Monte Carlo Sampling for Wave Functions Requiring Symmetrization or Antisymmetrization

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Many strongly correlated states, such as those arising in the fractional quantum Hall effect and spin liquids, are described by wave functions obtained by dividing particles into multiple clusters, constructing a readily evaluable wave function in each cluster, and (anti)symmetrizing across these clusters. We introduce a method to compute quantities such as energies and correlators, using Monte Carlo simulations for these states. Our framework overcomes the factorial scaling of explicit (anti)symmetrization, allowing for studies of systems beyond the reach of exact diagonalization.

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Introduction—Strongly interacting systems can exhibit phases characterized by topological order that lies beyond the conventional Landau paradigm of symmetry breaking of a local order parameter. These topological phases are characterized by long-range entanglement [1], ground-state degeneracy on nontrivial manifolds [2], and braiding of the anyonic quasiparticles that they host [3,4]. Experimentally, these phases are realized in the fractional quantum Hall effect (FQHE) [5], where electrons confined to two dimensions are subjected to a strong perpendicular magnetic field. In this regime, the single-particle spectrum organizes into discrete Landau levels (LLs), and within a partially filled LL, kinetic energy gets quenched, and interactions dominate. At selected rational fillings of an LL, interactions can open up a gap, resulting in incompressible FQHE phases. These states exhibit many interesting properties, foremost among which are the existence of fractionally charged excitations that exhibit anyonic statistics [6–10]. In certain FQHE states, these excitations exhibit non-Abelian braiding statistics that could, in principle, enable building a fault-tolerant topological quantum computer [4,11].

A prominently observed even-denominator state occurs at filling $\nu = 5/2$ [12], which is widely believed to be non-Abelian [13,14] since one of the leading candidates to describe this FQHE is the Moore-Read (MR) Pfaffian (Pf) [15] state or its hole conjugate the anti-Pf [16–18]. The MR is the $k = 2$ member of a broader class of k-clustered Read-Rezayi (RRk) states, which are non-Abelian for $k > 1$. Interestingly, these states can be written as conformal field theory (CFT) correlators of parafermionic primary fields, allowing for a direct study of their non-Abelian properties via conformal blocks [15,19–21]. Members of the RRk series could underpin some experimentally observed fractions in the second LL (SLL) (and its analog in bilayer graphene [22–26]); in particular, the $12/5$ state [27–31] has been proposed to be described by the hole conjugate of the RR3 state [21,32–36]. Furthermore, bosons in the lowest LL (LLL) interacting via the ultra-short-range delta-function or the long-range Coulomb interaction can stabilize the MR and the RR3 states [37–40].

The bosonic RRk wave function is obtained by symmetrizing over partitions of N particles into k clusters (N and $k > 1$ are positive integers with N divisible by k), where each cluster forms a bosonic $1/2$ Laughlin state [41]. Being a combinatorial operation, numerical construction of RRk wave functions by explicit symmetrization is computationally prohibitive except for very small systems. The RRk states can be alternatively constructed via exact diagonalization (ED) [21] and Jack polynomials [42,43], but these procedures are likewise limited to small sizes ($N \leq 25$). The RR3 state can also be generated using matrix product states on the quasi-two dimensions (2D) cylindrical geometry for fairly large systems [44,45] but not on the sphere [46], torus [47], or disk [48], which are the conventional 2D geometries for FQHE studies. Readily evaluable wave functions that lie in the same universality class as the hole conjugate of the fermionic RRk states exist [49], but they lack the desirable features of RRk states, such as the existence of a model Hamiltonian or being exact CFT

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correlators. It is therefore useful to develop an approach that enables the evaluation of quantities of interest for the RRk states for large systems in 2D geometries. Here, we present such a method, allowing efficient computation of quantities such as energies and correlation functions for the RRk states using Monte Carlo (MC). Our method is general and extendable to other wave functions that require explicit (anti)symmetrization and could be applicable in other domains, such as to quantum spin liquids [50], for computing electronic structures [51,52], and for describing molecules [53–55], etc.

