

# Noninteracting multiparticle quantum random walks applied to the graph isomorphism problem for strongly regular graphs

Kenneth Rudinger,<sup>1,\*</sup> John King Gamble,<sup>1</sup> Mark Wellons,<sup>2</sup> Eric Bach,<sup>2</sup> Mark Friesen,<sup>1</sup> Robert Joynt,<sup>1</sup> and S. N. Coppersmith<sup>1,†</sup>

<sup>1</sup>*Physics Department, University of Wisconsin–Madison, 1150 University Avenue, Madison, Wisconsin 53706, USA*

<sup>2</sup>*Computer Sciences Department, University of Wisconsin–Madison, 1210 West Dayton Street, Madison, Wisconsin 53706, USA*

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We investigate the quantum dynamics of particles on graphs (“quantum random walks”), with the aim of developing quantum algorithms for determining if two graphs are isomorphic (related to each other by a relabeling of vertices). We focus on quantum random walks of multiple noninteracting particles on strongly regular graphs (SRGs), a class of graphs with high symmetry that is known to have pairs of graphs that are hard to distinguish. Previous work has already demonstrated analytically that two-particle noninteracting quantum walks cannot distinguish nonisomorphic SRGs of the same family. Here, we demonstrate numerically that three-particle noninteracting quantum walks have significant, but not universal, distinguishing power for pairs of SRGs, proving a fundamental difference between the distinguishing power of two-particle and three-particle noninteracting walks. We show analytically why this distinguishing power is possible, whereas it is forbidden for two-particle noninteracting walks. Based on sampling of SRGs with up to 64 vertices, we find no difference in the distinguishing power of bosonic and fermionic walks. In addition, we find that the four-fermion noninteracting walk has greater distinguishing power than the three-particle walk on SRGs, showing that increasing the particle number increases the distinguishing power. However, we also show analytically that no noninteracting walk with a fixed number of particles can distinguish all SRGs, thus demonstrating a potential fundamental difference in the distinguishing power of interacting versus noninteracting walks.

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## I. INTRODUCTION

There has long been interest in algorithms that use random walks to solve a variety of mathematical and scientific problems [1–5]. Typically, the random walks in question have been classical random walks (CRWs). However, there is increasing interest in random walks with quantum walkers. In particular settings, these quantum random walks (QRWs) have been shown to have computational advantages over CRWs [6–8]. Certain algorithms utilizing QRWs have been proven to have faster run times than their best known classical counterparts [9–15].

Additionally, QRWs have been experimentally demonstrated in a variety of physical settings, such as ion traps [16], atom traps [17], quantum optics [18,19], and NMR systems [20]. Recent works have experimentally realized QRWs with two walkers, demonstrating the potential for implementing QRWs with many walkers [21–24]. Moreover, there are proposed methods for physically implementing nontrivial walks [25], indicating that there may be many QRW algorithms to be developed that would be both physically realizable and computationally powerful.

Often the context for QRWs is one in which the walks occur on graphs. It has been shown that QRWs are universal; any quantum algorithm can be mapped onto a QRW on such a graph [26]. It is also the case that many interesting computational problems are easily expressed in graph theoretic terms [27]. Thus there is considerable interest in further exploring QRWs on graphs, with the hope that we may be able to use such a framework to solve certain problems.

There are also interesting physical phenomena associated with many particles walking on a graph. It is known that QRWs of noninteracting bosons on graphs can give rise to effective statistical interactions [28–30]. It has even been shown that Bose–Einstein condensation can occur at a finite temperature in less than two dimensions if the bosons are placed on a particular kind of graph [30]. Therefore, there is motivation to further explore the dynamics of multiparticle ensembles on graphs.

This paper addresses the graph isomorphism (GI) problem, which is, given two graphs, to determine if they are isomorphic; that is, if one can be transformed into the other by a relabeling of vertices. This problem is of note for several reasons. While many graph pairs may be distinguished by a classical algorithm which runs in a time polynomial in the number of vertices of the graphs, there exist pairs which are computationally difficult to distinguish. Currently, the best general classical algorithm has a run time of  $O(c^{\sqrt{N} \log N})$ , where  $c$  is a constant and  $N$  is the number of vertices in the two graphs [31]. GI is believed to be similar to factoring in that both are thought to be NP-Intermediate problems [32]. Additionally, both problems may be approached as hidden subgroup problems, though this approach has had limited success for GI [33]. Due to these similarities, and the known quantum speedup available for factoring [34], there is hope that there similarly exists a quantum speedup for GI.

Strongly regular graphs (SRGs) are a particular class of graphs that are difficult to distinguish classically [31]. (See Sec. II B for a formal definition.) Shiao *et al.* showed that the single-particle continuous-time QRW fails to distinguish pairs of SRGs with the same family parameters [35]. Gamble *et al.* extended these results, proving that QRWs of two noninteracting particles will always fail to distinguish pairs of

\*rudinger@wisc.edu

†snc@physics.wisc.edu

nonisomorphic SRGs with the same family parameters [27]. They also demonstrated numerically the distinguishing power of the two-boson interacting QRW; it successfully distinguished all tested pairs of SRGs [27]. Since the publication by Gamble *et al.*, Smith proved that for any fixed number of bosons  $p$ , there exist nonisomorphic graph pairs which the  $p$ -boson interacting walk fails to distinguish [36]. These counterexample graphs are not strongly regular; whether or not the two-boson interacting walk successfully distinguishes nonisomorphic SRGs is still an open question.

Investigations into discrete-time QRW algorithms for GI have also been made [37–39]. Berry and Wang numerically showed that a discrete-time noninteracting QRW of two particles could distinguish some SRGs, something its continuous-time counterpart cannot do. However, this distinguishing power is not universal on SRGs, nor is an analytic explanation of the distinguishing power given [39]. The discrete-time algorithm proposed by Emms *et al.* successfully distinguished all tested SRGs [37], but it has been shown to not be universal [36]; it is unknown if it is universal on SRGs. Additionally, for the same number of particles, the discrete-time QRWs require Hilbert spaces larger than the ones required by continuous-time QRWs [39]. In an effort to relate discrete-time and continuous-time QRWs, it has been noted that the coin state of a discrete-time walk may be thought of as a relativistic particle’s internal degree of freedom; such a feature is absent from continuous-time QRWs [40]. The relationship between discrete-time and continuous-time QRWs in the context of the GI problem has been examined as well [41]. It remains an open question as to whether or not discrete-time walks in general have fundamentally greater distinguishing power than continuous-time walks or if they are better candidates for a universal GI algorithm.

