Classical shadows of fermions with particle number symmetry

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We consider classical shadows of fermion wavefunctions with \( \eta \) particles occupying \( n \) modes. We prove that all \( k \)-Reduced Density Matrices (RDMs) may be simultaneously estimated to an average variance of \( \epsilon^2 \) using at most \( \binom{n}{k} \left( 1 - \frac{2k}{n} \right)^k \frac{\pi n^2}{1 + n - k} / \epsilon^2 \) measurements in random single-particle bases that conserve particle number, and provide an estimator for any \( k \)-RDM with \( \mathcal{O}(k^2 \eta) \) classical complexity. Our sample complexity is a super-exponential improvement over the \( \mathcal{O}(\binom{n}{k} \sqrt{n}) \) scaling of prior approaches as \( n \) can be arbitrarily larger than \( \eta \), which is common in natural problems. Our method, in the worst-case of half-filling, still provides a factor of \( 4^k \) advantage in sample complexity, and also estimates all \( \eta \)-reduced density matrices, applicable to estimating overlaps with all single Slater determinants, with at most \( \mathcal{O}(\frac{1}{\epsilon}) \) samples, which is additionally independent of \( \eta \).

By representing fermions with qubits through, say, the Jordan-Wigner or Bravyi-Kitaev encoding [8], state tomography on fermions is reduced to one of the many optimal schemes for qubit tomography. The most compact encoding [9] then estimates all \( k \)-RDMs on \( n \) fermion modes using only \( \mathcal{O}(2n^k / \epsilon^2) \) samples. As bootstrapping to a qubit-based scheme incurs substantial overhead, directly randomizing the algebra of fermions, such as with fermionic gaussians, further reduces the samples required to only \( \left( \frac{n}{k} \right) \sqrt{\pi k / \epsilon^2} \) samples. As there are \( \mathcal{O}(n^{2k}) \) independent \( k \)-RDMs and \( \mathcal{O}(n^k) \) mutually commuting observables, this result is optimal, but does not realize the super-exponential improvement seen in the qubit setting.

Discovering an analogous super-exponential improvement would unlock for fermions many applications found in the toolbox of randomized qubit measurements [11]. A missing ingredient is the particle number symmetry present in many systems of interest, ranging from electronic structure to the Hubbard model. The design of random bases targeting number-conserving \( k \)-RDMs should account for this crucial prior that the fermion wavefunction has a definite number of \( \eta \) particles occupying \( n \) modes. As the condition that \( n \gg \eta \) also occurs naturally, such as in modeling dynamical correlation [12] or in plane-wave simulations [13, 14], a scheme that scales with \( \eta \) instead of \( n \) is highly desirable. However, prior approaches target all \( k \)-RDMs, both number-conserving and not. One solution is to choose random bases that are also number-conserving, but this appears challenging. For instance, prior attempts [10] required bootstrapping to qubit protocols to achieve tomographic completeness and ultimately achieved the same \( \mathcal{O}(n^k / \epsilon^2) \) sample complexity, or was able to prove scaling with \( \eta \) for only the \( k = 1 \) case [15].

In this work, we successfully exploit particle number symmetry. We find random bases that simultaneously estimate all \( \binom{n}{k} \) independent number-conserving \( k \)-RDMs

\[
\langle D^\eta_q \rangle = \text{Tr} \left[ D^\eta_q \rho \right], \quad D^\eta_q = a_1^\dagger a_2^\dagger \cdots a_p^\dagger a_{p+1} \cdots a_{q_1} \cdots a_{q_{\eta}} \cdot a_{q_{\eta+1}} \cdots a_{q_k}, \quad (1)
\]

of any quantum state \( \rho \) with an average variance of \( \epsilon^2 \) using only \( \mathcal{O}(\eta^k / \epsilon^2) \) samples, where the fermion operators satisfy the usual anti-commutation relations \( \{ a_j, a_k^\dagger \} = \cdots \)}
Theorem 1. For any \( \eta \)-particle \( n \)-mode fermion state \( \rho \), let the unitary single-particle basis rotation be

\[
U_\eta(u) \doteq e^{\sum_{p=r=1}^n \eta_p a^\dagger_p a^r} \in \mathbb{C}^{n \times n},
\]

where \( u \in \mathbb{C}^{n \times n} \) is a Haar random unitary. Measure \( U_\eta(u)P_{\eta}^0(u) \) to obtain the occupation \( \bar{z} \in S_{n, \eta} \doteq \{(z_1, \ldots, z_\eta) : \forall j \in [\eta], 1 \leq z_j < z_{j+1} \leq n\} \) with probability \( \langle \bar{z}|U_\eta(u)P_{\eta}^0(u)|\bar{z}\rangle \) and let \( v_{\bar{z}} \in \mathbb{Z}^{n \times n} \) be any permutation matrix that maps elements of \( [\eta] \) to \( \bar{z} \). Then the single-shot estimator of any \( k \)-RDM is

\[
\langle \hat{D}_q \rangle = \langle q \rangle U_k^\dagger(v_{\bar{z}}u)E_{\eta,k}U_k(v_{\bar{z}}u)\langle \hat{p} \rangle,
\]

\[
E_{\eta,k} = \sum_{\bar{r} \in S_{n,k}} |\bar{r}\rangle \langle \bar{r}| \left( \frac{(-1)^{S' + s'}}{k^{s'} - s'} \right),
\]

where \( s' = |\bar{r} \cap [\eta]| \) is the number of elements \( \bar{r} \) and \((1, \ldots, \eta)\) share in common, with average variance

\[
V = \mathbb{E}_{\bar{r}, \bar{z}}[\text{Var}(\langle \hat{D}_q \rangle)] \leq \frac{Tr\left[\frac{E_{\eta,k}^2}{(k^2)^n}\right]}{\left(\frac{n}{2}\right)^n} - \frac{(\frac{n}{2})^n}{(k)^n}. \tag{5}
\]

Importantly, the symmetries of our estimator allow it to be evaluated efficiently in \( O(k^2\eta) \) time [16], also independent of \( n \), even through the naive approach of multiplying dimension \((\frac{n}{2})^n \times (\frac{n}{2})^n \) matrices is efficient only for constant \( k \). This is through a reduction to evaluating Pfaffians corresponding to traces of products of fermionic gaussian [17, 18], which is similar to recent work [19] but significantly faster due to hidden structure in our number-conserving case.

We obtain our claim on sample complexity by averaging over \( N \) independent sampled pairs \((u, \bar{z})\). An upper bound on the variance in Equation (5) is

\[
V \leq \left(\frac{n}{k}\right) \left(1 - \frac{\eta - k}{n}\right)^k \left(1 + \frac{n + 1}{n - k}\right) \tag{6}
\]

In the worst-case of half-filling \( \eta = n/2 \), with large \( n \) and fixed \( k \), this bound also implies a sample complexity \( V \approx \frac{1}{\sqrt{\eta}} \left(1 + O\left(\frac{k^2}{n}\right)\right) \) which is an exponential factor of \( 4^k \) smaller than the prior approaches in the common case \( k^2 \ll n \). Even for small \( k \), this reduction is highly relevant to practical implementations of quantum algorithms such as the variational quantum eigenstates [20]. The case of very large \( k = \eta \) is also of interest to applications such as quantum-classical auxiliary-field quantum Monte Carlo [3], and we prove in that case \( V \approx \frac{4}{\sqrt{\eta}} \), compared to prior art of \( \tilde{O}(\sqrt{n}/2^k) \) [19]. Moreover, our scheme is practical as the quantum circuits implementing each basis rotation can have depth as little as \( O(n) \) [21]. Notably, measurements in random single-particle bases simultaneously reveals information on both local and non-local observables where \( k \) and \( \eta - k \) is small respectively.

The simple and exact expression for our estimator belies a complicated analysis. Prior qubit analyses are greatly simplified by how the easily implementable group of random Clifford bases are a unitary 3-design [22, 23] on the entire state space. Unfortunately for fermions, even though random single-particle rotations are generated by Haar random unitaries, they fail to be t-designs on the entire state space except when \( \eta = 1 \) [19] or \( k = 1 \) [24]. We prove Theorem 1 in four key steps.

In Section II, the basic observation in the classical shadows framework is that averaging over all classical shadows in the random basis \( U \in U \) defines a measurement channel

\[
\mathcal{M}_U[\rho] = \mathbb{E}_{\bar{z}, U}[U^\dagger |\bar{z}\rangle \langle \bar{z}| U] = \text{Tr}[I] \text{Tr}_1[U_{2, \eta} \rho \otimes I], \tag{7}
\]

expressed in terms of a t-fold twirling channel acting on the basis state \( |\bar{z}\rangle \langle \bar{z}| \) like

\[
\mathcal{T}_{t, \eta} \doteq \int (U |\bar{z}\rangle \langle \bar{z}| U^\dagger)^{\otimes t} \ dU_{\text{Haar}}(U). \tag{8}
\]

In our case \( U_\eta(u) \in U = \Lambda^n U_n \) is the group of single-particle rotations, where \( u \in U_n \) is the \( n \)-dimension unitary group. So long as \( U \) is tomographically complete for \( \rho \), the measurement channel may be inverted on any classical shadow to form a single-shot unbiased estimate of \( \rho = \mathbb{E}_{u, \bar{z}}[\hat{\rho}_{u, \bar{z}}] \), where

\[
\hat{\rho}_{u, \bar{z}} \doteq \mathcal{M}_{t, \eta}^{-1}[U_\eta(u)|\bar{z}\rangle \langle \bar{z}| U_\eta(u)]. \tag{9}
\]

Hence, we demonstrate in Theorem 2 that \( \Lambda^n U_n \) is tomographically complete, contrary to a previous negative result where the \( u \) are restricted to permutations [10]. In fact, it suffices to just invert the measurement channel on the state \([\eta]\langle [\eta] \rangle\), as

\[
\hat{\rho}_{u, \bar{z}} = U_\eta^\dagger(v_{\bar{z}}^\dagger u)\mathcal{M}_{t, \eta}^{-1}[[[\eta]] \langle [\eta]\rangle] U_\eta(v_{\bar{z}}^\dagger u), \tag{10}
\]

following the existence of a permutation \( v_{\bar{z}} \) such that \( |\bar{z}| = U_\eta(v_{\bar{z}}) |[\eta]\rangle \), and the invariance of Haar integration with respect to a change of variables.

In Section III, we find a closed-form expression for the twirling channel \( T_{2, \eta} \Lambda^n U_n \) for all \( n \) and \( \eta \). We leave the \( t = 3 \) case to future work, which would enable a per-k-RDM variance analysis rather than an average. This allows us to identify in Theorem 3 the eigenoperators \( \hat{n}_{\bar{x}, \bar{y}} \) of the measurement channel

\[
\mathcal{M}_U[\hat{n}_{\bar{x}, \bar{y}}] = \left(\frac{n + 1}{d}\right) \hat{n}_{\bar{x}, \bar{y}}, \tag{11}
\]

\[
\hat{n}_{\bar{x}, \bar{y}} \doteq \prod_{j=1}^d (\hat{n}_{x_j} - \hat{n}_{y_j}), \tag{12}
\]
where \( \tilde{n}_j = a_j^* a_j \) are number operators and \( x \cap y = \emptyset \). By expressing \( |[\eta] \rangle \langle [\eta]| = \sum_{x,y} \tilde{g}_{x,y} \tilde{h}_{x,y} \) as a linear combination of \( \tilde{g}_{x,y} \), we successfully find the inverse \( \mathcal{M}_U^{-1} [[[\eta]] \langle [\eta]] = (n+1) \sum_{x,y} \tilde{g}_{x,y} \tilde{h}_{x,y} \).

In Section IV, the estimate \( \tilde{\rho}_{\tilde{n},\tilde{z}} \) has exponentially large dimension, finding an expression for it does not guarantee the efficient computation of arbitrary observables \( O \). Fortunately, efficient computation is guaranteed if the estimate \( \tilde{O} = (n+1) \sum_{x,y} \tilde{g}_{x,y} \tilde{h}_{x,y} \langle \tilde{O} \rangle \) simplifies into an implicit sum over polynomially many terms without explicitly forming \( \tilde{\rho}_{\tilde{n},\tilde{z}} \). For any observable that is a linear combination of \( k \)-RDMs

\[
O = \sum_{\tilde{p},\tilde{q} \in \mathcal{S}_{n,k}} \sigma_{\tilde{p},\tilde{q}} \mathcal{D}_{\tilde{q}}^p,
\]

we show in Theorem 5 that for the estimator \( \hat{O} = \text{Tr} \left[ \frac{1}{\mathcal{M}_U} v^2 \rho E_{\tilde{p},\tilde{q}} U_k v^2 \rho U_k^d \right] \), with Equation (3) as a special case when \( O \) is a single \( k \)-RDM. This expression highlights how our estimator has no preferred basis. Though we specify \( k \)-RDMs in the computational basis, any basis rotated \( k \)-RDMs, e.g. \( U_k(w) \mathcal{D}_{\tilde{q}}^p U_k(w) \), which could contain exponentially many terms, may be estimated just as easily by absorbing \( v^2 \rho \rightarrow v^2 \omega \). One might also think that this estimator is computationally efficient only for constant \( k \) as \( U_k(u) \) has dimension \( (n^2)^k \). However, we show in Section IV A that any \( k \)-RDM may be evaluated in just \( O(k^2 \eta) \) time, which is also independent of \( n \).

Finally, in Section V, the classical shadows framework states that the variance of any observable for a given quantum state \( \text{Var} \left[ \langle \hat{O} \rangle \right] \leq \langle |O|^2 \rangle_{\rho} \) is bounded above by the square of a quantity called the shadow norm.

\[
\|O\|^2_{\rho} = \mathbb{E}_{\tilde{n},\tilde{z}} \left[ \langle \hat{O}_{\tilde{n}} \rangle^2 \right],
\]

where \( O_{\tilde{n}} \) is the trace-free component of \( O \). The convention is to express \( \|O\|^2_{\rho} = \text{Tr} \left[ \mathcal{T}_{A_n \wedge A_n} (\rho \otimes \mathcal{M}_U^{-1} (O_{\tilde{n}}) \otimes \mathcal{M}_U^{-1} (O_{\tilde{n}})) \right] \) in terms of the 3-fold twirling channel, which appears quite difficult to evaluate. We achieve some simplification by considering the case where \( O \) is a single \( k \)-RDM. Substituting our estimator Equation (3) into Equation (14), we obtain in Theorem 6 a state-independent equality on the squared shadow norm averaged over all \( k \)-RDMs

\[
\mathbb{E}_{\tilde{p},\tilde{q}} \left[ \|D_{\tilde{q}}^p\|^2 \right]_{\rho} = \frac{\text{Tr} \left[ E_{\eta,\eta}^2 \right]}{\left( \frac{n}{k} \right)^2} - \left( \frac{n-k}{n} \right)^2 \left( \frac{n}{k} \right)^2,
\]

seen in Equation (5) without needing to evaluate \( \mathcal{T}_{A_n \wedge A_n} \).

The upper bound Equation (6) on this exact expression for the squared average shadow norm is one that works reasonably well when \( \eta \ll n \). Given the variance, we note that taking the median-of-means \cite{[6]} or mean of multiple estimates \cite{[10]} furnishes the additive error bounds commonly seen in related work.

In Section VI, we discuss other implications of our results, such as estimating the overlap with all Slater determinants with \( \frac{m}{\eta^2} \) samples on average, and highlight possible future directions. We relegate some of our longer and highly technical proofs to the appendices. Appendix A evaluates \( \mathcal{T}_{A \wedge A_k} \) in closed-form by a combinatorial approach, and Appendix B evaluates certain triple- and quadruple-sums over hypergeometric terms related to finding the coefficients \( c_{\tilde{g},\tilde{y}} \) and entries of the estimation matrix. We define some commonly used notation in the remainder of this section.