Method—In this Letter, we demonstrate a way to do MC simulations of (anti)symmetrized wave functions that scales favorably with N, making it numerically tractable, unlike brute-force (anti)symmetrization. We use the $\nu = 1$ bosonic MR state [15] as an example to illustrate our idea. We write its wave function as [56]

$$\Psi_1^{\mathrm{MR}} = \mathbb{S}[\Phi_1^2(z_1, \ldots, z_{N/2})\Phi_1^2(z_{N/2+1}, \ldots, z_N)], \quad (1)$$

where $\Phi_1(z_1, \ldots, z_M) = \prod_{1\le i<j\le M}(z_i - z_j)$ is the $\nu = 1$ integer quantum Hall state. The wave function of Eq. (1) is obtained by dividing the particles into two clusters, forming the bosonic $\nu = 1/2$ Laughlin state [7] in each of the clusters, i.e., the Halperin (H)-(2,2,0) state [57],

$$\Psi_1^{\mathrm{H}(2,2,0)} = [\Phi_1^2(z_1, \ldots, z_{N/2})\Phi_1^2(z_{N/2+1}, \ldots, z_N)], \quad (2)$$

and symmetrizing over all particles, which the operator $\mathbb{S}$ implements. Here, one could write a Pf for MR, which can be evaluated efficiently. However, assuming that the Pf form was not known and one instead performs the explicit symmetrization, the computational complexity would scale poorly with increasing N. By contrast, it is easier to compute a matrix element like $\langle\Psi_1^{\mathrm{MR}}|\hat{O}|\Psi_1^{\mathrm{MR}}\rangle$, where $\hat{O}$ is a symmetric operator. Specifically, expectation values of interactions of the form $\hat{V} = \sum_{i<j} V_{i,j}$ such as the Coulomb interaction, where $V_{i,j} = 1/|z_i - z_j|$, are simpler to evaluate than the wave function itself since these interactions are invariant under particle permutations. To demonstrate this, we write the symmetrization as a sum over permutations,

$$\Psi_1^{\mathrm{MR}} = \frac{1}{N!}\sum_{P\in S_N} P\Psi_1^{\mathrm{H}(2,2,0)}, \quad (3)$$

where S_N is the symmetric group and $Pg(z_1, \cdots z_N) = g(z_{P(1)}, \ldots, z_{P(N)})$. [Note that the total number of permutations for the $k = 2$ case is fewer and equals $(N!)/\{2![(N/2)!]^2\}$, since permutations of indices within a cluster are identical and the two clusters can be exchanged overall.] Our matrix element is then

$$\langle\Psi_1^{\mathrm{MR}}|\hat{O}|\Psi_1^{\mathrm{MR}}\rangle = \left(\frac{1}{N!}\right)^2\sum_{P_1,P_2}\langle\Psi_1^{\mathrm{H}(2,2,0)}|P_1\hat{O}P_2|\Psi_1^{\mathrm{H}(2,2,0)}\rangle$$
$$= \frac{1}{N!}\sum_{P}\langle\Psi_1^{\mathrm{H}(2,2,0)}|\hat{O}P|\Psi_1^{\mathrm{H}(2,2,0)}\rangle, \quad (4)$$

which follows because $P_1\hat{O}P_2 = \hat{O}P_1P_2$, as $\hat{O}$ is invariant under permutations, i.e., particle-index exchanges. Hence, the double sum over P_1 and P_2 reduces to a single sum over all permutations P for a fixed base choice of $\Psi_1^{H(2,2,0)}$. [Here, we choose $(1, 2, \ldots, N/2)$ and $(N/2+1, \ldots, N)$ as the base set of the two clusters.] For a fixed base set, evaluating $\langle\Psi_1^{\mathrm{H}(2,2,0)}|\hat{O}P|\Psi_1^{\mathrm{H}(2,2,0)}\rangle$ yields only $\lfloor N/4\rfloor + 1$ distinct values, where $\lfloor x\rfloor = \mathrm{floor}(x)$ is the greatest integer $\le x$. This is because Φ_1^2 is already fully symmetric in its arguments. Similarly, the two clusters can be swapped overall as they form the same state. Consequently, the matrix element $\langle\Psi_1^{\mathrm{H}(2,2,0)}|\hat{O}P|\Psi_1^{\mathrm{H}(2,2,0)}\rangle$ gives the same result for any P which exchanges exactly m of the indices $(1, \ldots, N/2)$ into the set $(N/2+1, \ldots, N)$, where $m = 0, 1, \ldots, \lfloor N/4\rfloor$. Therefore, it suffices to evaluate the $\lfloor N/4\rfloor + 1$ distinct matrix elements by MC, and adding them with the appropriate combinatorial weights $C_{(N,m)}$ [see Supplemental Material (SM) [58]] gives us the full matrix element $\langle\Psi_1^{\mathrm{MR}}|\hat{O}|\Psi_1^{\mathrm{MR}}\rangle$ that we desire.

