = i\Omega_{kl} Y_j + i\Omega_{jl} Y_k . (20)$$

Then, the set of degree-k bosonic operators also satisfy the invariance property of Definition 2 for any $k \geq 1$. Like in the fermionic case, this means that we can take our set of operators to be given by low-degree products of the bosonic operators Q_j and P_j .

As a special case we could choose $S = \{P_1, P_2, \dots, Q_1, Q_2, \dots\}$. However, with this choice, one immediately arrives at the issue that \mathbf{H}_S is not Hermitian, since $[H, \vec{Y}] = -\mathrm{i}\mathbf{\Omega}\mathbf{\Gamma}\vec{Y}$ from Eq. (20), and $-\mathrm{i}\mathbf{\Omega}\mathbf{\Gamma}$ is not Hermitian in general. This operator is only Hermitian in the special case of number-conserving Hamiltonians, where all β_{jk} in Eq. (18) vanish, and this case was recently addressed in Ref. [BCS⁺24]. To circumvent this issue in our example, we consider a decomposition $\mathbf{\Gamma} = \mathbf{\Gamma}_1\mathbf{\Gamma}_2$ for some $\mathbf{\Gamma}_1$ of dimension $2n \times M$ and $\mathbf{\Gamma}_2$ of dimension $M \times 2n$, where $M \geq \mathrm{rank}(\mathbf{\Gamma})$. Then, transforming $\vec{Y} \mapsto \vec{O} := \mathbf{\Gamma}_2 \vec{Y}$ changes the coefficients in the commutators such that the invariance property reads $[H, \vec{O}] = -\mathrm{i}\mathbf{\Gamma}_2\mathbf{\Omega}\mathbf{\Gamma}_1\vec{O}$. The set of operators is now $S := \{O_1, \dots, O_M\}$, and we will be interested in instances where $\mathrm{i}\mathbf{\Gamma}_2\mathbf{\Omega}\mathbf{\Gamma}_1 \equiv \mathbf{H}_S$ is Hermitian.

One example is obtained when the matrix of interaction strengths is additionally positive semidefinite, i.e., $\Gamma \succeq 0$. It is possible to find a factorization where $\Gamma = \mathbf{B}\mathbf{B}^{\dagger}$ in this case, so that $\vec{O} := \mathbf{B}^{\dagger}\vec{Y}$, $H = \frac{1}{2}\vec{O}^T\vec{O}$, and $-\mathrm{i}\mathbf{B}^{\dagger}\mathbf{\Omega}\mathbf{B}$ is Hermitian, i.e., $\mathbf{H}_S = \mathrm{i}\mathbf{B}^{\dagger}\mathbf{\Omega}\mathbf{B} = \mathbf{H}_S^{\dagger}$. Note that to prepare the shadow state with respect to this S, we would like to simulate this \mathbf{H}_S efficiently, and this might require accessing \mathbf{B} or \mathbf{B}^{\dagger} efficiently. Reference [BBK⁺23] describes a way to do this for a collection of coupled classical oscillators; the same result applies to this case if the Hamiltonian is that of exponentially many coupled quantum harmonic oscillators, expressed as

$$H = \sum_{j} \frac{(P_j)^2}{2m_j} + \frac{\kappa_{jj}}{2} (Q_j)^2 + \sum_{k>j} \frac{\kappa_{jk}}{2} (Q_j - Q_k)^2.$$
 (21)

Here, $m_j > 0$ and $\kappa_{jk} \ge 0$ for all $j \in [n]$, $k \in [n]$, are the masses and spring constants. Given sparse access to matrices \mathbf{M} and \mathbf{K} that specify the m_j 's and κ_{jk} 's, the matrices \mathbf{B} , \mathbf{B}^{\dagger} , and \mathbf{H}_S can be accessed efficiently. This occurs when the graph underlying the interactions in the system is of bounded degree d. The factorization in Ref. [BBK+23] is such that M is at least the number of terms in Eq. (21). In this case, the vector of operators $\vec{O} = \mathbf{B}^{\dagger}\vec{Y}$ is the one with the first n entries being the $P_j/\sqrt{m_j}$'s, corresponding to the square roots of the first n terms in Eq. (21), and the remaining $\mathcal{O}(n^2)$ entries being either the $\sqrt{\kappa_{jj}}Q_j$'s or the $\sqrt{\kappa_{jk}}(Q_j - Q_k)$'s, corresponding to the square roots of the remaining terms in Eq. (21). The complexity of simulating the \mathbf{H}_S obtained through this factorization of $\mathbf{\Gamma}$ is almost linear in $t\sqrt{\aleph d}$, where $\aleph := \max_{j,k} \kappa_{jk}/\min_j m_j$, and polylog(n). This simulation is efficient and discussed in Ref. [BBK+23] in great detail.

Hence, choosing $S = \{O_1, \dots, O_M\}$ for this example, where the O_m 's are defined above, the

⁴Quadratic bosonic operators span the symplectic Lie algebra $\mathfrak{sp}(2n)$; see Section 3.4.

shadow state at any time with respect to S can be expressed as

$$|\rho(t); S\rangle = \frac{1}{\sqrt{A}} \sum_{m=1}^{M} \langle O_m(t) \rangle |m\rangle \equiv \frac{1}{\sqrt{A}} \left(\sum_{j=1}^{n} \frac{1}{\sqrt{m_j}} \langle P_j(t) \rangle |j\rangle |j\rangle + \sqrt{\kappa_{jj}} \langle Q_j(t) \rangle |j + n\rangle |j + n\rangle + \sum_{n+1 \le j < k \le 2n} \sqrt{\kappa_{jk}} \langle (Q_j(t) - Q_k(t)) \rangle |j\rangle |k\rangle \right) . \tag{22}$$

The expectations are with respect to the system's state $\rho(t)$ at time t. To prepare $|\rho(t); S\rangle$ efficiently, we also require the initial shadow state $|\rho(0); S\rangle$ to be efficiently preparable. This is not always possible, however, there are examples where this can be done. For illustration, consider the case of a bosonic product state ρ where $\langle Q_j(0)\rangle = 0$ and $\frac{1}{\sqrt{m_j}}\langle P_j(0)\rangle$ is the same constant for all $j \in [n]$. Then, $|\rho(0); S\rangle = \frac{1}{\sqrt{n}} \sum_{j=1}^{n} |j\rangle |j\rangle$ is a simple superposition state that can be prepared with $\mathcal{O}(\log(n))$ elementary gates. Like in the case of free-fermion systems, other shadow states can be considered by building upon this example.

