Fermionic Partial Tomography via Classical Shadows

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We propose a tomographic protocol for estimating any k-body reduced density matrix (k-RDM) of an n-mode fermionic state, a ubiquitous step in near-term quantum algorithms for simulating many-body physics, chemistry, and materials. Our approach extends the framework of classical shadows, a randomized approach to learning a collection of quantum-state properties, to the fermionic setting. Our sampling protocol uses randomized measurement settings generated by a discrete group of fermionic Gaussian unitaries, implementable with linear-depth circuits. We prove that estimating all k-RDM elements to additive precision ε requires on the order of $\binom{n}{k}k^{3/2}\log(n)/\varepsilon^2$ repeated state preparations, which is optimal up to the logarithmic factor. Furthermore, numerical calculations show that our protocol offers a substantial improvement in constant overheads for $k \geq 2$, as compared to prior deterministic strategies. We also adapt our method to particle-number symmetry, wherein the additional circuit depth may be halved at the cost of roughly 2–5 times more repetitions.

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Introduction.—One of the most promising applications of quantum computation is the study of strongly correlated systems such as interacting fermions. While quantum algorithms such as phase estimation [1,2] allow for directly computing important quantities such as ground-state energies with quantum speedup [3–5], current hardware limitations [6] have directed much attention toward variational methods. Of note is the variational quantum eigensolver (VQE) [7,8], where short-depth quantum circuits are repeatedly executed in order to estimate observable expectation values.

Initial bounds on the number of these circuit repetitions associated with fermionic two-body Hamiltonians were prohibitively high [9], spurring on much recent work addressing this problem. We roughly classify these strategies into two categories: those that specifically target energy estimates [8,10–29], referred to as Hamiltonian averaging, and more general techniques that can learn the k-body reduced density matrices (k-RDMs) of a quantum state [30–44]. (Not all works fit neatly into this dichotomy, e.g., Refs. [45–50].) Hamiltonian averaging is ultimately interested in a single observable, allowing for heavy exploitation in its structure. In contrast, reconstructing an RDM requires estimating all the observables that parametrize it.

Though generally more expensive than Hamiltonian averaging, calculating the k-RDM allows one to determine the expectation value of any k-body observable [51]. For example, the electronic energy of chemical systems is a linear functional of the 2-RDM, while in condensed-matter systems, effective models for electrons can require knowledge of the 3-RDM [52,53]. Beyond the energy, other important physical properties include pair-correlation functions and various order parameters [54,55]. The 2-RDM is also required for a host of error-mitigation techniques for near-term quantum algorithms [13,56,57], which have been experimentally demonstrated to be crucial in obtaining accurate results [58–61]. Additionally, promising extensions to VQE such as adaptive ansatz construction [62–65] and multireference- and excited-state calculations [56,57,66–69] can require up to the 4-RDM.

Motivated by these considerations, in this work we focus on partial tomography for fermionic RDMs. While numerous works have demonstrated essentially optimal sample complexity for estimating qubit RDMs [36,37,40–42], such approaches necessarily underperform in the fermionic setting. Recognizing this fundamental distinction, Bonet-Monroig *et al.* [37] and Jiang *et al.* [40] developed measurement schemes that achieve optimal scaling for fermions. However, the former construction is not readily generalizable for $k > 2$, while the latter requires a doubling in the number of qubits and a specific choice of fermion-to-qubit mapping.

In this Letter, we propose a randomized scheme that is free from these obstacles. It is based on the theory of classical shadows [42]: a protocol of randomly distributed measurements from which one acquires a partial classical representation of an unknown quantum state (its "shadow"). Classical shadows are sufficient for learning a limited collection of observables, making this framework ideal for partial state tomography. Our key results identify efficient choices for the ensemble of random measurements, suitable for the structure of fermionic RDMs.