A subtle issue arises even when the operator $\hat{O}$ is well behaved, i.e., is both Hermitian and invariant under the permutation of particles: the matrix elements that we evaluate are generally complex (not necessarily real or positive), which can result in poor convergence. There are two reasons for this: (a) the sampling function is different from the wave function of interest, i.e., we use $H(2, 2, 0)$ for sampling instead of the fully symmetrized wave function, and (b) for each configuration corresponding to m exchanges, which has $C_{(N,m)}$ terms in its ensemble [58], we evaluate only one representative term. While what we presented above is analytically correct, Metropolis MC using this approach is extremely slow to converge. This is because, when we choose a particular representation, we have artificially chosen some particles to be different from others (those in the two different groups and those that are exchanged between groups). Thus, we must wait for the MC to sample configurations where all types of particles exchange positions with all other types of particles so that the average of the chosen representative faithfully emulates its ensemble's average. While eventually MC will sample the entire space equitably, there can be an extremely long so-called mixing time.

In other words, if we include all terms in the full symmetrization, convergence to the expected value requires significantly fewer MC iterations. However, the cost per step becomes prohibitively expensive for large systems since the number of permutations scales factorially with N. On the other hand, approximating the many terms

associated with each exchange by a single representative term is computationally inexpensive, but it has a long mixing time and requires many MC iterations, which can again become time consuming as the system size grows. Thus, the problem effectively becomes a trade-off between the number of terms to be included and the number of MC iterations required for convergence. For the naive method of evaluating exchanges, we use the form given in Eq. (4) and do MC sampling using the readily evaluable wave function $\Psi_1^{\mathrm{H}(2,2,0)}$. We compute the quantity $r = \sum_m \mathcal{R}_{N,m}$, where $\mathcal{R}_{N,m} = C_{(N,m)} r_m$, and $r_m = (\Psi_1^{\mathrm{H}(2,2,0),m}/\Psi^{\mathrm{H}(2,2,0)})$, where $\Psi_1^{\mathrm{H}(2,2,0),m}$ is a representative of the Halperin $-(2,2,0)$ state, with m exchanges between the two clusters. Using this, we compute the expectation value of the operator $\langle O\rangle$ as the ratio of the unnormalized symmetrized state $[\langle O\rangle_{\mathrm{numerator}} = \sum_m C_{(N,m)} \hat{O} r_m]$ and the norm of the symmetrized state [by setting $\hat{O} = \mathbb{I}$, the identity operator, we have $\langle O\rangle_{\mathrm{denominator}} = \sum_m C_{(N,m)} r_m$].

In the refined version, we improve upon the naive method by strategically identifying and including additional terms to minimize error propagation. The key issue is that, even for a fixed N, the contribution or weight of each m-exchange is not uniform since $C_{(N,m)}$ increases with m. Thus, integrals for exchanges with smaller $C_{(N,m)}$ converge faster, since fewer correlations are encoded in them, than those with larger $C_{(N,m)}$. To mitigate this, we do a systematic correction by including more terms for larger $C_{(N,m)}$. This ensures that each m th exchange contributes roughly uniform error to $\langle \hat{O}\rangle$, enabling convergence to the expected value within a reasonable time frame. Thus, we define the matrix element obtained by symmetrization via refined exchanges as