As an application that uses the shadow state in Eq. (22), we consider the problem of estimating a semiclassical approximation to the (rescaled) kinetic or potential energies of a subset of masses or springs. This is essentially the same problem discussed in Ref. [BBK⁺23], and the reason why this becomes a semiclassical approximation here is because the expectation of a quadratic bosonic operator is not equal to the product of expectations of single operators in general. This estimation problem can be solved efficiently, also requiring $\mathcal{O}(1/\epsilon)$ preparations $|\rho(t); S\rangle$ and its inverse, where $\epsilon > 0$ is the allowed error.

To avoid this semiclassical approximation, we can consider instead a set of quadratic operators where now $S = \{O_m O_{m'}\}_{1 \leq m \leq M, 1 \leq m' \leq M}$, and each O_m is the same as in the prior example, being linear in the P_j 's and Q_j 's. This operator set also satisfies the invariance property. With this choice we have $|\rho; S\rangle = \frac{1}{\sqrt{A}} \sum_{m,m'} \langle O_m O_{m'} \rangle |m,m'\rangle$, where A>0 is for normalization. It can be shown that the Hamiltonian used to prepare the new shadow state at time t from that at time 0 is $H_S \otimes \mathbb{I}_M + \mathbb{I}_M \otimes H_S$, where H_S is the Hamiltonian described above, and which can be simulated efficiently under the assumptions. (Indeed, in Section 3.5 we provide a general result that proves this is the correct Hamiltonian in this example.) The energy of a subset of oscillators or springs is $\langle H_I \rangle = \frac{1}{2} \sum_{m \in I} \langle (O_m)^2 \rangle$, where $I \subseteq [M]$ denotes the subset. (Recall that each $\frac{1}{2}(O_m)^2$ corresponds to a term in Eq. (18).) This problem can also be reduced to an overlap estimation problem, since

$$\langle H_I \rangle = \frac{1}{2} \sqrt{A|I|} \langle \psi_I | \rho; S \rangle ,$$
 (23)

where $|\psi_I\rangle=\frac{1}{\sqrt{|I|}}\sum_{m\in I}|m,m\rangle$ is a unit quantum state of nonzero amplitudes only if m=m'. The overlap $\langle\psi_I|\rho;S\rangle$ can be obtained within additive error ϵ with $\mathcal{O}(1/\epsilon)$ uses of the unitary that prepares $|\rho;S\rangle$ and its inverse [KOS07]. If I is extensive, then |I| is proportional to n. However, the normalization constant A can be $\Omega(n^2)$ in general since the number of operators in S is now $\Theta(n^2)$ and all their expectations can be nonzero. (Note that $M \propto n$ if the interactions are of bounded degree.) This is inconvenient since, to be efficient, the quantum algorithm would output an estimate of $\langle H_I \rangle / n^{3/2}$, which approaches zero in the large n limit. Nevertheless, it is still possible to consider instances of the problem where the shadow state satisfies $A=\mathcal{O}(n)$, giving an efficient quantum algorithm to estimate $\langle H_I \rangle / n$. This quantity is $\mathcal{O}(1)$ if $\langle H_I \rangle$ is extensive. Examples of such shadow states are those corresponding to low-energy states ρ , where only $\mathcal{O}(n)$ expectations $\langle O_m O_{m'} \rangle$ contribute significantly to the normalization constant. Moreover, if S contains bosonic operators of

degree k > 2, we can perform other calculations like estimating the energies of interacting bosonic systems in the corresponding states.

We note that our shadow Hamiltonian simulation approach for this example is clearly different from other approaches aimed at simulating bosonic field theories formulated in the Schrödinger picture approach [JLP12, Som15]. Here, we did not perform any cutoff on the space dimension or other reductions to encode an infinite dimensional system in one that is finite dimensional, and the simulation is exact, in the sense that we provided a recipe to prepare $|\rho(t); S\rangle$ for exponentially many bosonic modes. This, however, comes at the expense of only being able to simulate the expectations of a restricted set of operators, which are linear combinations of (low-degree) products of the Q_j 's and P_j 's. At the same time, it is possible to consider larger degree products of the operators to encode more information of the states. We leave such investigations open.

3.2.1 From classical to quantum harmonic oscillators

There is an inherent relation between the quantum algorithm of Ref [BBK⁺23] for simulating exponentially many coupled classical oscillators and shadow Hamiltonian simulation of quantum oscillators. That quantum algorithm shares similar features in that we encoded the coordinates (position and momentum) of the oscillators in the amplitudes of a quantum state, which can be shown to evolve unitarily. While those are classical variables, it is simple to show that the dynamics of such a classical system is similar to the dynamics of the expectations of the corresponding operators of exponentially many coupled quantum oscillators. This can be seen as a consequence of Ehrenfest's theorem, which relates classical and quantum evolution, applied to quadratic bosonic systems.

More precisely, in classical Hamiltonian mechanics, the generalized coordinates q_j and p_j evolve according to

$$\frac{dq_j}{dt} = \{q_j, H_c\}_{PB}, \quad \frac{dp_j}{dt} = \{p_j, H_c\}_{PB}, \quad j = 1, \dots, n,$$
(24)

where $\{a,b\}_{PB}$ is the Poisson bracket and H_c is the classical Hamiltonian; for coupled classical oscillators, H_c is similar to Eq. (21), after replacing the operators by the classical coordinates, i.e., $Q_j \mapsto q_j$ and $P_j \mapsto p_j$. For these quadratic classical Hamiltonians, the Poisson brackets are linear in q_j and p_j , which follows from $\{q_j, p_k\}_{PB} = \delta_{jk}$ and $\{q_j, q_k\}_{PB} = \{p_j, p_k\}_{PB} = 0$. The equations of motion for the classical coordinates are then similar to those for the corresponding quantum operators in the Heisenberg picture, being a consequence of canonical quantization where $\{q_j, H_c\}_{PB} \to i[Q_j, H]$ and $\{p_j, H_c\}_{PB} \to i[P_j, H]$. Considering the expectations $\langle Q_j(t) \rangle$ and $\langle P_j(t) \rangle$, these evolve in the same way than the classical coordinates $q_j(t)$ and $p_j(t)$ evolve. As a consequence, the same quantum algorithm in Ref. [BBK+23] can be used to simulate an exponentially large system of quantum harmonic oscillators, where the amplitudes of the shadow states are the expectations of the corresponding linear combinations of Q_j and P_j , as described. In the other direction, shadow Hamiltonian simulation can give techniques for simulating other classical systems that follow a similar classical–quantum correspondence.

