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A Note on Observables for Counting Trails and Paths in Graphs

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Abstract We point out that the total number of trails and the total number of paths of given length, between two vertices of a simple undirected graph, are obtained as expectation values of specifically engineered quantum mechanical observables. Such observables are contextual with some background independent theories of gravity and emergent geometry. Thus, we point out yet another situation in which the mathematical formalism of a physical theory has some computational aspects involving intractable problems.

Keywords Enumeration · Paths · Cycles · Observables · Graphity models · Grassman variables

1 Introduction

When the length is part of the input, counting trails and paths in graphs is usually an expensive computational task. For example, counting the number of Eulerian trails and Hamiltonian cycles are $\#P$ problems (see [2] and [12], respectively).

In this note, we point out that the number of trails and the number of paths having generic given length can be obtained as expectation values of specifically engineered quantum mechanical observables. The observables arise from an operational construction used to associate energy to graphs in certain background independent models of gravity (see [6, 7]). The Hamiltonian of the system depends only on minimal information encoded in graphs, like, for example, the degrees sequence and

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the length of trails. The induced dynamics tends to maximize the number of trails of certain preferred lengths during the time evolution of the system. It has been argued that such models can exhibit a phase which describes a emergent geometry. We are interested in remarking some computational aspects of a physical model and it is out of our scope to propose any algorithm for #P problems.

The remainder of this article is structured as follows: in Section 2 we give the necessary definitions. Section 2.1 considers trails; Section 2.3, paths. Section 3 concludes the paper with a brief discussion.

2 Counting Trails and Paths

Let $G = (V, E)$ be a simple undirected graph, where $V(G) = \{1, ..., n\}$. A *walk* of *length* l in G is a non-empty sequence of vertices $v_1 v_2 \cdots v_l v_{l+1}$, such that $\{v_i, v_{i+1}\} \in E(G)$, for every $i < l$. The vertices v_1 and v_{l+1} are said to be the *initial* and *final* vertex of the walk, respectively. If $v_i = v_{l+1}$ then the walk is said to be *closed*. If $v_i \neq v_{l+1}$ then the walk is said to be *open*. When this is the case, we chose to omit the adjective. A *trail* is a walk in which no edges are repeated. A *Eulerian trail* is a trail of including all edges. A graph with a Euler trail is said to be *Eulerian*. A *path* is a trail in which no vertices are repeated. A *cycle* is a closed path. A *Hamiltonian cycle* is a cycle of length n, that is, a cycle including all vertices of G. A graph with a Hamiltonian cycle is said to be *Hamiltonian*. See the book by Diestel [4], for a reference on the concepts and terminology of graph theory.

The *adjacency matrix* of G is a binary $n \times n$ matrix, denoted by $A(G)$, with $A(G)_{u,v} = 1$ if $\{u, v\} \in E(G)$ and $A(G)_{u,v} = 0$, otherwise. Let $w(G, l, u, v)$ be the number of walks of length l in G, with initial vertex u and final vertex v. It is well-known that $w(G, l; u, v) = A(G)^l_{u,v}$, for all $u, v \in V(G)$, even if $u = v$. During our discussion, it is useful to define a *formal* adjacency matrix $\widetilde{A}(G)$, by replacing each $A(G)_{u,v} = 1$ with an independent variable $e_{u,v}$, where $[e_{u,v}, e_{w,z}] = 0$, for all $u, v, w, z \in V(G)$. For instance, for the 4-cycle C_4,

$$A(C_4) = \begin{pmatrix} 0 & 1 & 1 & 0 \\ 1 & 0 & 0 & 1 \\ 1 & 0 & 0 & 1 \\ 0 & 1 & 1 & 0 \end{pmatrix}$$

and

$$\widetilde{A}(C_4) = \begin{pmatrix} 0 & e_{12} & e_{13} & 0 \\ e_{21} & 0 & 0 & e_{24} \\ e_{31} & 0 & 0 & e_{34} \\ 0 & e_{42} & e_{43} & 0 \end{pmatrix}.$$

The walks of lengths 3 between vertex 1 and vertex 2 are given by $\widetilde{A}(C_4)^3_{1,2} = e^2_{1,3}e_{1,2} + e_{1,2}e^2_{2,4} + e_{1,3}e_{3,4}e_{2,4} + e^3_{1,2}$ and then $w(C_4, 3; 1, 2) = 4$. We denote by $t(G, l; u, v)$ and $p(G, l; u, v)$ respectively the number of trails and paths of length l in G, with initial vertex u and final vertex v.