Fermionic RDMs.—Consider a fixed-particle state ρ represented in second quantization on n fermion modes. The k-RDM of ρ, obtained by tracing out all but k particles, is typically represented as a $2k$-index tensor,

$$ {}^{k}D^{p_1\cdots p_k}_{q_1\cdots q_k} \coloneqq \mathrm{tr}(a^\dagger_{p_1}\cdots a^\dagger_{p_k} a_{q_k}\cdots a_{q_1}\rho), \tag{1}$$

where $a^\dagger_p$, a_p are fermionic creation and annihilation operators, $p \in \{0,\ldots,n-1\}$. By linearity, these matrix elements may be equivalently expressed using Majorana operators, starting with the definitions

$$\gamma_{2p} \coloneqq a_p + a^\dagger_p, \qquad \gamma_{2p+1} \coloneqq -i(a_p - a^\dagger_p). \tag{2}$$

Then for each $2k$-combination $\boldsymbol{\mu} \equiv (\mu_1,\ldots,\mu_{2k})$, where $0 \le \mu_1 < \cdots < \mu_{2k} \le 2n-1$, we define a $2k$-degree Majorana operator

$$\Gamma_{\boldsymbol{\mu}} \coloneqq (-i)^k \gamma_{\mu_1}\cdots\gamma_{\mu_{2k}}. \tag{3}$$

All unique $2k$-degree Majorana operators are indexed by the set of all $2k$ combinations of $\{0,\ldots,2n-1\}$, which we shall denote by $\mathcal{C}_{2n,2k}$. Because Majorana operators possess the same algebraic properties as Pauli operators (Hermitian, self-inverse, and Hilbert-Schmidt orthogonal), any fermion-to-qubit encoding maps between the two in a one-to-one correspondence.

The commutativity structure inherited onto $\mathcal{C}_{2n,2k}$ constrains the maximum number of mutually commuting (hence simultaneously measurable) operators to be $\mathcal{O}(n^k)$ [37]. As there are $\mathcal{O}(n^{2k})$ independent k-RDM elements, this implies an optimal scaling of $\mathcal{O}(n^k)$ measurement settings to account for all matrix elements.

Classical shadows and randomized measurements.—We briefly review the framework of classical shadows introduced by Huang *et al.* [42], upon which we build our fermionic extension and prove sampling bounds. Let ρ be an n-qubit state and $\{O_1,\ldots,O_L\}$ a set of L traceless observables for which we wish to learn $\mathrm{tr}(O_1\rho),\ldots,\mathrm{tr}(O_L\rho)$. Classical shadows require a simple measurement primitive: for each preparation of ρ, apply the unitary map $\rho \mapsto U\rho U^\dagger$, where U is randomly drawn from some ensemble $\mathcal{U}$; then perform a projective measurement in the computational basis, $\{|z\rangle | z \in \{0,1\}^n\}$.

Suppose we have an efficient classical representation for inverting the unitary map on postmeasurement states, yielding $U^\dagger|z\rangle\langle z|U$. Then the process of repeatedly applying the measurement primitive and classically inverting the unitary may be viewed, in expectation, as the quantum channel

$$\mathcal{M}_{\mathcal{U}}(\rho) \coloneqq \mathbb{E}_{U\sim\mathcal{U},|z\rangle\sim U\rho U^\dagger}[U^\dagger|z\rangle\langle z|U], \tag{4}$$

where $|z\rangle \sim U\rho U^\dagger$ is defined by the usual probability distribution from Born's rule, $\Pr[|z\rangle|U\rho U^\dagger] = \langle z|U\rho U^\dagger|z\rangle$. Informational completeness of $\mathcal{U}$ ensures that this channel is invertible, which allows us to define the classical shadow

$$\hat{\rho}_{U,z} \coloneqq \mathcal{M}^{-1}_{\mathcal{U}}(U^\dagger|z\rangle\langle z|U) \tag{5}$$

associated with the particular copy of ρ for which U was applied and $|z\rangle$ was obtained. Classical shadows form an unbiased estimator for ρ, and so they can be used to estimate the expectation value of any observable O:

$$\mathbb{E}_{U\sim\mathcal{U},|z\rangle\sim U\rho U^\dagger}[\mathrm{tr}(O\hat{\rho}_{U,z})] = \mathrm{tr}(O\rho). \tag{6}$$