3.3 Qubits

We apply shadow Hamiltonian simulation to systems composed of n qubits. The simplest example, which could be viewed as "free qubits", in analogy with the previous sections on free fermions and free bosons, is when the Hamiltonian H is a 1-local operator; that is, the Hamiltonian is a sum of terms, each acting non-trivially on only one qubit. In particular, such a Hamiltonian can always be written as a sum of operators in $S = \{1, X_1, Y_1, Z_1, \dots, X_n, Y_n, Z_n\}$, where the subscript

of an operator denotes the qubit that it acts on. It is easy to see that the invariance property is satisfied and that H_S is Hermitian due to the orthogonality of Pauli operators. But note that the dimension of the shadow state is only 3n+1, so we can encode a system of exponentially many qubits into a shadow state of exponential dimension, which uses only $\mathcal{O}(\log(n))$ many qubits. Due to the commutation relations of the Pauli operators, any operator in S can only have a nonzero commutator with at most two terms in the Hamiltonian (i.e., those operators that act on the same qubit as the chosen operator and are different from it) and hence the nonzero entries of the resulting Hamiltonian H_S are easy to compute if the terms in H are easy to compute. For example, $[H, X_1]$ will be a linear combination of Y_1 and Z_1 only, and hence H_S will be a 2-sparse Hamiltonian. Standard Hamiltonian simulation approaches can then be used to simulate H_S efficiently. The shadow states corresponding to some initial n-qubit states is also easy to prepare. For example, if ρ is the all-zero state $\rho = |0\rangle\langle 0|^{\otimes n}$, the only nonzero expectations are $\langle 1 \rangle = 1$ and $\langle Z_i \rangle = 1$ for all $j \in [n]$. The corresponding shadow state with respect to S is a superposition state that can be prepared with $\mathcal{O}(\log(n))$ gates. Other shadow states can also be prepared efficiently, even for cases where the states ρ are entangled. A downside with this example is that the qubits in the system do not interact, and hence the system might not be very interesting.

A different example is when we consider the set S of all n-qubit Pauli operators. Specifically, for $i, j \in \{0, 1\}^n$, let $P_{ij} := X_1^{i_1} Z_1^{j_1} \otimes \cdots \otimes X_n^{i_n} Z_n^{j_n}$ and let $S := \{P_{ij} : i, j \in \{0, 1\}^n\}$. Pauli operators are orthogonal and $|S| = 4^n$. For a state ρ , the shadow state with respect to S is

$$|\rho; S\rangle = \frac{1}{\sqrt{A}} \sum_{i,j \in \{0,1\}^n} \langle P_{ij} \rangle |i,j\rangle , \qquad (25)$$

where $\langle P_{ij} \rangle = \operatorname{tr}(\rho P_{ij})$ is the expectation. The normalization constant is $A = \sum_{ij} |\langle P_{ij} \rangle|^2 = 2^n \operatorname{tr}(\rho^2)$, being proportional to the purity of ρ . In particular, when $\rho = |\psi\rangle\langle\psi|$ is a pure state, $A = 2^n$.

Let V_S be the "Bell rotation", which maps between the Bell basis and the standard basis:

$$V_S^{\dagger}|i,j\rangle \mapsto (\mathbb{1}_N \otimes P_{ij}) \frac{1}{\sqrt{N}} \sum_{k=0}^{N-1} |k,k\rangle = (\mathbb{1}_N \otimes P_{ij}) \left(\frac{|00\rangle + |11\rangle}{\sqrt{2}}\right)^{\otimes n} , \qquad (26)$$

where $N=2^n$. Hence, V_S maps n Bell pairs to states in the computational basis. As we show in Lemma 9, the shadow state of a pure state is $|\rho; S\rangle = V_S |\psi\rangle \otimes |\overline{\psi}\rangle$, which is a special case of a more general result. The unitary V_S is efficient to implement and an example is given in Figure 1.

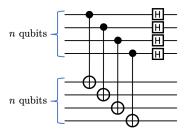


Figure 1: The operation V_S for a system of n=4 qubits. The two-qubit gates are CNOTs and H are Hadamard. When acting on n Bell pairs, these gates output a state in the computational basis, performing (the inverse of) Eq. (26).

Since V_S can be efficiently implemented, we can prepare the shadow state whenever we have an efficient circuit to prepare $|\psi\rangle$. We can also construct an efficient circuit for $|\overline{\psi}\rangle$ by complex conjugating all the elementary gates in the circuit for preparing $|\psi\rangle$. Similarly, it is possible to

perform Hamiltonian simulation or unitary evolution on the shadow state, since the shadow state corresponding to $U|\psi\rangle$ is simply $(U\otimes \overline{U})|\psi\rangle\otimes|\overline{\psi}\rangle$. The unitary $U\otimes \overline{U}$ has an efficient circuit when U does.

3.4 Lie algebras

The case of Lie algebras is a natural one to consider in shadow Hamiltonian simulation because the invariance property is automatically satisfied. More precisely, subspaces of operators on a Hilbert space sometimes form Lie algebras under the commutator, often corresponding to some physical symmetry in the system. We have seen three examples of this already: the set of quadratic fermionic operators span the Lie algebra $\mathfrak{so}(2n)$, quadratic bosonic operators span the symplectic Lie algebra $\mathfrak{sp}(2n)$, and Pauli operators acting on n qubits span the Lie algebra $\mathfrak{u}(2^n)$. Other examples are spin systems with associated Lie algebras $\mathfrak{su}(2)$ or, more generally, $\mathfrak{su}(n)$. This motivates us to consider the general case of Lie algebras.