### A. Notation

Let \( a_k^* \{0\} \equiv \{k\} \) be basis elements of a dimension \( n \) complex vector space \( V_n \). The basis elements of the \( \eta \) fermion space \( \wedge^\eta V_n \) are \( |\tilde{z}\rangle \equiv \wedge_{k=1}^\eta |z_k\rangle = |z_1 \rangle \wedge \cdots \wedge |z_\eta \rangle \) with dimension \( \dim \langle \wedge^\eta V_n \rangle = \binom{n}{\eta} \). These are indexed by the occupation number basis \( \tilde{z} \in S_{n,\eta} \), where

\[
S_{n,\eta} = \{ (z_1, \cdots, z_\eta) : \forall j \in [\eta], 1 \leq z_j < z_{j+1} \leq n \},
\]

is the set of \( \eta \) sorted integers between 1 and \( n \). For example, \( [\eta] = (1, \cdots, \eta) \in S_{n,\eta} \), and using the set complement notation, \( [n] \setminus \eta = (n+1, \cdots, n) \in S_{n,\eta} \). The basis state \( |\tilde{z}\rangle \) is an eigenvector of the number operators \( \tilde{n}_j = a_j^* a_j \), where products of \( d \) distinct number operators \( \tilde{n}_{p_1 \cdots p_d} \) satisfy

\[
\langle \tilde{z} | \tilde{n}_{p_1 \cdots p_d} | \tilde{z} \rangle = \left\{ \begin{array}{ll} 1, & \tilde{p} \subseteq \tilde{z}, \\ 0, & \text{otherwise}, \end{array} \right.
\]

and are rank-\( \binom{n-d}{\eta-d} \) projectors. For instance, for all \( \tilde{z} \in S_{n,\eta} \), the rank-1 projector

\[
|\tilde{z}\rangle \langle \tilde{z}| = \Pi_{\tilde{z}} = \hat{n}_{\tilde{z}}.
\]

We will often perform sums over combinations of \( \tilde{n}_{\tilde{z}} \) such as

\[
e_k (\tilde{n}_1 \cdots \tilde{n}_d) \equiv \sum_{\tilde{z} \in \mathcal{S}_{n,k}} \tilde{n}_{\tilde{z}} = \frac{1}{k!} \sum_{\tilde{p} \in \mathcal{S}_{d,k}} \tilde{n}_{\tilde{p}},
\]

which define elementary symmetric polynomials of degree \( k \) in \( d \) commuting variables, where we introduce \( S_{\tilde{p},k} \) as all permutations of \( k \) elements of \( \tilde{p} \). To simplify notation, we may replace the argument \( e_k \{ [\tilde{n}] \}_{d} \equiv e_k (\tilde{n}_1 \cdots \tilde{n}_d) \) with \( \tilde{n}_{[\tilde{n}]} \).

Let \( u \in U_n \) be a unitary operation on basis elements of the complex vector space \( \mathbb{C}^n \), that is \( |u_{jk}\rangle \equiv u_{jk} \). The representation \( U_\eta (u) \) on \( \wedge^\eta U_n \) is then a unitary fermion rotation applying

\[
U_\eta (u) |\tilde{z}\rangle = \bigwedge_{k=1}^\eta |u_{z_k}\rangle = \sum_{\tilde{p} \in S_{\eta,n}} \det [u_{\tilde{p} \tilde{z}}] |\tilde{p}\rangle,
\]

where \( u_{\tilde{p} \tilde{z}} \) denotes the submatrix formed by taking rows \( x_1, x_2, \cdots \) and columns \( y_1, y_2, \cdots \) of \( u \). In other words,
the determinant \( \det[u_{jk}] \) is the determinant of a matrix minor of \( u \). Fermion rotations are a homomorphism of \( U_n \) as

\[
U_\eta(v)U_\eta(u) = U_\eta(vu). \tag{21}
\]

Fermion rotations are also known as single-particle basis rotations as each creation operator is rotated to a linear combination of other creation operators as follows.

\[
U_\eta(u) a_k^\dagger U_\eta^\dagger(u) = \sum_j u_{jk} a_j^\dagger, \tag{22}
\]

\[
U_\eta^\dagger(u) a_k U_\eta(u) = \sum_j u_{kj}^* a_j^\dagger. \tag{23}
\]

Consider the special case where \( v, \omega \in \mathbb{Z}^{n \times n} \) is any permutation matrix such that \( |z_j\rangle = v|j\rangle \) for all \( j \in [\eta] \). Then

\[
|z\rangle = U_\eta(v_\omega)|[\eta]\rangle. \tag{24}
\]

We often rotate product of creation and annihilation operators. For any \( \vec{p}, \vec{q} \in S_{n,k} \), the rotated \( k\)-RDM is

\[
U_\eta(u) D_{\vec{q}}^\vec{p} U_\eta^\dagger(u) = \sum_{\vec{p}', \vec{q}' \in S_{n,k}} \det[u_{\vec{p}' \vec{p}}] D_{\vec{q}'}^\vec{p}' \det[(u^\dagger)^{\vec{q}' \vec{q}}]. \tag{25}
\]

Given a linear combination \( k\)-RDMs Equation (13), the rotated observable \( O' = U_\eta(u) O U_\eta^\dagger(u) \) is hence

\[
O' = \sum_{\vec{p}', \vec{q}' \in S_{n,k}} \left( \sum_{\vec{p}, \vec{q} \in S_{n,k}} \det[u_{\vec{p} \vec{p}'}] \delta_{\vec{p}', \vec{q}'} \det[(u^\dagger)^{\vec{q}' \vec{q}}] \right) D_{\vec{q}'}^\vec{p}'. \tag{26}
\]

Above, observe that conjugating \( O \) by the dimension \( \binom{n}{k} \) unitary \( U_\eta(u) \) is equivalent to conjugating \( O \) by the much smaller dimension \( \binom{k}{n} \) unitary \( U_k(u) \).

II. TOMOGRAPHIC COMPLETENESS

A well-determined inversion of the measurement channel requires the choice of random bases to be tomographically complete [6]. In other words, any Hermitian \( \eta \)-particle \( n \)-mode fermion state \( \rho \) must be shown to be some linear combination

\[
\rho = \sum_j \alpha_j U_\eta(u_j^\dagger) \Pi_{z_j} U_\eta^\dagger(u_j) = \sum_j \alpha_j U_\eta(u_j) \Pi_{[\eta]} U_\eta^\dagger(u_j), \tag{27}
\]

of fermion rotation \( U_\eta(u_j^\dagger) \) generated by unitaries \( u_j^\dagger \) with coefficients \( \alpha_j \). Note that we may replace \( \Pi_{z_j} \) with \( \Pi_{[\eta]} \), or in fact any diagonal operator without loss of generality, as there always exists a permutation matrix \( v \), such that \( \Pi_z = U_\eta(v_\omega) \Pi_{[\eta]} U_\eta^\dagger(v_\omega) \). We may then collect \( U_\eta(u_j^\dagger) U_\eta^\dagger(v_\omega) = U_\eta(u_j^\dagger) U_\eta^\dagger(v_\omega) = U_\eta(u_j) \) following the homomorphism Equation (21). We now prove that the decomposition of \( \rho \) in Equation (27) is always achievable.

**Theorem 2** (Tomographic completeness). Any \( n \)-mode \( \eta \)-particle fermion density matrix \( \rho \) is a linear combination of diagonal operators conjugated by some element \( U_\eta(u) \in \wedge^k U_n \). As in Equation (27).

**Proof.** First, observe that \( \rho = \sum_{\vec{p}, \vec{q} \in S_{n,n}} \rho_{\vec{p}, \vec{q}} |\vec{p}\rangle \langle \vec{q}| \) where \( |\vec{p}\rangle \langle \vec{q}| = D_{\vec{q}}^\vec{p} \) forms a complete basis for \( \rho \), and can be written as a sum of Hermitian operators \( D_{\vec{q}, \phi}^\vec{p} \) like

\[
D_{\vec{q}, \phi}^\vec{p} = \frac{1}{2} \left( D_{\vec{q}, \phi}^\vec{p} - i D_{\vec{q}, \phi}^\vec{p} \right), \tag{28}
\]

Hence for any \( \rho \), it suffices to show the existence of a decomposition

\[
D_{\vec{q}, \phi}^\vec{p} = \sum_j \alpha_j U_\eta(u_j) \Pi_{z_j} U_\eta^\dagger(u_j), \tag{29}
\]

for any \( \vec{p}, \vec{q}, \phi \).

Second, it suffices to consider \( \vec{k}\)-RDMs \( D_{\vec{q}}^\vec{p} \) where \( \vec{p} \) and \( \vec{q} \) have no elements in common. In the trivial case where \( \vec{p} = \vec{q} \), Equation (29) is automatically satisfied as \( D_{\vec{q}}^\vec{q} = \hat{n}_\vec{q} \) is diagonal. Otherwise, if \( \vec{p} \cap \vec{q} = \vec{z} \) has more than zero elements, we may always express \( D_{\vec{q}}^\vec{p} = (-1)^x \hat{n}_\vec{z} D_{\vec{q}}^\vec{p} \vec{z} \) with some sign depending on the order \( x \) of the permutation that anti-commutes out the number operators \( \hat{n}_\vec{z} \). Now assuming that \( D_{\vec{q}, \phi}^\vec{p} \) is of the form Equation (29) where \( u_j \) is identity on indices in \( \vec{z} \) implies that \( D_{\vec{q}, \phi}^\vec{p} \) also has the same representation as the number operators \( \hat{n}_\vec{z} \) are already linear combinations of some \( \Pi_{\vec{q}} \) and commute with \( U_\eta(u_j) \).

Third, it suffices to restrict the number of particles to \( \eta = k \). Suppose we have found some \( D_{\vec{q}}^\vec{p} = \sum_j \alpha_j U_\eta(u_j) \Pi_{[k]} U_\eta^\dagger(u_j) \) in the form of Equation (29). Note that \( \Pi_{[k]} \) is a product of number operators, and is diagonal. Hence Equation (25) implies that for any \( \vec{q} \), \( D_{\vec{q}}^\vec{p} = \sum_j \alpha_j U_\eta(u_j) D_{[2k]}^\vec{p} \Pi_{[k]} U_\eta^\dagger(u_j) \).

Finally, we show that in the space of \( \vec{k}\)-particles, the \( \vec{k}\)-RDM \( D_{\vec{q}, \phi}^\vec{p} \) has a rank-2 decomposition. It also suffices to assume that \( \vec{p} = [k] \) and \( \vec{q} = [2k]\setminus[k] = (k + 1, \ldots, 2k) \) as \( D_{\vec{q}, \phi}^\vec{p} = U_k(v) D_{[2k]}^\vec{p} \Pi_{[2k]\setminus[k] \phi} U_k^\dagger(v) \) for some permutation matrix \( v \). To diagonalize the \( D_{\vec{q}, \phi}^\vec{p} \), observe that it has only two eigenvectors \( |\phi_+\rangle = \frac{1}{\sqrt{2}} (|\vec{p}\rangle \pm e^{-i\phi/2} |\vec{q}\rangle) \), with non-zero eigenvalues. Hence

\[
D_{\vec{q}, \phi}^\vec{p} = |\phi_+\rangle \langle \phi_+| - |\phi_-\rangle \langle \phi_-|. \tag{30}
\]
Let us find a fermion rotation that rotates $U_k(w_\phi) |\bar{\phi}\rangle = |\phi_+\rangle$ and $U_k(w) |\bar{q}\rangle = |\phi_-\rangle$. From Equation (20), we see that $w_\phi$ must satisfy the following constraints

$$
\frac{1}{\sqrt{2}} \left( e^{i\phi/2} |\bar{\phi}\rangle + e^{-i\phi/2} |\bar{q}\rangle \right) = \sum_{\bar{p} \in S_n,k} \det \left[ (w_\phi)_{\bar{p}\bar{q}} \right] \left| \bar{p}\rangle \right>,
$$

where $I_k$ is the dimension-$k$ identity matrix.

$$
\frac{1}{\sqrt{2}} \left( e^{i\phi/2} |\bar{\phi}\rangle - e^{-i\phi/2} |\bar{q}\rangle \right) = \sum_{\bar{q} \in S_n,k} \det \left[ (w_\phi)_{\bar{q}\bar{q}} \right] \left| \bar{q}\rangle \right>.
$$

As the determinant is zero for linearly dependent columns or rows, we see by inspection that a solution is

$$
w_\phi = \frac{1}{\sqrt{2}} \begin{bmatrix}
                  e^{i\phi/2} I_k & e^{i\phi/2} I_k \\
                  e^{-i\phi/2} I_k & -e^{-i\phi/2} I_k 
\end{bmatrix},
$$

where $k$ is the dimension-$k$ identity matrix.

$$
D_{[2k]\{k\};\phi}^{[k]} = U(w_\phi) \left( \langle [k] | [k] \rangle - \langle [2k] | [k] \rangle \langle [2k] | [k] \rangle \right) U^\dagger(w_\phi).
$$

Altogether, we obtain the general case, where there $n$ modes and $\eta$ particles, the $k$-RDM $D_{[\bar{p},\bar{q}];\phi}^{[\bar{p},\bar{q}]}$ with parameters $\bar{p} \cap \bar{q} = \bar{z}$ corresponding to $\dim(\bar{z})$ elements in common and $\bar{k}' = k - \dim(\bar{z}) > 0$ element not in common, as follows.

$$
D_{[\bar{p},\bar{q}];\phi}^{[\bar{p},\bar{q}]} = U(v w_\phi) \left( \hat{n}_{[k]} - \hat{n}_{[2k] \{ k \}} \right) \hat{n}_{[2k'] + \dim(\bar{z})} \left| [2k] \{ k \} \right> \left< [2k] \{ k \} \right| U^\dagger(v w_\phi)
$$

$$
= \sum_{j \in (\bar{p},\bar{q})} U(v_j w_\phi) \hat{n}_{[k]} U^\dagger(v_j w_\phi)
$$

$$
w_\phi = \frac{1}{\sqrt{2}} \begin{bmatrix}
                  e^{i\phi/2} I_{k'} & e^{i\phi/2} I_{k'} \\
                  e^{-i\phi/2} I_{k'} & -e^{-i\phi/2} I_{k'} 
\end{bmatrix} \bigoplus \mathcal{I}_{\{[n] \{ 2k'\}}.
$$

Hence, we conclude that any $k$-RDM

$$
D_{[\bar{p},\bar{q}]}^{[\bar{p},\bar{q}]} = \begin{cases}
U_k(v) D_{[k]}^{[k]} U_k^\dagger(v), & k' = 0, \\
\sum_{j=1}^4 \alpha_j U(w) D_{[k]}^{[k]} U^\dagger(w), & k' > 0,
\end{cases}
$$

$$\alpha = \frac{1}{2} (1, 1, -i, -i),
$$

$$w = (v_p w_0, v_q w_0, v_p v_q w_{p/2}, v_q v_p w_{q/2}).
$$

is a linear combination of at most four diagonal $k$-RDMs $D_{[k]}^{[k]}$ conjugated by single-particle basis rotations $U(w_j)$.

III. INVERSE MEASUREMENT CHANNEL

In this section, we invert the measurement channel with the assurance from Section II that this is possible in principle given that single-particle rotations are tomographically complete. Following Equation (27), the measurement channel for any quantum state is

$$
\mathcal{M}_{\Lambda \cup \mathcal{U}_n} [\rho] = \mathcal{M}_{\Lambda \cup \mathcal{U}_n} \left[ \sum_j \alpha_j U_\eta(u_j) \Pi_{[\eta]} U_\eta^\dagger(u_j) \right]
$$

$$
= \sum_j \alpha_j U_\eta(u_j) \mathcal{M}_{\Lambda \cup \mathcal{U}_n} \left[ \Pi_{[\eta]} \right] U_\eta^\dagger(u_j).
$$

Above, we apply linearity of the measurement channel, and commute the fermion rotations out of the measurement channel by a change of variables in the Haar integral of the twirling channel Equation (8). Hence, for any state $\rho$, inverting the measurement channel reduces to evaluating $\mathcal{M}_{\Lambda \cup \mathcal{U}_n}^{-1} \left[ \Pi_{[\eta]} \right]$ on just a single basis state. Below, Theorem 3 evaluates $\mathcal{M}_{\Lambda \cup \mathcal{U}_n}^{-1} \left[ \Pi_{[\eta]} \right]$ in a useful form, first by finding the eigenoperators of $\mathcal{M}_{\Lambda \cup \mathcal{U}_n}$, and second by expressing $\Pi_{[\eta]}$ as a linear combination of these eigenoperators.

