Physically-motivated dynamical algorithms for the graph isomorphism problem

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Abstract

We investigate classical and quantum physics-based algorithms for solving the graph isomorphism problem. Our work integrates and extends previous work by Guðkov et al. (cond-mat/0209112) and by Rudolph (quant-ph/0206068). Guðkov et al. propose an algorithm intended to solve the graph isomorphism problem in polynomial time by mimicking a classical dynamical many-particle process. We show that this algorithm fails to distinguish pairs of non-isomorphic strongly regular graphs, thus providing an infinite class of counterexamples. We also show that the simplest quantum generalization of the algorithm also fails. However, by combining Guðkov et al.’s algorithm with a construction proposed by Rudolph in which one examines a graph describing the dynamics of two particles on the original graph, we find an algorithm that successfully distinguishes all pairs of non-isomorphic strongly regular graphs that we tested (with up to 29 vertices).

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Introduction. The graph isomorphism problem plays a central role in the theory of computational complexity and has importance in physics and chemistry as well. A graph is a set of $N$ points, or vertices, and a set of edges, or unordered pairs of those points. If two graphs differ only in the labelling of their points, then we say they are isomorphic, otherwise they are non-isomorphic. The graph isomorphism problem is to determine whether or not there is an algorithm that runs in polynomial time ($t \sim N^x$, with $x$ independent of $N$) that distinguishes non-isomorphic pairs with certainty. The efficient enumeration of possible distinct atomic clusters of size $N$, in which a cluster is defined by the bonds between its atoms, is the same problem in another guise.

Typical instances of graph isomorphism (GI) can be solved in polynomial time because two randomly chosen graphs with identical numbers of vertices and edges typically have different degree and eigenvalue distributions. Moreover, GI can be solved efficiently for restricted classes of graphs, such as trees, planar graphs, graphs with bounded degree, bounded eigenvalue multiplicity, and bounded average genus. However, no algorithm for solving GI for all graphs is presently known; the best existing upper bound is $\exp\sqrt{cN\log N}$. There is evidence that indicates that GI is not NP-complete: first, counting the number of isomorphisms is reducible to the decisional version of the problem, unlike the situation for all known NP-complete problems, and second, if GI were NP-complete then certain complexity classes that are believed to be different would be identical. Thus, it is believed that either GI is in P or else it is in the class of problems that are neither in P nor are NP-complete.

One way to solve GI is to solve the hidden subgroup problem for the permutation group. Unfortunately, though the hidden subgroup problem for abelian groups can be solved efficiently, no efficient algorithm for solving the hidden subgroup problem for the permutation group is known.

In this paper we investigate classical and quantum approaches to solving the graph isomorphism problem that are motivated by physical processes. Our work combines and extends ideas in Gudkov et al. and by Rudolph for attacking the GI problem using algorithms based on physical intuition. We show that the interesting classical dynamical algorithm proposed by Gudkov et al. fails to distinguish an infinite set of pairs of non-isomorphic graphs, and thus does not solve the GI problem in polynomial time. We trace this failure to certain algebraic properties of these particular pairs of graphs and show that
the simplest quantum generalizations of the Gudkov et al. algorithm also fails to distinguish these pairs of graphs. However, an algorithm obtained by combining the basic idea of the Gudkov et al. algorithm with a construction proposed by Rudolph[23] does distinguish all pairs of graphs that we have examined, including many with the same eigenvalue spectra.

The detailed statement of the GI problem is as follows. We are given two graphs. The first is a set of \( N \) vertices \( \{v_1, v_2, \ldots, v_N\} \), together with a set of edges, or unordered pairs \( \{e_1, e_2, \ldots\} \) connecting pairs of these vertices, while the second graph is a set of vertices \( \{v'_1, v'_2, \ldots, v'_N\} \), and a set of edges \( \{e'_1, e'_2, \ldots\} \). Each \( e_i \) is associated with a pair \( \{v_a, v_b\} \), and each \( e'_i \) is associated with a pair \( \{v'_a, v'_b\} \). We wish to determine whether there exists a permutation \( \mathcal{P} \) of the \( v_i \) such that the set of pairs \( \{\mathcal{P}v_a, \mathcal{P}v_b\} \) is identical with the set of pairs \( \{v'_a, v'_b\} \).