Definition 5. (Lie algebra) A Lie algebra \mathfrak{g} is a vector space with a Lie bracket binary operation $[\cdot,\cdot]:\mathfrak{g}\times\mathfrak{g}\to\mathfrak{g}$ satisfying

- (Bilinearity) [x, y + z] = [x, y] + [x, z] and [x + y, z] = [x, z] + [y, z].
- (Alternating) [x, x] = 0.
- (Jacobi) [x, [y, z]] + [y, [z, x]] + [z, [x, y]] = 0.

The following analyses focus on the specially interesting case where the Lie bracket is the commutator: [x, y] = xy - yx. If the Hamiltonian H of the system belongs to a Lie algebra \mathfrak{g} , this automatically implies that any discrete set S of operators in the Lie algebra \mathfrak{g} satisfy the invariance property in Definition 2. This provides a unifying framework for a broad class of situations where shadow Hamiltonian simulation is applicable. In the specific case where the dimension of the Lie algebra is polynomial in the system size, shadow Hamiltonian simulation is able to tackle quantum systems that are of exponential size.

The structure constants of a Lie algebra are important in shadow Hamiltonian simulation.

Definition 6. (Structure constants) Given a basis of anti-Hermitian operators $\{O_1, \ldots, O_M\}$ of a Lie algebra \mathfrak{g} , the structure constants of \mathfrak{g} are given by f_{jkl} in the equations

$$[O_j, O_k] = \sum_{l=1}^{M} f_{jkl} O_l . (27)$$

Let \mathfrak{g} be a real Lie algebra of dimension $M < \infty$, with an orthogonal basis of anti-Hermitian matrices $\{O_1, \ldots, O_M\}$, satisfying $\operatorname{tr}(O_m^{\dagger}O_{m'}) \propto \delta_{mm'}$. Given a Hamiltonian H such that $iH \in \mathfrak{g}$, we can write down the conditions under which efficient sparse access to H_S can be obtained:

- i) The structure constants f_{jkl} of \mathfrak{g} are d' = polylog(M)-sparse, i.e., given j and k at most d' structure constants are nonzero, and we have efficient sparse access to these constants.
- ii) The maximum number of terms p in H which do not commute with a given O_j is at most p = polylog(M), and we can efficiently compute these terms given any $j \in [M]$.

These conditions are sufficient but not necessary. Note that the entries of \mathbf{H}_S are determined by the structure constants and the interaction strengths in the Hamiltonian, which is $H = \mathrm{i} \sum_{m=1}^{M} \alpha_m O_m$,

 $\alpha_m \in \mathbb{R}$. In particular, $\|\boldsymbol{H}_S\|_{\max} \leq p \max_m |\alpha_m| \times \max_{j,k,l} |f_{jkl}|$, and \boldsymbol{H}_S is at most $d \leq pd'$ sparse. An example where these assumptions are satisfied is the case of free fermions in Section 3.1.

Certain shadow states can also be prepared efficiently in this case. Assume further that \mathfrak{g} is compact and semisimple. There is a special lowest-weight state $|lw\rangle$ that is a generalization of the bare vacuum state in Section 3.1 and has the following properties: it is an eigenstate of all diagonal operators, and it is annihilated by all lowering operators, when consider a particular decomposition of \mathfrak{g} referred to as the Cartan-Weyl decomposition. If h_i , $i \in [r]$, are the diagonal operators, then $h_i|\text{lw}\rangle = e_i|\text{lw}\rangle$, and the shadow state of $|\text{lw}\rangle$ is

$$|\rho; S\rangle = \frac{1}{\sqrt{A}} \sum_{i=1}^{r} e_i |i\rangle$$
 (28)

The eigenvalues e_i are purely imaginary and $A = \sum_i |e_i|^2$ is a normalization constant, which can often be computed efficiently. The shadow state can be prepared efficiently if the e_i 's can be described succinctly; this turns out to be the case in many examples like Eq. (16) for $\mathfrak{g} \equiv \mathfrak{so}(2n)$.

Other examples of efficiently preparable shadow states can be those corresponding to "generalized coherent" states of \mathfrak{g} , obtained as $e^{\mathfrak{g}}|\text{lw}\rangle$, where $e^{\mathfrak{g}}$ is a unitary in the group induced by \mathfrak{g} . These are the Gaussian fermionic states in Section 3.1 when $\mathfrak{g} \equiv \mathfrak{so}(2n)$. See Refs. [Fuc95, Per77] for more details on Lie algebras and coherent states.

3.5 Green's functions and other correlators

If H and S satisfy the invariance property, so does H and the operator set constructed from arbitrary degree products of the operators in S. This observation can be extended to encode expectations of products of different time-dependent operators in the amplitudes of a quantum state. This extension is most relevant in the Heisenberg picture, where the time-dependent expectation of an operator O on state $\rho(t)$ is alternatively described as the expectation of a time-dependent operator O(t)on the initial state $\rho(0)$. The evolution of the operator is determined by Heisenberg's equations: $\frac{\mathrm{d}}{\mathrm{d}t}O(t)=\mathrm{i}[H,O(t)],$ when H is time-independent. More generally, we can consider products of operators, each at a different time in the Heisenberg picture, e.g. $O_1(t)O_2(t')$. The following result extends shadow Hamiltonian simulation to this scenario.