**Theorem 3** (Inverse measurement channel). For any $\eta$ fermions on $n$-modes, the inverse measurement channel $\mathcal{M}_{\Lambda \cup \mathcal{U}_n}^{-1}$ has eigenoperators and eigenvalue

$$\forall \bar{x} \cap \bar{y} = 0, \quad \hat{n}_{\bar{x},\bar{y}} = \prod_{j=1}^d (\hat{n}_{x_j} - \hat{n}_{y_j}),
$$

$$\mathcal{M}_{\Lambda \cup \mathcal{U}_n}^{-1} \left[ \Pi_{[\eta]} \right] = \eta \sum_{d=0}^\eta \left( \begin{array}{c} n+1 \\ d \end{array} \right) \hat{n}_{\bar{x},\bar{y}}.
$$

**Proof.** From Equation (7), the measurement channel becomes

$$
\mathcal{M}_{\Lambda \cup \mathcal{U}_n} \left[ \Pi_{[\eta]} \right] = \left( \begin{array}{c} \eta \\ \eta \end{array} \right) \text{Tr}_1 \left[ \mathcal{T}_{2 \Lambda \cup \mathcal{U}_n} \left( \Pi_{[\eta]} \otimes I \right) \right],
$$

$$\mathcal{T}_{n \Lambda \cup \mathcal{U}_n} \equiv \int \left( U_\eta(u) \Pi_{[\eta]} U_\eta^\dagger(u) \right) \otimes \text{dHaar}(U_n).
$$

The first step is evaluating the twirling channel from Equation (8). In the second equality above, we use the fact that $|\bar{z}_\eta \rangle \langle \bar{z} | = U_\eta(x_\eta) \Pi_{[\eta]} U_\eta^\dagger(x_\eta)$ followed by a change of variables does not affect integration over the Haar measure. As $\Pi_{[\eta]}$ is diagonal, it suffices to evaluate only diagonal components of $\mathcal{T}_{2 \Lambda \cup \mathcal{U}_n}$. Each matrix entry of the fermion rotation $U_\eta(u)$ is a determinant of the $\eta \times \eta$ submatrix $u_{\bar{x},\bar{y}}$. By the Leibniz formula, det $[u_{\bar{x},\bar{y}}]$ is a
linear combination of \( \eta \) products of entries of \( u \). Hence \( \mathcal{T}_{\eta \land \mathcal{U}_n} \) is a linear combination of the Haar integral of \( 2^n \eta \) products of entries from \( u \) or \( u^\dagger \), which are in turn linear combinations of Weingarten functions [25]. Following an involved combinatorial proof in Theorem 8 of Appendix A, we find that diagonal components of the twirling channel are

\[
\mathcal{T}_{2, \land \mathcal{U}_n} = \sum_{\vec{p}, \vec{q} \in S_{n, \eta}} f(|\vec{p} \land \vec{q}|) \Pi_{\vec{p}} \otimes \Pi_{\vec{q}} + \cdots ,
\]

(48)

As \( f(|\vec{p} \land \vec{q}|) \) has the same value for all states with the same number of matching elements, the measurement channel separates into a sum of projectors

\[
\mathcal{M}_{\eta \land \mathcal{U}_n}[\Pi_{\vec{p}}] = \left( \binom{n}{\eta} \prod_{k=0}^{\eta} f(k) \text{Sim}_k (\Pi_{\vec{p}}) \right),
\]

(50)

\[
\text{Sim}_k (\Pi_{\vec{p}}) = \sum_{\vec{q} \in S_{n, \eta} : |\vec{p} \land \vec{q}| = k} \Pi_{\vec{q}}.
\]

(51)

In Lemma 4, we show that \( \text{Sim}_k (\Pi_{\vec{p}}) = \sum_{j=0}^{\eta} \binom{-1}{j+k} \binom{1}{\eta} \binom{n}{j} \binom{n+1}{\eta} \binom{\eta}{\eta} \) is a linear combination of elementary symmetric polynomials. Substituting into Equation (50) and applying the identity

\[
\sum_{k=0}^{\eta} \binom{-1}{j+k+1} \binom{1}{\eta-k} \binom{n}{k} = \binom{\eta}{j}^{-1},
\]

we get

\[
\mathcal{M}_{\eta \land \mathcal{U}_n}[\Pi_{\vec{p}}] = \sum_{j=0}^{\eta} \binom{\eta}{j} \binom{n+1}{\eta} \binom{n}{j},
\]

(52)

This representation allows us to identify the eigenoperators of \( \mathcal{M}_{\eta \land \mathcal{U}_n} \) by applying identity \( \text{Tr} e_k (A, X_2, \cdots) = e_k (B, X_2, \cdots) \) = \( (A - B) e_{\eta - 1} (X_2, \cdots) \). As \( \Pi_{\vec{p}} = \hat{\eta}_{p_1} \cdots \hat{\eta}_{p_\eta} = \eta \{ \{ \hat{\eta} \}_{\vec{p}} \} \), linearity of the measurement channel implies

\[
\mathcal{M}_{\eta \land \mathcal{U}_n} \left[ \prod_{j=1}^{d} (\hat{\eta}_{p_j} - \hat{\eta}_{g_j}) \hat{\eta}_{p_{d+1}} \cdots \hat{\eta}_{p_{\eta}} \right] = \prod_{j=1}^{d} (\hat{\eta}_{p_j} - \hat{\eta}_{g_j}) \sum_{j=d}^{\eta} \binom{\eta}{j} \binom{n+1}{\eta} \binom{n}{j}.
\]

(53)

Let us relabel the variables \( \vec{x} = (p_1, \cdots, p_d), \vec{z} = (p_{d+1}, \cdots, p_{\eta}). \) Note that \( \vec{x}, \vec{y}, \vec{z} \) have no elements in common. Hence,

\[
\mathcal{M}_{\eta \land \mathcal{U}_n} [\hat{\eta}_{\vec{x}, \vec{y}} | \hat{\eta}_{\vec{z}}] = \hat{\eta}_{\vec{x}, \vec{y}} \sum_{j=d}^{\eta} \binom{\eta}{j} \binom{n+1}{\eta} \binom{n}{j}.
\]

(54)

Without loss of generality, let \( \vec{x} \cup \vec{y} \) contain the last 2\( d \) elements of \( \eta \). Hence \( \vec{z} \in S_{n-2d, \eta-d} \). Now sum both sides over all values of \( \vec{z} \) using the summation identity

\[
\sum_{\vec{z} \in S_{n-2d, \eta-d}} \binom{n}{k} e_{\eta-d} (X_1, \cdots, X_{\eta}) = \binom{n-k}{\eta} e_{\eta-d} (X_1, \cdots, X_{\eta})
\]

on both sides. Hence,

\[
\mathcal{M}_{\eta \land \mathcal{U}_n} [\hat{\eta}_{\vec{x}, \vec{y}} | \hat{\eta}_{\vec{z}}] = \hat{\eta}_{\vec{x}, \vec{y}} \sum_{j=d}^{\eta} \binom{\eta}{j} \binom{n+1}{\eta} \binom{n}{j}.
\]

(55)

Observe that \( \hat{\eta}_{\vec{x}, \vec{y}} | \hat{\eta}_{\vec{z}} \) is non-zero only if \( \vec{z} \) contains \( \eta-d \) elements of \( \vec{x} \) and \( \vec{y} \). Hence for any state \( |\vec{p}\rangle \) where \( \vec{p} \) has \( \eta-d \) elements in \( [n-2d], e_{\eta-d} (\hat{\eta}_{1}, \cdots, \hat{\eta}_{n-2d}) |\vec{p}\rangle = \binom{\eta}{\eta-d} |\vec{p}\rangle \). Thus

\[
\mathcal{M}_{\eta \land \mathcal{U}_n} [\hat{\eta}_{\vec{x}, \vec{y}} | \hat{\eta}_{\vec{z}}] = \hat{\eta}_{\vec{x}, \vec{y}} \sum_{j=d}^{\eta} \binom{\eta}{j} \binom{n+1}{\eta} \binom{n}{j}.
\]

(56)

We then obtain Equation (42) by a trivial inversion.

Evaluating \( \mathcal{M}_{\eta \land \mathcal{U}_n}^{-1} [\hat{\eta}_{\vec{x}, \vec{y}}] \) requires us to express \( \Pi_{\vec{p}} \) as some linear combination of \( \hat{\eta}_{\vec{x}, \vec{y}} \). The symmetrized difference operators \( \hat{\eta}_{\vec{d}} \) Equation (45) are eigenoperators that enumerate over all combinations of \( \vec{x} \) and all permutations of \( \vec{y} \) consistent with \( \Pi_{\vec{p}} \). Hence, there exists a linear combination

\[
\Pi_{\vec{p}} = \sum_{d=0}^{\eta} d_{d} \hat{\eta}_{\vec{d}}, \quad d_{d} = \text{Tr} \left[ \Pi_{\vec{1}, \cdots, \eta} \hat{\eta}_{\vec{d}} \right] / \text{Tr} [\hat{\eta}_{\vec{d}}],
\]

(57)

where the last line follows from trace orthogonality \( \text{Tr} [\hat{\eta}_{\vec{d}}] \approx \delta_{\vec{d}} \).

It is helpful to expand \( \hat{\eta}_{\vec{d}} \) in terms of elementary symmetric polynomials.

\[
\hat{\eta}_{\vec{d}} = \sum_{j=0}^{d} (-1)^{j} \binom{d}{j} \left( \sum_{\vec{e} \in S_{d, \eta-j}} \left( \sum_{\vec{e} \in S_{d, d-j}} \binom{\eta-j}{\eta-j} \binom{n}{j} \right) \right. \\times \left. \sum_{\vec{e} \in S_{d, d-j}} \hat{\eta}_{e_1} \cdots \hat{\eta}_{e_{d-j}} \right) \hat{\eta}_{\eta+1} \cdots \hat{\eta}_{n}.
\]

(58)

To evaluate \( \text{Tr} \left[ \Pi_{\vec{1}, \cdots, \eta} \hat{\eta}_{\vec{d}} \right] \), note that \( \Pi_{\vec{1}, \cdots, \eta} e_{\eta} (\hat{\eta}_{1+1}, \cdots, \hat{\eta}_{n}) \) = \( \delta_{\vec{d}} \) for any basis state with \( \eta \) particles and that \( \text{Tr} \left[ \Pi_{\vec{1}, \cdots, \eta} e_{\eta} (\hat{\eta}_{1}, \cdots, \hat{\eta}_{\eta}) \right] = \binom{\eta}{\eta} \). Hence

\[
\text{Tr} \left[ \Pi_{\vec{1}, \cdots, \eta} \hat{\eta}_{\vec{d}} \right] = \binom{\eta}{\eta}! \binom{n}{n-\eta-d}! \binom{\eta}{\eta}.
\]

(59)

Evaluating \( \text{Tr} [\hat{\eta}_{\vec{d}}] \) is significantly more challenging, and we leave most details to Lemma 14. There, we show
that taking the square of Equation (58) leads to the sum,
\[
\text{Tr} \left[ \hat{n}_d^2 \right] = \frac{\eta![(n-\eta)!](\eta-s)!}{(n-\eta-s)!(\eta-d)!^2(n-\eta-d)!^2} \min(n,\eta-n) \times \sum_{s=0}^{\min(n,\eta-n)} f_{\eta,d}(s,j) \right)^2,
\]
and hence, from Equation (9), the estimator for any observable \(O\) is
\[
\langle \hat{O} \rangle = \text{Tr} \left[ OU_{\eta}^\dagger(u)M_{\lambda\eta \eta}^{-1} \Pi_{\omega} U_{\eta}(u) \right].
\]

However, this expression is not computationally efficient as the right-hand side of Equation (43) for \(M_{\lambda\eta \eta}^{-1} \Pi_{\omega} \) is a sum of exponentially many terms, and each operator in the trace above has exponentially large dimension \((\eta)^n \times (\eta)^n\). However, we now show below in Theorem 5 that for observables that are linear combination of \(k\)-RDMs, as in Equation (13), the estimator Equation (67) simplifies to multiplying at most 4 dimension \((\eta)^k \times (\eta)^k \times (\eta)^k \times (\eta)^k\) matrices, and is hence efficient for any fixed \(k\). We then go further in Section IV A to show that efficient evaluation with respect to \(k\) is also possible by modifying a recent technique based on polynomial interpolation of Pfaffians [19].

Furthermore in the special case where \(O = D_{ij}^p\) is just a single \(k\)-RDM, the single shot estimate Theorem 5 simplifies to
\[
\langle \hat{D}_{ij}^p \rangle = \langle \hat{q}| U_{k}^\dagger(v_s^z u) E_{\eta,k} U_k(v_s^z u) |\hat{p}\rangle.
\]

Hence the single evaluation of
\[
U_{k}^\dagger(v_s^z u) E_{\eta,k} U_k(v_s^z u) = \sum_{\hat{p}, \hat{q} \in S_{\eta,k}} |\hat{q}\rangle \langle \hat{p}| \langle \hat{D}_{ij}^p \rangle,
\]
simultaneously estimates all \(k\)-RDMs.

**Theorem 5 (Estimator for \(k\)-RDMs).** Let \((u, \tilde{z})\) be a classical shadow of \(p\). Let the observable \(O = \sum_{\hat{p}, \hat{q} \in S_{\eta,k}} o_{\hat{p}, \hat{q}} D_{ij}^p\). Then the single-shot estimator is
\[
\langle \hat{O} \rangle = \text{Tr} \left[ O U_{k}^\dagger(v_s^z u) \cdot E_{\eta,k} \cdot U_k(v_s^z u) \right],
\]
\[
E_{\eta,k} = \sum_{\hat{r}, \hat{s} \in S_{\eta,k}} |\hat{r}\rangle \langle \hat{s}| \langle \hat{q}| \langle \hat{p}| \langle \hat{D}_{ij}^p\rangle,
\]
when \(s' = |\hat{r} \cap \hat{q}|\) and \(v_{\tilde{z}}\) is any permutation that maps elements of \([\eta]\) to \(\tilde{z}\).

**Proof.** The inverse measurement channel on \(\Pi_{\tilde{z}} = U_{\eta}^\dagger(v_s^z \Pi_{[\eta]} U_{\eta}(v_s^z))\) can be expressed as one on \(\Pi_{[\eta]}\) through
\[
M_{\lambda\eta \eta}^{-1} \Pi_{\tilde{z}} = U_{\eta}^\dagger(v_s^z) M_{\lambda\eta \eta}^{-1} \Pi_{[\eta]} U_{\eta}(v_s^z). \tag{72}
\]
The estimator Equation (67) combined with the expression \(M_{\lambda\eta \eta}^{-1} \Pi_{[\eta]}\) from Theorem 3, is
\[
\langle \hat{O} \rangle = \sum_{d=0}^{\eta} a_d \left( \frac{n+1}{d} \right) \text{Tr} \left[ U_{\eta}(v_s^z u) O U_{\eta}^\dagger(v_s^z u) \tilde{n}_d \right]. \tag{73}
\]
To simplify notation, let \(w = v_s^z u\). As \(\tilde{n}_d\) is diagonal, only the diagonal components of \(U_{\eta}(w) O U_{\eta}^\dagger(w)\) have non-zero contributions to the trace. When \(O\) from Equation (13)

**IV. EFFICIENT ESTIMATION FROM FERMION SHADOWS**

In the previous section, we found an expression for the inverse measurement channel, which provides an unbiased single-shot estimate \(\hat{\rho}_{u,\tilde{z}}\) of the quantum state \(\rho\)
is a sum of $k$-RDMs, Equation (26) tells that diagonal components of
\[
U_n(w)OU_n^\dagger(w) = \sum_{\vec{r} \in S_{n,k}} \left( U_k(w) \cdot \eta \cdot U_k^\dagger(w) \right) \vec{r}_\eta + \cdots.
\]
(74)

Hence, the single-shot estimate is
\[
\langle \hat{O} \rangle = \text{Tr} \left[ U_k(w) \cdot \eta \cdot U_k^\dagger(w) \cdot E_{n,k} \right],
\]
\[
E_{n,k} = \sum_{\vec{r} \in S_{n,k}} |\vec{r} \rangle \langle \vec{r}| \text{Tr} \left[ \hat{n}_\eta \hat{n}_d \right].
\]
(75)

(76)

Using the cyclic property of the trace, this matches the form of Equation (70).