An equivalent but more useful formulation for our purposes is to represent each graph by its adjacency matrix \( A \). \( A_{ab} \) is an \( N \times N \) matrix such that \( A_{ab} = 1 \) if there is a pair \( e = \{v_a, v_b\} \) and \( A_{ab} = 0 \) otherwise. Two graphs are isomorphic if and only if there exists a permutation matrix \( P \) such that \( A' = PAP^{-1} \).

**Classical algorithm.** In the Gudkov et al. approach to this problem[22], each vertex of the graph is mapped into a point in an \( N \)–dimensional vector space. The vertex \( v_1 \) sits initially at the point \( \vec{r}_1 = (1, 0, 0, \ldots, 0) \), \( v_2 \) at \( \vec{r}_2 = (0, 1, 0, \ldots, 0) \), and so on. These are the vertices of an \( (N - 1) \)–dimensional simplex. We now view these as mass-points with forces acting pairwise among them. There is one force law if two particles are connected by an edge and a different force law if they are not. The forces are derived from potentials \( U_1 \) and \( U_2 \) that depend only on the distances between the points in the pair. From the initial configuration, the particles move in time according to the relaxational equations of motion

\[
\mu \frac{d\vec{r}_a(t)}{dt} = \vec{F}_a,
\]

where

\[
\vec{F}_a = -\nabla_{\vec{r}_a} U(\vec{r}_1, \vec{r}_2, \ldots)
\]

and

\[
U = \sum_{a>b} A_{ab} U_1(|\vec{r}_a - \vec{r}_b|) + \sum_{a>b} (1 - A_{ab}) U_2(|\vec{r}_a - \vec{r}_b|).
\]

(1)

The motion may be computed by any convenient algorithm. After a time \( T \) the positions are given by \( \vec{r}_a(T) \) for \( a = 1, 2, \ldots, N \). We now compute the set of \( N(N - 1)/2 \) distances...
\( d_{ab} = |\vec{r}_a(T) - \vec{r}_b(T)| \). Given a second graph, we compute \( d'_{ab} = |\vec{r}'_a(T) - \vec{r}'_b(T)| \) using the same prescription. The sets \( \{d_{ab}\} \) and \( \{d'_{ab}\} \), being non-negative real numbers, may be arranged in increasing order. If the resulting sets are identical, then it is conjectured that the graphs are isomorphic. Note that as long as \( T \) is not an exponentially long time, this is a polynomial-time algorithm. The sets \( d_{ab} \) and \( d'_{ab} \) can be computed, ordered, and compared efficiently. We wish to examine the claim that if \( \{d_{ab}\} \) and \( \{d'_{ab}\} \) are the same up to reordering, then their parent graphs are isomorphic.

For purposes of clarity, we shall initially consider a slightly simpler model, one in which a harmonic force acts only between particles connected by edges:

\[
\tilde{U} = -\mu \sum_{a>b} A_{ab} |\vec{r}_a - \vec{r}_b|^2 / 2.
\]

We then define an \( N \times N \) matrix \( X \), where the \( i \)-th coordinate of the \( a \)-th "particle" is denoted by \( X_{ai} \). Thus the above initial condition can be rewritten as

\[
X_{ai}(t = 0) = \delta_{ai},
\]

where \( \delta_{ai} \) is the Kronecker symbol: \( \delta_{ai} = 1 \) if \( a = i \) and \( \delta_{ai} = 0 \) otherwise. The equations of motion are

\[
\frac{dX_{ai}}{dt} = \sum_b F_{ab}^{(i)} = \sum_b A_{ab} (X_{ai} - X_{bi}) = -\sum_b A_{ab} X_{bi} + \sum_b \sum_c A_{ac} \delta_{ab} X_{bi} = \sum_b L_{ab} X_{bi},
\]

where

\[
L_{ab} = \delta_{ab} \sum_c A_{ac} - A_{ab} = D_{ab} - A_{ab},
\]

is the Laplacian matrix. The diagonal matrix \( D \) is the degree sequence matrix: \( D_{aa} \) is the number of edges incident to the vertex \( a \). Note that \( L \) is symmetric: \( L = L^T \). The algebraic isomorphism criterion mentioned in the introduction may also be put in terms of \( L \): two graphs defined by the Laplacian matrices \( L \) and \( L' \) are isomorphic if and only if there exists a permutation matrix \( P \) such that

\[
L' = PLP^T.
\]