2.1 Trails

Let $\mathcal{H}_2 \cong \mathbb{C}^2$ be a two-dimensional Hilbert space with the orthonormal basis $\{|0\rangle, |1\rangle\}$. Let a and $a^\dagger$ be operators obeying the relation

$$\{a, a^\dagger\} \equiv aa^\dagger + a^\dagger a = I.$$

These operators act on $\{|0\rangle, |1\rangle\}$ as follows: $a|0\rangle = 0|0\rangle$, $a^\dagger|0\rangle = |1\rangle$, $a|1\rangle = |0\rangle$ and $a^\dagger|1\rangle = 0|1\rangle$. The Hermitian combination $N = a^\dagger a$ is the so-called *particle number operator* and it has the property that

$$N|k\rangle = a^\dagger a|k\rangle = k|k\rangle,$$

for $k = 0, 1$. Each l-th ($l \geq 2$) normally ordered power of N gives $: N^l :\, |k\rangle = 0|k\rangle$. For instance,

$$: N^2 :\, |k\rangle = a^\dagger a^\dagger aa|k\rangle = 0|k\rangle.$$

This is equivalent to say $: N^l :$ only has zero eigenvalues. Let us now define the space

$$\mathcal{H}_{V^2} := \bigotimes_{u,v \in V(G)} (\mathcal{H}_2)_{u,v},$$

where $\dim \mathcal{H}_{V^2} = 2^{\binom{n}{2}}$. Each pair $\{u, v\}$ is associated to a space

$$(\mathcal{H}_2)_{u,v} \equiv \text{ span}\{|0_{u,v}\rangle, |1_{u,v}\rangle\}.$$

All vectors

$$|x\rangle = \bigotimes_{u,v \in V(G)} |x_{u,v}\rangle,$$

being $x_{u,v} \in \{0, 1\}$ and $x \in \{0, 1\}^{\binom{n}{2}}$ (*i.e.*, the set of binary strings of length $n(n-1)/2$) form an orthonormal basis of $\mathcal{H}_{V^2}$. The state in $\mathcal{H}_{V^2}$ corresponding to the graph G is the basis state $|\psi_G\rangle$, in which $|x_{u,v}\rangle \equiv |1\rangle$ if $\{u, v\} \in E(G)$ and $|0\rangle$, otherwise. The state $|\psi_G\rangle$ needs $n(n-1)/2$ qubits to be encoded. Operators acting on the space $\mathcal{H}_{V^2}$ can be defined by making use of the operators a and $a^\dagger$ acting on the individual spaces $(\mathcal{H}_2)_{u,v}$. In particular, it is possible to define number operators acting on each copy of $(\mathcal{H}_2)_{u,v}$. These operators are denoted by $N_{u,v}$ and are defined by $N_{u,v}|x\rangle = x_{u,v}|x\rangle$, for $x \in \{0, 1\}^{\binom{n}{2}}$. Each operator $N_{u,v}$ returns the occupation number $x_{u,v}$. More explicitly, $N_{u,v}$ is defined by

$$N_{u,v}|x\rangle = 1 \otimes 1 \otimes \cdots \otimes 1 \otimes a^\dagger a \otimes 1 \otimes \cdots \otimes 1|x\rangle = x_{u,v}|x\rangle.$$

Since the operators $N_{u,v}$ act on different subsystems of $\mathcal{H}_{V^2}$, they all commute with each other.