The number of repetitions M required to obtain an accurate estimate for each $\mathrm{tr}(O_j\rho)$ is controlled by the estimator's variance, which may be upper bounded by

$$\max_{\text{states }\sigma} \mathbb{E}_{\substack{U\sim\mathcal{U}\\ |z\rangle\sim U\sigma U^\dagger}} [\langle z|U\mathcal{M}^{-1}_{\mathcal{U}}(O_j)U^\dagger|z\rangle^2] \eqqcolon \|O_j\|^2_{\mathcal{U}}. \tag{7}$$

This quantity is referred to as the (squared) shadow norm. Then by median-of-means estimation, one may show that

$$M = \mathcal{O}\left(\frac{\log L}{\varepsilon^2}\max_{1\le j\le L}\|O_j\|^2_{\mathcal{U}}\right) \tag{8}$$

samples suffice to estimate all expectation values to within additive error ε. To minimize Eq. (8) for a fixed collection of observables, the only available freedom is in $\mathcal{U}$. One must therefore properly choose the ensemble of unitaries, with respect to the target observables.

Naive application to fermionic observables.—A natural ensemble for near-term considerations is the group of single-qubit Clifford gates, $\mathrm{Cl}(1)^{\otimes n}$ (i.e., Pauli measurements). For an ℓ-local Pauli observable P, Huang *et al.* [42] showed that $\|P\|^2_{\mathrm{Cl}(1)^{\otimes n}} = 3^\ell$, similar to the results of prior approaches also based on Pauli measurements [36,37,40,41]. Although optimal for qubit ℓ-RDMs, such strategies cannot achieve the desired $\mathcal{O}(n^k)$ scaling in the fermionic setting due to the inherent nonlocality of fermion-to-qubit mappings. Indeed, assuming that the n fermion modes are encoded into n qubits, the 1-degree Majorana operators necessarily possess an average qubit locality of at least $\log_3(2n)$ [40]. This implies that, under random Pauli measurements, the squared shadow norm maximized over all $2k$-degree Majorana operators cannot do better than $3^{2k\log_3(2n)} = 4^k n^{2k}$. In fact, for commonly used mappings such as the Jordan-Wigner [70] or Bravyi-Kitaev [71–74] transformations, the scalings are poorer (3^n and $\sim 9^k n^{3.2k}$, respectively).

Randomized measurements with fermionic Gaussian unitaries.—To obtain optimal scaling in the shadow norm for fermionic observables, we propose randomizing over a different ensemble: the group of fermionic Gaussian Clifford unitaries. First, the group of fermionic Gaussian unitaries $\mathrm{FGU}(n)$ comprises all unitaries of the form

$$U(e^A) \coloneqq \exp\left(-\frac{1}{4}\sum_{\mu,\nu=0}^{2n-1} A_{\mu\nu}\gamma_\mu\gamma_\nu\right), \tag{9}$$

where $A = -A^\mathsf{T} \in \mathbb{R}^{2n\times 2n}$. This condition implies that FGU(n) is fully characterized by the Lie group SO($2n$) [75]. In particular, the adjoint action

$$U(Q)^\dagger \gamma_\mu U(Q) = \sum_{\nu=0}^{2n-1} Q_{\mu\nu}\gamma_\nu \quad \forall\ Q \in \mathrm{SO}(2n) \tag{10}$$

allows for efficient classical simulation of this group [76–80]. Second, the Clifford group Cl(n) is the set of all unitary transformations that permute n-qubit Pauli operators among themselves. It also admits an efficient classical representation [81,82].

