# Geometric Algebra and Information Geometry for Quantum Computational Software

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The art of quantum algorithm design is highly nontrivial. Grover's search algorithm constitutes a masterpiece of quantum computational software. In this article, we use methods of geometric algebra (GA) and information geometry (IG) to enhance the algebraic efficiency and the geometrical significance of the digital and analog representations of Grover's algorithm, respectively. Specifically, GA is used to describe the Grover iterate and the discretized iterative procedure that exploits quantum interference to amplify the probability amplitude of the target-state before measuring the query register. The transition from digital to analog descriptions occurs via Stone's theorem which relates the (unitary) Grover iterate to a suitable (Hermitian) Hamiltonian that controls Schrodinger's quantum mechanical evolution of a quantum state towards the target state. Once the discrete-to-continuos transition is completed, IG is used to interpret Grover's iterative procedure as a geodesic path on the manifold of the parametric density operators of pure quantum states constructed from the continuous approximation of the parametric quantum output state in Grover's algorithm. Finally, we discuss the dissipationless nature of quantum computing, recover the quadratic speedup relation, and identify the superfluity of the Walsh-Hadamard operation from an IG perspective with emphasis on statistical mechanical considerations.

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#### I. INTRODUCTION

The goal of characterizing the problems that can be solved on a quantum computer [1], together with the efficiency with which problems can be solved, is of enormous theoretical interest and practical importance [2]. This goal, however, seems a daunting one. A quantum computer is a physical device wherein quantum algorithms are executed. Quantum algorithms are described in terms of quantum circuits that are constructed by assembling wires and discrete sets of quantum gates which carry information around and perform computational procedures, respectively. In realistic scenarios, algorithms are executed on imperfect physical components that implement mathematical operations. Imperfections and noise lead to errors that cause loss of efficiency and this may reduce the effectiveness of the information processing device. Error models, also known as channels, provide a mathematical description of errors occurring on bits being moved around from one point of the computer to another. Quantum error correcting codes [3–6] can be used to account for errors introduced by the imperfection of realistic devices at the cost of a reasonable amount of additional resources. It appears self-evident that imperfect gates lead to imperfect circuits which, in turn, lead to imperfect implementations of quantum algorithms. The propagation of imperfections from gates to circuits in realistic physical implementations of a quantum computer is likely to have consequences on the scaling of the amount of basic resources required to synthesize an algorithm.

The fundamental objective of theoretical physics is to describe and, to a certain extent, understand natural phenomena. To clearly describe a phenomenon, physicists must master a convenient mathematical language and must be aware of how it connects to physical reality. Improving the language is not limited to mathematics, it is indeed one of the main tasks of theoretical physics. In his Nobel Lecture [7], Feynman pointed out that, while working toward the development of the spacetime view of quantum electrodynamics, he always tried to increase the efficiency of his demonstrations and to see with more and more clarity why they worked. Enhanced clarity was achieved by reformulating the same physical concept in many different mathematical forms. Furthermore, observing that the same physical reality can be described by many different physical ideas, Feynman concluded that a good theoretical physicist might find it useful to have a wide range of physical viewpoints and mathematical expressions for the same theory available to her/him. Very challenging and unresolved problems in modern quantum information science require a very broad vision supported by quantitative knowledge of both applied mathematical methods and theoretical physics techniques. It is not unusual to seek answers to questions concerning a given difficult problem only after having recast it in a novel alternative form where answers can be found, ideally, in a simpler manner. For instance, uncovering optimal quantum circuits is of fundamental importance since computationally intensive problems may require the use

of quantum computers. This consideration motivated Nielsen and collaborators to describe and, to a certain degree, understand quantum computing as free fall in a curved geometry [8] (for a more explicit analysis, see Ref. [9]): finding the optimal circuit is equivalent to finding the shortest path between initial and final target points in an appropriate curved geometry.

The art of quantum algorithm design is highly nontrivial: it requires special techniques and special insights to uncover good algorithms [10, 11]. Part of the challenge resides in the fact that human beings have a natural intuition that is better suited for the classical world rather than the quantum world [12]. In [10], Shor presented his polynomial time quantum algorithm used for factoring integers into a product of primes (for instance,  $15 = 3 \times 5$ ) and for finding discrete logarithms [10]. From an applied perspective, this algorithm is essential for testing the security of cryptographic codes [13]. The first experimental realization of this algorithm was performed by means of nuclear magnetic resonance (NMR) techniques [14].

One of the basic problems in computational science is that of searching a very large database [15]. In [11], Grover presented a quantum algorithm for solving database search problems. Grover's search algorithm helps searching for an element in a list of N unsorted elements (for instance, searching a telephone directory when one knows the phone number but does not know the person's full name [16]). For the sake of completeness, we remark that factoring is a problem in the computational complexity class NP (non-deterministic polynomial time) and it is not known to be NP-complete. If it was NP-complete, all problems in the complexity class NP could be efficiently solved using quantum computers [12]. The traveling salesman problem is an example of an NP-complete problem. Furthermore, we also emphasize that Grover's algorithm does not solve NP-complete problems in polynomial time, nevertheless its range of applicability is extremely wide since essentially any difficult problem can be recast into the form of a search problem (Grover's algorithm solves an unstructured problem where no assumptions are made on the Boolean function being inverted). The first experimental implementation of Grover's algorithm was achieved using NMR methods by Chuang and collaborators in [17].

In this article, we aim to present a novel hybrid geometric characterization of Grover's search algorithm via the joint application of geometric algebra (GA, [18, 19]) and information geometry (IG, [20]). GA is a very powerful mathematical language with applications in physics, computer science, and engineering [19, 21, 22]. It is essentially the ordinary Clifford algebra with the powerful addition of a neat geometric interpretation. Applications of GA in physics span from quantum theory and gravity [23, 24] to classical electrodynamics [25–27]. IG is essentially differential geometry applied to probability calculus [20]. Applications of IG techniques include phase transitions in

statistical mechanical systems [28], quantum energy levels statistics [29], quantum entanglement [30], quantum aspects of chaoticity [31], and complex network science [32–34]. To the best of our knowledge, the first formal application of (non-geometric) Clifford algebra techniques to represent quantum algorithms appeared in [35]. In [36], there appears the first brief GA description of the Grover iterate with no mention to the GA of quantum states and operators. Using GA techniques, this latter aspect was addressed in part in [37, 38] where Grover's search process was interpreted as the precession of a spin- $\frac{1}{2}$  particle. In [39–41], using the *complex* projective Hilbert space ( $\mathbb{CP}$ ) of qubits, Grover's search algorithm was recast in differential geometric language with the notion of distance between pure states quantified in terms of the Fubini-Study metric. In particular, it was shown that Grover's dynamics is characterized by a geodesic of  $\mathbb{CP}$ . More specifically, the consequences of the removal of the assumption of temporal independence of the time evolution operator in Grover's algorithm were investigated in differential geometric terms in [39]. In [40], it was shown that, from a statistical standpoint, Grover's algorithm is described by a unitary and adiabatic process that preserves the Fisher information function. In [41], the notion of Fubini-Study metric was employed to investigate the role of entanglement in quantum search.