However, this evaluation is still not efficient as the estimation matrix $E_{n,k}$ is still a sum over exponentially many terms through $n_d = \sum_{\vec{r} \in S_{n,k}} \sum_{\eta \in S_{n||[\eta]} \cap \eta} \vec{n}_\eta \vec{r}_\eta$. The sum over permutations implies that the trace has a value that depends on $\vec{r}$ only through the number of elements that are not in $[\eta]$. Suppose $\vec{n}_\eta$ has $k - s = |\vec{r} \cap [\eta]|$ elements that overlap with $[\eta]$ and $s = |\vec{r} \setminus [\eta]|$ elements that overlap with $[n] \setminus [\eta]$. Then let
\[
E_{n,k} = \sum_{\vec{r} \in S_{n,k} : |\vec{r} \cap [\eta]| = s} \sum_{\eta \in S_{n||[\eta]} \cap \eta} |\vec{r} \rangle \langle \vec{r}|, \tag{77}
\]
\[
E_{n,k,s} = \text{Tr} \left[ \hat{n}_\eta \hat{n}_d \right] = \text{Tr} \left[ \hat{n}_{(k-s)} \hat{n}_\eta \eta_{[s]} \hat{n}_d \right].
\]
(78)

By expressing $\vec{n}_d$ in terms of elementary symmetric polynomials Equation (45), we obtain
\[
E_{n,k,s} = \sum_{d'=0}^{d} \frac{d!}{(d-d')!} \frac{(n-d)!}{(n-k)!} \times \frac{(n-s)!}{(n-k-s)!} \times \frac{(k-s)!}{(k-d)!}
\]
\[
\times \frac{(s)!}{(s-k)!} \times \left( \sum_{\vec{r} \in S_{n,k} : |\vec{r} \cap [\eta]| = s} \sum_{\eta \in S_{n||[\eta]} \cap \eta} |\vec{r} \rangle \langle \vec{r}| \right) \tag{79}
\]

Now, observe that $\vec{n}_\eta^2 = \vec{n}_j$ and that some of the number operators in $\hat{n}_{(k-s)} \hat{n}_\eta \eta_{[s]}$ may be identical to some of the terms in the symmetric polynomials. Thus we separate the sums in $e_{d-d'}(\cdot \cdot \cdot)$ and $e_{d'}(\cdot \cdot \cdot)$ into cases where the number operator indices contain $x'$ and $y'$ elements of $[k-s]$ and $[n-s]$ respectively, that is
\[
E_{n,k,s,d'} = \sum_{x'=0}^{k-s} \sum_{y'=0}^{s} \frac{(k-s)!}{(d-d')!} \frac{(n-s)!}{(n-k-s)!} \times \frac{(s)!}{(s-k)!} \tag{81}
\]
\[
\times \left( \sum_{\vec{r} \in S_{n,k} : |\vec{r} \cap [\eta]| = s} \sum_{\eta \in S_{n||[\eta]} \cap \eta} |\vec{r} \rangle \langle \vec{r}| \right).
\]

Combining all these expressions,
\[
E_{n,k,s} = \sum_{d=0}^{n} \sum_{d'=0}^{k-s} \sum_{x'=0}^{d} \sum_{y'=0}^{s} \cdots \tag{82}
\]
is a quadruple sum over hypergeometric terms that we simplify in Lemma 15 to obtain Equation (71).
to other linear combination of Majorana operators
\[ U(u)\gamma_p U^\dagger(u) = \sum_q \tilde{u}_{p,q} \gamma_q, \]  
\[ (\tilde{\gamma}_p)_{\gamma_q} = \sum_q \tilde{u}_{p,q} \gamma_q, \]  
(89)

More generally, given any real orthogonal matrix \( R \in O_{2n} \), let us overload the notation for \( U \) with
\[ U(R)\gamma_p U^\dagger(R) = \sum_q R_{p,q} \gamma_q. \]  
(91)

Elementary symmetric polynomials of number operators \( e_j' \) can be shown to be linear combinations of \( \{ \eta \} \) for \( j' \in [0, j] \). From the generating function
\[ \prod_{j=0}^{\eta} (\kappa - \lambda \hat{n}_j) = \sum_{j=0}^{\eta} \kappa^{n-j} (1-\lambda^j) \eta_j \{ \eta \} \],  
(92)

for elementary symmetric polynomials, one can show that
\[ \prod_{j=0}^{\eta} \left( \kappa - \frac{\lambda}{2} - i \frac{\lambda}{2} \right) \]  
\[ = \sum_{\alpha=0}^{\eta} \left( \kappa - \frac{\lambda}{2} \right)^{\eta-\alpha} \left( \frac{i}{\lambda} \right)^{\alpha} e_\alpha \{ \beta \} \eta. \]  
(93)

The estimate \( \hat{\rho} = \hat{\rho} (\Lambda \otimes Y) = \hat{\rho} [k] \) for \( k \) particles is then a linear combination of various degrees of elementary symmetric polynomials of Majorana bivectors
\[ \langle \hat{n}_{[k]} \rangle_{\gamma} = \sum_{j=0}^{\eta} \alpha_{n,k,j} \text{Tr}_k \left[ \hat{n}_{[k]} U_k^\dagger(u) \{ \beta \}_{\gamma} U_k(u) \right], \]  
(97)

\[ \alpha_{n,k,j} = (-1)^s \sum_{x=0}^{k} (-1)^s f_{k,s}(j)^{2s} F_{j,k,s}^{\dagger}. \]  
(98)

with some coefficients \( \alpha_{n,k,j} \). The speedup we present in this section arises from an improved method for computing in \( O(nk^2) \) time traces of the form
\[ \text{Tr}_k \left[ \hat{n}_{[k]} U(u) e_j \{ \beta \}_{\gamma} U^\dagger(u) \right]. \]  
(99)
Hence the following fermionic gaussian is a linear combination of the symmetric polynomials \( e_j (\{ \beta \}_{[\eta]} ) \) seen in Equation (95)

\[
\rho_{\eta}(\kappa) \doteq \rho (\kappa I_{[\eta]} \otimes Y) = \sum_{j=0}^{\eta} (i\kappa)^j e_j (\{ \beta \}_{[\eta]} ). \tag{107}
\]

Thus, a single evaluation of

\[
\text{Tr} \left[ \rho_k U_k (u) \rho_{\eta}(\kappa) U_k^\dagger (u) \right] = \sum_{j=0}^{\eta} (i\kappa)^j \text{Tr} [U(u) \hat{n}_{[\eta]} U^\dagger (u) e_j (\{ \beta \}_{[\eta]} )] , \tag{108}
\]

is some linear combination of the desired quantity Equation (99). Evaluating this on \( O(\eta) \) different values of \( \kappa \) then provides enough information to compute all \( \text{Tr} [\Pi_{[\eta]} U(v) e_j (\{ \hat{n} \}_{[\eta]} ) U^\dagger (v)] \), e.g. by polynomial interpolation.

In the second step, we avoid using polynomial interpolation and find a faster approach. Observe that the traces we compute turn out to be Pfaffians of appropriately defined matrices.

\[
\text{Tr} \left[ \rho_k U_k (u) \rho_{\eta}(\kappa) U_k^\dagger (u) \right] = (-1)^{n-k} \text{Pf} [A(\kappa)] . \tag{109}
\]

\[
A(\kappa) \doteq \kappa I_{[\eta]} \otimes Y - \hat{u}^T \Lambda \otimes \hat{u} \tag{110}
\]

By taking high-order derivatives with respect to \( \kappa \), we are able to isolate the traces with individual elementary symmetric polynomials. For instance,

\[
\partial_{\kappa}^n \text{Tr} \left[ \rho_k U_k (u) \rho_{\eta}(\kappa) U_k^\dagger (u) \right] |_{\kappa=0} = x^n \tau^2 \text{Tr}_k \left[ \hat{n}_{[\eta]} U(u) e_x (\{ \beta \}_{[\eta]} ) U^\dagger (u) \right] . \tag{111}
\]

In the following, we present an efficient method to compute all derivatives of the Pfaffian in Equation (109). Observe that the derivatives of a Pfaffian in general is

\[
\partial \text{Pf}(A) = \frac{1}{2} \text{Pf}(A) \text{Tr} [A^{-1} \partial A] . \tag{112}
\]

In our case, the derivatives are

\[
\partial_{\kappa} \text{Pf}(A(\kappa)) = \frac{1}{2} \text{Pf}(A) \text{Tr} [A^{-1} (I_{[\eta]} \otimes Y)] , \tag{113}
\]

\[
\partial_{\kappa}^2 \text{Pf}(A(\kappa)) = \frac{1}{2} \partial_{\kappa} \text{Pf}(A) \text{Tr} [A^{-1} (I_{[\eta]} \otimes Y)] - \frac{1}{2} \text{Pf}(A) \text{Tr} [A^{-1} (I_{[\eta]} \otimes Y) A^{-1} (I_{[\eta]} \otimes Y)] , \tag{114}
\]

\[
\vdots = \vdots
\]

\[
\partial_{\kappa}^n \text{Pf}(A(\kappa)) = \frac{1}{2} \sum_{j=0}^{n-1} \binom{n-1}{j} \partial_{\kappa}^{n-j-1} (-1)^j \text{Pf}(A) \text{Tr} \left[ (A^{-1} (I_{[\eta]} \otimes Y))^{j+1} \right] . \tag{115}
\]

This recursion allows us to compute higher-order derivatives from lower-order derivatives. After computing all the traces \( \text{Tr} \left[ (A^{-1} (I_{[\eta]} \otimes Y))^j \right] |_{\kappa=0} \), the recursion for all derivatives \( \forall x \in [\eta] \), \( \partial_{\kappa}^n \text{Pf}(A) |_{\kappa=0} \) can be solved in \( O(n^2) \) time.

We now evaluate the trace. Observe that

\[
A(0) = A^{-1}(0) = -\hat{u}^T \Lambda \otimes Y \hat{u} . \tag{116}
\]

Hence, the trace

\[
\text{Tr} \left[ (A^{-1} (I_{[\eta]} \otimes Y))^j \right] |_{\kappa=0} = (-1)^j \text{Tr} \left[ ((\Lambda \otimes Y) (\hat{u} I_{[\eta]} \otimes Y \hat{u}^T))^j \right] . \tag{117}
\]

In principle, it suffices to evaluate the all eigenvalues of \( (\Lambda \otimes Y) (\hat{u} I_{[\eta]} \otimes Y \hat{u}^T) \). Computing eigenvalues of a \( 2n \times 2n \) matrix takes \( O(n^2) \) time and would enable the straightforward computation of the trace. Indeed, a similar approach was taken in [19] for the non-particle conserving case. However, we now highlight optimizations for our particle-conserving case that reduces the problem to finding the eigenvalues of an even smaller \( 2k \times 2k \) matrix. Using the identity \( \Lambda = 2I_{[k]} - I_{[n]} \)
$$\text{Tr} \left[ (A^{-1}(I_{[n]} \otimes Y))^j \right] |_{k=0}$$
$$= (-1)^j \text{Tr} \left[ (2(\tilde{u}^T I_{[k]} \otimes Y \tilde{v})(I_{[n]} \otimes Y) - (\tilde{u}^T I_{[n]} \otimes Y \tilde{v})(I_{[n]} \otimes Y))^j \right]$$
$$= (-1)^j \text{Tr} \left[ (-2(\tilde{u}^T I_{[k]} \otimes I_{[2]} \tilde{u})(I_{[n]} \otimes I_{[2]})) + I_{[n]} \otimes I_{[2]} \right]^j \right], \quad (118)$$

where \( \tilde{u} = -\text{Im}[u] \otimes I_{[2]} + \text{Re}[u] \otimes Y \). Hence using the binomial expansion and the cyclic property of the trace,

$$\text{Tr} \left[ (A^{-1}(I_{[n]} \otimes Y))^j \right] |_{k=0} = (-1)^j \sum_{y=0}^{j} (-2)^y \binom{j}{y} \text{Tr} \left[ (I_{[n]} \otimes I_{[2]}) + I_{[n]} \otimes I_{[2]} \right]$$
$$= (-1)^j \left[ \text{Tr} \left[ (I_{[n]} \otimes I_{[2]}) \cdot \sum_{y=1}^{j} (-2)^y \binom{j}{y} \left( (\tilde{u}^T I_{[k]} \otimes I_{[2]} \tilde{u})(I_{[n]} \otimes I_{[2]})) \right) \right] \right]$$
$$= (-1)^j \left[ 2\eta + \sum_{y=1}^{j} (-2)^y \binom{j}{y} \left( (I_{[k]} \otimes I_{[2]}) (\tilde{u}^T I_{[n]} \otimes I_{[2]} \tilde{u})(I_{[n]} \otimes I_{[2]})) \right) \right]. \quad (119)$$

**V. ERROR OF ESTIMATION**

We now evaluate the variance of our estimator from Section IV for any \( k \)-RDM. For brevity, we use the notation for the expectation \( E_u \equiv E_{u \sim U_\mu} \) and \( E_{u,z} \equiv E_{u \sim U_\mu} E_{z \sim U_{\mu u}} \). Consider an observable \( O = O_{tr} + \alpha I \) where \( O_{tr} \) is traceless. From the definition of variance for any estimate \( \langle \hat{O} \rangle = \text{Tr} [O \hat{\rho}_{u,z}] \), the variance

$$\text{Var} \left[ \langle \hat{O} \rangle \right] = E_{u,z} \left[ |\text{Tr} [O \hat{\rho}_{u,z}] - \text{Tr} [O \rho]|^2 \right]$$
$$= E_{u,z} \left[ |\text{Tr} [O_{tr} \hat{\rho}_{u,z}]|^2 \right] \quad (121)$$

only depends on the traceless component. An upper bound on the variance is then the state-dependent shadow norm

$$|O|_{\alpha,\rho}^2 \equiv E_{u,z} \left[ \text{Tr} [O_{tr} \hat{\rho}_{u,z}]^2 \right]. \quad (122)$$

As the traceless component of any \( k \)-RDM is

$$(D_{\alpha q}^p)_{tr} = D_{\alpha q}^p - \delta_{\alpha q} \frac{(n-k)}{(n)} I, \quad (123)$$
the shadow norm of any $k$-RDM is then
\[ \|D_\rho^p\|^2_{s,p} = \mathbb{E}_{u,z} \left( \|D_\rho^p\|^2 \right) - \delta_{\tilde{p},\tilde{q}} \left( \frac{(n-k)}{\eta} \right)^2 \left( \frac{(n)}{\eta} \right)^2, \]
where $\langle D_\rho^p \rangle = \text{Tr} \left[ D_\rho^p \tilde{u}_{a\xi} \right]$ is our single-shot estimator from Equation (70) in the previous section that implicitly depends on the shadow $(u, z)$. One may also define a state-independent shadow norm by maximizing $\|O\|^2_k = \max_{\rho} \|O\|^2_{\rho}$. Below, we prove that the average variance of estimating all $k$-RDMs is also a quantity independent of $\rho$ and also small.

**Theorem 6 (Error of estimation).** For all $\eta$-particle $n$-mode fermion states $\rho$, the average variance over all $k$-RDMs is upper-bounded by the average squared shadow norm
\[ \mathbb{E}_{\tilde{p},\tilde{q}} \left( \|D_\rho^p\|^2 \right)_{s,p} \leq \left( \frac{\eta}{k} \right) \left( 1 - \frac{\eta - k}{\eta} \right)^k \left( \frac{1 + n}{1 + n - k} \right). \]

**Proof.** Consider the case $\tilde{p} = \tilde{q}$, where the cross-term $\mathbb{E}_{u,z} \left[ \langle D_\rho^p \rangle \right] = \mathbb{E}_{u,z} \left[ \text{Tr} \left[ \tilde{u}_{\rho a\xi} \right] \right]$ in Equation (124) appears. Using the identity $\sum_{\tilde{p} \in S_{n,k}} \tilde{u}_{\rho} = \sum_{\tilde{p} \in S_{n,k}} e_k(\tilde{n}_1, \ldots, \tilde{n}_n) = e_k(\tilde{n}_1, \ldots, \tilde{n}_n)$, observe that on the space of $\eta$-particle states,
\[ e_k(\tilde{n}_1, \ldots, \tilde{n}_n) = \frac{(n-k)!}{(\eta)\eta} \cdot I. \]

Hence, the sum
\[ K = \sum_{\tilde{p} \in S_{n,k}} \mathbb{E}_{u,z} \left( \langle D_\rho^p \rangle \right) \leq \left( \frac{\eta}{k} \right) \left( \frac{n-k}{\eta} \right) \left( \frac{n}{\eta} \right), \]
and the sum of shadow norms over all diagonal $k$-RDMs
\[ \sum_{\tilde{p} \in S_{n,k}} \|D_\rho^p\|^2_{s,p} = \sum_{\tilde{p} \in S_{n,k}} \mathbb{E}_{u,z} \left( \langle D_\rho^p \rangle \right)^2 - K, \]
and the sum of shadow norms over all $k$-RDMs
\[ \sum_{\tilde{p},\tilde{q} \in S_{n,k}} \|D_\rho^p\|^2_{s,p} = \mathbb{E}_{u,z} \left[ \text{Tr} \left[ \left( U_k(vz\tilde{u}) E_{n,k} U_k(vz\tilde{u})^\dagger \right)^2 \right] \right] - K \]
\[ = \mathbb{E}_{\tilde{u},\tilde{z}} \left[ \text{Tr} \left[ \left( U_k(vz\tilde{u}) E_{n,k} U_k(vz\tilde{u})^\dagger \right)^2 \right] \right] - K \]
\[ = \text{Tr} \left[ E_{n,k}^2 \right] - \left( \frac{n-k}{\eta} \right)^2 \left( \frac{n}{\eta} \right)^2, \]
is state-independent, where in the second line, we substitute the estimator Equation (70), and in the last line, we use the cyclic property of traces to cancel all adjacent unitaries $U_k(vz\tilde{u})U_k(vz\tilde{u})^\dagger = I$. We then obtain Equation (125) by dividing Equation (129) by the number of terms $(k)^2$ in the sum.