Because Majorana operators are equivalent to Pauli operators, we may deduce from Eq. (10) that a unitary that is both Gaussian and Clifford corresponds to Q being a signed permutation matrix. Note that this defines the full group of Majorana swap circuits [37]. As the signs are irrelevant for our purpose, we simply consider the group of $2n \times 2n$ permutation matrices with determinant 1, known as (the faithful matrix representation of) the alternating group, Alt($2n$).

Concretely, we set

$$\mathcal{U}_{\mathrm{FGU}} \coloneqq \{U(Q) \in \mathrm{FGU}(n) | Q \in \mathrm{Alt}(2n)\}. \tag{11}$$

Given the context of fermionic tomography, the motivation for studying FGU(n) is clear, as it preserves the degree of Majorana operators. On the other hand, the restriction to the discrete Clifford elements is valuable for practical considerations. As we show in Sec. II of the Supplemental Material [83], the permutational property of Clifford transformations necessarily implies that $\mathcal{M}_{\mathrm{FGU}}$, as a linear map on the algebra of fermionic observables, is diagonal in the Majorana-operator basis,

$$\mathcal{M}_{\mathrm{FGU}}(\Gamma_{\boldsymbol{\mu}}) = \lambda_{\boldsymbol{\mu}}\Gamma_{\boldsymbol{\mu}} \quad \forall\ \boldsymbol{\mu} \in \mathcal{C}_{2n,2k}, \tag{12}$$

with eigenvalues

$$\lambda_{\boldsymbol{\mu}} = \binom{n}{k} \Big/ \binom{2n}{2k} \equiv \lambda_{n,k}. \tag{13}$$

In this diagonal form, the channel is readily invertible. Thus one may obtain closed-form expressions for the classical shadows $\hat{\rho}_{Q,z}$, and, importantly, their corresponding estimators for $\mathrm{tr}(\Gamma_{\boldsymbol{\mu}}\rho)$:

$$\mathrm{tr}(\Gamma_{\boldsymbol{\mu}}\hat{\rho}_{Q,z}) = \lambda_{n,k}^{-1} \sum_{\boldsymbol{\nu}\in\mathcal{C}_{2n,2k}} \langle z|\Gamma_{\boldsymbol{\nu}}|z\rangle \det[Q_{\boldsymbol{\nu},\boldsymbol{\mu}}]. \tag{14}$$

Here, $Q_{\boldsymbol{\nu},\boldsymbol{\mu}}$ denotes the submatrix of Q formed from its rows and columns indexed by $\boldsymbol{\nu}$ and $\boldsymbol{\mu}$, respectively [98]. Because Q is a permutation matrix, for each $\boldsymbol{\mu}$ there is exactly one $\boldsymbol{\nu}'$ such that $\det[Q_{\boldsymbol{\nu}',\boldsymbol{\mu}}] \neq 0$. Thus Eq. (14) is nonzero if and only if that $\Gamma_{\boldsymbol{\nu}'}$ is diagonal (i.e., maps to a Pauli-Z operator under a fermion-to-qubit transformation). In other words, the Clifford operation $U(Q)$ sends $\Gamma_{\boldsymbol{\mu}}$ to $\pm\Gamma_{\boldsymbol{\nu}'}$, which can be estimated only if it is diagonal in the computational basis.

From Eq. (7), the eigenvalues $\lambda_{n,k}^{-1}$ of the inverse channel $\mathcal{M}_{\mathrm{FGU}}^{-1}$ determine the shadow norm. The sample complexity of our approach then follows from Eq. (8). We summarize this first key result with the following theorem.