In [42], we investigated the utility of GA methods in quantum information science. For instance, using the multiparticle spacetime algebra (MSTA, that is, the geometric algebra of a relativistic configuration space), we presented
an explicit algebraic description of one and two-qubit quantum states together with a MSTA characterization of one
and two-qubit quantum computational gates. We concluded that the MSTA approach leads to a useful conceptual
unification where the complex qubit space and the complex space of unitary operators acting on them become united,
with both being comprised solely of multivectors in real space. We also reported that the GA approach to rotations
based on the rotor group does bring conceptual and computational advantages compared to standard vectorial and
matrix approaches. In [43, 44], we presented a preliminary IG characterization of Grover's quantum search algorithm
[11]. First, we quantified the notion of quantum distinguishability between parametric density operators by means of
the Wigner-Yanase quantum information metric. We then showed that the quantum search problem can be recast in
an information geometric framework where Grover's dynamics is characterized by a geodesic on the manifold of the
parametric density operators of pure quantum states constructed from the continuous approximation of the parametric
quantum output state in Grover's algorithm. Combining the geometric intuition and the algebraic power of both IG
and GA in quantum search algorithms from a unifying standpoint (digital, digital-to-analog, and analog viewpoints)
remains unexplored.

Here, inspired by the findings reported in [35–41] and improving on our lines of investigations presented in [42–44], we

aim to improve upon our understanding of Grover's search algorithm. We start by observing that the two main physical intuitions that originally lead Grover to the development of his quantum searching algorithm were the discretization of Schrodinger's equation and the gravitation towards lower potential energy regions of a uniform quantum superposition [45]. To sharpen our understanding of his two intuitions, we use in this article GA and IG methods to enhance the algebraic efficiency and the geometrical significance of the digital and analog representations of Grover's algorithm, respectively. Specifically, GA is used to describe both the Grover iterate, viewed as a rotation defined by the product of two reflections (corresponding to the inversion about the mean and the oracle operators, respectively), as well as the discretized iterative procedure that exploits quantum interference to amplify the probability amplitude of the target-state before measuring the query register. The transition from digital to analog descriptions occurs via Stone's theorem which relates the (unitary) Grover iterate to a suitable (Hermitian) Hamiltonian that controls Schrodinger's quantum mechanical evolution of a quantum state towards the target state. Once the discrete-to-continuous transition is completed, IG is used to interpret Grover's iterative procedure as a geodesic on the manifold of the parametric density operators of pure quantum states constructed from the continuous approximation of the parametric quantum output state in Grover's algorithm. In particular, we discuss the dissipationless nature of quantum computing, recover the quadratic speedup relation, and confirm the superfluity of the Walsh-Hadamard operation from an IG perspective with emphasis on statistical mechanical considerations.

The layout of the article is as follows. In Section II, the concepts of quantum parallelism, quantum interference, and entanglement responsible for supra-classical performances in quantum computing are briefly introduced. In Section III, in preparation for the GA language translation and the IG analysis, we reexamine the standard mathematical steps that characterize Grover's quantum search algorithm. Special focus is devoted to the quadratic speedup behavior and to the matrix representations of the Grover iterate viewed as a rotation defined in terms of a product of two reflections. Some technical details on the inversion about the mean operator appear in Appendix A. In Section IV, after introducing the concepts of reflection and rotation in GA terms, we provide a GA description of the Grover iterate and recover the approximate asymptotic quadric speedup relation. Further details on the GA of physical space, spacetime, and quantum states and quantum operators appear in Appendix B. In Section V, we consider the continuous-time Hamiltonian version of the quantum search problem. We focus on a specific Hamiltonian model which we study by means of both matrix and geometric algebra techniques. Some technical details concerning the unitary time-evolution operator appear in Appendix C. In Section VI, after introducing some basic elements of IG, we recast the quantum search problem in terms of finding geodesic paths on manifolds of density matrices. In particular,

we discuss the dissipationless nature of quantum computing, recover the quadratic speedup relation, and verify the superfluity of the Walsh-Hadamard operation from an IG perspective. In Section VII, we also present several insights on Grover's fixed point phase- $\frac{\pi}{3}$  quantum search algorithm [46, 47] that arise from either GA or IG standpoints. Some technical details on the Fisher information function, the mechanical kinetic energy, the minimization of the action functional in differential geometric terms, and the steps on information geometric paths appear in Appendix D, Appendix E, Appendix F, and Appendix G, respectively. Finally, a summary of our findings together with limitations, improvements, and future lines of investigations appear in our Final Remarks located in Section VIII.

#### II. QUANTUM MECHANICAL CONCEPTS

In this section, we briefly mention several physical quantum effects responsible for computational speedups: parallelism, interference, and entanglement [48–53]. Recall that the dimensionality of the state space of multiparticle quantum systems grows exponentially with the number of particles. The reason why this happens is because in order to model the correlations among particles, the Hilbert space of a system of distinguishable particles must be taken as the tensor product of the Hilbert spaces of the individual particles.

### A. Parallelism

Quantum parallelism is the ability of a quantum computer to encode multiple computational results into a quantum state in a single quantum computational step [54]. Consider a Boolean function f with an n-bit domain and a one-bit range,

$$f: \{0,1\}^n \ni x \longmapsto f(x) \in \{0,1\}.$$
 (1)