Now, let us define a matrix $\mathbf{N}$ with elements

$$\mathbf{N}_{u,v} = \begin{cases} N_{u,v}, & \text{if } u \neq v; \\ 0, & \text{otherwise.} \end{cases}$$

Note that the matrix $\mathbf{N}$ is not an operator on $\mathcal{H}_{V^2}$ in the usual sense; it is the elements of $\mathbf{N}$ that act naturally on $\mathcal{H}_{V^2}$. Thus, the action of $\mathbf{N}$ on a state should be understood

as occurring entry-wise. The evaluation of the matrix $\mathbf{N}$, using the state $|\psi_G\rangle$, gives the same entries of the adjacency matrix, that is,

$$\langle\psi_G|\mathbf{N}_{u,v}|\psi_G\rangle := \langle\psi_G|N_{u,v}|\psi_G\rangle = A(G)_{u,v}.$$

Powers of $\mathbf{N}$ can be defined recursively as $\mathbf{N}^l = \mathbf{N}\mathbf{N}^{l-1}$. The entries of $\mathbf{N}^l$ are sums of sequences of number operators acting on different subspaces. By considering the expectation values of the normally ordered entries, we can state the following proposition: (Recall that a trail is a walk in which no edges are repeated.)

Proposition 1 *Given a graph G, the total number of trails of length l in G, with initial vertex u and final vertex v is*

$$t(G, l; u, v) = \langle\psi_G| : \mathbf{N}^l_{u,v} : |\psi_G\rangle. \tag{1}$$

Proof (Sketch) Keeping in mind the formal adjacency matrix $\widetilde{A}(G)$, we need to point out the following two facts only:

- If a product of number operators in one of the terms $\mathbf{N}^l_{u,v}$ contains a member acting on a pair of nonadjacent vertices then the operator yields zero and that term does not contribute to the expectation value.
- When a term in $\mathbf{N}^l_{u,v}$ contains more than one copy of a number operator acting on a particular edge, that term also does not contribute to the expectation value, because $: N^l : |k\rangle = 0|k\rangle$.

It follows that the only combinations of number operators that do not give a vanishing contribution to $t(G, l, u, v)$ correspond to trails with initial vertex u and final vertex v. Thus, Eq. 1 gives this number of trails as an expectation value of a quantum mechanical operator. □

Notice that $: \mathbf{N}^m_{u,u} :$ counts the number of Eulerian trails in G, if $|E(G)| = m$.

It is noteworthy to remark that the logarithm of the dimension of the space $\mathcal{H}_{V^2}$ is polynomial in the number of vertices. Also, notice that the operators $\mathbf{N}^l_{u,v}$ are independent of G. For the purpose of counting trails in a specific graph, a similar procedure may be applied taking a Hilbert space

$$\mathcal{H}_E := \bigotimes_{\{u,v\}\in E(G)} (\mathcal{H}_2)_{u,v},$$

where $\dim \mathcal{H}_E = 2^{|E(G)|}$. In this case, the matrix of operators $\mathbf{N}$ needs to be slightly modified so that some of its entries are zero from the beginning, rather than number operators acting on empty states.

Proposition 1 is based on the equation $: N^l : |k\rangle = 0|k\rangle$. It may be worth remarking that there is way of counting trails without making use of normal ordering. This can be done by defining the matrices

$$\mathbf{D}_{u,v} = \begin{cases} a_{u,v}, & \text{if } u \neq v; \\ 0, & \text{otherwise.} \end{cases}$$

It is in the same spirit of matrix $\mathbf{N}_{u,v}$, but the entries are annihilation operators, $a_{u,v}$, rather than number operators $N_{u,v}$. This matrix of operators is not Hermitian, *i.e.*, $\mathbf{D}^\dagger \neq \mathbf{D}$. Here the Hermitian conjugate is defined entry-wise by $(\mathbf{D}^\dagger)_{u,v} = \left(\mathbf{D}_{u,v}\right)^\dagger$. It can be shown that

$$\begin{aligned} t(G, l; u, v) &= \langle \psi_G | : \mathbf{N}^l_{u,v} : | \psi_G \rangle \\ &= \langle \psi_G | \left(\mathbf{D}^l_{u,v}\right)^\dagger \mathbf{D}^l_{u,v} | \psi_G \rangle. \end{aligned}$$