This paper extends the results of [27] to address continuous-time multiparticle noninteracting quantum walks on SRGs, with a particular focus on understanding the role of particle number in determining the distinguishing power of the walks. We have several main results. We numerically demonstrate that three-particle noninteracting walks have significant (but not universal) distinguishing power on hard-to-distinguish pairs of SRGs. Additionally, we find that a four-fermion noninteracting walk has even greater (but still not universal) distinguishing power on SRG pairs. We explain analytically where this distinguishing power comes from and how these multiparticle noninteracting walks are fundamentally different from single-particle and two-particle noninteracting walks. This is done by showing that a particular feature present in the smaller walks which limits their distinguishing power is not present in walks of three or more noninteracting particles. Further, we analytically show that, even though the distinguishing power of noninteracting walks increases with particle number, there is no noninteracting walk with a fixed number of particles that can, with our comparison algorithm, distinguish all SRGs.

This paper is organized as follows. Section II covers the requisite background, including graph theoretic definitions and concepts, a review of SRGs, and a formal definition of the QRW. In Sec. III, we first demonstrate analytically how two-particle noninteracting walks are fundamentally different from three-particle noninteracting walks. We then present the numerical results for noninteracting three-particle

and four-particle walks on SRGs. In the final part of Sec. III, we demonstrate that a  $p$ -particle noninteracting QRW cannot distinguish all SRGs for any fixed  $p$ . We discuss our conclusions in Sec. IV.

Appendix A discusses a fundamental difference between noninteracting walks of two particles and noninteracting walks of more than two particles. Appendix B provides details necessary to show that a noninteracting  $p$ -particle walk cannot distinguish all SRGs for a fixed  $p$ . In Appendix C, we show that the number of unique evolution operator elements for a  $p$ -particle noninteracting walk is superexponential in  $p$ . Finally, we explain in Appendix D how we ensure numerical stability and determine numerical error in our simulations.

## II. BACKGROUND

### A. Basic graph definitions

Here we develop the background and definitions necessary to discuss multiparticle QRWs on graphs. This paper only considers simple, undirected graphs. A graph  $G = (V, E)$  is a set of vertices  $V$  and edges  $E$ . The vertices are a set of labels, usually integers, and the edges are a list of unordered pairs of vertices. If a pair of vertices appears in  $E$ , then the vertices are connected by an edge; otherwise there is no edge between the vertices and they are considered disconnected. The terms “adjacent,” “neighboring,” and “connected” may be used interchangeably to refer to a vertex pair which shares an edge. It is convenient to represent a graph by its adjacency matrix  $\mathbf{A}$ , defined as

$$A_{ij} = \begin{cases} 1 & \text{if vertices } i \text{ and } j \text{ are connected.} \\ 0 & \text{if vertices } i \text{ and } j \text{ are disconnected.} \end{cases} \quad (1)$$

A graph of  $N$  vertices has an  $N \times N$  adjacency matrix. For the undirected and simple graphs considered here,  $\mathbf{A}$  is symmetric, with zeros on the diagonal.

Two graphs are isomorphic if one graph is transformed into the other by a relabeling of vertices. More formally, given two adjacency matrices  $\mathbf{A}$  and  $\mathbf{B}$ , the graphs represented by  $\mathbf{A}$  and  $\mathbf{B}$  are isomorphic if and only if a permutation matrix  $\mathbf{P}$  exists such that  $\mathbf{B} = \mathbf{P}^{-1}\mathbf{A}\mathbf{P}$ .

### B. Strongly regular graphs

This paper addresses SRGs, which we examine because they are difficult to distinguish classically and because of their simple algebraic properties [31,42]. An SRG is characterized by four parameters, denoted  $(N, k, \lambda, \mu)$ .  $N$  is the number of vertices in the graph, and each vertex is connected to  $k$  other vertices (the graph is  $k$  regular or has degree  $k$ ). Each pair of neighboring vertices shares  $\lambda$  common neighbors, while each pair of nonadjacent vertices shares  $\mu$  common neighbors. The set of SRGs sharing the same set of four parameters is referred to as an SRG *family*; correspondingly, the four parameters are often called the family parameters. While some SRG families may have only one nonisomorphic member, there are many families of SRGs with multiple nonisomorphic graphs. These are the families which are of interest to us.

The adjacency matrix of any SRG has at most three eigenvalues. As these eigenvalues and their multiplicities are functions of the family parameters, the adjacency matrices

of SRGs in the same family are always cospectral [42]. This contributes to the difficulty of distinguishing nonisomorphic SRGs.

The adjacency matrix of any SRG satisfies the particularly useful algebraic identity [42]

$$\mathbf{A}^2 = (k - \mu)\mathbf{I} + \mu\mathbf{J} + (\lambda - \mu)\mathbf{A}, \quad (2)$$

where  $\mathbf{I}$  is the identity and  $\mathbf{J}$  is the matrix of all ones. Because  $\mathbf{J}^2 = N\mathbf{J}$ ,  $\mathbf{J}\mathbf{A} = \mathbf{A}\mathbf{J} = k\mathbf{A}$ , and  $\mathbf{I}$  acts trivially on  $\mathbf{I}$ ,  $\mathbf{J}$ , and  $\mathbf{A}$ , we see that  $\{\mathbf{I}, \mathbf{J}, \mathbf{A}\}$  forms a commutative three-dimensional algebra, so we conclude that, for any positive integer  $n$ ,

$$\mathbf{A}^n = \alpha_n\mathbf{I} + \beta_n\mathbf{J} + \gamma_n\mathbf{A}, \quad (3)$$

where  $\alpha_n$ ,  $\beta_n$ , and  $\gamma_n$  depend only on  $n$  and the family parameters.

### C. Defining the quantum random walk

Now we discuss how we form a continuous-time noninteracting QRW on a graph. As in [27], we use the Hubbard model, where each site corresponds to a graph vertex. A particle can move from one vertex to another if the two vertices are connected. Thus, for a graph on  $N$  vertices with adjacency matrix  $\mathbf{A}$ , our noninteracting Hamiltonian is given by

$$\mathbf{H} = - \sum_{i,j}^N A_{ij} c_i^\dagger c_j, \quad (4)$$

where  $c_i^\dagger$  and  $c_i$  are the creation and annihilation operators, respectively, for a boson or (spinless) fermion at site  $i$ . For bosons, they satisfy the commutation relations  $[c_i, c_j^\dagger] = \delta_{ij}$  and  $[c_i, c_j] = [c_i^\dagger, c_j^\dagger] = 0$ . For fermions, they satisfy the anticommutation relations  $\{c_i, c_j^\dagger\} = \delta_{ij}$  and  $\{c_i, c_j\} = \{c_i^\dagger, c_j^\dagger\} = 0$ .