Roughly speaking, quantum computers can evaluate the function f(x) for many different values of x simultaneously thanks to quantum parallelism that manifests itself in the ability of the computer to be in superpositions of different states. Note that the same task can be accomplished on a classical computer using classical parallelism. In the latter case, unlike the single-circuit quantum scenario, the multiple circuits built to evaluate f(x) for each value of x are executed simultaneously. Consider a two qubit quantum computer in the initial state  $|x,y\rangle$  where x and y denote the data and target registers, respectively. Assume a function f with an n-bit input x and one-bit output. The quantum parallel evaluation of f can be achieved as follows. First, prepare the n+1 qubit state  $|x,y\rangle = |0\rangle^{\otimes n} |0\rangle$ . Second, apply the Walsh-Hadamard transform  $H^{\otimes n} = H \otimes ... \otimes H$  (that is, the n-fold tensor product of n Hadamard

transforms) to the first n qubits. Finally, apply a unitary transformation  $U_f$  such that

$$U_f|x,y\rangle = |x,y \oplus f(x)\rangle,$$
 (2)

where  $\oplus$  denotes modulo-2 bitwise addition (for instance,  $1101 \oplus 0111 = 1010$ ). The sequence of these operations lead to the state [54],

$$\left[U_f \circ \left(H^{\otimes n} \otimes I\right)\right] |0\rangle^{\otimes n} |0\rangle = \frac{1}{\sqrt{2^n}} \sum_{x=0}^{n-1} |x\rangle |f(x)\rangle, \tag{3}$$

where  $|x\rangle \in \mathcal{H}_2^n$ ,  $|f(x)\rangle \in \mathcal{H}_2^1$ ,  $I \stackrel{\text{def}}{=} I_{\mathcal{H}_2^1}$  is the identity operator on the single-qubit Hilbert space  $\mathcal{H}_2^1$ , and the symbol of denotes the ordinary composition of maps. In the remainder of the article, for the sake of notational simplicity, we shall suppress use of the composition of maps symbol. Quantum parallelism allows for a simultaneous evaluation of all possible values of f(x). However, measuring the superposition state in Eq. (3) would yield only f(x) for a single value of x. In order to extract some global property of the function f(x) from the state in Eq. (3), one needs to exploit the fact that multiple alternatives can interfere with one another. This leads to the concept of quantum interference.

#### B. Interference

Assume that  $|0\rangle$  and  $|1\rangle$  are the computational basis states while  $\alpha$  and  $\beta$  are *complex* numbers whose modulus is not greater than unity. Then, a qubit  $|q\rangle$  is a coherent quantum mechanical superposition that can be written as,

$$|q\rangle \stackrel{\text{def}}{=} \alpha |0\rangle + \beta |1\rangle,$$
 (4)

where  $\alpha$  and  $\beta$  are known as probability amplitudes. We note that while in classical information theory a bit can have only one out of two alternative outcomes, 0 or 1, a qubit can exhibit an infinity of possible outcomes (states). To a given probability amplitude there corresponds a probability obtained by computing its modulus squared. Calculating probabilities in this manner endows quantum computing with the nonclassical feature of quantum interference. For example, note that to an amplitude probability  $\alpha + \beta$  there corresponds a probability given by,

$$|\alpha + \beta|^2 = |\alpha|^2 + |\beta|^2 + \alpha^* \beta + \alpha \beta^*, \tag{5}$$

where  $\alpha^*$  denotes the *complex* conjugate of  $\alpha$ . In the language of probabilistic classical computation adapted to quantum mechanics, from Eq. (5) one concludes that the probability of the quantum computational path with amplitude  $\alpha + \beta$  depends not only separately on the paths with amplitude  $\alpha$  and  $\beta$  but also, and this is the key

aspect, on the interference of such paths [55]. Indeed, it was also thanks to the constructive interference of quantum amplitudes that Grover was capable of designing quantum operations enhancing the presence of the searched target state [16]. A clever choice of the function to be evaluated together with a final transformation that allows efficient determination of useful global information about the function itself can be regarded as the essence of quantum algorithm design [12]. For an experimental realization of the quantum interference phenomenon in terms of photons on a silicon chip produced from a single ring-resonator source, we refer to [56].

### C. Entanglement

Entanglement is a physical property of composite quantum systems and emerges as non-local correlations that are absent in composite classical systems. From a practical standpoint, consider a bipartite quantum system S composed of two subsystems A and B which may themselves be composite systems. Let  $\mathcal{H}_A$  and  $\mathcal{H}_B$  be the  $N_A$ -dimensional and  $N_B$ -dimensional Hilbert spaces for A and B, respectively. If  $\{|a_i\rangle\}_{i=1,\ldots,N_A}$  and  $\{|b_j\rangle\}_{j=1,\ldots,N_B}$  are orthonormal bases for  $\mathcal{H}_A$  and  $\mathcal{H}_B$ , respectively, then an orthonormal basis for S is  $\{|a_ib_j\rangle\}_{i=1,\ldots,N_A;\ j=1,\ldots,N_B}$ . A normalized pure state  $|\psi\rangle \in \mathcal{H}_S$  of S,

$$|\psi\rangle \stackrel{\text{def}}{=} \sum_{i,j} c_{ij} |a_i b_j\rangle,$$
 (6)

represents an entangled state if it cannot be expressed as a direct product of states  $|\psi_A\rangle \in \mathcal{H}_A$  and  $|\psi_B\rangle \in \mathcal{H}_B$ ,

$$|\psi\rangle \neq |\psi_A\rangle |\psi_B\rangle$$
. (7)

From a conceptual standpoint, entanglement can be understood by investigating the various ways in which information, one of the most fundamental concepts in quantum physics, can be distributed within a composite system. First, assume that information contained in any system, be it composite or individual, is not infinite. Second, assume that the information contained in a composite system can be partitioned into the information encoded in the individual subsystems and into the information carried by the correlations between observations performed on the individual subsystems. The essence of quantum entanglement can be explained as follows. For a classical composite system, knowledge of all properties of each individual subsystem of the composite system allows one to draw conclusions about how much information is contained in the correlations. For a quantum entangled system, such a conclusion cannot be reached any longer: entangled quantum states can carry more information in joint properties than what may be concluded from knowledge of the individual subsystems [57]. In recent years, entanglement has undergone foundational investigations [58], more theoretically oriented studies of relativistic nature [59, 60], and very practical

investigations [61]. For an experimental realization of quantum entanglement in terms of orbital angular momentum states of photons, we refer to [62]. For a detailed review on quantum entanglement, we refer to [63] and [64].

#### III. GROVER'S ITERATIVE PROCEDURE

In what follows, we report what Grover's algorithm roughly does by following very closely Grover's pedagogical description [45]. Take into consideration the following problem from a crossword puzzle (solution: computer),

$$- - M - - T E -.$$
 (8)

If we limit ourselves to a classical computer and to an online dictionary with  $N=10^6$  words arranged alphabetically, we could write a classical software that finds the solution after inspecting about  $N/2=5\times 10^5$  words. However, if we use a quantum computer and the same online dictionary, we could write a quantum software (Grover's quantum search algorithm) that solves the puzzle in about  $\sqrt{N}=10^3$  steps. In what follows, we describe the iterative procedure that characterizes Grover's quantum search algorithm in standard mathematical terms [11, 12, 45, 54].