$$\langle \hat{O}\rangle_{\Psi_1^{\mathrm{MR}}} = \frac{1}{N!}\left\langle \Psi_1^{\mathrm{H}(2,2,0)} | \hat{O} \sum_m \frac{C_{(N,m)}}{\mathcal{N}_{(N,m)}} \sum_{t=0}^{\mathcal{N}_{(N,m)}} |\Psi_1^{\mathrm{H}(2,2,0),m_t}\right\rangle, \tag{5}$$

where $\mathcal{N}_{(N,m)}$ denotes the number of terms retained for the m th exchange and t corresponds to a unique choice of m exchanges between the two clusters. In other words, we group the large number of permutations into a much smaller number of equivalent groups. We then sample a few representative terms from each group and combine them with the correct combinatorial weights to obtain the matrix element.

Next, we explain how we choose $\{\mathcal{N}_{(N,m)}\}$ using the example of $N = 20$. The values of $C_{(20,m)}$ are 1,100,2025,14400,44100,31752 for $m = 0, 1, 2, 3, 4, 5$, respectively. From a preliminary MC run, we observed that each exchange contributes roughly equally to the expectation $\langle \hat{O}\rangle$ for many observables $\hat{O}$. Since the combinatorial weight factor increases with increasing m, the numerator $\hat{O} r_m$, or r_m, decreases with increasing m. As a result, r_5 contributes the most error to $\langle O\rangle$ since its inaccuracy gets amplified when multiplied by its large combinatorial weight. To ensure that the error in each r_m is of the same order, we define the number of terms to be computed for the m th exchange [see Eq. (5)] as $\mathcal{N}_{(N,m)} = \lceil C_{(N,m)}/s_{\mathrm{rep}} \rceil$, where $\lceil x\rceil = \mathrm{ceil}(x)$ and s_{rep} is a parameter that is chosen to get to a desired accuracy. Based on the observation that r_5 has a value of the order of MC error, $\sim 10^{-2}$, after 20 million MC steps, which results in an error in the first significant digit, we choose $s_{\mathrm{rep}} = 1000$ so that of the order ten additional terms are now included for r_5 which pushes the error in it down to the next significant digit. Accordingly, $\mathcal{N}_{(20,m)} = \lceil C_{(20,m)}/1000 \rceil$, so that any $\mathcal{N}_{(20,m)} > 1$ corresponds to including multiple representations (chosen arbitrarily) of the exchange of m indices between the two clusters in the Halperin $-(2,2,0)$ state. As a result, instead of computing $\lfloor N/4\rfloor + 1 = 5$ ratios r_m, we compute a total of $\sum_m \mathcal{N}_{(N,m)} = 97$ ratios, with $\mathcal{N}_{(N,m)}$ unique ratios for each m. This number is still much less than the minimal set of permutations, i.e., $20!/[(10!)^2 2!] = 92378$.

Without refinement, the naive symmetrization has to be run for $\sim$100 times more MC steps to achieve the same level of accuracy, i.e., to reduce the MC error to the next order. Note that, since the naive method involves fewer terms per step and is therefore computationally faster than the refined method, it allows for more MC iterations in the same time. However, the refined method can be substantially accelerated through parallelization, yielding faster convergence with the same run-time, whereas multicore processing offers limited benefits for the naive method. We explicitly show this in Fig. 1 by computing the pair-correlation function for $N = 20$ using three methods: (i) naive, (ii) refined, and (iii) the full symmetrization. For each method, we run ten MC chains, each for ten minutes on a dual-Intel Xeon Platinum 8358@2.6 GHz, 32-core processor. Additionally, the corresponding LLL Coulomb energies computed using these three methods are presented in Table I. In SM [58], we provide a detailed error analysis explaining why the refined method

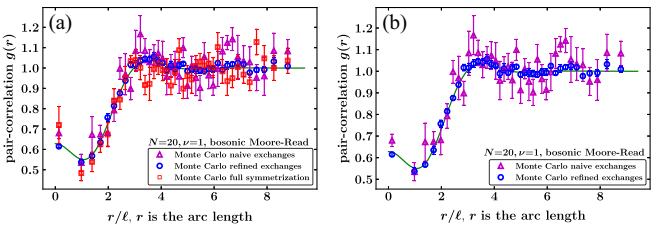

FIG. 1. (a) Pair-correlation function for the $\nu = 1$ Moore-Read state of $N = 20$ bosons on the sphere obtained with different methods keeping the same computational resources and run-time. (b) Same as (a), except, for clarity, results from only the refined and naive methods are shown.