For walks of  $p$  bosons, we use basis states of the form  $|j_1 \dots j_p\rangle_B$ , which is the appropriately symmetrized basis state with bosons on vertices  $j_1$  through  $j_p$ . These vertices need not be distinct, since vertices may be multiply occupied. Similarly, for walks of  $p$  fermions, we use basis states of the form  $|j_1 \dots j_p\rangle_F$ , which is the appropriately antisymmetrized basis state with fermions on vertices  $j_1$  through  $j_p$ . These vertices must be distinct, because the Pauli exclusion principle implies that no vertex can be occupied by multiple fermions. We refer to these bases as the particles-on-vertices bases.

Following [27,36], it is straightforward to show that the elements of the  $p$ -boson or  $p$ -fermion noninteracting Hamiltonian ( $\mathbf{H}_{p,B}$  and  $\mathbf{H}_{p,F}$ , respectively) are, in their respective particles-on-vertices bases,

$$\begin{aligned} {}_B \langle i_1 \dots i_p | \mathbf{H}_{p,B} | j_1 \dots j_p \rangle_B \\ = - {}_B \langle i_1 \dots i_p | \mathbf{A}^{\oplus p} | j_1 \dots j_p \rangle_B, \end{aligned} \quad (5)$$

$$\begin{aligned} {}_F \langle i_1 \dots i_p | \mathbf{H}_{p,F} | j_1 \dots j_p \rangle_F \\ = {}_F \langle i_1 \dots i_p | \mathbf{A}^{\oplus p} | j_1 \dots j_p \rangle_F, \end{aligned} \quad (6)$$

where

$$\begin{aligned} \mathbf{A}^{\oplus p} = & \underbrace{\mathbf{A} \otimes \mathbf{I} \otimes \mathbf{I} \dots \otimes \mathbf{I}}_p \\ & + \mathbf{I} \otimes \mathbf{A} \otimes \mathbf{I} \dots \otimes \mathbf{I} + \dots + \mathbf{I} \otimes \mathbf{I} \otimes \mathbf{I} \dots \otimes \mathbf{A}. \end{aligned} \quad (7)$$

The evolution operator is defined in the standard manner,

$$\mathbf{U}(t) = e^{-it\mathbf{H}}, \quad (8)$$

where  $\hbar = 1$  for convenience.

### D. Comparison algorithm

Our method for comparing two graphs in an attempt to determine whether or not they are isomorphic is the same as the one used in [27]. Given two graphs with adjacency matrices  $\mathbf{A}$  and  $\mathbf{B}$ , we compute, in the particles-on-vertices basis,  $\mathbf{U}_A(t)$  and  $\mathbf{U}_B(t)$ , respectively, for the same number and type of particle, as well as the same time  $t$ . The absolute values of each element of  $\mathbf{U}_A(t)$  and  $\mathbf{U}_B(t)$  are written to lists  $\mathbf{X}_A$  and  $\mathbf{X}_B$ , respectively. Both lists are sorted, and we compute the distance between the lists,  $\Delta$ :

$$\Delta = \sum_v |\mathbf{X}_A[v] - \mathbf{X}_B[v]|. \quad (9)$$

We say that  $\mathbf{A}$  and  $\mathbf{B}$  are distinguished by a particular walk if and only if that walk yields  $\Delta \neq 0$ ; isomorphic graphs and nonisomorphic nondistinguished graphs both yield  $\Delta = 0$  [27]. We note that we lose phase information by taking the absolute value of the elements, but it makes our comparison procedure more tractable and seems to do no harm (see [27]). Finally, for all simulations presented in this paper,  $t = 1$ .

## III. QUANTUM RANDOM WALKS ON STRONGLY REGULAR GRAPHS

### A. Comparing the distinguishing power of two- and three-particle noninteracting walks

In this subsection we show analytically that there is a fundamental difference between two-particle noninteracting walks and three-particle noninteracting walks on SRGs, because three-particle noninteracting walks are capable of distinguishing SRGs from the same family, unlike two-particle noninteracting walks. To show this difference, we recall the proof used by Gamble *et al.* to demonstrate the inadequacy of two-particle walks [27].

The proof by Gamble *et al.* first shows that the value of every element in the two-particle evolution operators ( ${}_B \langle ij | \mathbf{U}_{2B}(t) | kl \rangle_B$  or  ${}_F \langle ij | \mathbf{U}_{2F}(t) | kl \rangle_F$ ) must be a function only of the SRG family parameters and the time  $t$ . Then it is shown that the multiplicity of each element value in the evolution operator is also a function of the SRG family parameters. We begin similarly here for the three-particle walk and find that while the values of the elements are all functions of the SRG family parameters, the multiplicities of the values are not.

We first address the element values. We refer to each element of each evolution operator (computed in the particles-on-vertices basis) as a *Green's function*, following the nomenclature of Gamble *et al.* [27]. Because the three-particle walk in question is noninteracting, we know that the evolution operator for the walk factorizes into three single-particle evolution

operators:

$${}_B \langle ijk | \mathbf{U}_{3B} | lmn \rangle_B = {}_B \langle ijk | \mathbf{U}_{1P}^{\otimes 3} | lmn \rangle_B, \quad (10)$$

$${}_F \langle ijk | \mathbf{U}_{3F} | lmn \rangle_F = {}_F \langle ijk | \overline{\mathbf{U}}_{1P}^{\otimes 3} | lmn \rangle_F, \quad (11)$$

where  $\mathbf{U}_{1P}^{\otimes 3} = \mathbf{U}_{1P} \otimes \mathbf{U}_{1P} \otimes \mathbf{U}_{1P}$ ;  $\mathbf{U}_{1P}$  is the evolution operator for the single-particle walk, that is,  $\mathbf{U}_{1P} = e^{iAt}$  and  $\overline{\mathbf{U}}_{1P} = e^{-iAt}$ .

Recalling Eq. (3), and expanding  $e^{iAt}$  as a Taylor series in powers of  $At$ , we note that

$$\mathbf{U}_{1P} = \alpha \mathbf{I} + \beta \mathbf{J} + \gamma \mathbf{A}, \quad (12)$$

where  $\alpha$ ,  $\beta$ , and  $\gamma$  are functions of the family parameters and the time  $t$ . Therefore, we conclude that all possible values of the elements of  $\mathbf{U}_{3B}$  and  $\mathbf{U}_{3F}$  (the Green's functions) are determined by the family parameters. Thus, the set of all potential values for the Green's functions are the same for any two graphs in the same family. Any distinguishing power of the walks must come from the existence of at least one Green's function with different *multiplicities* for nonisomorphic graphs in the same family.