The solution to the equation of motion for the particles defined by \( \tilde{U} \) is

\[
X_{ai}(t) = (e^{Lt})_{ab} X_{bi}(t = 0) = (e^{Lt})_{ai}.
\]
so the final positions are

\[ X(T) = e^{LT}, \]

in a matrix notation. In order to compute the distances, we note that the set of dot products between the position vectors may be written as:

\[ S_{ab} = \sum_i X_{ai} X_{bi} \]

which is the matrix

\[ S = XX^\text{Transpose} = X^2 = e^{2Lt} = 1 + 2tL + \frac{(2t)^2}{2!}L^2 + ... \]

Another graph would be characterized by a different dot product matrix

\[ S' = e^{2L't}. \]

Since the \( N^2 \) distances \( d_{ab} \) satisfy \( d_{ab}^2 = S_{aa} + S_{bb} - 2S_{ab} \), comparing the set of numbers in the matrices \( S \) and \( S' \) is essentially the same as comparing the distances. (We shall consider the relationship more carefully below.)

If the graphs are isomorphic, then clearly \( S' \) is a rearrangement of \( S \):

\[ S' = e^{2L'T} = e^{2PLP^{-1}T} = Pe^{2Lt}P^{-1} = PSP^{-1}. \]

The interesting question is whether the converse is also true.

In fact there do exist many interesting graph pairs for which the algorithm works. Because \( S \) is most easily computed by diagonalizing the real symmetric matrix \( L \), it is natural to ask whether pairs of non-isomorphic but isospectral graphs can be distinguished by the method. Isospectral graphs are those for which the eigenvalues of \( A \) and \( A' \) are the same. We have investigated this question for some small graphs that are isospectral but not isomorphic. A simple illustrative pair is shown in Fig. [I]

We take the total time interval as \( T = 1 \) and compute numerically the dynamics of the simple harmonic model for 10 steps of length 0.1 using the first-order Euler algorithm and finally obtain a normalized \( X(T) \). The sorted \( d_{ab}^2 \) and \( d'_{ab}^2 \) for two graphs \( G \) and \( G' \) in Fig. [I] are respectively

\[ d_{ab}^2 = \{ [0]^5, [0.0785]^{12}, [3.9685]^8 \}. \]

\[ d'_{ab}^2 = \{ [-1.9216]^8, [-0.2570]^4, [0]^5, [0.1406]^8 \}. \]
In these expressions the superscripts denote the multiplicity of the number in square brackets.

Thus the algorithm of Ref. [22] works for this non-isomorphic isospectral pair. The dynamical algorithm also distinguishes successfully some pairs of graphs that have both identical degree distributions and identical Laplacian spectra [29].

It has been known for decades, however, that certain classes of graphs are difficult to distinguish by elementary methods. An important intransigent class is the so-called “strongly regular graphs” (SRG’s) [24, 25]. A SRG with parameters \((N, k, \lambda, \mu)\) is a graph with \(N\) vertices in which each vertex has \(k\) neighbors, each pair of adjacent vertices has \(\lambda\) neighbors in common, and each pair of non-adjacent vertices has \(\mu\) neighbors in common. An example known as \(L_2(3)\) with parameters \((9, 4, 1, 2)\) is shown in Fig. 2. Many pairs of nonisomorphic SRGs with the same parameter set are known. [30]

The adjacency matrix \(A\) of a SRG has some interesting algebraic properties. For a general graph, the \((a, b)\) entry of \(A^2\) is the number of vertices adjacent to both \(a\) and \(b\). For SRGs, this number is \((A^2)_{ab} = k\) if \(a = b\), \((A^2)_{ab} = \lambda\) if \(a\) is adjacent to \(b\), and \((A^2)_{ab} = \mu\) if \(a\) is not adjacent to \(b\). Hence

\[
A^2 = kI + \lambda A + \mu(J - I - A),
\]