Theorem 1.—Consider all $2k$-degree Majorana operators $\Gamma_{\boldsymbol{\mu}}$ on n fermionic modes, labeled by $\boldsymbol{\mu} \in \mathcal{C}_{2n,2k}$. Under the ensemble $\mathcal{U}_{\mathrm{FGU}}$ defined in Eq. (11), the shadow norm satisfies

$$\|\Gamma_{\boldsymbol{\mu}}\|_{\mathrm{FGU}}^2 = \binom{2n}{2k} \Big/ \binom{n}{k} \approx \binom{n}{k}\sqrt{\pi k} \tag{15}$$

for all $\boldsymbol{\mu} \in \mathcal{C}_{2n,2k}$. Thus the method of classical shadows estimates the fermionic k-RDM of any state ρ, i.e., $\mathrm{tr}(\Gamma_{\boldsymbol{\mu}}\rho)\ \forall\ \boldsymbol{\mu} \in \cup_{j=1}^{k} \mathcal{C}_{2n,2j}$, to additive error ε, given

$$M = \mathcal{O}\left[\binom{n}{k}\frac{k^{3/2}\log n}{\varepsilon^2}\right] \tag{16}$$

copies of ρ. Additionally, there is no subgroup $G \subset \mathrm{FGU}(n) \cap \mathrm{Cl}(n)$ for which $\|\Gamma_{\boldsymbol{\mu}}\|_G < \|\Gamma_{\boldsymbol{\mu}}\|_{\mathrm{FGU}}$.

The proof is presented in the Supplemental Material [83], Sec. II. Furthermore, noting from Eq. (14) that $|\mathrm{tr}(\Gamma_{\boldsymbol{\mu}}\hat{\rho}_{Q,z})| \leq \lambda_{n,k}^{-1}$, we also show in the Supplemental Material that Bernstein's inequality [99] guarantees the above sample complexity via standard sample-mean estimation, rather than requiring the median-of-means technique proposed in the original work on classical shadows [42].

This result has an intuitive conceptual interpretation. In the computational basis, there are precisely $\binom{n}{k}$ diagonal Majorana operators within $\mathcal{C}_{2n,2k}$, corresponding to the unique k-fold products of occupation-number operators (e.g., $\prod_{j=1}^{k} a_{p_j}^\dagger a_{p_j}$) on n modes. As a permutation on $\mathcal{C}_{2n,2k}$, each element of $\mathcal{U}_{\mathrm{FGU}}$ defines a different basis in which some other subset of $\binom{n}{k}$ operators are diagonal. Then, one may expect to account for all $|\mathcal{C}_{2n,2k}| = \binom{2n}{2k}$ Majorana operators by randomly selecting on the order of $\binom{2n}{2k}/\binom{n}{k}$ such bases; Theorem 1 makes this claim rigorous.

Fermionic Gaussian circuits have a well-studied compilation scheme based on a Givens-rotation decomposition [100–102]. For a general element of $\mathcal{U}_{\mathrm{FGU}}$, we require a circuit depth of at most $2n$ with respect to this decomposition [102]. Additionally, as pointed out in Ref. [37], Gaussian unitaries commute with the global parity operator $\Gamma_{(0,\ldots,2n-1)}$, allowing for error mitigation via symmetry verification [103,104].

Such compilation schemes make use of a group homomorphism property, $U(Q_1)U(Q_2) = U(Q_1Q_2)$. Therefore, if the circuit preparing ρ itself features fermionic Gaussian operations at the end, then we may further compile the measurement unitary into the state-preparation circuit [57]. In the case of indefinite particle number, this concatenation is essentially free. However, rotations with particle-number symmetry have depth at most n [101,102], so they must be embedded into the larger Gaussian unitary of depth $2n$. This observation motivates us to explore classical shadows over the number-conserving (NC) subgroup of $\mathrm{FGU}(n)$.

Modification based on particle-number symmetry.—Fermionic Gaussian unitaries that preserve particle number are naturally parametrized by $\mathrm{U}(n)$. We express an element of this NC subgroup as

$$U(e^{\kappa}) \coloneqq \exp\left(\sum_{p,q=0}^{n-1} \kappa_{pq} a_p^\dagger a_q\right), \tag{17}$$

where $\kappa = -\kappa^\dagger \in \mathbb{C}^{n\times n}$, hence $e^{\kappa} \in \mathrm{U}(n)$. Because the particle-number symmetry manifests as a global phase factor $e^{\mathrm{tr}\,\kappa/2} \in \mathrm{U}(1)$, without loss of generality we may consider $\mathrm{tr}\,\kappa = 0$, or equivalently, $e^{\kappa} \in \mathrm{SU}(n)$. Such unitaries are also called orbital-basis rotations, owing to their adjoint action,

$$U(u)^\dagger a_p U(u) = \sum_{q=0}^{n-1} u_{pq} a_q \quad \forall\ u \in \mathrm{SU}(n). \tag{18}$$

This action on Majorana operators follows by linear extension.