Gamble *et al.* prove that the multiplicity of each Green's function for two-particle noninteracting walks is a function of the SRG family parameters. In Appendix A, we show that there exist Green's functions for the three-particle noninteracting walk on SRGs whose multiplicities are *not* functions of the family parameters. This is because the multiplicity of a Green's function in a  $p$ -particle walk depends on how many shared neighbors a collection of up to  $p$  vertices has. For  $p = 2$ , strong regularity uniquely determines the number of shared neighbors:  $\lambda$  if the vertices are connected and  $\mu$  if they are not. However, for  $p \geq 3$ , the multiplicity is dependent on the number of shared neighbors among sets of  $p$  vertices. Thus the multiplicity is not uniquely determined by strong regularity, so the multiplicity for such a Green's function need not be a function of the family parameters.

The definition of SRGs does not directly constrain the number of neighbors of a set of  $p$  vertices with  $p \geq 3$ . However, this difference from the two-particle case does not guarantee that walks of three or more particles can distinguish nonisomorphic SRGs, only that they have the potential to do so. Our numerical investigations of the distinguishing power of these walks are presented in Sec. III B.

## B. Numerical results

In this subsection, we present our numerical results for three-particle and four-fermion walks on SRGs. To simulate a walk on a graph, we compute the appropriate Hamiltonian and exponentiate it to compute its corresponding evolution operator, following the algorithm described in Sec. II D. Then, to compare pairs of nonisomorphic graphs from the same family, we compute the list distance  $\Delta$ , defined in Eq. (9). We find our error on  $\Delta$  to be no greater than  $10^{-6}$ , so two nonisomorphic graphs are considered distinguished if and only if  $\Delta > 10^{-6}$ . Further details of numerical error analysis are provided in Appendix D.

Because the Hamiltonians are very large, we must use a sparse matrix exponentiation routine [43] to make exponentiation computationally tractable. (The largest evolution opera-

TABLE I. Numerical results for three-particle noninteracting walks in 12 families of SRGs. The first column lists the family parameters for the particular SRG family examined. The second column lists the number of graphs in the family that we compared. This number  $S$  is equal to the number of graphs in the family, with the exception of (49, 18, 7, 6), where we examined only a subset of the family. The third column gives the number of comparisons made for each family, equal to  $S$  choose 2. The fourth and fifth columns list the number of graph pairs which the three-boson and three-fermion walks fail to distinguish, respectively. We see that, of 70 712 graph comparisons, both the boson and the fermion walks fail a total of 256 times, corresponding to a success rate of greater than 99.6%.

SRG family ( $N, k, \lambda, \mu$ )	No. of graphs	Comparisons	Boson failures	Fermion failures
(16,6,2,2)	2	1	0	0
(16,9,4,6)	2	1	0	0
(25,12,5,6)	15	105	0	0
(26,10,3,4)	10	45	1	1
(28,12,6,4)	4	6	0	0
(29,14,6,7)	41	820	0	0
(35,18,9,9)	227	25 651	38	38
(36,14,4,6)	180	16 110	89	89
(40,12,2,4)	28	378	8	8
(45,12,3,3)	78	3 003	7	7
(49,18,7,6)	147	10 731	21	21
(64,18,2,6)	167	13 861	92	92

tors we compute have a dimension of 91 390 and correspond to four-fermion walks on graphs of 40 vertices.) Additionally, in order to be able to perform these exponentiations sufficiently quickly, we parallelize the computations, utilizing the Open Science Grid and the University of Wisconsin–Madison's Center for High Throughput Computing Cluster.

Our numerical results for three-particle walks are presented in Table I. For the 70 712 pairs of SRGs compared, boson and fermion walks distinguish all but 256 pairs, corresponding to a success rate of greater than 99.6%. Thus we see that both three-boson and three-fermion walks have significant (but not universal) distinguishing power on SRGs, while two-particle noninteracting walks fail on *all* pairs of nonisomorphic graphs in the same family [27].

Bosonic and fermionic walks fail to distinguish the same pairs of nonisomorphic graphs that we tested; we have found no graph pair wherein one kind of particle successfully distinguishes while the other does not. Thus, despite having a state space of smaller dimension (due to Pauli exclusion), the three-fermion walk has the same distinguishing power as the three-boson walk on all tested graph pairs. It remains an open question whether graph pairs exist for which this is not true.

Having identified some graph pairs that three noninteracting particles fail to distinguish, we want to know if noninteracting walks exist that can distinguish these graphs. However, it is computationally expensive (even with the speedup provided by parallelization) to simulate four-particle walks. We therefore simulated only fermion walks, and only on a subset of the three-particle counterexample graph pairs. Our results are summarized in Table II. We simulated four-fermion noninteracting walks on 136 counterexample pairs, finding that all but one pair are distinguished.

TABLE II. Numerical results for four-fermion noninteracting walks in 136 graph pairs that are not distinguished by three-particle noninteracting walks. Of the 136 graph pairs tested, only 1 pair is not successfully distinguished. We therefore see that increasing the number of noninteracting particles beyond 3 continues to increase the distinguishing power of the noninteracting QRWs.

Family $(N, k, \lambda, \mu)$	3-particle failures	4-fermion failures
(26,10,3,4)	1	0
(35,18,9,9)	38	0
(36,14,4,6)	89	1
(40,12,2,4)	8	0

Since increasing the number of noninteracting particles in the walk apparently increases the distinguishing power, it is natural to ask, “Does there exist a  $p$  such that the  $p$ -particle noninteracting walk can distinguish all SRGs?” The next subsection shows that the answer to this question is no.

**C. Limitations of noninteracting walks**

In this subsection, we show that pairs of nonisomorphic SRGs exist that are not distinguished by any  $p$ -particle noninteracting quantum walk with fixed  $p$  in conjunction with the comparison algorithm described by Eq. (9). This is because for a fixed  $p$ , there exists an  $N$  such that the number of SRGs with  $N$  vertices is larger than the maximum number of graphs distinguishable by the  $p$ -particle noninteracting walk.

To prove this claim, we define  $S(N)$ , the number of SRGs in a particular family with  $N$  vertices, and  $Z(p, N)$ , the number of distinct “graph fingerprints” that the  $p$ -boson walk can generate for an SRG family whose graphs have  $N$  vertices. By a graph fingerprint, we mean a sorted list of the absolute value of every element of an evolution operator [Eq. (10)]. We examine the boson walk here, because its state space is strictly larger than that of a fermion walk of the same number of particles. Thus the  $p$ -boson walk generates more fingerprints than the  $p$ -fermion walk (even though we have seen no evidence yet that it distinguishes more graph pairs). Therefore,  $Z(p, N)$  bounds from above the maximum number of SRGs with  $N$  vertices in a particular family that noninteracting walks of either  $p$  fermions or bosons can distinguish.