FIG. 1: Two isospectral graphs

FIG. 2: \(L_2(3)\) (9, 4, 1, 2)
where $I$ is the identity matrix and $J$ is the matrix consisting entirely of 1’s. $J^2 = NJ$. $A$ and $J$ also have the properties that

$$AJ = JA = kJ.$$ 

This follows from the fact that multiplication of a matrix by $J$ has the effect of adding the rows or columns of the matrix. For $A$, this sum is just the number of neighbors. The Laplacian matrix for a SRG is

$$L = kI - A$$

These equations show that the three matrices $\{I, J, L\}$ form a commutative, associative algebra. The elements of the algebra have the form $R = fI + gJ + hL$, where $f$, $g$ and $h$ are real numbers. The multiplication rule is:

$$RR' = R'R = (fI + gJ + hL)(f'I + g'J + h'L)$$

$$= \{ff' - [k^2 - k(\lambda - \mu + 1) + \mu]hh'\} I + (fg' + gf' + Ngg' + \mu hh')J$$

$$+ [fh' + hf' + (2k + \mu - \lambda)hh']L$$

The structure of the algebra is therefore independent of the precise form of the $L$ matrix, depending only on the $(N, k, \lambda, \mu)$ parameters.

We now consider two non-isomorphic graphs characterized by Laplacian matrices $L$ and $L'$ that share a set $(N, k, \lambda, \mu)$. Let the corresponding dot product matrices be $S = \exp(2LT)$ and $S' = \exp(2L'T)$. Since $L$ and $L'$ define the same algebra, we have

$$S(N, k, \lambda, \mu, T) = f(N, k, \lambda, \mu, T)I + g(N, k, \lambda, \mu, T)J + h(N, k, \lambda, \mu, T)L$$

and

$$S'(N, k, \lambda, \mu, T) = f(N, k, \lambda, \mu, T)I + g(N, k, \lambda, \mu, T)J + h(N, k, \lambda, \mu, T)L'$$

where the $f, g, h$ are definite functions of the parameters — the point being that the
functions are the same for the two graphs. More explicitly, we have that

\[
S = \begin{pmatrix}
  f + g + kh & g - hA_{12} & g - hA_{13} & \ldots \\
  g - hA_{21} & f + g + kh & g - hA_{23} & \ldots \\
  g - hA_{31} & g - hA_{32} & f + g + kh & \ldots \\
  \vdots & \vdots & \vdots & \ddots \\
\end{pmatrix}
\]

The same relation holds when \(S\) is replaced by \(S'\) and \(A\) is replaced by \(A'\). In any row or column of \(A\) or \(A'\), precisely \(k\) entries are equal to 1 and \(N - k\) entries are equal to 0. It now follows that, considered as a set of numbers, \(S\) has \(N\) entries equal to \(f + g + kh\), \(Nk\) entries equal to \(g - h\), and \(N(N - k - 1)\) entries equal to \(g\). The same holds true for \(S'\).

The \(N^2\) squared distances satisfy \((d^2)_{ab} = S_{aa} + S_{bb} - 2S_{ab} = 2(f + kh) + 2hA_{ab}\), and \((d^2)_{ab}' = S'_{aa} + S'_{bb} - 2S'_{ab} = 2(f + kh) + 2hA'_{ab}\) with \(a \neq b\). For \(a = b\), \((d^2)_{ab} = (d^2)_{ab}' = 0\). There are \(Nk\) nonzero entries of \(A_{ab}\) and \(A'_{ab}\) with \(a \neq b\). Hence, for both graphs there will be \(Nk\) distances \(2(f + kh) + 2h\), \(N(N - k - 1)\) distances equal to \(2(f + kh)\), and \(N\) distances equal to 0. Thus it is impossible to distinguish this pair of non-isomorphic graphs by this simplified algorithm.