TABLE I. Density-corrected [63] per-particle Coulomb energies for $N = 20$ bosons in the $\nu = 1$ Moore-Read state, computed in the spherical geometry by different methods with identical computational resources and the same run-time. The number in the parentheses is the statistical uncertainty coming from the Monte Carlo computations.

ν	N	ED	MC naive	MC refined	MC full symm
1	20	−0.45422	−0.44(1)	−0.457(3)	−0.43(2)

outperforms the naive one. Hereafter, we will only show results obtained using the refined method.

We now turn our attention to the RR3 state. Interestingly, its excitations, Fibonacci anyons, can be used to carry out universal topological quantum computation, in contrast to the Ising anyons of the MR state, which lack the necessary degrees of freedom to achieve universality [64,65]. Importantly, unlike the MR state, where the Pf provides a more efficient alternative to full symmetrization, the RR3 wave function can only be evaluated by symmetrization. This makes our method particularly well suited for calculating observables for the RR3 state. As in the $k = 2$ case, we must group permutations corresponding to equivalent matrix elements. However, owing to the presence of three clusters, distinct matrix elements cannot be identified by just exchanges. To overcome this hurdle, we recast the problem in terms of set partitions, which, along with exhaustively enumerating all permutations, help identify unique matrix elements. Each set partition maps to a 3×3 doubly stochastic integer matrix, which serves as a representative of its equivalence class. These equivalence classes allow us to aggregate terms with identical matrix elements and compute their weights, as detailed in SM [58]. In the $k = 2$ case, the 2×2 doubly stochastic integer matrix analysis reduces to using exchanges [58].

Results—In Fig. 2 and Table II, we show the pair-correlation function and tabulate the LLL Coulomb energies, respectively, for $N = 30$ bosons for the $\nu = 1$ MR and $N = 24$ bosons for the $\nu = 3/2$ RR3 states, obtained in the spherical geometry [46]. For each system, we run 20 independent MC chains. For comparison, MC computations using the Pf and ED results are also shown on the same plot. For $N = 30$ at $\nu = 1$, we set $s_{\mathrm{rep}} = 50000$, which results in a total of $\sum_m \mathcal{N}_{(30,m)} = 1558$ terms, while for $N = 24$ at $\nu = 3/2$, we set $s_{\mathrm{rep}} = 10^6$, which results in a total of $\sum_n \mathcal{N}_{(24,n)} = 1603$ terms (here n labels the equivalence classes). Our approach is easily extended to the fermionic RRk states since those are related to the bosonic ones by a multiplicative factor of Φ_1. In Fig. 2 and Table II, we also show results for the fermionic MR and RR3 states at $\nu = 1/2$ and $3/5$, respectively, for which we choose the same systems and parameters as the analogous bosonic ones. In all cases, we find fairly good agreement with the results obtained from the Pf or ED.

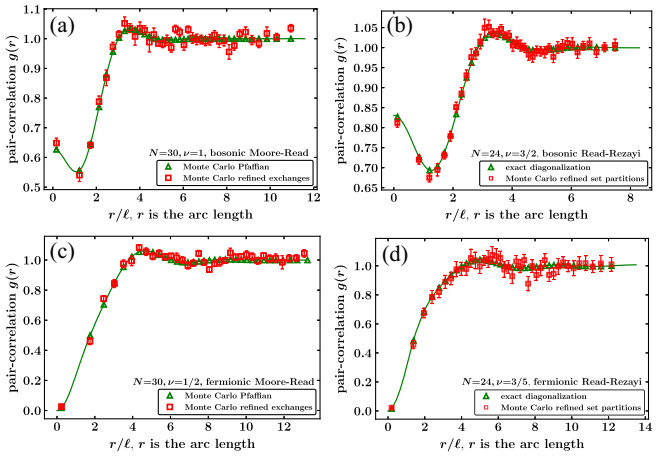

FIG. 2. Pair-correlation function $g(r)$ for the Moore-Read state of (a) bosons at $\nu = 1$ and (c) fermions at $\nu = 1/2$ for $N = 30$ particles, and the 3-cluster Read-Rezayi state of (b) bosons at $\nu = 3/2$ and (d) fermions at $\nu = 3/5$ for $N = 24$ particles obtained in the spherical geometry by different methods.