Theorem 7. Let H be a Hamiltonian and $S = \{O_1, \ldots, O_M\}$ a set of operators. Assume that H and S satisfy the invariance property. Let ρ be the initial state of the system and $O_m(t)$, $m \in [M]$, be the corresponding time-evolved operators. Define the (pure) state

$$|\rho; S(t, t')\rangle = \frac{1}{\sqrt{A}} \begin{pmatrix} \langle O_1(t)O_1(t')\rangle \\ \langle O_1(t)O_2(t')\rangle \\ \vdots \\ \langle O_M(t)O_{M-1}(t')\rangle \\ \langle O_M(t)O_M(t')\rangle \end{pmatrix}, \tag{29}$$

where $\langle O_m(t)O_{m'}(t')\rangle$ are the expectations with respect to the initial state ρ . Then, $|\rho; S(t,t')\rangle$ satisfies the differential equations:

$$\frac{\partial}{\partial t} |\rho; S(t, t')\rangle = -\mathrm{i}(\mathbf{H}_S \otimes \mathbb{1}_M) |\rho; S(t, t')\rangle , \qquad (30)$$

$$\frac{\partial}{\partial t'} |\rho; S(t, t')\rangle = -\mathrm{i}(\mathbb{1}_M \otimes \mathbf{H}_S) |\rho; S(t, t')\rangle . \qquad (31)$$

$$\frac{\partial}{\partial t'}|\rho; S(t,t')\rangle = -\mathrm{i}(\mathbb{1}_M \otimes \boldsymbol{H}_S)|\rho; S(t,t')\rangle . \tag{31}$$

Proof. Let $\vec{O}(t) = (O_1(t), \dots, O_M(t))^T$ and consider the vector of M^2 operators $\vec{O}(t) \otimes \vec{O}(t')$. Heisenberg's equations imply

$$\frac{\partial}{\partial t}\vec{O}(t)\otimes\vec{O}(t') = i[H,\vec{O}(t)]\otimes\vec{O}(t') = -i(\boldsymbol{H}_S\vec{O}(t))\otimes\vec{O}(t') = -i(\boldsymbol{H}_S\otimes\mathbb{1}_M)(\vec{O}(t)\otimes\vec{O}(t')). \quad (32)$$

A corresponding equation can be obtained applying $\frac{\partial}{\partial t'}$. We can compute the expectation with respect to the initial state ρ on either side of this equation and obtain Eq. (30), since we can alternatively express $|\rho; S(t,t')\rangle$ as the vector $\frac{1}{\sqrt{A}}\langle \vec{O}(t) \otimes \vec{O}(t')\rangle$.

Theorem 7 allows us to encode two-time correlators and Green's functions in the amplitudes of a quantum state. To prepare $|\rho; S(t,t')\rangle$ from $|\rho; S(0,0)\rangle$ efficiently, it suffices to have efficient sparse access to \mathbf{H}_S . The procedure involves evolving with \mathbf{H}_S acting on the first register for time t and evolving with the same \mathbf{H}_S acting on the second register for time t'. In addition, it is often possible to prepare the initial state $|\rho; S(0,0)\rangle$ efficiently, as in the examples discussed above where the set of initial expectations contains structure that can be expressed succinctly.

Importantly, Theorem 7 can be generalized in two directions. First, we can encode higher order correlation functions $\langle O_{m_1}(t_1) \dots O_{m_q}(t_q) \rangle$, where all the O_{m_j} 's are in the same operator set S and evolve under H. For this case there are q registers and, to evolve the expectations, we apply the Hamiltonian H_S on each register for the corresponding time. This gives a straightforward generalization of Theorem 7 to the case of q > 2. Second, the operators in the product can belong to different operator sets S_1, \dots, S_q , and these can evolve with their own distinct Hamiltonians H_1, \dots, H_q . Assume that each H_j and S_j satisfy the invariance property. Then, to evolve the expectations of products of time-dependent operators, we apply a Hamiltonian H_{S_1} on the first register for time t_1 , a Hamiltonian H_{S_2} on the second register for time t_2 , and so on. Each H_{S_j} is obtained from the commutation relations between H_j and the operators S_j , as in Eq. (3).

3.6 Operators in the Heisenberg picture

In shadow Hamiltonian simulation, we encode the expectations of certain operators with respect to the evolved state $\rho(t)$, in the amplitudes of a different state. However, it is possible to extend the method to encode a representation of the time-evolved operators themselves in the Heisenberg picture, rather than their expectations, without making reference to the state of the system. We present a quantum algorithm for this problem.

Consider the operator set $S = \{O_1, \ldots, O_M\}$ and let $Z := \sum_{m=1}^M z_m O_m$ be another operator, where $z_m \in \mathbb{C}$ for all $m \in [M]$. The time-evolved version in the Heisenberg picture is Z(t) and, if the Hamiltonian H is time-independent, Heisenberg's equation of motion is $\frac{\mathrm{d}}{\mathrm{d}t}Z(t) = \mathrm{i}[H,Z(t)]$. If H and S further satisfy the invariance property of Definition 2, we can express $Z(t) = \sum_{m=1}^M z_m(t)O_m$, where $z_m(t) \in \mathbb{C}$. These coefficients evolve according to

$$\frac{\mathrm{d}}{\mathrm{d}t}z_{m}(t) = -\mathrm{i}\sum_{m'=1}^{M} h_{m'm}z_{m'}(t) , \qquad (33)$$

which is a direct consequence of Heisenberg's equation of motion. The coefficients $h_{m'm}$ are the entries of the matrix \mathbf{H}_S in Definition 2.

Note that Eq. (33) is also a Schrödinger equation when H_S is Hermitian, and it is natural to consider the operator-vector mapping $Z(t) \mapsto |Z(t)\rangle \propto \sum_{m=1}^{M} z_m(t)|m\rangle$. In this way, we can encode the time-evolved operator in a quantum state, and Eq. (33) gives rise to Hamiltonian evolution:

$$\frac{\mathrm{d}}{\mathrm{d}t}|Z(t)\rangle = -\mathrm{i}\overline{\boldsymbol{H}_S}|Z(t)\rangle . \tag{34}$$

A quantum algorithm that prepares $|Z(t)\rangle$ involves then preparing the initial state $|Z(0)\rangle$ and performing time evolution with the Hamiltonian $\overline{H_S}$ for time t. The algorithm is efficient when these two steps can be implemented efficiently. This could let us probe many interesting properties of the system, such as operator growth and operator scrambling. For example, in the case where S consists of all products of Pauli operators on n qubits, and when Z(0) is a local operator, we can use the algorithm to measure the support of the evolved operator (related to the Hamming weight of $|m\rangle$). Similar to Section 3.5, we can also consider the evolution of products of operators and two-time correlators by encoding them in quantum states.