To extend this to the actual algorithm of Gudkov et al., we examine their general equations of motion \((1)\). From a SRG defined by \(L\), these equations produce a matrix \(X(T)\) which starts life as \(X(t = 0) = I\). Any numerical solution of the differential equation is simply a finite sequence of matrix multiplications and additions. All such operations belong to the algebra defined by \(I, J, L\). The dot product matrix \(S\) also belongs to this algebra. Thus the result is again characterized by only three numbers \(f, g, h\). For a different SRG defined by \(L'\) but with the same parameter set, the algorithm produces the same \(f, g, h\),

\[
\begin{array}{cccc}
1 & 2 & 3 & 4 \\
2 & 1 & 4 & 3 \\
3 & 4 & 1 & 2 \\
4 & 3 & 2 & 1 \\
\end{array}
\quad
\begin{array}{cccc}
1 & 2 & 3 & 4 \\
2 & 3 & 4 & 1 \\
3 & 4 & 1 & 2 \\
4 & 1 & 2 & 3 \\
\end{array}
\]

FIG. 3: Latin squares \(L_3(4) (16, 9, 4, 6)\) \([26]\)
since the algebra for the two graphs is the same. The above argument for the simplified algorithm then goes through without further modification.

To illustrate the breakdown of the algorithm, we shall apply it to the smallest pair of non-isomorphic SRGs. These are the “Latin square” graphs with size \( N = 16 \). Latin squares are two-dimensional \( M \times M \) arrays of the numbers 1 to \( M \), arranged so that in each row and column no number is repeated. Two examples are shown in Fig. 3. Latin square graphs are constructed from Latin squares as follows: Given a Latin square of order \( M \), the vertices are the \( N = M^2 \) cells. Two vertices are adjacent if they lie in the same row or column or if they share the same integer label.

We use the following non-harmonic potential \( U_1 \) to calculate normalized \( X(T) \) and \( d_{ab}^2 \) again using the first-order Euler algorithm for the two non-isomorphic Latin square graphs drawn from Fig. 3.

\[
U_1 = -A \sum (r_a - r_b)^2 + B \sum (r_a - r_b)^4,
\]

where the sum is over pairs of connected vertices. Again taking time interval \( T = 1 \) with step of length 0.1, we obtain the distances \( d_{ab}^2 \) for \( A = 1 \), \( B = 1 \)

\[
d_{ab}^2 = \left\{ [0]^{16}, [1.8641]^{96}, [2.3129]^{144} \right\}.
\]

\[
d_{ab}^{2'} = \left\{ [0]^{16}, [1.8641]^{96}, [2.3129]^{144} \right\}.
\]

\( f^{(t)}, h^{(t)} \) are computed from \( d_{ab}^{2(t)} \)

\[
f = f' = -1.0876
\]

\[
h = h' = 0.2244
\]

\( g = g' \), but these quantities do not affect the distances. We have also verified that the two sets are identical at each of the discrete time steps. As one would expect, the multiplicity of each distinct distance depends only on \( N \) and \( k \) and are independent of time.

For completeness we tried a different non-harmonic attractive(repulsive) potential \( U_1(\vec{r}_a - \vec{r}_b)(U_2(\vec{r}_a - \vec{r}_b)) \) whose force is expressed as

\[
\vec{F}_{1a} = -\nabla_{\vec{r}_a} U_1(\vec{r}_a - \vec{r}_b) = \frac{\vec{r}_a - \vec{r}_b}{1 + |\vec{r}_a - \vec{r}_b|^2}.
\]

\[
\vec{F}_{1a} = -\vec{F}_{2a}.
\]
Using this potential and still taking $T = 1$, we obtain the distances
\[ d_{ab}^2 = \{[0]^{16}, [1.4991]^{96}, [2.4486]^{144}\} \]
\[ d_{ab}^{2'} = \{[0]^{16}, [1.4991]^{96}, [2.4486]^{144}\} \]
with $f^{(t)}, h^{(t)}$
\[ f = f' = -3.5482 \]
\[ h = h' = 0.4748 \]

Thus, using a non-harmonic potential does not enable the dynamical algorithm to distinguish these graphs.

Because we have identified two non-isomorphic graphs that result in the same list of distances, we have disproved the conjecture of Ref. [22]. There are an infinite number of nonisomorphic pairs of SRGs with identical parameter sets, so the number of counterexample pairs is infinite.