We now define the ratio  $R(p, N)$ :

$$R(p, N) = \frac{S(N)}{Z(p, N)}. \tag{13}$$

We show that for any fixed  $p$ ,  $R > 1$  for large enough  $N$ , thus demonstrating that there exist more SRGs than the  $p$ -particle walk can distinguish.

It is shown in [44] that there is a mapping between Latin squares of size  $n$  and SRGs of size  $n^2$  with family parameters  $(n^2, 3(n - 1), n, 6)$ . The results of [44,45] imply that when  $N$  is large enough, the number of nonisomorphic Latin square SRGs of size  $N$  is bounded below by

$$S(N) \geq \frac{1}{6} (\sqrt{N}!)^{2\sqrt{N}-3} N^{\frac{N}{2}}. \tag{14}$$

As for  $Z(p, N)$ , we show in Appendix B that for a fixed  $p$ ,  $Z$  satisfies the inequality

$$Z(p, N) < N^{2X_p(p+1)}, \tag{15}$$

where  $X_p$  is the number of unique values a Green’s function for a  $p$ -boson walk can assume. While it can be shown that  $X_p$  is superexponential in  $p$ , it does not depend on  $N$ . This is because the value of a Green’s function for a noninteracting  $p$ -particle QRW on an SRG is determined by a configuration of up to  $2p$  vertices in that SRG, as discussed in Sec. III A and Appendix A.

To examine the behavior of  $R$  in the limit of large  $N$ , we use Stirling’s formula:

$$x! = \sqrt{2\pi} e^{-x} x^{x+1/2} [1 + O(x^{-1})]. \tag{16}$$

This allows us compute a lower bound for  $R$  in the limit of large  $N$ :

$$\lim_{N \rightarrow \infty} R \geq \frac{1}{6} (2\pi)^{\sqrt{N}-\frac{3}{2}} e^{-2N+3\sqrt{N}} N^{\frac{N}{2}-\sqrt{N}-\frac{3}{4}-2X_p(p+1)}. \tag{17}$$

Taking the logarithm of Eq. (17) yields:

$$\lim_{N \rightarrow \infty} \ln R(p, N) \geq \lim_{N \rightarrow \infty} \frac{N}{2} \ln N + O(N), \tag{18}$$

which diverges as  $N \rightarrow \infty$ . Therefore, for a fixed  $p$ ,  $R$  approaches  $\infty$  as  $N$  increases, showing that no  $p$ -particle noninteracting walk can distinguish all SRGs.

One can let  $p$  grow slightly with  $N$  and achieve the same result. Indeed, we show in Appendix C that

$$\log_2(X_p) = p^2 + O(p \log p). \tag{19}$$

Using this, we find that our argument remains valid for  $p < C\sqrt{\log_2 N}$ , for any  $C < 1$ .

We can contrast these results with those of Gamble *et al.* They found that the hard-core two-boson walk distinguished all graph pairs in a data set of more than 500 million pairs of SRGs [27]. This distinguishing power was shown to arise from an underlying algebra that is fundamentally different from that of noninteracting two-boson or two-fermion walks. As we see no obvious way to extend the proof presented in this section to include hard-core walks, it is an open question whether or not the two-boson hard-core walk has universal distinguishing power on SRGs. Even if does not, it is still possible that there exists a fixed  $p > 2$  such that the  $p$ -boson hard-core walk could distinguish all SRGs. If this is the case, then this would be a marked difference between noninteracting and hard-core walks.

**IV. DISCUSSION**

We have shown how three-particle noninteracting QRWs are qualitatively different from two-particle noninteracting QRWs; the latter will always fail to distinguish nonisomorphic SRGs from the same family, whereas the former successfully distinguish many (but not all) nonisomorphic pairs of SRGs. We have analytically identified a fundamental difference between these two classes of quantum walks. Three-particle walks have potential distinguishing power because the shared connectivity of triples of vertices in SRGs is not governed by the SRG family parameters. We have also demonstrated

numerically that three-particle noninteracting walks have significant, but not universal, distinguishing power on SRGs. We observe numerically that bosonic and fermionic walks distinguish the same pairs of nonisomorphic pairs of graphs. Increasing the number of noninteracting fermions to four further increases the distinguishing power. However, this distinguishing power is not limitless; we have shown that for any fixed number of noninteracting particles, there exist nonisomorphic pairs of SRGs that cannot be distinguished.

Finally, we discuss the implications of these results in terms of the computational complexity of the GI problem. Not only are there graph pairs on which three- and four-particle walks fail, but also we know that for any fixed particle number, there will be SRGs that such noninteracting walks cannot distinguish. It is still possible that, given any nonisomorphic SRG pair of a fixed size  $N$ , there exists a  $p$  such that the  $p$ -particle noninteracting walk will succeed in distinguishing the graphs. However, the lower bound given at the end of Sec. III C rules out the possibility of our algorithm providing a classical polynomial-time solution to GI for SRGs.

#### ACKNOWLEDGMENTS

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#### APPENDIX A: COMPUTING MULTIPLICITIES OF VALUES OF MATRIX ELEMENTS OF THE EVOLUTION OPERATOR FOR STRONGLY REGULAR GRAPHS

Here we discuss how to compute the multiplicities of values of elements of evolution operators, or Green's functions, for SRGs. We show in this Appendix that the multiplicity of a noninteracting three-particle Green's function is in general not a function of the SRG family parameters. This result is used in Sec. III A to demonstrate how two-particle and three-particle noninteracting walks have different distinguishing powers for SRGs.