The analysis can be extended to time-dependent Hamiltonians. In that case, it can be shown that the transformation that takes $|Z(0)\rangle$ to $|Z(t)\rangle$ is the evolution operator with the Hamiltonian $\overline{H_S(t-s)}$, where the final time t is fixed and s is increased from 0 to t. This resembles the evolution of the operator in the Heisenberg picture that evolves backwards in time. Since that case is equivalent to a quantum circuit, where quantum gates can be interpreted as evolutions with time-dependent Hamiltonians, we provide the analysis for the latter. Let $G = G^L \dots G^1$ be the quantum circuit composed of L unitary gates G^j . The requirement for these gates and S to satisfy the invariance property is given in Eq. (9). Accordingly, to study the evolution of an operator $Z = \sum_{m=1}^M z_m O_m$, we define the operators $Z_l := (G^{L+1-l})^{\dagger} \dots (G^L)^{\dagger} Z G^L \dots G^{L+1-l}$ for all $l \in [L]$. Also $Z_0 := Z$, i.e., $z_{0,m} = z_m$ for all $m \in [M]$. These Z_l 's are basically a (backwards) transformation of Z when acting with the last l gates of the circuit, and we are interested in Z_L , which is the operator transformed by all gates.

The invariance property implies $Z_l = \sum_{m=1}^M z_{l,m} O_m$, with coefficients $z_{l,m} \in \mathbb{C}$. Then Eq. (9) gives

$$Z_{l+1} = (G^{L-l})^{\dagger} Z_l G^{L-l} = \sum_{m=1}^{M} z_{l,m} \sum_{m'=1}^{M} g_{mm'}^{L-l} O_{m'} \implies z_{l+1,m} = \sum_{m'=1}^{M} z_{l,m'} g_{m'm}^{L-l} . \tag{35}$$

Let G_S^j be the matrix of entries $g_{mm'}^j$. When this is unitary—the analogue of requiring H_S be Hermitian—Eq. (35) denotes a unitary transformation on the vector of coefficients $z_{l,m}$, for each l. We then consider the operator-vector mapping $Z_l \mapsto |Z_l\rangle \propto \sum_{m=1}^M z_{l,m}|m\rangle$. This provides an encoding of the time-evolved operators Z_l in a quantum state, and Eq. (35) implies

$$|Z_{l+1}\rangle = (G_S^{L-l})^T |Z_l\rangle , \quad l = 0, \dots, L-1 .$$
 (36)

A quantum algorithm that prepares $|Z_L\rangle$ is then a sequence of the unitaries $(G_S^1)^T \dots (G_S^L)^T$ acting on $|Z_0\rangle$. Note that applying the transpose of G_S^{L-l} is the analogue to evolving with $\overline{H}_S(t-s)$.

3.6.1 Comparison with the transfer matrix method

The quantum algorithm shares some similarities with the "transfer matrix" method used for time-evolving Pauli operators acting on n qubits under the action of a quantum circuit. This is a classical algorithm that describes the evolution of the operator, and is also applied to studying the growth of light cones and operator scrambling, even under the presence of noise [BKP19, AGLV23]. In the noiseless case, at each step of a quantum circuit (also evolving backwards in time), the operator is represented by a vector of dimension 4^n , and this is acted on by a $4^n \times 4^n$ unitary that provides the vector at the next step and corresponds to a gate in the circuit (i.e., the unitary $(\mathbf{G}_S^{L-l})^T$). Depending on the choice of operator basis, this unitary may also be called the super-operator [WBC15] or Pauli transfer matrix [Gre15]. The quantum algorithm described in Section 3.6 performs essentially the same evolution, but where the 4^n -dimensional vector is encoded in a quantum state of 2^n qubits in this case, and where each $4^n \times 4^n$ unitary matrix $(\mathbf{G}_S^{L-l})^T$ is implemented with a quantum circuit.

4 Properties of the shadow state

We now discuss some properties and alternate representations of the shadow state $|\rho; S\rangle$ for finite dimensional systems, without reference to any time-evolution problem one might wish to solve with this state.

Standard basis. Let $\rho = |\psi\rangle\langle\psi| \in \mathbb{C}^{N\times N}$ be a pure quantum state of a system of dimension $N < \infty$, and let S be an orthogonal basis of the space $\mathbb{C}^{N\times N}$. In this case, $|\rho;S\rangle$ is related to other standard representations of the state $|\psi\rangle$. One example is the standard basis, $S_{\text{SB}} = \{O_{ij} : i, j = 0, \dots, N-1\}$, where $O_{ij} = |j\rangle\langle i|$. Then,

$$|\rho; S_{\rm SB}\rangle = \sum_{i,j=0}^{N-1} \langle O_{ij} \rangle |i,j\rangle = \sum_{i,j=0}^{N-1} \left(\langle \psi | j \rangle \langle i | \psi \rangle \right) |i,j\rangle = \sum_{i=0}^{N-1} |i\rangle \langle i | \psi \rangle \otimes \sum_{j=0}^{N-1} |j\rangle \overline{\langle j | \psi \rangle} = |\psi\rangle \otimes |\overline{\psi}\rangle. \quad (37)$$

This is already an interesting state that is different from the "standard" representation $|\psi\rangle$. Clearly we can create $|\psi\rangle$ given one copy of $|\psi\rangle\otimes|\overline{\psi}\rangle$, but the reverse is not possible. In fact, there exist problems that can be solved using only one copy of $|\psi\rangle\otimes|\overline{\psi}\rangle$ that would require exponentially many copies of $|\psi\rangle$ alone to solve.

Theorem 8. Consider the problem of deciding if an n-qubit state $|\psi\rangle$ satisfies $|\langle\psi|\overline{\psi}\rangle| \leq 1/3$ or $|\langle\psi|\overline{\psi}\rangle| \geq 2/3$, promised that one of these holds. Any quantum algorithm that solves this problem using only copies of $|\psi\rangle$ must use $\Omega(2^{n/2})$ copies, but the problem can be solved with one copy of $|\psi\rangle \otimes |\overline{\psi}\rangle$ with constant success probability.