Taking the intersection with the Clifford group requires that u be an $n \times n$ generalized permutation matrix, with nonzero elements taking values in $\{\pm 1, \pm i\}$. This corresponds to the group of fermionic swap circuits [71,101]. Again, the phase factors on the matrix elements are irrelevant, so we shall restrict to $u \in \mathrm{Alt}(n)$. By itself, this ensemble is insufficient to perform tomography. To see this, consider an arbitrary reduced density operator $A_{\boldsymbol{p}}^\dagger A_{\boldsymbol{q}} \coloneqq a_{p_1}^\dagger \cdots a_{p_k}^\dagger a_{q_k} \cdots a_{q_1}$, where $\boldsymbol{p}, \boldsymbol{q} \in \mathcal{C}_{n,k}$. Such operators are diagonal in the computational basis only if $\boldsymbol{p} = \boldsymbol{q}$. Informational completeness thus requires that there exists some $U(u)$ that maps $A_{\boldsymbol{p}}^\dagger A_{\boldsymbol{q}}$ to $A_{\boldsymbol{r}}^\dagger A_{\boldsymbol{r}}$, for some $\boldsymbol{r} \in \mathcal{C}_{n,k}$. Because $u \in \mathrm{Alt}(n)$, conjugation by $U(u)$ simply permutes $\boldsymbol{p}$ and $\boldsymbol{q}$ independently. However, as permutations are bijective, it is not possible to permute both $\boldsymbol{p}$ and $\boldsymbol{q}$ to the same $\boldsymbol{r}$ if $\boldsymbol{p} \neq \boldsymbol{q}$.

Therefore, this ensemble will necessarily require operations beyond either the NC or Gaussian constraints. The simplest option for maintaining the low-depth structure of the basis rotations is to append Pauli measurements at the end of the circuit. Although the resulting circuit no longer preserves particle number, this addition incurs only a single layer of single-qubit gates. Specifically, we define the ensemble

$$\mathcal{U}_{\mathrm{NC}} \coloneqq \{V \circ U(u) | V \in \mathrm{Cl}(1)^{\otimes n}, u \in \mathrm{Alt}(n)\}. \tag{19}$$

By virtue of introducing the notion of "single-qubit" gates, this method is dependent on the choice of fermion-to-qubit mapping. Let $\mathrm{loc}(\Gamma_{\boldsymbol{\mu}})$ denote the qubit locality of $\Gamma_{\boldsymbol{\mu}}$ under some chosen mapping. While Pauli measurements incur a factor of $3^{\mathrm{loc}(\Gamma_{\boldsymbol{\mu}})}$ in the variance, the randomization over fermionic swap circuits effectively averages this quantity over all same-degree Majorana operators (rather than depending solely on the most nonlocal operator). Formally, we find that the shadow norm here is

$$\|\Gamma_{\boldsymbol{\mu}}\|_{\mathrm{NC}}^2 = \mathbb{E}_{u\sim\mathrm{Alt}(n)}[3^{-\mathrm{loc}[U(u)^\dagger \Gamma_{\boldsymbol{\mu}} U(u)]}]^{-1}. \tag{20}$$

Although this expression does not possess a closed form, the following theorem provides a universal upper bound.