#### A. Standard mathematical description

Step- $\theta$ : Initialization of the quantum registers. Prepare the query and target registers. Suppose we set the target register to  $|0\rangle \in \mathcal{H}_2^1$  and the query register to  $|0\rangle^{\otimes n} \in \mathcal{H}_2^n$  with  $N \stackrel{\text{def}}{=} 2^n$ . The composite state of the registers becomes,

$$|\Psi_{\text{step-0}}\rangle = |0\rangle^{\otimes n} |0\rangle.$$
 (9)

Step-1: Application of the Walsh-Hadamard transform,  $H^{\otimes n}$ . Apply the Walsh-Hadamard transform  $H^{\otimes n}$  to the query register and the transformation  $H\sigma_x$  to the target register where  $\sigma_x$  is the bit-flip operator. The composite state of the registers becomes,

$$|\Psi_{\text{step-1}}\rangle = \frac{1}{\sqrt{N}} \sum_{x=0}^{N-1} |x\rangle \left[ \frac{|0\rangle - |1\rangle}{\sqrt{2}} \right] = \frac{1}{\sqrt{N}} \sum_{x=0}^{N-1} |x\rangle \left[ \frac{1}{\sqrt{2}} \sum_{y=0}^{1} (-1)^y |y\rangle \right].$$
 (10)

The effect of the Walsh-Hadamard transform is that of generating a uniform superposition of basis states  $\{|x\rangle\}_{x=0,1,...,N-1}$ . The effect of  $H\sigma_x$  on  $|0\rangle$  is that of producing a new target state  $H|1\rangle = |-\rangle \stackrel{\text{def}}{=} (|0\rangle - |1\rangle)/\sqrt{2}$ . The usefulness of the latter effect will become clear in step-2.

Step-2: Application of the oracle,  $U_{f_{\bar{x}}}$ . Assume that the set of all query values  $\mathcal{X} \stackrel{\text{def}}{=} \{0, 1..., N-1\}$  can be partitioned in two sets,  $\mathcal{X}_{good}$  and  $\mathcal{X}_{bad}$  with

$$\mathcal{X}_{\text{good}} \stackrel{\text{def}}{=} \{\bar{x}\}, \text{ with } f_{\bar{x}}(x) = 1,$$
 (11)

and,

$$\mathcal{X}_{\text{bad}} \stackrel{\text{def}}{=} \mathcal{X} \setminus \{\bar{x}\}, \text{ with } f_{\bar{x}}(x) = 0.$$
 (12)

Applying the operator  $U_{f_{\bar{x}}}$  to  $|\Psi_{\text{step-1}}\rangle$ , one obtains

$$|\Psi_{\text{step-2}}\rangle = \frac{1}{\sqrt{2N}} \sum_{x=0}^{N-1} (-1)^{f_{\bar{x}}(x)} |x\rangle \sum_{y=0}^{1} |y\rangle.$$
 (13)

Note also that the probability amplitude of  $|\bar{x}\rangle$  picks up a -1 phase shift after the application of  $U_{f_{\bar{x}}}$ . As a consequence, the mean value of the amplitudes slightly decreases. Note that the flip of the target state in step-1 is cleverly exploited in step-2 since the target register is in an eigenstate and can be therefore ignored. This allows one to focus only on the query register. Furthermore, observe that the action of  $U_{f_{\bar{x}}}$  on  $|\Psi_{\text{step-1}}\rangle$  can be rewritten as,

$$|\Psi_{\text{step-2}}\rangle = U_{f_{\bar{x}}} |\Psi_{\text{step-1}}\rangle = \left(U_{\bar{x}} \otimes I_{\mathcal{H}_{2}^{1}}\right) |\Psi_{\text{step-1}}\rangle.$$
 (14)

The quantity  $I_{\mathcal{H}_2^1}$  is the identity operator acting on the target register while  $U_{\bar{x}}$  is the operator that flips the amplitude of the marked state in the query register and is defined as,

$$U_{\bar{x}} |x\rangle \stackrel{\text{def}}{=} (I_{\mathcal{H}_{2}^{n}} - 2 |\bar{x}\rangle \langle \bar{x}|) |x\rangle = \begin{cases} |x\rangle, & x \neq \bar{x} \\ \\ \\ -|\bar{x}\rangle, & x = \bar{x} \end{cases}$$

$$(15)$$

where  $I_{\mathcal{H}_2^n}$  denotes the identity operator acting on the query register.

Step-3: Application of the inversion about the mean operator,  $U_{\psi^{\perp}}$ . Focusing on the query register state, consider the state

$$|\psi\rangle \stackrel{\text{def}}{=} H^{\otimes n} |0\rangle^{\otimes n} = \frac{1}{\sqrt{N}} \sum_{n=0}^{N-1} |x\rangle, \qquad (16)$$

together with the vector spaces  $V_{\psi} \stackrel{\text{def}}{=} Span\{|\psi\rangle\}$  and  $V_{\psi}^{\perp} \stackrel{\text{def}}{=} Span\{H|x\rangle\}$  with  $x \neq 0...0$ . Note that  $V_{\psi}^{\perp}$  is orthogonal to  $V_{\psi}$  since  $\langle 0...0 | H^{\dagger}H | x \rangle = 0$ ,  $\forall x \neq 0...0$  since  $H^{\dagger} = H^{-1} = H$ . We wish to introduce an operator  $U_{\psi^{\perp}}$  such that it acts like the identity on  $V_{\psi} \subset \mathcal{H}_2^n$  and like a phase shift of -1 on states in  $V_{\psi}^{\perp} \subset \mathcal{H}_2^n$ . The operator acting on the joint space of both registers that exhibits these properties is the so-called inversion about the mean operator defined as,

$$U_{\psi^{\perp}} \stackrel{\text{def}}{=} \left( H^{\otimes n} \otimes I_{\mathcal{H}_{2}^{1}} \right) U_{f_{\bar{x}} = 0} \left( H^{\otimes n} \otimes I_{\mathcal{H}_{2}^{1}} \right), \tag{17}$$

that is, using Eq. (14) and the properties of tensor products,

$$U_{\psi^{\perp}} = \left(H^{\otimes n} U_{\bar{x}=0} H^{\otimes n}\right) \otimes I_{\mathcal{H}_{2}^{1}} = \left(2 \left|\psi\right\rangle \left\langle\psi\right| - I_{\mathcal{H}_{2}^{n}}\right) \otimes I_{\mathcal{H}_{2}^{1}}.\tag{18}$$

Applying  $U_{\psi^{\perp}}$  in Eq. (18) to  $|\Psi_{\text{step-2}}\rangle$  yields,

$$|\Psi_{\text{step-3}}\rangle = U_{\psi^{\perp}} |\Psi_{\text{step-2}}\rangle.$$
 (19)