**Quantum algorithms.** The same argument can also be used to show that a simple one-particle quantum random walk algorithm also fails to solve the GI problem. Consider the vertices of the graph as states $|j\rangle$ in a Hilbert space. The Hamiltonian for the walk is
\[ H = -\sum_{ab} A_{ab} c_a^\dagger c_b, \]
where the operator $c_a^\dagger c_b$ is defined by \[ \langle i | c_a^\dagger c_b | j \rangle = \delta_{ia} \delta_{bj}. \] In physics terms, this is simply a tight-binding model with bonds on the vertices of the graph. We now consider $N$ possible starting wavefunctions
\[ |\psi_1(t = 0)\rangle = |1\rangle, \quad |\psi_2(t = 0)\rangle = |2\rangle, \ldots \]
and we evolve these forward in time according to the usual time-dependent Schrödinger equation
\[ i \frac{d |\psi\rangle}{dt} = H |\psi\rangle \] (2)
for a time $T$. We then compute the $N \times N$ matrix of overlaps
\[ O_{ij} = \langle \psi_i(0) | \psi_j(T) \rangle. \]
We might then conjecture that this matrix, considered as a set of complex numbers, is different for non-isomorphic graphs. It can distinguish isospectral graphs, since it uses
information about the eigenvectors of $H$, not just information about the spectrum. However, our algebraic argument is trivially extended to the now complex algebra defined by $I, J, L$. For non-isomorphic SRG’s with identical parameter sets, we again find that the two matrices of overlaps are the same after a rearrangement, so the conjecture is invalid.

Though the two strongly regular Latin square graphs of Fig. 3 are not distinguished by the algorithm of Ref. [22], they can be distinguished in polynomial time by using a construction proposed by Rudolph [23], in which the original adjacency matrix is interpreted as the Hamiltonian of a tight-binding model. The original graph with $N$ vertices describes the possible states (positions) of a single particle. However, we can also consider the quantum-mechanical motion of many particles on the same graph. Rudolph uses symmetric wavefunctions but forbids double occupancy of any site, corresponding to a hard-core boson model. Rudolph showed that the spectra of the 3-particle matrices obtained from two non-isomorphic regular graphs with identical single-particle spectra are different, demonstrating that the multiparticle construction does increase the power of the algorithm to distinguish similar graphs.

Here we combine Rudolph’s multiparticle construction with the dynamical algorithm for wavefunction overlaps; this hybrid algorithm has the advantage that it can distinguish nonisomorphic strongly regular graphs using the 2-particle matrices, as opposed to 3-particle matrices needed if the matrix eigenvalues are examined. In addition to Rudolph’s original case of hard-core bosons, we also examine non-hard-core bosons and noninteracting spinless fermions.

For bosons we consider a simple Hubbard Hamiltonian [27], in which each boson can hop between two vertices if and only if the vertices are connected by an edge, and in addition there is an energy cost $U$ if two bosons are on the same site. Using as a basis the states $|ij\rangle$ with particles at vertices $i$ and $j$, the matrix $K$ for the level 2 (i.e. two-particle) graph for bosons is specified by the Hamiltonian matrix elements

$$K_{ij, kl}^B = -\langle ij | H | kl \rangle$$

$$= \delta_{il}A_{kj} + \delta_{jk}A_{il} + \delta_{ik}A_{jl} + \delta_{jl}A_{ik} \quad \text{if } i \neq j \text{ and } k \neq l$$

$$= U\delta_{ik} \quad \text{if } i = j \text{ and } k = l$$

$$= \frac{1}{\sqrt{2}}(\delta_{il}A_{kj} + \delta_{jk}A_{il} + \delta_{ik}A_{jl} + \delta_{jl}A_{ik}) \quad \text{if } i = j \text{ or } k = l,$$
where for bosonic statistics we have $N(N + 1)/2$ initial two-particle states

$$|ij⟩ = |11⟩, |12⟩, |13⟩, ... |1N⟩, |22⟩, |23⟩, |24⟩, ..., |NN⟩.$$ 

In the hard core limit $U → ∞$ the basis states with doubly-occupied sites can be ignored, the Hilbert space has $N(N − 1)/2$ dimensions, and the Hamiltonian matrix elements are

$$K^{HCB}_{ij, kl} = −⟨ij|H|kl⟩ = \delta_{il}A_{kj} + \delta_{jk}A_{il} + \delta_{ik}A_{jl} + \delta_{jl}A_{ik},$$

where now we require $i \neq j$ and $k \neq l$.