From Equation (129), an upper bound on the average shadow norm is just $\mathbb{E}_{\tilde{p},\tilde{q}} \left( \|D_\rho^p\|^2 \right)_{s,p} \leq \frac{\text{Tr} \left[ E_{\eta,n,k}^2 \right]}{(n)^2} \leq Q_{n,\eta,k}$. From Theorem 5, $(\tilde{p} \parallel E_{n,k} \parallel \tilde{p}) = (-1)^{s} (k-s) \left( n^{n-\eta} \right)$, where $s = |\tilde{p} \setminus [\eta]|$. By writing the sum $\sum_{\tilde{p} \in S_{n,k}} \cdots = \sum_{s=0}^{k} \left( n-\eta \right) \left( n-\eta \right) \cdots$ and collecting terms,
\[ Q_{n,\eta,k} = \frac{n}{\eta} \sum_{s=0}^{k} \left( \frac{n}{\eta} \right) \left( \frac{n}{\eta} \right) \cdots \]
\[ \leq Q_{n,\eta,k} = \frac{n}{\eta} \sum_{s=0}^{k} \left( \frac{n}{\eta} \right) \left( \frac{n}{\eta} \right) \cdots \leq \frac{1}{\eta^n} \left( \frac{n}{\eta} \right) \left( \frac{n}{\eta} \right) \cdots \]
\[ \leq \frac{1}{\eta^n} \left( \frac{n}{\eta} \right) \left( \frac{n}{\eta} \right) \cdots \]
We arrive at the bound in Equation (125) by observing that the product on the right $\prod_{j=0}^{k} \left( \frac{n}{\eta} \right) \left( \frac{n}{\eta} \right) \cdots$ is state-independent, where in the second line, we substitute the estimator Equation (70), and in the last line, we use the cyclic property of traces to cancel all adjacent unitaries $U_k(vz\tilde{u})U_k(vz\tilde{u})^\dagger = I$. We then obtain Equation (125) by dividing Equation (129) by the number of terms $(k)^2$ in the sum.

**VI. CONCLUSION**

We have presented a technique to estimate all $k$-RDMs of fermion states extremely efficiently with an average error that depends only on the number of particles, in contrast to all prior methods which depend on the number of modes. Our main assumption that the state of interest has a definite number of particles applies to very
many systems of interest. On a quantum computer, our scheme may be applied with any fermion-to-qubit mapping so long as the random number-conserving single-particle rotations can be applied. Implementing our approach in the second-quantized representation also facilitates a straightforward approach to error mitigation by symmetry verification [27, 28] and can detect multiple errors—simply check that the measured state \( |z \rangle \) has \( n \)-particles.

Our estimator is also computationally efficient for all parameters. Many observables such as electronic structure or nuclear Hamiltonians only require \( k \leq 3 \). However, there are natural applications for large \( k \) as well. Consider the problem of estimating overlaps with arbitrary Slater determinants \( |q^\prime \rangle = U_\eta(w)|q \rangle \) for any \( w \in \mathcal{U}_n \), a key component of quantum-classical auxiliary-field quantum Monte Carlo [3]. For any pure state \( |\psi \rangle = \sum_{\vec{p} \in S_{n,\eta}} \psi_{\vec{p}} |\vec{p} \rangle \), add \( \eta \) more modes and prepare the state
\[
|\psi'\rangle = \frac{|\psi\rangle + |n + [\eta]\rangle}{\sqrt{2}}.
\]
Then the \( \eta \)-RDM \( U_\eta(w)D^{n+|\eta|}_q U_\eta^\dagger(w) \) has expectation
\[
\text{Tr} \left[ U_\eta(w)D^{n+|\eta|}_q U_\eta^\dagger(w) |\psi'\rangle \langle \psi'| \right] = \frac{\psi_{\eta}^2}{2}, \tag{133}
\]
which is half of the desired overlap with the Slater determinant \( |q^\prime \rangle \). Our approach simultaneously estimates all \( \eta \)-RDMs extremely efficiently using only \( 2^{n/\eta} \) samples on average according to Equation (131), which compares favorably to very recent work [19] that performs the same task using exponentially more \( O(\sqrt{n}/c^2) \) samples, through with a stronger per-RDM error guarantee rather than an average. Many variations on this idea are possible future directions to pursue. For instance, the number of additional modes required may also be reduced to as few as 1 by preparing \( |\psi'\rangle = \frac{|\psi\rangle + |n - [\eta + 1]\rangle}{\sqrt{2}} \) and estimating \( D^{n-[\eta+1]|\eta|}_q U_\eta^\dagger(w) \), or even to 0 when the sign is not important by estimating \( U_\eta(w)D^{n}_q U_\eta^\dagger(w) \).

As our estimator has no preferred basis, any rotated \( k \)-RDM \( U_\eta(w)D^{n}_q U_\eta^\dagger(w) \) may be estimated just as efficiently and easily as \( D^{n}_q \) even if they contain exponentially many terms in the computational basis. Even more general \( k \)-RDMs of the form \( U_\eta(w)D^{n}_q U_\eta^\dagger(w') \) where \( w \neq w' \) may also be estimated following Equation (70), though we leave the Pfaffian method in Section IV A for this case to a future analysis. This suggests that our approach is tailored to estimating observables of the form
\[
O = \sum_{j \in [\eta]} \alpha_j U_\eta(w_j)D^{n}_q U_\eta^\dagger(w_j'),
\]
similar to Equation (27), that either have a low-rank structure or are well-approximated by it, meaning that \( R \) is small and \( |\tilde{a}|_2 \) is minimized. As the upper-bound on the variance of our estimator was evaluated using the 2-fold twirling channel, this approach bounded the average variance across all \( k \)-RDMs rather than each \( k \)-RDM individually. We leave to future work the task of obtaining the shadow norm of linear combinations of \( k \)-RDMs such as \( O \), which would require a challenging evaluation of the 3-fold twirling operator for the group \( \Lambda \mathcal{U}_n \), followed by understanding the covariance of \( k \)-RDM estimation.

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other words, where

Theorem 8. For a Hermitian observable $\hat{f}$ acting on $\mathbb{C}^n$, the twirling operator $T_{\mathcal{U}}$ with respect to the Haar measure in $S_n$, is given by

$$T_{\mathcal{U},\mathbb{H}} \equiv \int \langle U(u) | \hat{f} | U(u) \rangle \otimes U(u) \text{d}u_{\text{Haar}}(\mathcal{U}),$$

where $|\hat{f}\rangle = |\hat{f}\rangle \rangle = \bigotimes_{k=1}^{n} |\hat{f}\rangle$ is a basis vector of $\mathcal{U}[n]$, and $|k\rangle$ are orthonormal bases for $\mathcal{U}_n$.

Definition 7 (Twirling operator). The twirling operator of degree $t$ on $\bigwedge_{k=1}^{n} \mathcal{U}_n$ with respect to the Haar measure on $\mathcal{U}_n$ is

$$T_{t,\mathcal{U}} \equiv \int \langle U(u) | \hat{f} \rangle \langle \hat{f} | U(u) \rangle \otimes U(u) \text{d}u_{\text{Haar}}(\mathcal{U}_n),$$

where $|\hat{f}\rangle = |\hat{f}\rangle \rangle = \bigotimes_{k=1}^{n} |\hat{f}\rangle$ is a basis vector of $\bigwedge_{k=1}^{n} \mathcal{U}_n$ and $|k\rangle$ are orthonormal bases for $\mathcal{U}_n$.

Theorem 8. Twirling operator

$$T_{2,\bigwedge\mathcal{U}_n} = \sum_{\vec{p}, \vec{q} \in S_n^2} f(\vec{p} \cap \vec{q}) \Pi_{\vec{p}} \otimes \Pi_{\vec{q}} + \sum_{\vec{p}, \vec{q} \in S_n^2} f(\vec{p}, \vec{q}) \langle \vec{p} \rangle \otimes \langle \vec{q} \rangle,$$

where for the diagonal terms, the structure factor $f(k) = \frac{1}{n^k} \langle \hat{f} \rangle$ and the form of $f(\vec{p}, \vec{q})$, of lesser interest, is detailed in Lemma 10.
Our derivation begins by expressing the twirling operator in the basis of Weingarten integrals.

**Definition 9** (Weingarten integral [25, Equation (1)]). The basis \( (\vec{i},\vec{j},\vec{j}') \) Weingarten integral of degree \( t \) on \( U_n \) is

\[
\int_{u \sim U_n} u_{i_1 j_1} \cdots u_{i_n j_n} u_{i'_1 j'_1} \cdots u_{i'_n j'_n} \, du = \sum_{\pi \in S_q} \delta_{\pi,\pi(j)} \delta_{\xi^{-1}(j),j} W_{\xi^{-1}} (\pi \xi^{-1}), \quad (A3)
\]

where \( S_q \) is the symmetric group on \( q \) elements, and \( W_{\pi^{-1}} (\xi^{-1}) = W_{\pi} (\xi^{-1}) = W_{\pi} (\xi^{-1}) \) is the so-called Weingarten function, which depends only on the conjugacy class of the permutation.

With the help of Weingarten integrals, we may evaluate the twirling operator and express then in a simpler form. We use the notation \( \vec{x} \oplus \vec{y} = (x_1, \ldots, x_{\dim(\vec{x})}, y_1, \ldots, y_{\dim(\vec{y})}) \) for list concatenation, and \( S_k \) for the symmetric group on \( k \) elements.

**Lemma 10** (Twirling operator structure factor). The twirling operator evaluates to

\[
\mathcal{T}_{t,\wedge U_n} = \sum_{\vec{p}, \vec{q} \in S_n, \eta} f(\vec{p}, \vec{q}) \bigotimes_{\theta \in [t]} |\vec{p}_\theta \rangle \langle \vec{q}_\eta|, \quad (A5)
\]

\[
f(\vec{p}, \vec{q}) = \sum_{\mu \in S_n^\wedge} \sum_{\nu \in S_n^\wedge} \sum_{\xi \in S_n} (-1)^{\mu} \prod_{\theta \in [t]} \det \left[ \Delta_{\vec{q}_\eta, \vec{p}_\theta} \right] W_{\mu \xi}(\mu \nu \xi), \quad (A6)
\]

where \( f \) is the structure factor, \( \vec{p} \equiv \bigoplus_{j \in [t]} \vec{p}_j \), \( \vec{q} \equiv \bigoplus_{j \in [t]} \vec{q}_j \), \( \Delta_{ij} = \delta_{ij} \), and \( \bigoplus_{j \in [t]} \vec{p}_j = \xi(\vec{p}) \), \( \mu = \bigoplus_{j \in [t]} \mu_j \), \( \nu = \bigoplus_{j \in [t]} \nu_j \).

\[
\mu \left( \bigoplus_{\theta \in [t]} \vec{x}_\theta \right) = \begin{pmatrix} x_{\mu,1}(1) & \cdots & x_{\mu,1}(t) \\ \vdots & \ddots & \vdots \\ x_{\mu,\eta}(1) & \cdots & x_{\mu,\eta}(t) \end{pmatrix}, \quad \nu \left( \bigoplus_{j \in [t]} \vec{x}_j \right) = \begin{pmatrix} x_{\nu,1}(1) & \cdots & x_{\nu,1}(t) \\ \vdots & \ddots & \vdots \\ x_{\nu,\eta}(1) & \cdots & x_{\nu,\eta}(t) \end{pmatrix}. \quad (A7)
\]

**Proof.** The twirling operator from Definition 7 is \( \mathcal{T}_{t,\wedge U_n} \equiv \int_{u \sim U_n} \left( U(u) |\vec{p} \rangle \langle \vec{q}| U^\dagger(u) \right) \otimes_t du. \) By expanding the fermion rotation using Equation (20),

\[
\mathcal{T}_{t,\wedge U_n} = \sum_{\vec{p}, \vec{q} \in S_n, \eta} \left[ \prod_{\theta \in [t]} \det [u_{\vec{p}_\theta \eta}]\det [u_{\eta \vec{q}_\theta}] \right] \int_{u \sim U_n} \prod_{\theta \in [t]} \det [u_{\eta \vec{q}_\theta}] \, du \bigotimes_{\theta \in [t]} |\vec{p}_\theta \rangle \langle \vec{q}_\eta|.
\]

Note that transposing a matrix does not change its determinant. We now expand the determinants into Weingarten integrals Definition 9 using the Leibniz formula

\[
\det [u_{\eta \vec{x}}] = \sum_{\tau \in S_n} (-1)^{\tau} \prod_{i \in [\eta]} (u^\dagger_{\tau(i) \eta} \vec{x}) = \sum_{\tau \in S_n} (-1)^{\tau} \prod_{i \in [\eta]} u^\dagger_{\tau(i) \eta} x_i, \quad (A9)
\]

\[
\det [u_{\vec{x} \eta}] = \sum_{\sigma \in S_n} (-1)^{\sigma} \prod_{i \in [\eta]} (u_{\sigma(\vec{x}) \eta}) = \sum_{\sigma \in S_n} (-1)^{\sigma} \prod_{i \in [\eta]} u_{x_{\sigma(i)} \eta}, \quad (A10)
\]

where \( (-1)^{\sigma} = \text{sgn}(\sigma) \) is parity of the permutation \( \sigma \). Above, we use the notation \( (\sigma(\vec{x}))_j = x_{\sigma(j)} = j \) for any vector \( \vec{x} \in \mathbb{Z}^n \). In particular, \( (\sigma(\vec{y}))_j = \eta_{\sigma(j)} = \sigma(j) \) since \( \vec{y} = (1, 2, \ldots, \eta) \). The following identity will be useful

\[
\det [\Delta_{\vec{x}, \vec{y}}] = \sum_{\sigma \in S_n} (-1)^{\sigma} \delta_{\vec{x}, \sigma(\vec{y})} = \sum_{\sigma \in S_n} (-1)^{\sigma} \prod_{i \in [\eta]} \delta_{x_i, y_{\sigma(i)}} = \begin{cases} (-1)^{\sigma}, & \vec{y} = \sigma(\vec{x}), \\ 0, & \text{otherwise}. \end{cases} \quad (A11)
\]
Hence the structure factor
\[
\begin{align*}
f(\vec{p}, \vec{q}) &= \int_{U^n} \sum_{\sigma, \tau} \frac{\det [\Delta_{\vec{p}_\sigma, \vec{q}_\tau}]}\det [\Delta_{\vec{p}_\sigma, \vec{q}_\tau}]}Wg^{\mu^n} (\xi \pi) \\
&= \sum_{\eta \in S_{\mu}^n} \frac{\det [\Delta_{\vec{p}_\eta, \vec{q}_{\pi \eta}^{\pi \eta}}]}\det [\Delta_{\vec{p}_\eta, \vec{q}_{\pi \eta}^{\pi \eta}}]}Wg^{\mu^n} (\xi \pi) \\
&= \sum_{\eta \in S_{\mu}^n} \frac{\det [\Delta_{\vec{p}_\eta, \vec{q}_{\pi \eta}^{\pi \eta}}]}\det [\Delta_{\vec{p}_\eta, \vec{q}_{\pi \eta}^{\pi \eta}}]}Wg^{\mu^n} (\xi \pi) \\
&= \sum_{\eta \in S_{\mu}^n} \frac{\det [\Delta_{\vec{p}_\eta, \vec{q}_{\pi \eta}^{\pi \eta}}]}\det [\Delta_{\vec{p}_\eta, \vec{q}_{\pi \eta}^{\pi \eta}}]}Wg^{\mu^n} (\xi \pi), \quad (A12)
\end{align*}
\]

Above, we use the notation \( \bigoplus_{\theta \in [t]} \vec{\varphi} = \pi(\vec{\varphi}^{\text{out}}) \) and \( \bigoplus_{\theta \in [t]} \vec{\varphi}^\xi = \xi(\vec{\varphi}) \).

We may simplify further as \( \det [\Delta_{\vec{p}_\eta, \vec{q}_{\pi \eta}^{\pi \eta}}] \) is non-zero only when \( \pi(\vec{\varphi}^{\text{out}}) = \bigoplus_{\theta \in [t]} \mu_\theta(\vec{\eta}) \) is a permutation that preserves the same set of terms \( \{ k \}_{k \in [n]} \) for each \( j \). The number of unique valid \( \pi \) is thus \( n! \eta_1 \eta_2 \cdots \eta_t \). Hence valid \( \pi \) decompose into \( \pi = \mu \nu \), where \( \nu \in S_{\nu}^{\nu} \) which swaps elements at the same position between different copies of \( \vec{\eta} \), and \( \mu \in S_{\mu}^{\mu} \) permutes within each \( \vec{\eta} \). More precisely,
\[
\begin{align*}
\mu \left( \bigoplus_{\theta \in [t]} \vec{x}_\theta \right) &= \left( \begin{array}{c}
x_{1, \mu_1(1)} \cdots x_{t, \mu_1(1)} \\
\vdots \quad \vdots \\
x_{1, \mu_\nu(\eta)} \cdots x_{t, \mu_\nu(\eta)}
\end{array} \right), \\
\nu \left( \bigoplus_{j \in [t]} \vec{x}_j \right) &= \left( \begin{array}{c}
x_{1, \nu_1(1)} \cdots x_{t, \nu_1(1)} \\
\vdots \quad \vdots \\
x_{1, \nu_t(\eta)} \cdots x_{t, \nu_t(\eta)}
\end{array} \right).
\end{align*}
\]

This decomposition exactly characterizes valid permutations without any over-counting as \( |S_{\nu}^{\nu}| |S_{\mu}^{\mu}| = (t!)^\nu (\eta t)!^\nu \).