To compute the multiplicity of each value of the Green's function in a noninteracting three-particle walk, we first note that Eqs. (10) through (12) imply that the value of a given Green's function depends on the relationships between the vertices in the final state (the bra;  $\{i, j, k\}$ ) and the vertices in the initial state (the ket;  $\{p, q, r\}$ ). For each pair of indices  $(x, y)$ , with  $x$  from the bra ( $x \in \{i, j, k\}$ ) and  $y$  from the ket ( $y \in \{p, q, r\}$ ), there are three possible relations. The vertices can be connected ( $A_{xy} = 1$ ), the vertices can be the same ( $\delta_{xy} = 1$ ), or the vertices can be different and disconnected ( $A_{xy} = \delta_{xy} = 0$ ). Therefore, we may think of each Green's function as corresponding to a generalized subgraph of the original graph. We say "generalized subgraph" because the Green's function is unaffected by internal connections within the initial or final

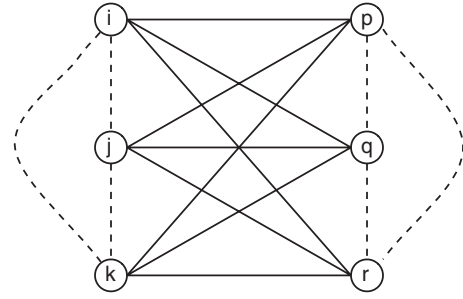


FIG. 1. Sketch of a generalized subgraph, or “widget,” used to calculate the values and degeneracy of a Green's function for a three-particle quantum walk on an SRG. Vertices on the right side correspond to the vertices the particles are on to begin with (the ket  $|pqr\rangle_B$  or  $|pqr\rangle_F$ ), and vertices on the left side correspond to the vertices the particles end up on (the bra  ${}_B\langle ijk|$  or  ${}_F\langle ijk|$ ), after application of the evolution operator  $U$ . A solid line between vertex  $x$  and vertex  $y$  indicates that  $A_{xy} = 1$ . A dashed line between  $x$  and  $y$  means that the value of  $A_{xy}$  does not affect the value of the Green's function. Thus, for bosons, the depicted widget corresponds to the Green's function  ${}_B\langle ijk| \mathbf{U}_{3B} |pqr\rangle_B$  when all six vertices are distinct and when  $A_{xy} = 1$  for all  $x \in \{i, j, k\}$  and  $y \in \{p, q, r\}$ . Equations (10) and (12) show that the value of this Green's function, or widget, is  ${}_B\langle ijk| \mathbf{U}_{3B} |pqr\rangle_B = 6(\beta + \gamma)^3$ .

state; we adopt the more compact terminology of referring to these generalized subgraphs as “widgets.”

To illustrate this point, let us consider the widget shown in Fig. 1. Solid lines in the widget indicate that the sites are connected in the graph, while dashed lines indicate that the value of the widget does not depend on whether or not those sites are connected. Thus, two widgets are considered the same whether or not sites that are connected by dashed lines are actually adjacent. To evaluate  ${}_B\langle ijk| \mathbf{U}_{3B} |pqr\rangle_B$  for the widget shown in Fig. 1, we note that all six vertices ( $\{i, j, k, p, q, r\}$ ) are distinct. We can then use Eqs. (10) and (12) to find that  ${}_B\langle ijk| \mathbf{U}_{3B} |pqr\rangle_B = 6(\beta + \gamma)^3$ , where  $\beta$  and  $\gamma$ , defined in (12), are functions of the SRG family parameters. The multiplicity of this particular value for a particular graph is given by the number of times its corresponding widget occurs in the graph.

To compute the multiplicity,  $M$ , of  $6(\beta + \gamma)^3$  in  $\mathbf{U}_{3B}$ , we count the number of occurrences of this widget in the graph. To do this, we perform the following combinatorial sum, generalizing the procedure outlined in Appendix B of Gamble *et al.* [27].

$$\begin{aligned}
 M &= \sum_{i < j < k} \sum_{p < q < r} A_{ip} A_{iq} A_{ir} A_{jp} A_{jq} A_{jr} A_{kp} A_{kq} A_{kr} \\
 &= \frac{1}{36} \sum_{ijkpqr} A_{ip} A_{iq} A_{ir} A_{jp} A_{jq} A_{jr} A_{kp} A_{kq} A_{kr} (1 - \delta_{ij}) \\
 &\quad \times (1 - \delta_{ik})(1 - \delta_{jk})(1 - \delta_{pq})(1 - \delta_{pr})(1 - \delta_{qr}).
 \end{aligned} \tag{A1}$$

The analogous sums considered by Gamble *et al.*, who examine only two-particle walks, can be decomposed into

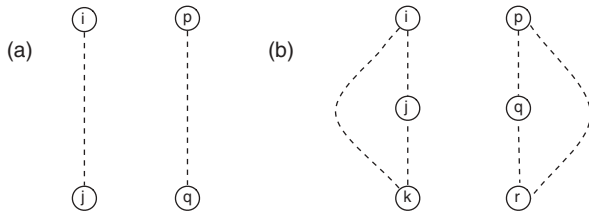


FIG. 2. Empty widgets for two-particle and three-particle noninteracting walks. In both widgets, all vertices are distinct and no vertex in the initial state is adjacent to any vertex in the final state. The values of the widgets depend only on the family parameters for both (a) and (b), while the degeneracies of these values depend only on family parameters for two particles but not for three. The multiplicity of each widget's respective Green's function for a particular SRG is equal to the number of times that widget appears in the SRG. (a) The empty widget for two particles. The number of times this widget appears in an SRG is a function of the SRG family parameters, as is the case for all two-particle widgets [27]. (b) The empty widget for three particles. The number of times this widget appears in an SRG is *not* a function solely of SRG family parameters. This is demonstrated by the graphs in Fig. 3. An analytic explanation for this phenomenon is given in the text following Eq. (A2).

sums and traces over powers of the adjacency matrix. Such operations are given by contracting over two occurrences of the same index in the summand. Conveniently, these quantities are expressible in terms of SRG family parameters, as illustrated by Gamble *et al.* Things are not as simple, however, for three-particle walks. By inspection, we see that Eq. (A1) contains contractions over three occurrences of the same index. Such contractions correspond to neither matrix multiplication nor computation of the trace and cannot in general be massaged into forms expressible in terms of SRG family parameters, as evidenced by the fact that three-particle walks have distinguishing power over many pairs of SRGs.

However, the above statement does not give us analytic proof that there exist Green's functions whose multiplicities are not functions of the family parameters; up to this point, we are still relying on the numerical results as proof. Below, we analytically demonstrate that there exist widgets whose multiplicities *cannot* be determined by family parameters. To demonstrate this, we take a step back to the two-particle walk. Consider the widget shown in Fig. 2(a). We can determine this widget's multiplicity for an arbitrary SRG with family parameters  $(N, k, \lambda, \mu)$  by performing the combinatorial sum analogous to Eq. (A1), or equivalently, we can actually count the number of times we can fit this widget on the SRG. To begin, we pick two sites in the graph to serve as sites  $i$  and  $j$ ; these sites may be adjacent or not, as indicated by the dashed line between them in the figure. Now we must count, given our choice of  $i$  and  $j$ , how many sites we may pick as  $p$  and  $q$ . If  $i$  and  $j$  are connected, there are  $\binom{N-2k+\lambda}{2}$  choices for  $p$  and  $q$ , whereas if  $i$  and  $j$  are disconnected, there are  $\binom{N-2-2k+\mu}{2}$  choices for  $p$  and  $q$ . There are  $\frac{Nk}{2}$  choices for connected sites that can serve as  $i$  and  $j$  and  $\binom{N}{2} - \frac{Nk}{2}$  disconnected sites. Thus, the number of four-vertex empty widgets occurring in a