We point out that the action of the operator  $2|\psi\rangle\langle\psi|-I_{\mathcal{H}_2^n}$  on an arbitrary vector  $|\phi\rangle$  in  $\mathcal{H}_2^n$ ,

$$|\phi\rangle = \sum_{x=0}^{N-1} \alpha_x |x\rangle, \qquad (20)$$

with  $\alpha_x \in \mathbb{C}$  for any  $x \in \mathcal{X}$  is given by,

$$(2|\psi\rangle\langle\psi| - I_{\mathcal{H}_2^n})|\phi\rangle = \sum_{x=0}^{N-1} (2\mu_\alpha - \alpha_x)|x\rangle, \qquad (21)$$

where  $\mu_{\alpha}$  is the mean of the amplitudes defined as,

$$\mu_{\alpha} \stackrel{\text{def}}{=} \frac{1}{N} \sum_{x=0}^{N-1} \alpha_x. \tag{22}$$

For a detailed derivation of Eq. (21), we refer to Appendix A. We point out that this explicit derivation was useful since it allows to identify and correct a typographical error that appears in [54]. Eq. (21) justifies the terminology of inversion about the mean operator associated to  $2|\psi\rangle\langle\psi|-I_{\mathcal{H}_2^n}$ . The net effect of this operator is that of enhancing the amplitude of the target state  $|\bar{x}\rangle$  and slightly lowering the amplitudes of all the remaining basis states. At this point, we can finally define the Grover iterate operator G in terms of  $U_{f_{\bar{x}}}$  and  $U_{\psi^{\perp}}$  as follows,

$$G \stackrel{\text{def}}{=} U_{\psi^{\perp}} U_{f_{\bar{x}}}. \tag{23}$$

Step-4: Iterations of the Grover iterate,  $G^k$  with  $G = U_{\psi^{\perp}} U_{f_{\bar{x}}}$ . This step requires the application of the quantum search iterate a number of k-times. This number is approximately estimated by requiring that for  $N \gg 1$  the probability of the amplitude of the target state  $|\bar{x}\rangle$  approaches unity,

$$\left|\left\langle \bar{x}\left|G^{k}\right|\psi\right\rangle \right|^{2} \stackrel{N\to\infty}{\longrightarrow} 1. \tag{24}$$

Grover uncovered that [11, 45],

$$k_{\text{Grover}}(N) \stackrel{N \gg 1}{\approx} \frac{\pi}{4} \sqrt{N}.$$
 (25)

Eq. (25) ends our standard mathematical treatment. The explicit derivation of Eq. (25) appears in the next subsection.

## B. The quadratic speedup

We begin by applying the Walsh-Hadamard transform  $H^{\otimes n}$  to the state  $|0\rangle^{\otimes n}$  in order to construct a uniform amplitude initial state  $|\psi\rangle$  given in Eq. (16),

$$|\psi\rangle \stackrel{\text{def}}{=} \frac{1}{\sqrt{N}} \sum_{x=0}^{N-1} |x\rangle.$$
 (26)

We note that  $|\psi\rangle$  can be decomposed as,

$$|\psi\rangle = \frac{1}{\sqrt{N}} \sum_{x=0}^{N-1} |x\rangle = \frac{1}{\sqrt{N}} |\bar{x}\rangle + \sqrt{1 - \frac{1}{N}} \sum_{x \in \mathcal{X} \setminus \{\bar{x}\}} |x\rangle, \qquad (27)$$

that is,

$$|\psi\rangle = \frac{1}{\sqrt{N}} |\bar{x}\rangle + \sqrt{\frac{N-1}{N}} |\psi_{\text{bad}}\rangle,$$
 (28)

where  $|\bar{x}\rangle$  is the target state,  $\mathcal{X}$  is the set previously defined, and

$$|\psi_{\text{bad}}\rangle \stackrel{\text{def}}{=} \sum_{x \in \mathcal{X} \setminus \{\bar{x}\}} |x\rangle.$$
 (29)

Observe that the application of the Grover iterate G onto  $|\psi\rangle$  yields states that belong to  $Span\{|\bar{x}\rangle, |\psi_{\text{bad}}\rangle\}$ , a two-dimensional subspace of  $\mathcal{H}_2^n$ . Furthermore, it happens to be convenient to introduce an additional basis of such a two-dimensional space in order to better understand the iterative procedure proposed by Grover. Specifically, consider the orthogonal states  $|\psi\rangle$  in Eq. (26) and  $|\bar{\psi}\rangle$  where,

$$|\bar{\psi}\rangle \stackrel{\text{def}}{=} \sqrt{\frac{N-1}{N}} |\bar{x}\rangle - \frac{1}{\sqrt{N}} |\psi_{\text{bad}}\rangle.$$
 (30)

To quantify the relation between the two orthogonal bases  $\{|\bar{x}\rangle, |\psi_{\rm bad}\rangle\}$  and  $\{|\psi\rangle, |\bar{\psi}\rangle\}$ , introduce an angle  $\theta$  such that

$$\sin\left(\theta\right) \stackrel{\text{def}}{=} \frac{1}{\sqrt{N}}, \text{ and } \cos\left(\theta\right) \stackrel{\text{def}}{=} \sqrt{\frac{N-1}{N}}.$$
 (31)

Using Eqs. (28), (30), and (31), it follows that

From Eq. (32), it is straightforward to verify that

$$\begin{pmatrix} |\bar{x}\rangle \\ |\psi_{\text{bad}}\rangle \end{pmatrix} = \begin{pmatrix} \sin(\theta) & \cos(\theta) \\ \cos(\theta) & -\sin(\theta) \end{pmatrix} \begin{pmatrix} |\psi\rangle \\ |\bar{\psi}\rangle \end{pmatrix}.$$
(33)

The iterative procedure begins in the state  $|\psi\rangle$ ,

$$|\psi\rangle = \sin\left(\theta\right)|\bar{x}\rangle + \cos\left(\theta\right)|\psi_{\text{bad}}\rangle.$$
 (34)

Let us consider the first iteration by computing  $G|\psi\rangle = U_{\psi^{\perp}}U_{f_{\bar{x}}}|\psi\rangle$ . Using Eqs. (14) and (34) together with the orthogonality of states  $|\bar{x}\rangle$  and  $|\psi_{\rm bad}\rangle$ , we obtain

$$U_{f_{\bar{x}}} |\psi\rangle = \cos(2\theta) |\psi\rangle - \sin(2\theta) |\bar{\psi}\rangle. \tag{35}$$