As an application of our method, we consider the competition between the bosonic RR3 and Jain states at $\nu = 3/2$ with the hard-core delta-function, equivalently, the V_0 Haldane-pseudopotential [46], interaction. For small systems, the exact V_0 ground state has a high overlap with the bosonic RR3, indicating that RR3 could be stabilized for this interaction [39]. Here, we go beyond the system sizes accessible to ED and obtain a reliable thermodynamic-limit estimate by evaluating the V_0 energies of the two states from their density-density correlation, i.e., the static structure factor [66,67] (the two-body interaction energy of a state is just a weighted sum over the different components of its static structure factor). For the bosonic RR3 state, this is done using Monte Carlo with our refined method, while for the Jain state we use standard Monte Carlo [68,69]. The wave function of the Jain state is evaluated as the fermionic 3/5 Jain state [70] over Φ_1 [71,72], since this form is amenable to large-scale numerical evaluation via the Jain-Kamilla projection [73–77]. The bosonic RR3 extrapolates to a lower zero relative angular momentum pair amplitude than the Jain

TABLE II. Density-corrected [63] per-particle Coulomb energies for N bosons and fermions in the $\nu = 1$ and $\nu = 1/2$ Moore-Read and the $\nu = 3/2$ and $\nu = 3/5$ 3-cluster Read-Rezayi states computed in the spherical geometry by different methods. The number in the parentheses is the statistical uncertainty stemming from the Monte Carlo (MC) computations.

ν	N	ED or Pf-MC	MC refined
1	30	−0.45295(1)	−0.450(2)
1/2	30	−0.457956(2)	−0.4586(7)
3/2	24	−0.42533	−0.428(3)
3/5	24	−0.4882	−0.487(1)

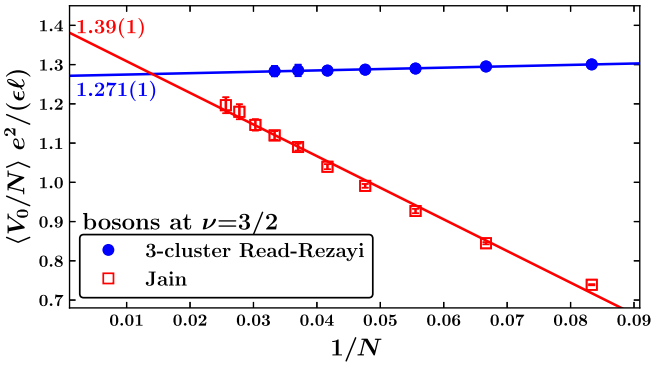

FIG. 3. Competition between the bosonic $k = 3$ Read-Rezayi and Jain states at $\nu = 3/2$ for the hard-core V_0 interaction.

state, consistent with RR3 being stabilized for the V_0 interaction [39] [see Fig. 3].

Discussion—The ideas that we presented can be readily generalized to more clusters. An interesting future direction is to test the competition between the 2/5 Bonderson-Slingerland [78] and the hole conjugate of the fermionic RR3 [21] states for the 12/5 FQHE. Since this competition is very tight [79], it requires an extremely accurate evaluation of the energies of the RR3 state. Extracting topological quantities via this method could be an interesting avenue to explore. For instance, our technique can extend previous studies of braiding statistics [20,80–83] to the RR3 state, to establish that its excitations are Fibonacci anyons [84]. This method can also be used to compute wave functions where full (anti)symmetrization is needed, such as at 5/2 with LL mixing, where the LLL is filled and the second LL is half filled, or when constructing bipartite or tripartite composite fermion states [85–87]. Our approach can be further augmented by improving the sampling efficiency of the MC using Hamiltonian or hybrid MC methods [88,89]. We leave an exploration of this and other directions to future work.

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Data availability—All data from this work are available at [91].

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