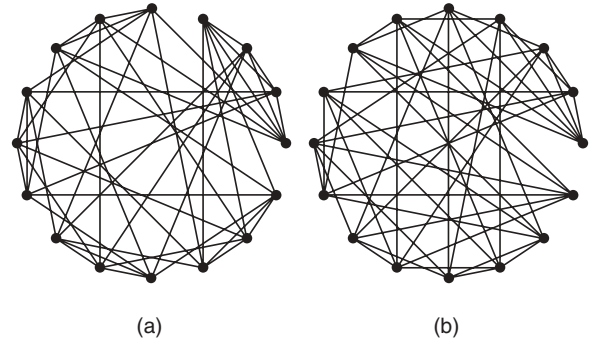


FIG. 3. The two nonisomorphic graphs of the SRG family (16,6,2,2). The widget in Fig. 2(b) appears in the graph shown in (a) 608 times, whereas the same widget appears in the graph shown in (b) 512 times. Thus we see that the same three-particle widget can have different multiplicities in graphs of the same family, so the three-particle noninteracting walk can distinguish at least some nonisomorphic graphs from the same SRG family.

two-particle noninteracting walk is

$$M_{2,\text{empty}} = \frac{Nk}{2} \binom{N-2k+\lambda}{2} + \left[ \binom{N}{2} - \frac{Nk}{2} \right] \binom{N-2-2k+\mu}{2}, \quad (\text{A2})$$

in agreement with the result of Gamble *et al.* for this particular widget [27]. Thus we see that this widget's multiplicity is, as expected, a function of the family parameters. Let us see what happens when we try this same approach for the corresponding widget in three-particle walks, shown in Fig. 2(b). Again, we consider the multiplicity of the widget in an arbitrary SRG by counting the number of times we can fit this widget on the graph. Now we pick three sites to serve as  $i$ ,  $j$ , and  $k$ . We want to count, given our choice of  $i$ ,  $j$ , and  $k$ , the number of sites that can serve as  $p$ ,  $q$ , and  $r$ . To do this, we need to know how  $i$ ,  $j$ , and  $k$  are connected among themselves, just as we did in the previous example. There are four possible nonisomorphic connectivities, as there can be between zero and three connections among these sites. In order to count the multiplicity of this widget, we must consider for each of these four cases how many sites in the graph are mutually disconnected from sites  $i$ ,  $j$ , and  $k$ . In the previous example, we could answer the analogous question via the family parameters, as illustrated above. However, this is because the family parameters  $\mu$  and  $\lambda$  tell us how many common neighbors *pairs* of vertices have. There are no family parameters which encode this information for *triples* of vertices, as strong regularity does not place absolute constraints on shared connectivities for triples of vertices.

We illustrate this point with an example in Fig. 4. Two copies of the Petersen graph, an SRG with family parameters (10,3,0,1), are depicted. The first copy highlights three mutually nonadjacent vertices; this particular triple of vertices has one common neighbor. The second copy also highlights a triple of mutually nonadjacent vertices, but this triple has *no* shared neighbors. Thus we have demonstrated by example that strong regularity cannot in general uniquely determine the shared connectivity for triples of vertices.

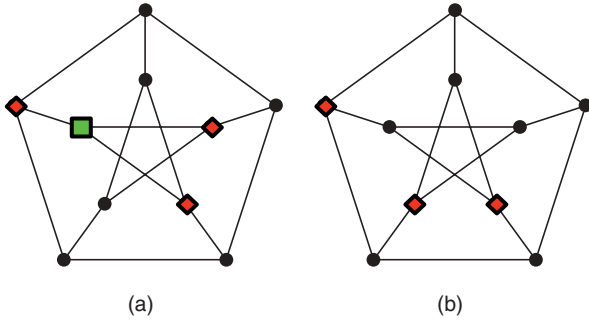


FIG. 4. (Color online) Two copies of the Petersen graph, an SRG with parameters  $(10,3,0,1)$ . In each graph, three mutually nonadjacent vertices are highlighted as (red) diamonds. In (a), the three vertices share one common neighbor, shown as the (green) square. In (b), the three vertices share no common neighbors. This demonstrates that the number of neighbors common to a triple of vertices in a strongly regular graph is not strictly a function of the SRG family parameters, thus showing why widget multiplicity is not strictly governed by family parameters when  $p \geq 3$ .

Moreover, we can see that counting the multiplicity of the widget shown in Fig. 2(b) can be used to distinguish two non-isomorphic graphs from the same SRG family. Figure 3 shows the two non-isomorphic graphs in the SRG family  $(16,6,2,2)$ . The widget in Fig. 2(b) appears 512 times in the first graph and 608 times in the second graph, thus distinguishing them.

We conclude, then, that there exist three-particle widgets whose multiplicities *cannot* be functions of family parameters. Thus, three-particle noninteracting walks are *not* forbidden from distinguishing nonisomorphic SRGs from the same family, unlike two-particle noninteracting walks.

#### APPENDIX B: COMPUTING THE NUMBER OF SRG FINGERPRINTS

In Sec. III C, it is shown that quantum walks of  $p$  noninteracting particles cannot distinguish all nonisomorphic pairs of SRGs. This is done by showing that  $Z(p,N)$ , the number of graph fingerprints given by the  $p$ -boson walk on an SRG family with  $N$  vertices, is less than the number of no-isomorphic SRGs with  $N$  vertices, in the limit of large  $N$ . This subsection presents the calculation of  $Z(p,N)$ .