Proof. The problem can be solved with constant success probability using one copy of $|\psi\rangle \otimes |\overline{\psi}\rangle$ by using the well-known swap test. The success probability can be made arbitrarily close to 1 using a constant number of copies of $|\psi\rangle \otimes |\overline{\psi}\rangle$ by standard error reduction via majority vote.

For the lower bound, we observe that any state with all real amplitudes satisfies $|\langle \psi | \psi \rangle| = 1$ and that a Haar-random state has $|\langle \psi | \overline{\psi} \rangle| = o(1)$ with high probability. The lower bound follows from Ref. [BS19] that shows that a binary phase state (i.e., a uniform superposition state where all phases are uniformly random in $\{\pm 1\}$) is indistinguishable from a Haar-random state unless we have $\Omega(2^{n/2})$ copies of the state. Similarly, [CHM21] shows that distinguishing a Haar-random state with real entries from a standard Haar-random state requires $\Omega(2^{n/2})$ copies of the state.

The state $|\psi\rangle\otimes|\overline{\psi}\rangle$ is also related to another well-known alternate representation of quantum states that uses only real amplitudes. In this "real representation" of quantum states, the state $|\psi\rangle$ is represented by the quantum state $|0\rangle|\Re(\psi)\rangle + |1\rangle|\Im(\psi)\rangle$, where $|\Re(\psi)\rangle$ and $|\Im(\psi)\rangle$ are the quantum states where each amplitude is replaced by the real and imaginary parts of the corresponding amplitude of $|\psi\rangle$, respectively. Up to a Hadamard on the first qubit, this state is also $|0\rangle|\psi\rangle + |1\rangle|\overline{\psi}\rangle$.

Orthonormal bases. For the standard basis $S_{\rm SB}$, the shadow state is $|\psi\rangle \otimes |\psi\rangle$. More generally, the shadow state for any orthonormal basis S is a unitary transformation V_S applied to $|\psi\rangle \otimes |\overline{\psi}\rangle$.

Lemma 9. Let $S = \{O_{ij} : i, j = 0, ..., N-1\}$ be an orthonormal basis of $\mathbb{C}^{N \times N}$. Let V_S be the unitary on $\mathbb{C}^N \otimes \mathbb{C}^N$ defined by

$$V_S^{\dagger}|i,j\rangle = (\mathbb{1}_N \otimes O_{ij}) \sum_{k=0}^{N-1} |k,k\rangle.$$
(38)

Then, if $\rho = |\psi\rangle\langle\psi|$ is pure, we have

$$|\rho; S\rangle = V_S |\psi\rangle \otimes |\overline{\psi}\rangle.$$
 (39)

Proof. First, we show that V_S is indeed unitary. Observe that

$$\langle i', j' | V_S V_S^{\dagger} | i, j \rangle = \sum_{k,k'=0}^{N-1} \langle k', k' | (\mathbb{1}_N \otimes O_{i'j'}^{\dagger} O_{ij}) | k, k \rangle = \sum_{k=0}^{N-1} \langle k | O_{i'j'}^{\dagger} O_{ij} | k \rangle = \operatorname{tr}(O_{i'j'}^{\dagger} O_{ij}) = \delta_{ii'} \delta_{jj'}, \tag{40}$$

since the operators O_{ij} are orthogonal. We obtain

$$\langle O_{ij} \rangle = \operatorname{tr}(|\psi\rangle\langle\psi|O_{ij}) = \sum_{k=0}^{N-1} \langle k|\psi\rangle\langle\psi|O_{ij}|k\rangle = \sum_{k=0}^{N-1} \langle k|\psi\rangle\langle k|O_{ij}^{\dagger}|\overline{\psi}\rangle = \sum_{k=0}^{N-1} \langle k,k|(\mathbb{1}_{N}\otimes O_{ij}^{\dagger})|\psi\rangle\otimes|\overline{\psi}\rangle. \tag{41}$$

Using the definition of V_S , we get that $\langle O_{ij} \rangle = \langle i, j | V_S | \psi \rangle \otimes | \overline{\psi} \rangle$, which gives

$$|\rho;S\rangle = \sum_{i,j=0}^{N-1} \langle O_{ij}\rangle |i,j\rangle = \sum_{i,j=0}^{N-1} \langle i,j|V_S|\psi\rangle \otimes |\overline{\psi}\rangle |i,j\rangle = \left(\sum_{i,j=0}^{N-1} |i,j\rangle\langle i,j|\right) V_S|\psi\rangle \otimes |\overline{\psi}\rangle = V_S|\psi\rangle \otimes |\overline{\psi}\rangle.$$

$$\Box \quad (42)$$

So far we have only considered pure states. But observe that the lemma can equivalently be restated as asserting that $|\rho; S\rangle = V_S |\rho; S_{SB}\rangle$. Since both sides of the equation are linear in ρ , we have the straightforward corollary that $|\rho; S\rangle = V_S |\rho; S_{SB}\rangle$ holds for all mixed states ρ .

To understand the form of $|\rho; S_{\rm SB}\rangle$, note that Eq. (37) equivalently implies that $|\rho; S_{\rm SB}\rangle$ equals $\operatorname{vec}(\rho)$ when $\rho = |\psi\rangle\langle\psi|$, where vec is the operation that maps $\sum_{j,k} a_{jk} |j\rangle\langle k| \mapsto \sum_{j,k} a_{jk} |j\rangle\langle k|$ [Wat18]. When ρ is mixed, $|\rho; S_{\rm SB}\rangle$ is the state whose entries are proportional to $\operatorname{vec}(\rho)$ with the normalization constant equal to the square root of the purity of ρ , $\sqrt{\operatorname{tr}(\rho^2)}$. Alternatively, if $\rho = \sum_{\ell} p_{\ell} |\psi_{\ell}\rangle\langle\psi_{\ell}|$, then $|\rho; S_{\rm SB}\rangle \propto \sum_{\ell} p_{\ell} |\psi_{\ell}\rangle \otimes |\overline{\psi_{\ell}}\rangle$.