Thus
\[
\begin{align*}
f(\vec{p}, \vec{q}) &= \sum_{\nu \in S_{\nu}^{\nu}} \sum_{\mu \in S_{\mu}^{\mu}} \sum_{\eta \in S_{\eta}^{\eta}} (-1)^\mu \det [\Delta_{\vec{p}_\eta, \vec{q}_{\pi \eta}^{\pi \eta}}] Wg^{\mu^n} (\xi \nu \mu) \\
&= \sum_{\nu \in S_{\nu}^{\nu}} \sum_{\mu \in S_{\mu}^{\mu}} \sum_{\eta \in S_{\eta}^{\eta}} (-1)^\mu Wg^{\mu^n} (\mu \nu \xi), \\
\end{align*}
\]

and we then apply the cyclic property \( Wg^{\mu^n} (\xi \nu \mu) = Wg^{\mu^n} (\mu \nu \xi). \)

We find for the structure factor \( f(\vec{p}, \vec{q}) \) that the case where \( \vec{q} \) is some permutation of \( \vec{p} \) occurs quite frequently. We may further simplify the twirling operator in this case.

**Lemma 11** (Twirling operator diagonal structure factor). The coefficient of diagonal components of the twirling operator
\[
\begin{align*}
\mathcal{T}_{\Lambda^n U^n} = \sum_{\vec{p} \in S_{\vec{p}}^{\vec{p}}} f(\vec{p}) |\vec{p}_\eta\rangle \langle \vec{p}_\eta| + \sum_{\vec{p} \neq \vec{q} \in S_{\vec{p}}^{\vec{q}}} f(\vec{p}, \vec{q}) \otimes |\vec{p}_\eta\rangle \langle \vec{q}_\eta|, \\
\end{align*}
\]
is the diagonal structure factor
\[
\begin{align*}
f(\vec{p}) &= \sum_{\nu \in S_{\nu}^{\nu}} \sum_{\gamma \in S_{\nu}^{\gamma}} \sum_{\mu, \chi \in S_{\mu}^{\mu}} (-1)^{\mu \chi} Wg^{\mu^n} (\mu \nu \gamma), \\
\end{align*}
\]
where \( \nu \in S_{\vec{p}}^{\vec{p}}, \ldots \), \( \gamma \) swaps matching elements between \( t \) copies of \( \vec{p} \), and \( \gamma \in S_{\nu}^{\nu} \), \( \vec{p} \) swaps matching elements between the \( t \) vectors \( \vec{p}_j \).

**Proof.** Observe that the twirling operator has unit trace, \( \text{Tr} [\mathcal{T}_{\Lambda^n U^n}] = 1 \). Using the expression for it from Lemma 10,
\[
\text{Tr} [\mathcal{T}_{\Lambda^n U^n}] = \sum_{\vec{p} \in S_{\vec{p}}^{\vec{p}}} f(\vec{p}, \vec{p}). \quad (A17)
\]

Let us define \( f(\vec{p}) \equiv f(\vec{p}, \vec{p}) \). Hence
\[
\begin{align*}
f(\vec{p}) &= \sum_{\mu \in S_{\mu}^{\mu}} \sum_{\nu \in S_{\nu}^{\nu}} \sum_{\eta \in S_{\eta}^{\eta}} (-1)^\mu \det [\Delta_{\vec{p}_\eta, \vec{p}_\eta}] Wg^{\mu^n} (\mu \nu \xi), \\
\end{align*}
\]
Now observe that \( \det \left[ \Delta_{\vec{p}_i, \vec{q}_j} \right] \) is non-zero only when \( \bigoplus_{\theta \in [\ell]} \vec{p}_\theta = \xi \left( \bigoplus_{\theta \in [\ell]} \vec{p}_\theta \right) \) is a permutation that preserves the same set of terms in \( \vec{p}_\theta \). Similar to the derivation of Equation (A13), valid \( \xi \) decomposes into \( \xi = \chi \gamma, \gamma \in S_{\vec{p}_1, \cdots, \vec{p}_i} \) which swaps matching elements between different \( \vec{p}_j \), and \( \chi \in S_{\vec{q}_1}^\ell \) permutes within each \( \vec{p}_j \). Thus

\[
f(\vec{p}) = \sum_{\nu \in S_t^\eta} \sum_{\gamma \in S_{\vec{p}_1, \cdots, \vec{p}_i}} \sum_{\mu, \chi \in S_{\vec{q}_1}^\ell} (-1)^{\mu \chi} W_{\gamma}^{\mu \chi} (\mu \nu \chi). \tag{A19}
\]

The diagonal structure factor in Lemma 11 contains many instances of Weingarten functions, each depending on permissible swaps between the vectors \( \vec{p}_j \). We now show that for each \( \eta \), there is only one unique sum.

**Lemma 12.** For all \( \eta \geq 0, t = 2, \vec{p}_1, \vec{p}_2 \in S_{n, \eta}, \)

\[
f(\vec{p}) = g_\eta (| \vec{p}_1 \cap \vec{p}_2 |) \Xi_{n, \eta}, \quad \Xi_{n, \eta} = \sum_{\nu \in S_t^\eta} \sum_{\mu, \chi \in S_{\eta}^\ell} (-1)^{\mu \chi} W_{\gamma}^{\mu \chi} (\mu \nu \chi), \tag{A20}
\]

\[
g_\eta(k) = (\eta!)^2 \frac{\eta + 1}{\eta - k + 1}. \tag{A21}
\]

**Proof.** We make use of the fact that the Weingarten function depends only on cycle structure of the permutation, which is uniquely determined by its conjugacy class. Hence we have the identities such as

\[
W_{\gamma}^{\mu \chi} (abc) = W_{\gamma}^{\mu \chi} (cab) = W_{\gamma}^{\mu \chi} (e^{-1}b^{-1}a^{-1}). \tag{A22}
\]

From Lemma 11, the structure factor

\[
f(\vec{p}) = \sum_{\nu \in S_t^\eta} \sum_{\gamma \in S_{\vec{p}_1, \vec{p}_2}} \sum_{\mu, \chi \in S_{\vec{q}_1}^\ell} (-1)^{\mu \chi} W_{\gamma}^{\mu \chi} (\mu \nu \chi). \tag{A23}
\]

Let us insert an identity term \( \mu \nu \chi \gamma = \mu \nu \chi \gamma^{-1} \chi \) and substitute \( \chi \mu \rightarrow \mu \) to obtain

\[
f(\vec{p}) = \sum_{\chi \in S_{\eta}^\ell} \sum_{\gamma \in S_{\vec{p}_1, \vec{p}_2}} \Xi_{n, \eta} (\chi \gamma^{-1}), \tag{A24}
\]

\[
\Xi_{n, \eta} (\tau) = \sum_{\mu \in S_{\eta}^\ell} \sum_{\nu \in S_{\vec{q}_1}^\ell} (-1)^{|\mu \nu \chi|} W_{\gamma}^{\mu \chi} (\mu \nu \tau). \tag{A25}
\]

Whereas \( \gamma \in S_{\vec{p}, \vec{q}} \) is a product of up to \( k = | \vec{p} \cap \vec{q} | \) 2-cycles \( (p_j, q_j) \) that transposes matching elements of \( \vec{p}, \vec{q} \), let the set \( \Theta_k \ni \gamma \gamma^{-1} \) represents all possible transpositions \( (p_j, q_j) \) between up to any \( k \) elements of \( \vec{p}, \vec{q} \). As the cycle structure is invariant under conjugation, cycles \( \gamma \gamma^{-1} \) = cycles \( \gamma \). Let the set

\[
\Theta_{\eta, j} = \left\{ \chi \gamma \gamma^{-1} : \chi \in S_{\eta}^\ell, \gamma \in S_{\vec{p}}^\gamma, \text{2-cycles (\( \gamma \)) = } j \right\}, \tag{A26}
\]

\[
|\Theta_{\eta, j}| = \left( \eta! \right) \left( (\eta)(\eta - 1) \cdots (\eta - j + 1) \right) / j! = \left( \eta! \right) / (\eta - j)!, \tag{A27}
\]

be the distinct elements generated by any \( \gamma \) with a cycle structure of \( (2, \cdots, 2, \cdots) \). Then

\[
\Theta_k = \bigcup_{j=0}^{k} \Theta_{\eta, j}, \quad |\Theta_k| = \sum_{j=0}^{k} \left( \eta! \right) / (\eta - j)!^2. \tag{A28}
\]

As there are fewer elements in \( |\Theta_k| \) than there are permutations in \( |S_{\eta}^\ell| \), the map from \( (\chi, \gamma) \rightarrow \tau \) is injective with multiplicity

\[
\Theta^{-1}_{\eta, k} (\tau) = \left\{ (\mu, \nu) : \tau = \mu \nu \mu^{-1}, \mu \in S_{\eta}^\ell, \nu \in S_{\eta}^\ell \right\}, \tag{A29}
\]

\[
|\Theta^{-1}_{\eta, j} (\tau)| = |\Theta^{-1}_{\eta, k} (\tau)| = \left( k \right)^2 / (k - j)!^2. \tag{A30}
\]
The elements of \((\mu, \cdot) \in \Theta_k^{-1}(\tau)\) are permutations within each vector \(\vec{p}, \vec{q}\).

This allows us to express the structure factor Weingarten sum over distinct elements in \(\Theta_n\):

\[
\Xi_{n,\eta,j} = \sum_{\tau \in \Theta_{n,j}} \Xi_{n,\eta}(\tau), \tag{A31}
\]

\[
\Rightarrow f(k) = \sum_{j=0}^{k} \left| \Theta_{k,j}^{-1} \right| \Xi_{n,\eta,j}. \tag{A32}
\]

We now evaluate \(\Xi_{n,\eta,j+1}\) in terms of \(\Xi_{n,\eta,j}\). Observe that the case \(j = 0\) corresponds to \(\tau \in \Theta_{n,0} = \{e\}\). Hence

\[
\Xi_{n,\eta,0} = \Xi_{n,\eta}(e) = \Xi_{n,\eta}. \tag{A33}
\]

For any \(j > 0\), observe that any element of \(\tau_{j+1} \in \Theta_{n,j+1}\) is the product of a transposition and an element \(\tau_j \in \Theta_{n,j}\). Let \(G_{\tau_j} = \{(j k) : (j k) \notin \tau_j\}\) be the set of transpositions between any element of \(\vec{p}\) and \(\vec{q}\), excluding those contained in \(\tau\). There are \(|G_{\tau_j}| = (\eta - j)^2\) such transpositions. Hence

\[
\Xi_{n,\eta,j+1} = \sum_{\tau \in \Theta_{n,j+1}} \Xi_{n,\eta}(\tau) = \sum_{\tau \in \Theta_{n,j}} \sum_{g \in G_{\tau}} \Xi_{n,\eta}(g \tau). \tag{A34}
\]

When \(j = 1\), consider all transpositions \(g \in G_\epsilon\) in the sum

\[
\Xi_{n,\eta,1} = \sum_{g \in G_\epsilon} \Xi_{n,\eta}(g) = \sum_{g \in G_\epsilon} \sum_{\nu \in S_{\eta}^{\oplus 2}} \sum_{\mu \in S_{\eta}^{\oplus 2}} (-1)^\mu W_{g}^{H_{\mu}}(\mu \nu \eta).
\]

Observe that only the \(\eta\) elements \(g \in S_{\eta}^{\oplus 2} \cap G\) leave the sum unchanged as seen by a change of variables \(\nu g \rightarrow \nu \in S_{\eta}^{\oplus 2}\). For all other transpositions in \(G_{\epsilon}/S_{\eta}^{\oplus 2}\), consider the transposition \((l_j r_k)\) representing swapping elements \(p_{1,j} \leftrightarrow p_{2,k}\) where \(j \neq k\). For every \(\nu \in S_{\eta}^{\oplus 2}\), with \(k\) 2-cycles, e.g. for \(k = 1\), \(g \nu = (l_j r_k)(l_{r_j} r_{r_k})\) consider the \(\nu\) with one more or less \(2\) cycles where the added cycle shares an index with \(g\). E.g., \((l_j r_k)(l_{r_j} r_{r_k}) = (l_k l_j r_k)(l_{r_j} r_{r_k})\) or \((l_j r_k)(l_{r_j} r_{r_k})(l_j r_k) = (l_j r_k)(l_{r_j} r_{r_k})(l_{r_j} r_{r_k})\). There is always an odd permutation \(\mu' \in S_{\eta}^{\oplus 2}\) that converts the 3-cycle back into a 2-cycle. For instance, \((r_j r_k)(l_j r_k r_j) = (l_j r_k)\). Thus the sum \(\sum_{\mu \in S_{\eta}^{\oplus 2}} (-1)^\mu W_{g}^{H_{\mu}}(\mu \nu \eta) = -\sum_{\mu \in S_{\eta}^{\oplus 2}} (-1)^\mu W_{g}^{H_{\mu}}(\mu \nu \eta) = 0\), and

\[
\Xi_{n,\eta,1} = \eta \Xi_{n,\eta,0} = \eta \Xi. \tag{A36}
\]

For any \(j > 0\), a similar argument holds – only \(\eta - j\) transpositions in \(G_{\tau_j}\) do not cancel. All other elements \(g \nu\) have a matching \(\mu' \nu \eta\) with exactly the same cycle structure where \(\mu'\) is odd. Hence

\[
\Xi_{n,\eta,j+1} = (\eta - j) \Xi_{n,\eta,j} = \frac{\eta!}{(\eta - j)!} \Xi_{n,\eta} = j! \frac{\eta!}{j!} \Xi_{n,\eta}. \tag{A37}
\]

Now substituting our result for \(\Xi_{n,\eta,j}\) into the structure factor,

\[
f(k) = \sum_{j=0}^{k} \frac{k! (\eta - j)!^2 \eta!}{(k - j)! (\eta - j)!} \Xi_{n,\eta} = \eta! \sum_{j=0}^{k} \frac{k! (\eta - j)!}{\eta! (k - j)!} \Xi_{n,\eta} = (\eta!)^2 \frac{\eta + 1}{\eta - k + 1} \Xi_{n,\eta}. \tag{A38}
\]

Above, we use the fact \(A(\eta, k) = \sum_{j=0}^{k} \frac{k! (\eta - j)!}{\eta! (k - j)!} = \frac{\eta + 1}{\eta - k + 1}\), which may be proven by induction. Assuming \(A(\eta, k) = \frac{\eta + 1}{\eta - k + 1}\) is true. Then \(A(\eta, 0) = \sum_{j=0}^{0} \frac{0! (\eta - j)!}{\eta! (0 - j)!} = 1\) is true. Observe that

\[
A(\eta, k) = \sum_{j=0}^{k} \frac{k! (\eta - j)!}{\eta! (k - j)!} = \frac{\eta + 1}{k + 1} \sum_{j=1}^{k+1} \frac{(k + 1)! (\eta - j)!}{(k + 1 - j)!} \tag{A39}
\]

\[
\frac{k + 1}{\eta + 1} \left( A(\eta, k) + \frac{\eta + 1}{k + 1} \right) = A(\eta + 1, k + 1) \tag{A40}
\]

Now \(A(\eta, k) = \frac{\eta + 1}{\eta - k + 1}\) is true implies that

\[
\frac{k + 1}{\eta + 1} \left( \frac{\eta + 1}{\eta - k + 1} + \frac{\eta + 1}{k + 1} \right) = \frac{\eta + 2}{\eta - k + 2}, \tag{A41}
\]

and \(A(\eta + 1, k + 1)\) is true. By iterating from \(A(\eta, 0)\) for all \(\eta\), hence \(A(\eta, k)\) is true for all \(k \leq \eta\).
With the partially evaluated twirling operator, we may evaluate some useful sums of Weingarten functions.