Theorem 2.—Under the ensemble $\mathcal{U}_{\mathrm{NC}}$ defined in Eq. (19), the shadow norm obeys

$$\max_{\boldsymbol{\mu}\in\mathcal{C}_{2n,2k}} \|\Gamma_{\boldsymbol{\mu}}\|_{\mathrm{NC}}^2 \leq 9^k \binom{n}{2k} \Big/ \binom{n-k}{k} = \mathcal{O}(n^k) \tag{21}$$

for a fixed integer k and for all fermion-to-qubit mappings. Thus the method of classical shadows with $\mathcal{U}_{\mathrm{NC}}$ estimates the k-RDM to additive error ε with sample complexity

$$M = \mathcal{O}\left(\frac{n^k \log n}{\varepsilon^2}\right). \tag{22}$$

We provide derivations for the above results in the Supplemental Material [83], Sec. III. Note that we have fixed k as a constant here, so the asymptotic notation may hide potentially large prefactors depending on k. To understand such details, we turn to numerical studies.

Numerical calculations.—Instead of drawing a new circuit for each repetition, here we employ a simplification more amenable to practical implementation. Fixing some integer $r \geq 1$, we generate a random collection $\{U^{(j)} \sim \mathcal{U}\}_{j=1}^{K_r}$ of K_r unitaries such that all target observables are covered at least r times. We say a Majorana operator $\Gamma_{\boldsymbol{\mu}}$ is covered by the measurement unitary U if $U\Gamma_{\boldsymbol{\mu}}U^\dagger$ is diagonal in the computational basis. Because the ensembles considered here consist of Gaussian and Clifford unitaries, we can determine all covered operators efficiently. Additionally, for the $\mathcal{U}_{\mathrm{NC}}$ calculations, the qubit mappings were automated through OpenFermion [105].

To achieve precision corresponding to $S = \mathcal{O}(1/\varepsilon^2)$ samples per observable, one repeats each circuit $\lceil S/r \rceil$ times. The total number of circuit repetitions for our randomized protocols is then $\lceil S/r \rceil K_r$. For practical purposes, we fix $r = 50$ in this work (see Sec. V of the

SORTED INSERTION	n-qubit Clifford circuits $C \sim \mathcal{O}(n^{2k-1})$ (empirical)
Majorana clique cover	Ferm. Gaussian circuits $C = \mathcal{O}(n^k)$ $(k \leq 2)$
Fermionic swap networks	Basis-rotation circuits $C = \tilde{\mathcal{O}}(n^k)$
Classical shadows (FGU)	Ferm. Gaussian circuits $K_r/r = \tilde{\mathcal{O}}(n^k)$
Classical shadows (NC)	Basis-rotation circuits $K_r/r = \tilde{\mathcal{O}}(n^k)$ (JW) (BK)

Note: $\tilde{\mathcal{O}}(\cdot)$ denotes an upper bound scaling, suppressing polylogarithmic factors.