2.2 Example

We consider the 4-cycle C_4: the set of vertices is $V(C_4) = \{1, 2, 3, 4\}$; the set of edges is $E(C_4) = \{\{1, 2\}, \{1, 3\}, \{2, 4\}, \{3, 4\}\}$. Since $|V(C_4)| = 4$, we associated to this graph an Hilbert space $\mathcal{H}_{V^2}$ of dimension $2^6 = 64$. Specifically,

$$\mathcal{H}_{V^2} = (\mathcal{H}_2)_{1,2} \otimes (\mathcal{H}_2)_{1,3} \otimes \cdots \otimes (\mathcal{H}_2)_{3,4}\,.$$

The state associated to C_4 is

$$|\psi_G\rangle = |110011\rangle.$$

Regarding the operators $N_{u,v}$, we have, for instance

$$N_{1,2}|110011\rangle = 1|110011\rangle$$

and

$$N_{1,4}|110011\rangle = 0|110011\rangle.$$

In fact,

$$\langle 110011|N_{1,2}|110011\rangle = A(C_4)_{1,2} = 1$$

and

$$\langle 110011|N_{1,4}|110011\rangle = A(C_4)_{2,4} = 0$$

Observe that $\widetilde{A}(C_4)^3_{1,2} = e^2_{1,3}e_{1,2} + e_{1,2}e^2_{2,4} + e_{1,3}e_{3,4}e_{2,4} + e^3_{1,2}$. For the vertices 1 and 2, we have,

$$\begin{aligned} \langle \psi_G | : \mathbf{N}^3_{1,2} : | \psi_G \rangle &= \langle \psi_G | : N^2_{1,3}N_{1,2} : | \psi_G \rangle \\ &\quad + \langle \psi_G | : N_{1,2}N^2_{2,4} : | \psi_G \rangle \\ &\quad + \langle \psi_G | : N_{1,3}N_{3,4}N_{2,4} : | \psi_G \rangle \\ &\quad + \langle \psi_G | : N^3_{1,2} : | \psi_G \rangle \\ &= \langle \psi_G | : N_{1,3}N_{3,4}N_{2,4} : | \psi_G \rangle \\ &= 1 \end{aligned}$$

Indeed, $t(C_4, 3; 1, 2) = p(C_4, 3; 1, 2) = 1$, something that $: \mathbf{N}^3_{1,2} :$ is able to detect even if $w(C_4, 3; 1, 2) = 4$.

2.3 Paths

In this section, our working space is $\mathcal{H}_V := \bigotimes_{v\in V(G)}(\mathcal{H}_2)_v$, where $\dim \mathcal{H}_V = 2^n$, given that $|V(G)| = n$. This is the space usually assigned to networks of spin 1/2 quantum mechanical particles. The space $(\mathcal{H}_2)_v$ is associated to the vertex v and $(\mathcal{H}_2)_v \equiv \text{span}\{|0_v\rangle, |1_v\rangle\}$. All vectors $|x\rangle = \bigotimes_{v\in V(G)} |x_v\rangle$, being $x_v \in \{0, 1\}$ and $x \in \{0, 1\}^n$, form an orthonormal basis of $\mathcal{H}_V$. The state in $\mathcal{H}_V$ corresponding to the graph G is the basis state $|11...1\rangle = \bigotimes_n |1\rangle$. As we have done in the previous subsection, we can define number operators acting on each $(\mathcal{H}_2)_v$. These operators are denoted by N_v.

Let $\mathbf{M}$ be a matrix of operators with entries defined as follows:

$$\mathbf{M}_{u,v} = \begin{cases} N_{\max(u,v)}, & \text{if } \{u, v\} \in E(G) \text{ and } v > u; \\ N_{\min(u,v)}, & \text{if} \{u, v\} \in E(G) \text{ and } u > v; \\ 0, & \text{otherwise.} \end{cases}$$

As in the previous subsection, the elements of $\mathbf{M}$ are still number operators, but this time acting on $\mathcal{H}_V$. However, unlike the adjacency matrix, $\mathbf{M}$ is not symmetric. Powers of $\mathbf{M}$ are defined via matrix multiplication, for example, by the recursion $\mathbf{M}^l = \mathbf{M}\mathbf{M}^{l-1}$. Recall that a path is a trail in which no vertices are repeated.