**Lemma 13.** The sum of Weingarten functions

\[
\Xi_{n,\eta} = \sum_{\nu \in S_{n,\eta}^<} \sum_{\mu \in S_n} (-1)\mu W^d \mu (\mu \nu) = \frac{1}{(\eta!)^2 \binom{n+1}{\eta}}.
\]  

(A42)

*Proof.* We use the fact that the twirling operator has unit trace \(\text{Tr} [\mathcal{T}_{2,\eta \land \mathcal{U}_n}]\). From its expression in Lemma 11 combined with the form for the structure factor \(f(\tilde{p}) = g_\eta (|\tilde{p}_1 \cap \tilde{p}_2|) \Xi_{n,\eta}\), where \(g_\eta (k) = (\eta!)^2 \frac{n+1}{\eta - k + 1}\) in Lemma 12,

\[
\text{Tr} [\mathcal{T}_{2,\eta \land \mathcal{U}_n}] = \sum_{\tilde{p} \subseteq S_{n,\eta}^<} g_\eta (|\tilde{p}_1 \cap \tilde{p}_2|) \Xi_{n,\eta} = \Xi_{n,\eta} \sum_{k=0}^{\eta} g_\eta (k) \sum_{\tilde{p}_1 \subseteq S_{n,\eta}^< \text{Sim}(\tilde{p}_1, \tilde{p}_2) = k} 1.
\]  

(A43)

The combinatorial factor

\[
\sum_{\tilde{p}_1 \subseteq S_{n,\eta}^<} \sum_{|\tilde{p}_1 \cap \tilde{p}_2| = k} 1 = \binom{n}{\eta} \binom{n-\eta}{k}.
\]  

(A44)

Hence

\[
\text{Tr} [\mathcal{T}_{2,\eta \land \mathcal{U}_n}] = \Xi_{n,\eta} \binom{n}{\eta} (\eta!)^2 \sum_{k=0}^{\eta} \frac{\eta+1}{\eta-k+1} \frac{\eta}{k} \binom{n-\eta}{\eta-k} = 1.
\]  

(A45)

We now evaluate the sum

\[
A = \sum_{k=0}^{\eta} \frac{\eta+1}{\eta-k+1} \frac{\eta}{k} \binom{n-\eta}{\eta-k} = \sum_{k=0}^{\eta} \frac{\eta+1}{\eta-k+1} \binom{n-\eta}{\eta-k}.
\]  

(A46)

Using the recurrence relation \(\binom{n}{k} = \frac{n+1-k}{k} \binom{n}{k-1}\) implies \(\frac{n+1}{k} \binom{n}{k-1} = \binom{n}{k} + \binom{n}{k-1} = \binom{n+1}{k}\). Hence the term \(\frac{1}{k+1} \binom{n-\eta}{k} = \frac{1}{n-\eta+1} \binom{n-\eta+1}{k}\), and

\[
A = \frac{\eta+1}{n-\eta+1} \sum_{k=0}^{\eta} \left( \frac{n-\eta+1}{k+1} \right) \binom{\eta}{k} = \frac{\eta+1}{n-\eta+1} \sum_{k=0}^{\eta} \left( \frac{n-\eta+1}{\eta-k+1} \right) \binom{\eta}{k}.
\]  

(A47)

We perform the sum using the Chu-Vandermonde identity \(\sum_{k=0}^{\eta} \binom{n-\eta}{k} \binom{\eta}{k} = \binom{n+1}{\eta}\), to obtain

\[
A = \frac{\eta+1}{n-\eta+1} \binom{n+1}{\eta} = \binom{n+1}{\eta}.
\]  

(A48)

Substituting \(A\) back into Equation (A45), we obtain \(\Xi_{n,\eta} = \frac{1}{(\eta!)^2} \binom{n+1}{\eta}^{-1} \binom{n}{\eta}^{-1}\). \(\square\)

**Appendix B: Hypergeometric sums**

In this section we evaluate the hypergeometric sums associated with \(\text{Tr} [\hat{n}_d^2\mathbf{1}]\) in Equation (60) of Theorem 3 and the estimation matrix entries \(E_{\eta,k,s}\) in Equation (82) of Theorem 5.

**Lemma 14.** For all integers \(n \geq \eta \geq 0\), \(d \in [0, \min(n, n-\eta)]\),

\[
\text{Tr} [\hat{n}_d^2\mathbf{1}] = \frac{\sum_{s=0}^{\min(n, n-\eta)} \binom{\eta}{\eta-s} \binom{n-\eta}{s} \sum_{j=\max(0, s+d-\eta)}^{\min(d, s)} (-1)^{j+1} (n+1)! (n-j)! \binom{\eta-s}{d-j}^2}{(n+d)! (n-\eta)! (n-d)!}.
\]  

(B1)
Proof. From Equation (58), \( \hat{n}_d = \sum_{j=0}^{d} (-1)^j \frac{(\eta-d+j)}{(\eta-j)!} \frac{(n-\eta-j)}{(n-\eta)!} e_{d-j}(\hat{n}_1, \ldots, \hat{n}_\eta) e_j(\hat{n}_{\eta+1}, \ldots, \hat{n}_n) \). Hence, the trace of its square

\[
\text{Tr}_{\eta} \left[ \hat{n}_d^2 \right] = \text{Tr}_{\eta} \left[ \sum_{j,k=0}^{d} (-1)^{j+k} \frac{(\eta-d+j)!}{(\eta-j)!} \frac{(n-\eta-j)!}{(n-\eta)!} e_{d-j}(\hat{n}_1, \ldots, \hat{n}_\eta) e_j(\hat{n}_{\eta+1}, \ldots, \hat{n}_n) e_k(\hat{n}_{\eta+1}, \ldots, \hat{n}_n) \right] \tag{B2}
\]

Let |\( \eta, s \rangle \) be any state with \( s \) fermions supported on the number operators \( \hat{n}_{\eta+1}, \ldots, \hat{n}_n \), that is \( \sum_{j=0}^{[n]} \hat{n}_j |\eta, s \rangle = s |\eta, s \rangle \) and \( \sum_{j=\eta}^{[n]} \hat{n}_j |\eta, s \rangle = n-\eta |\eta, s \rangle \). Note that there are \( \binom{n-\eta}{s} \) such states. Observe that

\[
e_j(\hat{n}_1, \ldots, \hat{n}_\eta) |\eta, s \rangle = \begin{pmatrix} \eta-s \\ j \end{pmatrix} |\eta, s \rangle, \quad e_k(\hat{n}_{\eta+1}, \ldots, \hat{n}_n) |\eta, s \rangle = \binom{s}{k} |\eta, s \rangle. \tag{B4}
\]

Hence the trace

\[
t_{\eta,d,j,k} = \sum_{s=0}^{\min(n,\eta-n)} \binom{n-\eta}{s} \binom{n-s}{j} \binom{s}{k} \binom{\eta-s}{d-j} \binom{\eta-s}{d-k}. \tag{B5}
\]

Substituting into Equation (B2), and noting that the summand is zero when \( d-j > \eta-s \) due to the term \( \binom{\eta-s}{d-j} \) and similarly for \( \binom{\eta-s}{d-k} \), we obtain the sum

\[
\text{Tr}_{\eta} \left[ \hat{n}_d^2 \right] = \sum_{s=0}^{\min(n,\eta-n)} \sum_{j,k=\max(0,s+d-\eta)}^{\min(d,s)} F_{n,\eta,d}(s,j,k) \frac{(\eta-d)!}{(n-\eta)!} \frac{(n-\eta)!}{(n-\eta)!} \tag{B6}
\]

where the summand

\[
F_{n,\eta,d}(s,j,k) = (-1)^{j+k} \frac{(\eta-d+j)!}{(\eta-j)!} \frac{(n-\eta-j)!}{(n-\eta)!} \frac{(\eta-s)!}{(n-\eta-s)!} \frac{(n-s)!}{(n-\eta-s)!} \frac{(\eta-s)!}{(n-\eta-s)!} \frac{(n-s-k)!}{(n-\eta-s-k)!} \tag{B7}
\]

By recognizing the double sum over \( j, k \) as the square of a sum,

\[
\text{Tr}_{\eta} \left[ \hat{n}_d^2 \right] = \frac{\eta!(n-\eta)!(\eta-s)!}{(n-\eta-s)!(n-\eta)!} \frac{\sum_{s=0}^{\min(n,\eta-n)} \left( \sum_{j=\max(0,s+d-\eta)}^{\min(d,s)} f_{n,\eta,d}(s,j) \right)^2}{(n-\eta-s)!} \tag{B8}
\]

The above sum holds for all non-negative integers satisfying \( \eta \leq n, d \leq \min(n, \eta-n) \). This proves the first equality in Equation (B2).

We find it convenient to define

\[
F_{n,\eta,d}(j,k) = \sum_{s=0}^{\min(d,s)} F_{n,\eta,d}(s,j,k), \tag{B10}
\]

\[
F_{n,\eta,d}(k) = \sum_{j=\max(0,s+d-\eta)}^{\min(d,s)} F_{n,\eta,d}(j,k), \tag{B11}
\]

\[
F_{n,\eta,d} = \sum_{k=\max(0,s+d-\eta)}^{\min(d,s)} F_{n,\eta,d}(k). \tag{B12}
\]
where we apply the Chu-Vandermonde identity 

This allows the telescoping sum and canceling poles when 

For example, the sum simplifies when 

is zero whenever the number of factorials with negative arguments in the denominator is greater than that in the numerator. Hence 

where the difference operators are 

and second to find a linear recurrence in \( n \) satisfied by \( F_{n,\eta,d} \) with \( F_{2n,\eta,0} \) as the initial condition. A more direct proof would find a linear recurrence in \( d \) satisfied by \( F_{n,\eta,d} \), but we were unable to do so in reasonable time. Let the shift operator on the variable \( x \) be \( S_x f(x) = f(x+1) \). From the definition of the summand, it is straightforward to verify that it is annihilated like \( Q_i(s,j,k)F_{n,\eta,d}(s,j,k) = 0 \) by the difference operators 

The amazing method of creative telescoping by Wilf and Zeilberger [29] guarantees the existence of \( s \)-free \( Q_i(j,k) \) that do not depend on \( s \) and some certificate \( R_i(s,j,k) \) that annihilate this proper hypergeometric summand according to 

The \( s \)-free property of \( Q \) allows us to perform a sum over \( s \) in \([s_0, s_1]\), 

Hence \( Q \) defines the linear recurrence that the sum \( \sum_{s=s_0}^{s_1} F_{n,\eta,d}(s,j,k) \) satisfies. A key insight in evaluating the right-hand side is that the summand has compact support. Using the Euler’s reflection formula \((-z)! = \pi / (z-1)! \sin(\pi z)\) and canceling poles when \( z \) approaches an integer, observe that 

is zero whenever the number of factorials with negative arguments in the denominator is greater than that in the numerator. Hence we may change the summation limits to, for instance, 

This allows the telescoping sum \( \sum_{s=-1}^{\min(n-n-\eta)} (S_s - 1) R_i(s,j,k) F_{n,\eta,d}(s,j,k) = 0 \) due to the natural boundaries of \( F_{n,\eta,d}(s,j,k) \). Thus \( Q_i(j,k) \) defines a recurrence satisfied by \( F_{n,\eta,d}(j,k) \). By recursing the procedure and finding \( (s,j) \)-free \( Q_i(k) \) and then \( (s,j) \)-free \( Q_i \), we then obtain the desired recurrence for \( F_{n,\eta,d} \) as follows 

\[
\sum_k [Q_i(k) + (S_j - 1) R_i(j,k)] F_{n,\eta,d}(j,k) = Q_i(j,k) F_{n,\eta,d}(j) = 0,
\]

\[
\sum_j [Q_i + (S_k - 1) R_i(k)] F_{n,\eta,d}(j) = Q_i(j,k) F_{n,\eta,d} = 0,
\]
At each iteration $x$ of the recursion, the operators $R(x, \cdots)$ are also called certificates as the correctness of $Q(\cdots)$ may be readily verified by reducing each equation $[Q_i(\cdots) + (S_x - 1)R_i(x, \cdots)]$ with respect to the annihilators $Q_i(x, \cdots)$ of the preceding iteration. For instance, reducing Equation (B15) with respect to the annihilators Equation (B14) may be done by hand, through verification of later iterations should be done by computer.

We now state the recurrences $[\tilde{Q}_i(\cdots) + (S_x - 1)\tilde{R}_i(s, \cdots)] F_{2n,\eta,d}(x, \cdots) = 0$ with respect to $d, s, j, k$. These were all computed in Mathematica by the HolonomicFunctions package [30]. The $s$-free operators and certificates are

$$\tilde{Q}(j, k) = \{ (d - j)(d - \eta - j - 1)(d - \eta - j + k) - (k - 1)(k - \eta)(\eta - d - j + k + 1)S_k, \]
$$

$$(d - j)(d - \eta - j - 1)(d - \eta + j - k) - (j + 1)(j - \eta)(\eta - d + j - k + 1)S_j, \]
$$

$$(d - \eta)(d - j + k)(d - \eta - j + k) - 2(2d - 2\eta + 1)(d - j + 1)(d - \eta - j)(d - \eta - k)S_d \}, \]

(B22)

$$\tilde{R}(s, j, k) = \{ \frac{(d - k)(s - j)(k - s)(d - \eta - k - 1)}{d - \eta - k + s - 1}, \frac{(d - j)(j - s)(s - k)(d - \eta - j - 1)}{d - \eta - j + s - 1}, \]

$$\frac{(j - s)(s - k)(3\eta - 3d + j + k - 2s)}{. \] \]

(B23)

The $(s, j)$-free operators and certificates are

$$\tilde{Q}(k) = \{ (2 + k)(1 + k - \eta)S_k^2 + (-2 + 2(-2 + d)k - 2k^2 + d(3 - d + \eta)) \}
$$

$$(1 - d + k + \eta), \]

$$2(1 + d)(-1 - d - k)(-1 + d - 2\eta)(1 + 2d - 2\eta)(-d + k + \eta)S_d + (1 + k)(k - \eta)(-1 - 3d + 2k + 2\eta)S_k - \eta (8d^2 - 9dk + d + 4k^2 + k - 1) \]

+ (2d - k)(-3dk + d(2d - 1) + 2k^2 + k - 1) + \eta^2(4d - 2k + 2) \}, \]

(B24)

$$\tilde{R}(k) = \{ \frac{j(-d - k)(-1 + 2d - 2\eta)(-1 + j - \eta)(d - j + k - \eta)(1 - d + k + \eta)}{(1 + k)(k - \eta)(1 - d - j + k + \eta)(2 - d - j + k + \eta)}, \]

$$((-1 - d + j)(-1 + d + j - k - \eta)(-d + j + \eta))^{-1} j(-1 + j - \eta)(-d + j - k + \eta) \]

$$\times \{ (-2 + d(5 + 17d) + j - 5dj + 2(-2 - 7d + 2)k + 2k^2) \eta + (-2d + k)(-1 + d + 4d^2 - 2dj + (-1 - 3d + 2j)k + (-3 - 11d + 2j + 4k)\eta^2 + 2\eta^3) \}. \]

(B25)

The $(s, j, k)$-free operators and certificates are

$$\tilde{Q} = \{ (2d - 2\eta - 1) + (d + 1)(d - 2\eta - 1)(2d - 2\eta + 1)S_d \}, \]

(B26)

$$\tilde{R}(k) = \{ \frac{(1 + 3d - 2k - 2\eta)(1 + k)(k - \eta)S_k + (-2dk + 2k^2 + d(-1 + d - \eta))}{2(-1 - d + k)(-d + k + \eta)} \}. \]

(B27)

Hence, $\tilde{Q}$ defines the recurrence satisfied by

$$F_{2n,\eta,d} = \frac{(\eta - d + 3/2)}{d(2\eta - d + 2)(\eta - d + 1/2)} F_{2n,\eta,d-1} \]

$$= \frac{(\eta + 1/2)!}{d!(\eta - d + 1/2)!} \frac{(2\eta - d + 1)!}{(2\eta + 1)!} \frac{(\eta - d - 1/2)!}{(\eta - 1/2)!} F_{2n,\eta,0} \]

$$= \frac{(2\eta - d + 1)!}{d!(2\eta - 2d + 1)(2\eta)!} F_{2n,\eta,0} \]

$$= \eta^{1/2} \frac{(2\eta - d + 1)!}{d!(2\eta - 2d + 1)} . \]

(B28)

We now state the recurrences $[Q_i(\cdots) + (S_x - 1)R_i(s, \cdots)] F_{n,\eta,d}(x, \cdots) = 0$ with respect to $n, s, j, k$ and their cer-
tificates. The $s$-free operators and certificates are

$$Q(j, k) = \{$$
$$\eta - n - 1)(d - j - k - 1)(d^2 - dj - \eta(3d + k - 2(n + 1)) + dn + jk - k^2 + kn - n^2 - n)$$
$$+ (k + 1)(\eta - n + 1)(n + k - n)(\eta - d - j + k + 1)S_k + (n - 2\eta)(\eta - d + k + 1)S_n,$$
$$(\eta - n - 1)(d - j - 1)(d^2 + d(-3\eta + k + n) - j^2 + j(-\eta + k + n) - (n + 1)(n - 2\eta))$$
$$+ (j + 1)(\eta - n + 1)(\eta - j - n)(\eta - d + k + 1)S_j + (n - 2\eta)(\eta - d + j + 1)S_n,$$
$$(n - \eta + 2)(d^2 - d(4\eta + j + k - 2n - 2) - \eta^2 - \eta(j + k - 4n + 6) + (n + 1)(j + k - 2n - 3)) S_n$$
$$- (2d - n - 1)(n - \eta + 1)(n - \eta + 2)(\eta + j - n - 1)(\eta + k - n - 1) + (n - 2\eta + 1)S_n^2\},$$

(B29)

$$R(s, j, k) = \{\frac{(j - s)(k - s)(-\eta + n + 1)(s - 1 - \eta)(-d + \eta + k + 1)(d - 2\eta - k + n)}{\eta - n + s + 1}(d - \eta - k + s - 1)}$$
$$\frac{\eta - n + s - 1)(-d + \eta + j - s + 1)}{(j - s)(s - k)(-\eta + n + 1)(s - 1 - \eta)(-d + \eta + j + 1)(d - 2\eta + j - n)}$$
$$\frac{(j - s)(k - s)(\eta - n - 2)(\eta - n - 1)(s - 1 - \eta)(\eta + j - n - 1)(\eta + k - n - 1)}{(\eta - n + s - 2)(\eta - n + s - 1)}\}.$$  