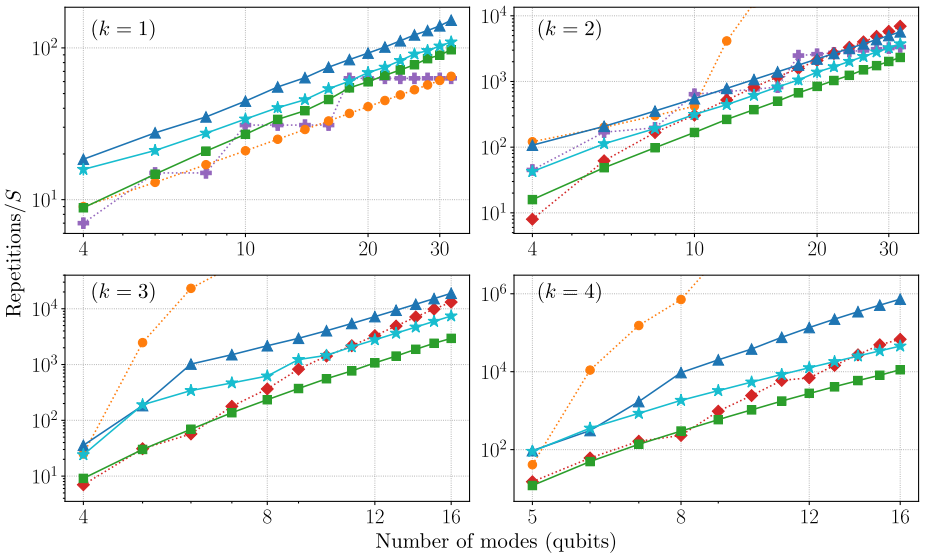

FIG. 1. (Left) Summary of the methods compared here, cataloging their required circuit types and scalings in the number of measurement settings. Because graph-based methods [33–35,38] are resource intensive, we employ SORTED INSERTION [17] as a more tractable alternative. The Majorana clique cover [37], which employs the same class of fermionic Gaussian Clifford circuits as our classical shadows (FGU) unitaries, possesses optimal asymptotic scaling; however, it exhibits jumps at powers of 2 due to a divide-and-conquer approach. Furthermore, the construction exists only for $k \leq 2$. The measurement strategy using fermionic swap networks is a generalization of the optimal 1-RDM strategy introduced in Ref. [61], which we describe in Sec. IV of the Supplemental Material [83]. (Right) Numerical performances (log-log scale). Note that SORTED INSERTION and the Majorana clique cover are equivalent for $k = 1$. Because our scheme uses randomization, we include error bars of 1 standard deviation, averaged over 10 instances. However, they are not visible at the scale of the plots, indicating the consistency of our method.

Supplemental Material [83] for further details). To compare against prior deterministic strategies, we compute $S \times C$ for each such strategy, where C is the number of sets of commuting observables constructed by a given strategy.

For the comparisons presented in Fig. 1, we focus on the most competitive prior strategies applicable to fermionic RDM tomography. Because the 1-RDM has a relatively simple structure, optimal strategies are known [37,61], and so randomization underperforms for $k = 1$. However, the advantage of our $\mathcal{U}_{\mathrm{FGU}}$-based method becomes clear for $k \geq 2$. When comparing against the Majorana clique cover, which features asymptotically optimal $\mathcal{O}(n^2)$ scaling for the 2-RDM [37], we find a roughly twofold factor improvement by our approach.

For the $\mathcal{U}_{\mathrm{NC}}$ case, we observe a trade-off between circuit size and measurement efficiency. As expected, the choice of fermion-to-qubit mapping matters here; the Jordan-Wigner (JW) mapping performs worse than Bravyi-Kitaev (BK), as the former possesses more qubit nonlocality. Although more measurement settings are required compared to the $\mathcal{U}_{\mathrm{FGU}}$ ensemble (e.g., a factor of $\sim 2-5$ under BK, depending on k), each circuit itself requires only half the depth of general fermionic Gaussian circuits. Notably, however, $\mathcal{U}_{\mathrm{NC}}$ classical shadows for the 2-RDM under the BK mapping is closely comparable to the Majorana clique cover.

Conclusions.—We have adapted the framework of classical shadows to the efficient tomography of fermionic k-RDMs, applicable for all k. Numerical calculations demonstrate that our approach consistently outperforms prior strategies using measurement circuits of comparable sizes when $k \geq 2$, despite the logarithmic factor in the sample complexity (a consequence of rigorously bounding the worst-case probabilistic instances). The power of randomization here lies in avoiding the NP-hard problem of partitioning observables into commuting cliques [32–35]. Instead, we show that a highly overlapping cover of the observables suffices to perform partial tomography efficiently, as a factor of $\mathcal{O}(1/\varepsilon^2)$ repetitions is already required for this task.

An outlook for further applications is to adapt these ensembles, e.g., for Hamiltonian averaging. As expected, our method is less efficient in this context than those tailored for the task (see Sec. V C of the Supplemental Material [83] for preliminary numerical calculations). Possible modifications may include biasing the distribution of unitaries [22,27–29], or derandomization techniques [25].

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