Proposition 2 *Given a graph G, the total number of paths of length l in G, with initial vertex u and final vertex v is*

$$p(G, l; u, v) = \langle 11...1| : \mathbf{M}^l_{u,v} : |11...1\rangle.$$

Proof (Sketch) The operators $\mathbf{M}^l_{u,v}$ are sums of products of number operators. Since the entries in $\mathbf{M}$ are nonzero only in the positions where the adjacency matrix is nonzero, each of the terms in $\mathbf{M}^l_{u,v}$ also correspond to walks. Due to the normal ordering convention, a term in which the same vertex appears more than once does not contribute to the expectation value. Thus, $\langle\varphi_G| : \mathbf{M}^l_{u,v} : |\varphi_G\rangle$ has the desired interpretation. □

A similar construction could be made up with a "symmetric version" of $\mathbf{M}$.

With respect to the Hilbert space $\mathcal{H}_V$, we define a matrix of operators $\mathbf{F}$ with entries

$$\mathbf{F}_{u,v} = \begin{cases} a_{\max(u,v)} & \text{if } \{u, v\} \in E(G) \text{ and } v > u; \\ a_{\min(u,v)} & \text{if } \{u, v\} \in E(G) \text{ and } u > v; \\ 0 & \text{otherwise.} \end{cases}$$

Notice that $\mathbf{F}_{u,v}$ depends on $E(G)$ and thus on the graph G. Then, the transition amplitude

$$p(G, l; u, u) = \langle 00...0|\mathbf{F}^l_{u,u}|11...1\rangle,$$

is the number of cycles of length l containing the vertex u. Taking $l = n$, we have $p(G, n; u, u) > 0$ if and only if the graph G used to construct $\mathbf{F}_{u,u}$ is Hamiltonian.

3 Conclusion

For the purpose of counting trails and paths, we have described quantum observables in Hilbert spaces whose logarithm of the dimension is a polynomial in the number of vertices. The numbers of trails and paths can be obtained as expectation values of these observables. The states involved are the pure states $|11...1\rangle$ and $|\psi_G\rangle$. These states can be prepared efficiently. While it is clear that the observables raise no issues about uncertainty, it is most likely that these are not efficiently implementable in a quantum computer (*e.g.*, by phase estimation). The reason behind this thought is based on the fact that our observables are used to approach $\#P$ problems. Despite this, it may still be instructive to describe their form for special classes of graphs, to determine their complexity, and to describe the physics required for the implementation.

It is valuable to point out that the literature contains so far a number of examples of quantum observables for solving computational task, which are either not known to be efficiently implementable or implementable with poor accuracy. Among these, observables for the graph isomorphism problem [5] and for the permanent [11] (see also [13]). It has also be shown that some *mathematically well-defined* observables allow to solve the halting problem, in contradiction with the Church-Turing thesis [9]. Recall that the Church-Turing thesis asserts that every function which can be computed by what we would naturally regard as an algorithm is a computable function, and *viz*.

In the present notes, we have highlighted yet another situation in which the mathematical formalism of a physical theory has some computational aspects involving intractable problems. On the other hand, the computational complexity side may suggest some potential limitations on the physical picture (see [1], for a detailed survey on these ideas)—that is, the physical picture is simply not plausible.—With the same perspective of [8], it is legitimate to study the properties of background independent models of gravity and emergent geometry as computational devices (as cellular automata, for instance). Indeed, in the model studied in [6], the Hamiltonian of the system keeps track of trails of given lengths. Still this is inline with natural phenomena of self-organization at the microscopic scale. For example, the folded 3-dimensional conformation of a protein is believed to be its lowest free energy state. The 3-dimensional models describing the folding process of a protein as free energy minimization problems are NP-hard (see, *e.g.*, [3]). Finally, since the entries of the observables described in this paper can be seen as Grassmann numbers (because corresponding to fermionic operators), the observables may have some analogy to certain matrix model (see, *e.g.*, [10]), where the partition function is given by their weighted sums.

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