Applying  $U_{\psi^{\perp}}$  in Eq. (18) to  $U_{f_{\bar{x}}} | \psi \rangle$  in Eq. (35) together with standard trigonometric relations, we find

$$G|\psi\rangle = U_{\psi^{\perp}} U_{f_{\bar{x}}} |\psi\rangle = \sin(3\theta) |\bar{x}\rangle + \cos(3\theta) |\psi_{\text{bad}}\rangle. \tag{36}$$

Using some mathematical reasoning, it is straightforward to verify that after k-iterations of G, the angle  $\theta_k$  that specifies  $G^k$  is such that  $\theta_{k+1} = \theta_k + 2\theta$  and  $\theta_1 = 3\theta$ . Therefore, it follows that  $\theta_k = (2k+1)\theta$  and  $G^k |\psi\rangle$  becomes

$$G^{k} |\psi\rangle = \sin\left[\left(2k+1\right)\theta\right] |\bar{x}\rangle + \cos\left[\left(2k+1\right)\theta\right] |\psi_{\text{bad}}\rangle. \tag{37}$$

From Eq. (37), the probability of the amplitude of the target state  $|\bar{x}\rangle$  becomes,

$$\left|\left\langle \bar{x}\left|G^{k}\right|\psi\right\rangle \right|^{2} = \sin^{2}\left[\left(2k+1\right)\theta\right]. \tag{38}$$

Observe that the probability in Eq. (38) approaches unity when  $(2k+1)\theta$  approaches  $\pi/2$ . From the first relation in Eq. (31), in the limit of  $N \gg 1$ , we obtain

$$\frac{\pi}{2} = (2k+1)\theta \stackrel{N \gg 1}{\approx} \frac{(2k+1)}{\sqrt{N}} \stackrel{N \gg 1}{\approx} \frac{2}{\sqrt{N}} k, \tag{39}$$

that is, finally,

$$k_{\text{Grover}}(N) \stackrel{N \gg 1}{\approx} \frac{\pi}{4} \sqrt{N}.$$
 (40)

Eq. (40) concludes our formal reexamination of the quadratic speedup relation. As a side remark, we point out that within the framework of quantum amplitude amplification techniques [65], quantum operations allow to amplify the amplitudes of good output states. Since the corresponding probabilities are defined as the squares of the amplitudes, the amplification is quadratically faster than in the classical case. Having said that, the quadratic improvement in the complexity of Grover's search algorithm can be explained also by observing that Grover's search is a special case of the amplitude amplification technique [65].

## C. Matrix representation of the Grover iterate

Observe that the action of the oracle  $U_{f_{\bar{x}}}$  in Eq. (14) on the state  $|\psi\rangle = \sin(\theta) |\bar{x}\rangle + \cos(\theta) |\psi_{\text{bad}}\rangle$  in Eq. (34) is given by,

$$U_{f_{\bar{x}}} |\psi\rangle = -\sin(\theta) |\bar{x}\rangle + \cos(\theta) |\psi_{\text{bad}}\rangle. \tag{41}$$

Therefore,  $U_{f_{\bar{x}}}$  describes a reflection about the vector  $|\psi_{\text{bad}}\rangle$  in the plane defined by  $|\bar{x}\rangle$  and  $|\psi_{\text{bad}}\rangle$ . Similarly, we note that the action of  $U_{\psi^{\perp}}$  in Eq. (18) on the state  $|\bar{x}\rangle = \sin(\theta) |\psi\rangle + \cos(\theta) |\bar{\psi}\rangle$  in Eq. (33) is given by,

$$U_{\psi^{\perp}} |\bar{x}\rangle = \sin(\theta) |\psi\rangle - \cos(\theta) |\bar{\psi}\rangle. \tag{42}$$

Therefore,  $U_{\psi^{\perp}}$  performs a reflection about the vector  $|\psi\rangle$  in the plane defined by  $|\bar{x}\rangle$  and  $|\psi_{\rm bad}\rangle$  because  $Span\{|\bar{x}\rangle, |\psi_{\rm bad}\rangle\} = Span\{|\psi\rangle, |\bar{\psi}\rangle\}$ . Since the Grover iterate G is the composition of two reflections, it is a rotation. In particular, after some straightforward algebra, the matrix representation [G] of the operator G restricted to the two-dimensional space spanned by  $|\psi_{\rm bad}\rangle$  and  $|\bar{x}\rangle$  becomes,

$$[G] = \begin{pmatrix} \langle \psi_{\text{bad}} | G | \psi_{\text{bad}} \rangle & \langle \psi_{\text{bad}} | G | \bar{x} \rangle \\ \langle \bar{x} | G | \psi_{\text{bad}} \rangle & \langle \bar{x} | G | \bar{x} \rangle \end{pmatrix} = \begin{pmatrix} \cos(2\theta) & -\sin(2\theta) \\ \sin(2\theta) & \cos(2\theta) \end{pmatrix}. \tag{43}$$

Note that [G] is an orthogonal matrix since  $\det([G]) = +1$  and  $[G]^t[G] = [G][G]^t = I_{2\times 2}$  where  $I_{2\times 2}$  denotes the  $2\times 2$  identity matrix and the symbol t denotes the transposition operation. Therefore, [G] does indeed represent a rotation. In summary: i) the Grover iterate is the product of two reflections; ii) the product of two reflections is a rotation; iii) the Grover iterate is a rotation in the two-dimensional space spanned by  $|\psi_{\rm bad}\rangle$  and  $|\bar{x}\rangle$  that rotates state vectors by  $2\theta$  radians. For the sake of completeness, we also point out that, following the same computational steps needed to compute [G] in Eq. (43), the matrix representations  $[U_{\psi^{\perp}}]$  and  $[U_{f_{\bar{x}}}]$  of the operators  $U_{\psi^{\perp}}$  and  $U_{f_{\bar{x}}}$  restricted to the two-dimensional space spanned by  $|\psi_{\rm bad}\rangle$  and  $|\bar{x}\rangle$  are given by,

$$\begin{bmatrix} U_{\psi^{\perp}} \end{bmatrix} = \begin{pmatrix} \langle \psi_{\text{bad}} | U_{\psi^{\perp}} | \psi_{\text{bad}} \rangle & \langle \psi_{\text{bad}} | U_{\psi^{\perp}} | \bar{x} \rangle \\ \langle \bar{x} | U_{\psi^{\perp}} | \psi_{\text{bad}} \rangle & \langle \bar{x} | U_{\psi^{\perp}} | \bar{x} \rangle \end{pmatrix} = \begin{pmatrix} \cos(2\theta) & \sin(2\theta) \\ \sin(2\theta) & -\cos(2\theta) \end{pmatrix}$$
(44)

and,

$$[U_{f_{\bar{x}}}] = \begin{pmatrix} \langle \psi_{\text{bad}} | U_{f_{\bar{x}}} | \psi_{\text{bad}} \rangle & \langle \psi_{\text{bad}} | U_{f_{\bar{x}}} | \bar{x} \rangle \\ \langle \bar{x} | U_{f_{\bar{x}}} | \psi_{\text{bad}} \rangle & \langle \bar{x} | U_{f_{\bar{x}}} | \bar{x} \rangle \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \tag{45}$$

respectively. Observe that from Eqs. (43), (44), and (45), one obtains, as expected, that

$$[G] \stackrel{\text{def}}{=} \left[ U_{\psi^{\perp}} U_{f_{\bar{x}}} \right] = \left[ U_{\psi^{\perp}} \right] \left[ U_{f_{\bar{x}}} \right]. \tag{46}$$