Examples of V_S . When $S = S_{SB}$, observe that $V_S \equiv \mathbb{1}_{N^2}$, where $N = 2^n$. More interestingly, let S be the set of Pauli operators on n qubits, $\{P_{ij}\}_{i,j\in\{0,1\}^n}$, where P_{ij} are tensor products of n Pauli operators as discussed in Section 3.3. In this case, the state $(\mathbb{1}_N \otimes P_{ij}) \frac{1}{\sqrt{N}} \sum_{k=0}^{N-1} |k,k\rangle$ are tensor products of n Bell pairs. Thus the operator V_S is a Bell rotation and can be achieved by the sequence of n entangling gates shown in Figure 1.

As another example, let S be the set of Heisenberg-Weyl operators of dimension N. This is a group of N^2 unitary matrices spanned by the generators X and Z, where $X|j\rangle = |j+1 \pmod N\rangle$ and $Z|j\rangle = e^{-\mathrm{i}2\pi j/N}|j\rangle$. In this case, the unitary V_S can be constructed from the discrete Fourier transform matrix of size $N\times N$, and the conditional shift operator $\sum_{j=0}^{N-1}|j\rangle\langle j|\otimes X^j$, both of which have efficient quantum circuits. In these examples, the unitary V_S was efficient to implement as a quantum circuit. In general, this may not be the case.

Incomplete bases. In many of the applications considered in this article, S is not a complete basis of the space, but an incomplete set of orthonormal operators. In this case, $|\rho; S\rangle$ may not contain all the information contained in $|\psi\rangle$ and hence it will not simply be a unitary transformation applied to $|\psi\rangle \otimes |\overline{\psi}\rangle$. However, the state $|\rho; S\rangle$ can still be viewed as a unitary transformation and projection of this state, justifying the name "shadow" state.

More precisely, even when S is not a complete basis, the same proof of Lemma 9 can be followed, except for the last equation where $\sum_{i,j=0}^{N-1} |i,j\rangle\langle i,j|$ is not identity in this case: the sum is not over all i,j. This sum becomes an orthogonal projector P_S . Thus, when $\rho = |\psi\rangle\langle\psi|$ is pure, we have $|\rho;S\rangle = P_S V_S |\psi\rangle \otimes |\overline{\psi}\rangle$.

5 Summary and future directions

We devised a novel approach to quantum simulation that uses other representations of quantum states, being complementary to the traditional approach based on simulating the full quantum state. Our shadow Hamiltonian simulation approach allows us to encode limited information about a system's quantum state, like the expectations of a relevant set of operators at any time, in the amplitudes of a different "shadow state". In cases where the number of these operators is exponentially smaller than the space dimension of the system, we can leverage the exponential growth of the quantum computer's dimension and encode, for example, the expectations of operators acting on systems of exponential size (i.e., the system's dimension is doubly exponential). By doing so we unveiled natural applications to quantum systems like free-fermions and free-bosons with an exponential number of modes. We described computations that can be carried efficiently via shadow Hamiltonian simulation, while these computations can be hard for traditional approaches, as preparing the full states would require exponential resources.

Additionally, we demonstrated how the ideas underlying shadow Hamiltonian simulation can be applied to a broader range of problems. In one example, we extended these concepts and described how to encode the expectations of two-time correlators or other products of time-dependent operators in a different quantum state. Furthermore, we described an approach for encoding operators in the Heisenberg picture in quantum states, without referencing to the state of the system. These developments enable the solution to other problems; an example is studying the growth of the light cone associated with an evolving operator.

We anticipate future directions based on similar ideas. For instance, we mentioned that quantum algorithms for differential equations might be used when the invariance property is satisfied but H_S is not Hermitian, and understanding when such algorithms are efficient would be important. Another interesting direction is the simulation of open quantum system dynamics, and whether shadow states can be used to perform these simulations more efficiently or address questions that traditional approaches are unable to resolve. Furthermore, many classical systems have an underlying Lie algebra structure (e.g., under the Poisson bracket like in classical harmonic oscillators), and it would be interesting to discover other classical systems whose dynamics can be efficiently simulated on a quantum computer using shadow states. Also, we discussed some applications to operator scrambling, but a more thorough characterization of what related problems can be solved efficiently would be interesting.

Shadow Hamiltonian simulation could be simulated classically, although such a simulation would be inefficient in the worst case. Nevertheless, properties like locality of interactions could be exploited, potentially enabling efficient classical simulations of the dynamics of certain expectations of correlators, or operators.

We also note that is possible to prove a robust version of Theorem 3, which applies to cases where the invariance property is "almost" satisfied. In this case, the commutations $[H, O_m]$ are not necessarily linear combinations of the operators in S, but if this "leakage" outside S is bounded and small, we can still satisfy Eq. (4) approximately, potentially allowing the simulation of larger classes of systems. One interesting example could be simulating the dynamics of quantum field theories, extending the results in Section 3.2. It might be possible to perform a cutoff in the degree of the operator set given by polynomials of Q_j and P_j , and attempt a simulation using shadow states, which encode less information than the full states.

In addition, there is a plethora of encodings from states and operators to other "shadow states" that one might consider. For example, when the system's state $\rho = \sum_{\ell} p_{\ell} |\psi_{\ell}\rangle\langle\psi_{\ell}|$ is mixed, the

⁵One simple example is the simulation of exponentially many and non-interacting magnetic dipoles under the influence of an external field.

amplitudes of $|\rho; S\rangle$ are linear in ρ and might not reveal anything useful (e.g., if the state is highly mixed, many expectations can become too small). However, one can consider an alternative encoding where ρ maps to a *mixed* shadow state, e.g., to each pure state $\rho_{\ell} := |\psi_{\ell}\rangle\langle\psi_{\ell}|$ we assign a shadow state $|\rho_{\ell}; S\rangle$, and then take the convex combination of such shadow states, e.g., $\sum_{\ell} p_{\ell} |\rho_{\ell}; S\rangle\langle\rho_{\ell}; S|$. For problems where the goal is to compute expectations of quantities that are quadratic in the pure-state expectations $\operatorname{tr}(\rho_{\ell} O_m)$'s, this type of encoding can be advantageous.

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