To calculate  $Z(p,N)$ , we note that if there are  $X_p$  possible Green's function values for the  $p$ -boson walk, and  $Y$  elements of the evolution operator  $U$ , then computing the number of unique fingerprints is equivalent to computing the number of ways one can put  $Y$  indistinguishable balls in  $X_p$  labeled bins, so that [46]

$$Z(p,N) = \binom{X_p + Y - 1}{X_p - 1}. \quad (\text{B1})$$

We recall that  $X_p$  is a function of  $p$ , but not of  $N$ . (We may think of  $X_p$  as the number of uniquely valued widgets that appear in the  $p$ -boson walk.) However,  $Y$ , the number of elements in the evolution operator, will depend on both  $p$  and  $N$ , and we henceforth write it as  $Y_{p,N}$ . The dimension of the evolution operator is computed by determining how many different ways  $p$  bosons can be put on  $N$  vertices, which is the same problem as computing the number of ways to put

$p$  indistinguishable balls into  $N$  labeled bins. The number of elements in the evolution operator is just the square of its dimension, so we find that

$$Y_{p,N} = \binom{N + p - 1}{p}^2. \quad (\text{B2})$$

Using Eqs. (B1) and (B2), we now compute an upper bound for  $Y_{p,N}$  and  $Z$ . It can be shown that  $\binom{n+k-1}{k-1} \leq n^k$  when  $n \geq 2$  and  $k \geq 1$ . Thus

$$Y_{p,N} < \binom{N + p}{p}^2 \leq N^{2(p+1)} \quad (\text{B3})$$

and

$$Z(p,N) \leq (Y_{p,N})^{X_p} < N^{2X_p(p+1)}. \quad (\text{B4})$$

Therefore, the maximum number of unique graphs the  $p$ -boson walk can distinguish is bounded above by  $N^{2X_p(p+1)}$ . We use this result in Sec. III C to show that there exist SRGs that a particular  $p$ -particle walk cannot distinguish.

#### APPENDIX C: BOUNDING THE NUMBER OF WIDGETS IN THE NONINTERACTING $p$ -PARTICLE WALK

Here, we show that  $\log_2 X_p \sim p^2$ , where  $X_p$  is the number of distinct widgets for the noninteracting  $p$ -boson walk. First, Auluck proved that there are  $e^{O(p^{2/3})}$  widgets with no edges [47]. [He counted bipartitions of  $(p,q)$ , which may be considered to be edgeless widgets when  $p = q$ .] Since there are at most  $2^{p^2}$  ways to add edges to one of these, we have the upper bound  $X_p \leq 2^{p^2 + O(p^{2/3})}$ . To get a lower bound, it will suffice to consider the widgets with  $2p$  distinct indices. The edges in one of these can be specified by a  $p \times p$  array of bits, and the widgets isomorphic to it are obtained by permuting rows, permuting columns, or transposing the matrix. Therefore, by Burnside's counting lemma [48], the number of isomorphism classes of widgets of this type is

$$\frac{1}{|F|} \sum_{f \in F} [\text{No. of arrays fixed by } f],$$

where the finite group  $F$  is the semidirect product of  $S_p \times S_p$  by  $S_2$ . ( $S_p$  and  $S_2$  are the symmetric groups on  $p$  and 2 objects, respectively.) This is lower bounded by the term coming from  $f = 1$ , which is  $2^{p^2}/[2(p!)^2]$ , and this is  $2^{p^2 + O(p \log p)}$  by Stirling's formula. From these two estimates the result of Eq. (19) follows.

#### APPENDIX D: ERROR ANALYSIS FOR NUMERICAL COMPUTATIONS

When comparing two graphs, we compute  $\Delta$ , a measure of the distance between the lists of matrix elements of the evolution operators for the two graphs, as defined in Eq. (9). Computing  $\Delta$  requires comparing two lists of numbers that are each exponentially large in particle number  $p$ . An evolution operator for a walk of  $p$  noninteracting fermions on a graph with  $N$  vertices has  $\binom{N}{p}^2$  elements, and the boson equivalent has  $\binom{N+p-1}{p}^2$  elements. For example, the evolution operator



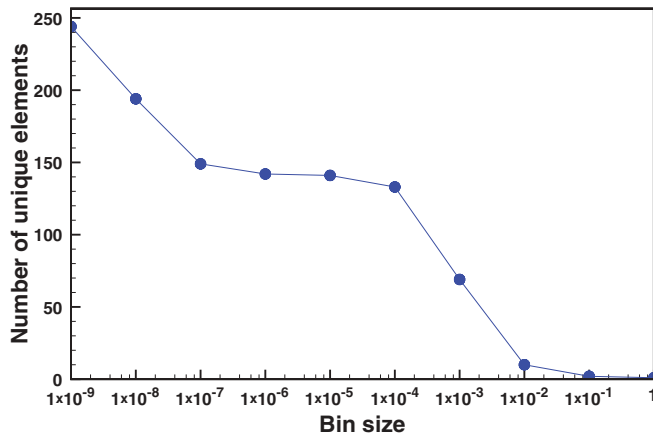


FIG. 5. (Color online) The number of numerically distinguished elements in the evolution operator  $U(t)$ , defined in Eq. (8) as a function of the bin size used in grouping the elements. This plot is for the noninteracting three-fermion walk on a graph in the SRG family (16,6,2,2). We see that the actual number of unique elements is about 150, which can be obtained by using a bin size in the range of  $10^{-7}$  to  $10^{-4}$ .

for the noninteracting four-fermion walk on a graph of 35 vertices has more than 2.7 billion elements.

Comparison of the lists can be made much more efficient by exploiting the fact that the values in the list are highly degenerate. Instead of comparing the entries in a list, we make histograms of element values and their multiplicities. We then compute  $\Delta$  by comparing these histograms. When

constructing the histograms, it is important to determine the correct bin size. Choosing a bin size that is too large results in falsely grouping distinct elements together, while choosing a bin size that is too small results in falsely distinguishing elements. By constructing a series of histograms with different bin sizes for the same evolution operator, we are able to determine a range of bin sizes which are neither too large nor too small. This is illustrated in Fig. 5, which shows that for a noninteracting three-fermion walk on a graph in (16,6,2,2), an appropriate bin size is between  $10^{-7}$  and  $10^{-4}$ .

Because we compute  $\Delta$  via numerical simulation, we expect there to be some numerical noise floor. That is, for any two permutations of the same graph, we expect  $\Delta > 0$ . It is important to determine how big this quantity, which we denote  $\Delta_{\text{iso}}$ , will be. We consider two nonisomorphic graphs to be distinguished only if they yield a  $\Delta$  which satisfies  $\Delta \gg \Delta_{\text{iso}}$ .

We numerically compute  $\Delta_{\text{iso}}$  using double-precision arithmetic for a variety of random permutations on our graphs, and we find the maximum  $\Delta_{\text{iso}}$  to be approximately  $10^{-6}$ . Thus, only graph pairs which yield a  $\Delta > 10^{-6}$  are considered distinguished. We find  $\Delta_{\text{iso}}$  to be relatively insensitive to graph size and particle number.

In practice, we see a gap for  $\Delta$  between distinguished graph pairs and nondistinguished graph pairs. For distinguished graphs, we find  $\Delta$  to be at least two orders of magnitude larger than  $\Delta_{\text{iso}}$  (usually much larger); nondistinguished graph pairs have values of  $\Delta$  that are approximately equal to, or even smaller than,  $\Delta_{\text{iso}}$ .

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