Finally, notice that  $[U_{\psi^{\perp}}]$  and  $[U_{f_{\bar{x}}}]$  are orthogonal matrices with det  $([U_{\psi^{\perp}}]) = \det([U_{f_{\bar{x}}}]) = -1$ . Therefore,  $[U_{\psi^{\perp}}]$  and  $[U_{f_{\bar{x}}}]$  do indeed represent reflections.

### IV. GEOMETRIC ALGEBRA AND THE DIGITAL DESCRIPTION

From the standard mathematical description of Grover's algorithm, we realize that some of the key concepts that need to be translated into the GA language are those of reflection, rotation, quantum state, and quantum operators. In what follows, we introduce the strictly necessary GA tools needed to provide a GA description of the key aspects of Grover's search algorithm. For the sake of completeness, some additional details appear in Appendix B.

A GA is a graded linear space whose elements are known as multivectors. For instance, a scalar is a grade-0 multivector, a vector is a grade-1 multivector, a bivector is a grade-2 multivector, and so on. The so-called pseudoscalar is the highest-grade element in the algebra. Multivectors can be either homogeneous or non-homogeneous. In the former case, they only contain elements of a single grade. In the latter case, they contain elements with multiple grades. Furthermore, homogeneous vectors form a subspace which is closed under scalar multiplication and addition. For further details, we shall refer to our Appendix B. For more foundational purposes, we refer to more extensive works on the use of GA in quantum information processing [19, 66–70].

# A. Reflections

Recall from Section III that the Grover iterate is a rotation defined in terms of the product of two reflections. GA offers a powerful platform for handling rotations and reflections by means of bivectors (a grade-2 multivector). Let us consider two vectors a and b that belong to the GA of physical space  $\mathfrak{cl}(3)$  (for further details, see Appendix B). Let us further assume that a and b diverge by an angle  $b \in (0, \pi)$ . Using the GA formalism, the vector a can be written as a superposition of two vectors  $a_{\parallel}$  and  $a_{\perp}$  as follows,

$$a = a_{\parallel} + a_{\perp},\tag{47}$$

where,

$$a_{\parallel} = (a \cdot b) \frac{b}{|b|^2} = (a \cdot b) b^{-1},$$
 (48)

and,

$$a_{\perp} = a - a_{\parallel} = a - (a \cdot b) b^{-1} = (ab - a \cdot b) b^{-1} = (a \wedge b) b^{-1}.$$
 (49)

Vectors  $a_{\parallel}$  and  $a_{\perp}$  denote vectors parallel and perpendicular to b, respectively. The reflection of a vector v across the line a is obtained by sending  $v = v_{\parallel} + v_{\perp}$  to the mirror image  $v' = v_{\parallel} - v_{\perp}$ ,

$$v' = v_{\parallel} - v_{\perp} = (v \cdot a) a^{-1} - (v \wedge a) a^{-1}$$

$$= (v \cdot a - v \wedge a) a^{-1}$$

$$= (a \cdot v + a \wedge v) a^{-1}$$

$$= ava^{-1},$$
(50)

that is,

$$v \to v' = ava^{-1}$$
: single reflection. (51)

Note that the composition of two reflections of v, first across a and then across b is defined as,

$$v \to v' = ava^{-1} \to v'' = bv'b^{-1} = bava^{-1}b^{-1} = (ba)v(ba)^{-1},$$
 (52)

therefore,

$$v \to v'' = (ba)v(ba)^{-1}$$
: composition of two reflections. (53)

For further details on reflections, we refer to [19].

# B. Rotations

To keep a smooth reading flow, we refer to Appendix B for further mathematical and notational details. Using GA, the unit vector  $e_{\theta} \in \mathfrak{cl}(3)$  obtained from  $e_1$  by a rotation by an angle  $\theta$  in the  $e_1e_2$  plane is given by [19],

$$e_{\theta} = e_1 \cos(\theta) + e_2 \sin(\theta)$$

$$= e_1 \left[\cos(\theta) + e_1 e_2 \sin(\theta)\right]$$

$$= e_1 \exp\left[e_1 e_2 \theta\right]$$

$$= \exp\left[e_2 e_1 \theta\right] e_1, \tag{54}$$

that is,

$$e_1 \to e_\theta \stackrel{\text{def}}{=} \mathcal{R}_{e_1 e_2}(\theta) e_1 = \exp\left[e_2 e_1 \theta\right] e_1.$$
 (55)

The quantity  $\mathcal{R}_{e_1e_2}(\theta)$  in Eq. (55) denotes the bivector operator that describes the rotation by  $\theta$  of  $e_1$  in the  $e_1e_2$  plane. The rotation of a vector v that does not necessarily belong to the rotation plane  $e_1e_2$  can be described as,

$$v \to v' = \mathcal{R}_{e_1 e_2}(\theta) v = \exp\left[e_2 e_1 \frac{\theta}{2}\right] v \exp\left[e_1 e_2 \frac{\theta}{2}\right] : \text{rotation}$$
 (56)

For the sake of completeness, we point out that  $e_1$  belongs to the rotation plane  $e_1e_2$ , and

$$\exp\left[e_2 e_1 \theta\right](e_1) = \exp\left[e_2 e_1 \frac{\theta}{2}\right](e_1) \exp\left[e_1 e_2 \frac{\theta}{2}\right]. \tag{57}$$

Let us now demonstrate the equivalence of a rotation to a pair of successive reflections in intersecting planes. Observe that from  $e_{\theta}$  in Eq. (54), we obtain

$$e_1 e_\theta = \exp\left[e_1 e_2 \theta\right] = \cos\left(\theta\right) + e_1 e_2 \sin\left(\theta\right). \tag{58}$$