For Fermi statistics, since two fermions cannot occupy the same vertex, the Hilbert space has $N(N − 1)/2$ dimensions, and we can choose the basis states $|ij⟩, i \neq j$. The Hamiltonian matrix elements are

$$K^F_{ij, kl} = \delta_{il}A_{kj} + \delta_{jk}A_{il} − \delta_{ik}A_{jl} − \delta_{jl}A_{ik}.$$ 

Thus we extend an adjacency matrix of rank $N$ to a matrix $K$ of higher rank, either $N(N + 1)/2$ (for non-hard-core bosons) or $N(N − 1)/2$ (for hard-core bosons and for fermions). Technically, except for hard core bosons, the matrix $K$ is not an adjacency matrix since it has elements other than 0 and 1. For fermionic statistics, some entries of $K$ are equal to $-1$, while for soft-core bosons some entries are equal to $\sqrt{2}$ and others to $U$. $K$ can be pictured basically as a matrix in which every off-diagonal element represents the probability amplitude for particles to hop from one state to another state. Accordingly, the information of the adjacency matrix $A$ is embedded in the corresponding $K$.

Again we evolve forward the initial two-particle states in time according to the quantum mechanical evolution Eq. (2) and ask whether any pair of nonisomorphic graphs has two distinct sets of $O_{ij}(T)$. The test of isomorphism is whether the sets $O_{ij}$ and $O'_{ij}$ are the same after rearranging. It is of course possible to order these sets first by their real parts and then by their imaginary parts. A simple way to compare the ordered sets is to compute the numbers $R$ and $I$ defined as

$$R(T) = \sum_{i,j} |\text{Re}\tilde{O}_{ij}(T) − \text{Re}\tilde{O}'_{ij}(T)| \quad (3)$$

$$I(T) = \sum_{i,j} |\text{Im}\tilde{O}_{ij}(T) − \text{Im}\tilde{O}'_{ij}(T)| \quad (4)$$
FIG. 4: Variation of the numbers $R$ and $I$ (defined in Eqs. 3 and 4) as a function $U$ (potential) for the two non-isomorphic Latin square graphs with $N=16$. As $U$ goes to zero, $R$ and $I$ vanish.

where $\tilde{O}_{ij}$, $\tilde{O}'_{ij}$ are the elements of $O_{ij}$, $O'_{ij}$ ordered by their real parts, while $\hat{O}_{ij}$, $\hat{O}'_{ij}$ are ordered by their imaginary parts. If either $R(T)$ or $I(T)$ is nonzero, the graphs are non-isomorphic. The numbers $R$ and $I$ are sufficient to distinguish the non-isomorphic graphs in this paper.

To probe this approach, we again take pairs of non-isomorphic strongly regular graphs, two examples being the pairs of non-isomorphic Latin square graphs in Figs. 3 and 5. For each graph in a given pair, we find numerically the eigenvectors and eigenvalues of $K$ and use them to calculate the $O_{ij}$, $O'_{ij}$ and then $R(T)$ and $I(T)$ for $T = 1$. The qualitative behavior does not depend on the choice of $T$. Table I shows that for all these pairs of graphs both $R$ and $I$ vanish for noninteracting bosons, but both $R$ and $I$ are nonzero for hard core bosons and for noninteracting fermions. We find also that $R$ and $I$ are nonzero for graphs with nonzero but finite $U$. An illustration of this is shown in Fig. 4, the pair with $N = 16$. Note that the linear term in $U$ is sufficient to distinguish these graphs.