(B30)

The $(s, j)$-free operators and certificates are

$$Q(k) = \{(\eta + n + 1)(d^2 + d(\eta - 2n - 3) + k^2 + k(\eta - n) + (n + 1)(-\eta + n + 1))$$
$$+ (d + \eta - n - 1)S_n - ((k + 1)(-\eta + n + 1)(\eta + k - n))S_k,$$
$$(\eta + n + 2)(d^2 + d(3\eta + 2k - 4n - 7) + (n + 2)(-2k - k + 2n + 3)) S_n$$
$$+ (d - n - 2)(2d - n - 1)(n - \eta + 1)n - \eta + 2)(\eta + k - n - 1)$$
$$+ (d + \eta + k - n - 2)S_n^2\},$$

(B31)

$$R(j, k) = \{\frac{j(d - n - 1)(\eta + n + 1)(\eta + j - n - 1)}{d - \eta + j - k - 1}\}$$
$$\frac{(n - 2\eta + 1)^{-1}[j(n - 2d + 1)(\eta - j - n + 2)(\eta + j - n - 1)(\eta - k + n + 1)$$
$$+ (d^2 - d(2n + j + k - n - 1) + \eta^2 - \eta(k + j + 2n - 2) + (n + 1)(j - n - 1)) ]}{\eta(n - 2)}S_n\}.$$  

(B32)

The $(s, j, k)$-free operators and certificates are

$$Q = \{(d - n - 2)(2d - n - 1)(\eta + n + 1) + (2d - n - 2)S_n\}, \quad R(k) = kS_n.$$  

(B33)

Hence, $Q$ defines the recurrence satisfied by

$$F_{n, \eta, d} = \frac{(n - d + 1)(n - 2d)(n - \eta)}{(n - 2d + 1)} F_{n-1, \eta, d}$$
$$= \frac{(n - d + 1)!}{(2\eta - d + 1)!} \frac{(n - 2d)!}{(\eta)!} \frac{(n - \eta)!}{(n - 2d + 1)!} F_{2\eta, \eta, d}$$
$$= \frac{(n - d + 1)!}{(2\eta - d + 1)!} \frac{(n - \eta)!}{(\eta)!} \frac{(2n - 2d + 1)!}{(n - 2d + 1)!} F_{2n, \eta, d}$$
$$= \frac{(n - d + 1)!}{(2\eta - d + 1)!} \frac{(n - \eta)!}{(\eta)!} \frac{(2\eta - 2d + 1)!}{(n - 2d + 1)!} \frac{\eta^2(2\eta - d + 1)!}{d!(2\eta - 2d + 1)}$$
$$= \eta(n - \eta)! \frac{(n - d + 1)!}{(n - 2d + 1)!}.$$  

(B34)

We complete the proof by dividing $\text{Tr}_n \left[ \hat{n}_d^2 \right] = \sum_{s, j, k} F_{n, \eta, d, s, j, k} \frac{F_{n, \eta, d, s, j, k}}{(n - d)!^2(n - \eta - d)!^2}.$
We now apply the same technique to evaluate the estimation matrix entries $E_{n,k,s}$ from Equation (82). In the following, the sum $t_{n,\eta,k,s} = E_{n,k,s}$ following a change of variables $d' \to d'$. 

**Lemma 15.** The sum

$$t_{n,\eta,k,s} = \sum_{d=0}^{\eta} \sum_{d'=0}^{d} \sum_{x''=0}^{k} \sum_{y''=0}^{s} F_{n,\eta,k,s}(d,d',x'',y'') = (-1)^s \binom{k}{s} \binom{n-\eta+k-s}{k-s}, \quad \text{(B35)}$$

where the summand

$$F_{n,\eta,k,s}(d,d',x'',y'') = a_d \binom{n+1}{d} (-1)^{d-d'} \binom{\eta-d'}{\eta-d} \binom{n-\eta-d+d'}{n-\eta-d} \binom{k-s}{d-d''} \binom{\eta+k-s}{d''-x''} \binom{s}{y''} \times \binom{n-\eta-s}{d-d'-y''} \binom{n-(d+k-x''-y'')}{n-\eta} \binom{1}{s}.$$

**Proof.** As $F_{n,\eta,k,s}(d,d',x'',y'')$ is zero outside the domain of summation in $\sum_{d=0}^{\eta} \sum_{d'=0}^{d} \sum_{x''=0}^{k} \sum_{y''=0}^{s}$, we may replace the summation limits with a sum over all integers

$$t_{n,\eta,k,s} = \sum_{d} \sum_{d'} \sum_{x''} \sum_{y''} F_{n,\eta,k,s}(d,d',x'',y''). \quad \text{(B37)}$$

We find it convenient to define

$$t_{n,\eta,k,s} = \sum_{d,c,a,b} F_{n,\eta,k,s}(d,c,a,b). \quad \text{(B38)}$$

The sum simplifies when $k = s = 0$ to

$$t_{n,\eta,0,0} = t_{n,\eta,0,0}(0,0,0,0) = 1. \quad \text{(B39)}$$

Our proof strategy is to first find a linear recurrence in $k$ satisfied by $t_{n,\eta,k,0}$ with $t_{n,\eta,0,0}$ as the initial condition, and second to find a linear recurrence in $s$ satisfied by $t_{n,\eta,k,s}$ with $t_{n,\eta,k,0}$ as the initial condition. As with the proof of Lemma 14, we exhibit a sequence of $y''$-free, $x''$-free, $d'$-free, and finally $d$-free operators $Q$ that annihilate the summand $QF_{n,\eta,k,s}(d,d',x'',y'')$ together with certificates $R$ that verify their correctness.

When $s = 0$, $t_{n,\eta,0,0} = \sum_{d,d',x''} F_{n,\eta,k,s}(d,d',x'',0)$ is a triple sum. We now state the recurrences

$$[Q_i(\cdots) + (S_x - 1)\tilde{R}_i(x,\cdots)] F_{n,\eta,k,s}(x,\cdots,0) = 0 \text{ with respect to } k, d, d', x'' \text{ and their certificates.}$$

The $d'$-free operators and certificates are

$$Q(d,a) = \left\{ (-1 + d - k)(a - d + k + n)S_k + (1 + k)(a - d + k + \eta), \right.$$
$$\left. (1 + a)(1 + d - k + \eta)S_a - (a - d)(1 + d - a + k + n), \right.$$ 
$$\left. - (-1 + a - d)(1 + d)(1 + 2d - n)(a - d - k + n)(d - \eta)S_d ight.$$ 
$$\left. + (d - k)(1 + 2d - n)(1 - d + n)^2(a - d - k + \eta) \right\}, \quad \text{(B40)}$$

$$R(d,c,a) = \left\{ \frac{(a - c)(1 + k)}{(-1 + a - k)(k - \eta)} \right.$$ 
$$\left. \frac{(a - c)(1 + a - d - k + n)(-1 + c - \eta)}{1 + a - c - k + \eta}, \right.$$ 
$$\left. \frac{(a - c)(1 + 2d - n)(1 - d + n)^2(-1 + c - \eta)(-a + d + k - \eta)}{-1 + c - d} \right\}. \quad \text{(B41)}$$

The $(d',x'')$-free operators and certificates are

$$Q(d) = \left\{ (-1 + d - k)(d + k - n)S_k + (1 + k)(k - \eta), \right.$$ 
$$\left. (1 + d)^2(1 - 2d + n)(d + k - n)(d - \eta)S_d + (d - k)(1 + 2d - n)(1 - d + n)^2(d - n + \eta) \right\}, \quad \text{(B42)}$$

$$R(d,a) = \left\{ \frac{a(1 + k)(a - d + k + \eta)}{-a + d + k + n}, \right.$$ 
$$\left. \frac{a(d - k)(1 + 2d - n)(1 - d + n)^2(-1 + a - 2d - k + n)(a - d - k + \eta)}{-1 + a - d)(a - d - k + n)} \right\}. \quad \text{(B43)}$$
The \((d, d', x')\)-free operators and certificates are

\[
Q = \left\{ (-1 - k) S_k + (1 + k + n - \eta) \right\}, \tag{B44}
\]
\[
R(d) = \left\{ \frac{d^2(-1 + d - \eta)}{(-1 + d - k)(-1 + 2d - n)} \right\}. \tag{B45}
\]

Hence, we solve the first order recurrence defined by \(Q t_{n, \eta, k, 0}\) to obtain

\[
t_{n, \eta, k, 0} = \frac{n - \eta + k}{k} t_{n, \eta, k-1, 0} \quad \text{and} \quad t_{n, \eta, 0, 0} = \frac{(n - \eta + k)!}{k!(n - \eta)}. \tag{B46}
\]

For the case \(s > 0\), we now state the recurrences \(\hat{Q}_i(\cdots) + (S_\eta - 1)\hat{R}_i(x, \cdots)\) \(F_{n, \eta, k, s}(x, \cdots, 0) = 0\) with respect to \(s, d, d', x', y'\) and their certificates. The \(y'\)-free operators and certificates are

\[
Q(d, c, a) = \left\{ (a - d - k + n)(1 - a + k - s)(k - s - \eta)S_k + (1 + k - s)(a - c + k + \eta)(a - d - k + s + \eta), \right.
\]
\[
(1 + s)(1 - a + d + k - s - \eta)S_k + (a - k + s)(-1 + k - s - \eta), \quad
\]
\[
(1 + c - d)(1 + d)(-1 + 2d - n)(a - d - k + n)S_d
\]
\[
- (1 + 2d - n)(1 + d - n)^2(a - d - k + s + \eta), \quad
\]
\[
(1 + a)(1 + a - c - k + \eta)(1 + a - d - k + s + \eta)S_a
\]
\[
- (a - c)(1 + a - d - k + n)(a - k + s) \}, \tag{B47}
\]
\[
R(d, c, a, b) = \left\{ -\frac{b(k - s - 1)(a + b - d + \eta - k)(b + c - d - \eta + n - s)}{a + b - d - k + n}, \right.
\]
\[
\frac{b(a - k + s)(\eta - k + s + 1)(a + b - d + \eta - k)(b + c - d - \eta + n - s)}{(b - s - 1)(\eta - n + s)(a - c + \eta - k + s + 1)},
\]
\[
((b + c - d - 1)(c - d - \eta + n)(a + b - d - k + n))^{-1} b(2d - n + 1)(-d + n + 1)^2
\]
\[
\times (a + b - d + \eta - k)(a + b + c - 2d - k + n - 1)(-b - c + d + \eta - n + s), \quad
\]
\[
b(a + b - d + \eta - k),
\]
\[
b(c - a)(a - k + s)(b + c - d - \eta + n - s)
\]
\[
a - c + \eta - k + s + 1 \}. \tag{B48}
\]

The \((d', y')\)-free operators and certificates are

\[
Q(d, a) = \left\{ (1 - d + k)(a - d - k + n)(1 - a + k - s)(k - s - \eta)S_k + (a - 1 - k)(1 + k - s)(k - \eta)(a - d - k + s + \eta), \right.
\]
\[
(1 + a - d)(1 + d)(-1 + 2d - n)(a - d - k + n)(d - \eta)S_d
\]
\[
- (d - k)(1 + 2d - n)(1 + d + n)^2(a - d - k + s + \eta), \quad
\]
\[
(1 + a)(k - a)(1 + a - d - k + s + \eta)S_a + (a - d)(1 + a - d - k + n)(a - k + s),
\]
\[
(s - k)(-1 + a + d + k - s - \eta)S_s - (a - k + s)(-1 + k - s - \eta) \}, \tag{B49}
\]
\[
R(d, a, c) = \left\{ (a - c)(1 + k - s)(-1 + c - \eta)(a - d - k + s + \eta)
\right.
\]
\[
\frac{(a - c)(1 + 2d - n)(1 + d + n)^2(-1 + c - \eta)(a - d - k + s + \eta)}{-1 + c - d}
\]
\[
\frac{(a - c)(1 + a - d - k + n)(a - k + s)(1 - c + \eta)}{1 + a - c - k + \eta}, \tag{B50}
\]
The \((d', x'', y'')\)-free operators and certificates are

\[
Q(d) = \{- (1 + d - n)(2d - n)(1 + 2d - n)(k - s)(n - s - \eta)S_s \\
+ (1 + d)^2(-1 + 2d - n)(d + k - n)(d - \eta)S_d \\
+ (d^3 + d^2(k - 1 - n - 2s - \eta) + k(n + ns - \eta) - ns(1 + s + \eta) \\
+ d(2s + \eta + (n + 2s)(s + \eta) - k(1 + 2s + \eta))(-1 + d - n)(1 + 2d - n), \\
(1 + d)(2 + d)^2(1 - 2d + n)(2d - n)(1 + d + k - n)(1 + d - \eta)S_d^2 \\
+ (n(n(-1 + k - s) + 2s) + d^2(2k + n - 4s - 2\eta) - d(-1 + n)(2k + n - 4s - 2\eta) + 2n\eta - k(2 + n)\eta) \\
\times (1 + d)(n - d)(-1 + 2d - n)(3 + 2d - n)S_d \\
+ (d - k)(d - n)(2 + 2d - n)(3 + 2d - n)(1 - d + n)^2(d - n + \eta)\}, \tag{B51}
\]

\[
R(d, c) = \{- ((-1 + a - d)(a - d - k + n))^{-1}a(-1 + a - k)(-1 + d - n)(1 + d - n)\frac{-d^3 + k^2 - kn + k^2n + n^2}{-kn^2 - ks - kns + n^2s - (k + kn - n^2)\eta + d^2(1 - 2k + 3s + 3\eta) + a(d^2 - k(1 + n) \\
+ d(-1 + k - 2s - 2\eta) + n(1 + s + \eta)) + d\frac{-k^2 + s + \eta - 3n(1 + s + \eta) + k(2 + 3n + s + \eta)}{}}}, \\
((-2 + a - d)(-1 + a - d - k + n)(a - d - k + n)(d - \eta))^{-1}a(-1 + a - k)(-1 + d - n)(d - n) \\
\times (3 + 2d - n)(1 - d + n)^2(a - d - k + s + \eta)[4d^4 - 2(-2 + a)(-1 + a - k)\eta \\
- d(a^2(-2 + n) + 3k^2n + (-1 + n)(4 + 3n - 8s + 5ns) - k(4 + n(-8 + 5n + 3s)) \\
+ a(6 + k(2 - 4n) - 4s + n(-4 + n + 4s))) - 2d(9 + a^2 - a(7 + k - 4n) + k(3 - 2n) + n(-11 + 3n))\eta \\
+ n^3(1 - k + s + \eta) - 2d^3(-6 + 3a - 3k + 2n + 3s + 4\eta) + (-2 + a)n(-2s + (-5 + a - k)\eta) \\
+ n^2((3 - a + k)(-1 + k - s) - (5 - 2a + k)\eta) + d^2(2a^2 + 2k^2 - k(-10 + 9n + 2s + 4\eta) \\
+ a(-12 - 4k + 5n + 4s + 8\eta) - 2(-6 + 7s + 11\eta) + n(-5 + n + 9s + 12\eta))\}, \tag{B52}
\]

The \((d', x'', y'')\)-free operators and certificates are

\[
Q = \{- (n - \eta + k - s)S_s - (\eta + s - k + 1)\}, \tag{B53}
\]

\[
R(d) = \{- \frac{d(1 + d)^2(d + k - n)(d - \eta)((-1 + d - k - s - \eta)S_d}{(-1 + d - n)(2d - n)(1 + 2d - n)(k - s)(n - s - \eta) \\
- ((-1 + 2d - n)(2d - n)(n - s - \eta))^{-1}d \\
\times (d^4 + d^3(-2 + 2k - n - 3s - 2\eta) + (1 + n)(1 - k + s + \eta)(ns + k(-n + \eta)) \\
+ d^2(1 + k^2 + n + 5s + 3n + (s + \eta)(2n + 4s + \eta) - k(3 + n + 5s + 3n)) \\
- d(k^2(1 + 2n - \eta) + (1 + s + \eta)(2s + 4ns + \eta + n\eta) + k(-1 - 3 s + \eta(s + \eta) - 3n(1 + 2s + \eta)\} \}. \tag{B54}
\]

Hence, we solve the first order recurrence defined by \(Q_{n,q,k,s}\) to obtain

\[
\begin{align*}
\tilde{t}_{n,q,k,s} &= \frac{(\eta + s - k)}{(n - \eta + k - s + 1)}\tilde{t}_{n,q,k,s-1} \\
&= (-1)^s\frac{(\eta + s - k)!}{(n - \eta + k - s)!}\frac{(n - \eta + k - s)!}{(n - \eta + k)!}t_{n,q,k,0} \\
&= (-1)^s\frac{(\eta + s - k)!}{(n - \eta + k - s)!}k!(n - \eta)\eta \\
&= (-1)^s\left(\frac{k}{s}\right)^{-1}\left(\eta + s - k\right)\left(n - \eta + k - s\right). \tag{B55}
\end{align*}
\]