Thus, we find that all the non-isomorphic pairs of strongly regular graphs that we have examined (with size $N = 16, 25, 26, 28, 29$) can be distinguished by using two-fermion and the interacting boson algorithms. It is necessary to examine all matrix elements of $K$, not just the spectrum of $K$. The $K$ matrices of the two non-isomorphic graphs still share the same set of eigenvalues. In physical terms, this is due to the additivity of energies for
TABLE I: Table of results for hybrid dynamical algorithm for pairs of nonisomorphic strongly regular graphs for non-interacting fermions, non-interacting bosons, and hard-core bosons. Each pair of graphs has the same parameters \((N, k, \lambda, \mu)\), where \(N\) is the number of vertices, each vertex has \(k\) neighbors, each pair of adjacent vertices has \(\lambda\) neighbors in common, and each pair of non-adjacent vertices has \(\mu\) neighbors in common. The algorithm distinguishes the nonisomorphic pairs when using either hard-core bosons or fermions, but not when using noninteracting bosons.

| graph specification | fermions | noninteracting bosons | hard-core bosons |
|---------------------|----------|-----------------------|------------------|
| (16,9,4,6)         | \(R=1.37\) | \(R=0\)               | \(R=110.66\)    |
|                     | \(I=3.01\) | \(I=0\)               | \(I=81.53\)     |
| (25,12,5,6)        | \(R=1.24\) | \(R=0\)               | \(R=129.66\)    |
|                     | \(I=1.93\) | \(I=0\)               | \(I=198.53\)    |
| (26,10,3,4)        | \(R=1.91\) | \(R=0\)               | \(R=14.88\)     |
|                     | \(I=0.65\) | \(I=0\)               | \(I=23.47\)     |
| (28,12,6,4)        | \(R=1.82\) | \(R=0\)               | \(R=87.27\)     |
|                     | \(I=1.25\) | \(I=0\)               | \(I=95.11\)     |
| (29,14,6,7)        | \(R=3.50\) | \(R=0\)               | \(R=28.69\)     |
|                     | \(I=3.73\) | \(I=0\)               | \(I=42.51\)     |

non-interacting particles.

**Conclusion.** Our work suggests two conjectures for the solution of the GI problem. The first, which we doubt but have not been able to disprove, is that the two-particle quantum algorithm with computation of overlaps solves GI. A more plausible conjecture is that the motion of \(N_p\) quantum-mechanical fermions or interacting bosons on the graph, where \(N_p \sim N\), say \(N_p = N/2\), solves GI. From the standpoint of efficiency, we must

FIG. 5: Latin squares \(L_3(5)\) (25, 12, 5, 6)\[^{26}\]
distinguish whether the algorithm is run on a classical or a quantum computer. The two-particle algorithms already run in polynomial time on a classical computer. The $O_{ij}$ matrix contains $O(N^4)$ entries, each of which is computed in a time of $O(N^4)$. If this algorithm is sufficient to distinguish all graphs, then GI is in $P$. If, on the other hand, we must consider the motion of $N_p$ particles, where $N_p \sim N$, then the time is roughly $(\binom{N}{N_p}) \sim \binom{N}{N/2}$, which is exponential in $N$. The question of efficiency on a quantum computer is more interesting. The motion of $N_p \sim N$ particles can be mapped onto the Heisenberg model of a spin system at a fixed magnetization, which is nothing more than the dynamics of $N$ qubits with a constraint. Thus the evolution takes place in polynomial time on a quantum computer. On the other hand, we need an exponential number of overlaps if a naive algorithm is chosen. However, since all we need to do is ask whether the evolution of the two systems is in some sense similar, there may exist a preparation that entangles the graphs and a measurement that captures the needed information.

In conclusion, we have shown that strongly regular graphs provide a useful testbed for both classical and quantum dynamical algorithms that aim to solve the graph isomorphism problem. Pairs of graphs in this class cannot be distinguished by the classical algorithm of Gudkov et al. [22], but quantum algorithms combining the dynamical evolution of Gudkov et al.’s algorithm with a construction of Rudolph [23] using interacting bosons as well as noninteracting fermions can distinguish pairs of SRGs of order $\leq 29$, while a two-boson noninteracting algorithm fails. [28] Interesting open questions include whether either a $N_p$-fermion or $N_p$-hard-core-boson algorithm solves the GI problem, and if so, what value of $N_p$ suffices, and whether an algorithm with $N_p \sim N$ can be implemented efficiently on a quantum computer.

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