Therefore, using Eqs. (56) and (58), we find

$$v' = \exp\left[e_2 e_1 \frac{\theta}{2}\right] v \exp\left[e_1 e_2 \frac{\theta}{2}\right]$$

$$= \left(e_{\frac{\theta}{2}} e_1\right) v \left(e_1 e_{\frac{\theta}{2}}\right)$$

$$= \left(e_{\frac{\theta}{2}} e_3\right) \left(e_3 e_1\right) v \left(e_1 e_3\right) \left(e_3 e_{\frac{\theta}{2}}\right), \tag{59}$$

that is, the rotated vector v' becomes

$$v' = \left(e_{\frac{\theta}{2}}e_3\right)(e_3e_1)v(e_1e_3)\left(e_3e_{\frac{\theta}{2}}\right). \tag{60}$$

From Eq. (60), we observe that

$$v' = \left[ \operatorname{rotation}_{e_1 e_2} (\theta) \right] (v) = \operatorname{reflection}_{e_{\frac{\theta}{2}} e_3} \left[ \operatorname{reflection}_{e_3 e_1} (v) \right], \tag{61}$$

where,

$$\theta = 2\cos^{-1}\left[n_{e_{\frac{\theta}{2}}e_3} \cdot n_{e_3e_1}\right],\tag{62}$$

with  $n_{\pi}$  denoting the unit normal to the plane  $\pi$ . From Eqs. (60) and (62), it becomes transparent using GA that a rotation is equivalent to a pair of successive reflections in intersecting planes where the angle of rotation is twice the angular opening between the planes that characterize the reflections. Observe that it is straightforward to verify within GA that both rotations and reflections are orthogonal (linear) transformations since they both preserve the inner product. Furthermore, while rotations are proper orthogonal transformations with det (rotation) = +1, reflections are improper orthogonal transformations with det (reflection) = -1. Within GA, these last two statements

can be explained as follows. First, we point out that the mirror image of an arbitrary vector x in the plane through the origin with normal n is called the reflection along n and is given by x' = -nxn [71]. As a consequence, it so happens that the product of three transformed vectors becomes

$$xyz \to x'y'z' = -n(xyz)n, \tag{63}$$

where,

$$xyz = x(yz) = x[y \cdot z + y \wedge z] = x(y \cdot z) + x(y \wedge z)$$

$$= (y \cdot z)x + x \cdot (y \wedge z) + x \wedge (y \wedge z)$$

$$= (y \cdot z)x + (x \cdot y)z - (x \cdot z)y + x \wedge y \wedge z$$

$$= (y \cdot z)x - (x \cdot z)y + (x \cdot y)z + x \wedge y \wedge z,$$

$$(64)$$

that is,

$$xyz = (y \cdot z) x - (x \cdot z) y + (x \cdot y) z + x \wedge y \wedge z. \tag{65}$$

The trivector part of the multivector xyz is given by,

$$\langle xyz \rangle_{\text{grade-3}} = x \wedge y \wedge z,$$
 (66)

where, under reflection,

$$x \wedge y \wedge z \to -n (x \wedge y \wedge z) n = -x \wedge y \wedge z, \tag{67}$$

since vectors in the GA of physical space  $\mathfrak{cl}(3)$  commute with all pseudoscalars. Second, an outermorphism of a linear transformation  $\mathcal{R}$  is a transformation on  $\mathfrak{cl}(3)$  which is linear, grade-preserving, and preserves the outer product [71]. Since for linear transformations  $\mathcal{R}$  on  $\mathfrak{cl}(3)$  the determinant is specified in terms of the action of its outermorphism  $\mathcal{R}$  on trivectors (that is, the pseudoscalars),

$$\underline{R}(x \wedge y \wedge z) = \det(\mathcal{R}) x \wedge y \wedge z, \tag{68}$$

from Eq. (67) we conclude that det (reflection) = -1 (improper orthogonal transformation). Furthermore, since a rotation is a composition of two reflections, det (reflection) = +1 (proper orthogonal transformation). Observe that  $x \wedge y \wedge z$  denotes an oriented volume of a parallelepiped with edges x, y, z. Therefore, det ( $\mathcal{R}$ ) is a factor that represents an induced change in scale of the volume. In what follows, we shall employ the relevant GA considerations presented here to understand the structure of the Grover iterate, namely a rotation defined in terms of the product of two reflections as evident from Eqs. (43), (44), and (45).

### C. The Grover iterate and the quadratic speedup

Let us briefly recall that the Grover iterate is given by  $G = U_{\psi^{\perp}} U_{f_{\bar{x}}}$  where  $U_{f_{\bar{x}}}$  describes a reflection about the vector  $|\psi_{\rm bad}\rangle$  in the plane defined by  $|\bar{x}\rangle$  and  $|\psi_{\rm bad}\rangle$ ,  $U_{\psi^{\perp}}$  represents a reflection about the vector  $|\psi\rangle$  in the plane defined by  $|\bar{x}\rangle$  and  $|\psi_{\rm bad}\rangle$ , and, finally, G is a rotation by  $2\theta$  in the two-dimensional space spanned by  $|\bar{x}\rangle$  and  $|\psi_{\rm bad}\rangle$ . In what follows, a quantum state in the Hilbert space  $\mathcal{H}_2^n$  will be replaced by a multivector belonging to the reduced even subalgebra space  $\left[\mathfrak{cl}^+(3)\right]^n/E_n$  where  $E_n$  denotes the n-particle correlator defined in Eq. (B24) (for further details, see Appendix B). Using the GA language, the quantum state  $|\psi\rangle$  in Eq. (26) can be recast as

$$e_{\psi} = \frac{1}{\sqrt{N}} \sum_{i=0}^{N-1} e_i = \frac{1}{\sqrt{N}} e_{\bar{x}} + \sqrt{\frac{N-1}{N}} e_{\text{bad}}.$$
 (69)

After the application of the first above-mentioned reflection and using Eq. (51), the multivector  $e_{\psi}$  becomes

$$e_{\psi} \to e_{\text{bad}} e_{\psi} e_{\text{bad}}^{-1} = e_{\text{bad}} e_{\psi} \frac{e_{\text{bad}}}{|e_{\text{bad}}|^2} = e_{\text{bad}} e_{\psi} e_{\text{bad}}, \tag{70}$$

since  $|e_{\text{bad}}|^2 = 1$ . After the application of the second above-mentioned reflection and employing Eq. (53), we obtain

$$e_{\text{bad}}e_{\psi}e_{\text{bad}} \to e_{\psi}\left(e_{\text{bad}}e_{\psi}e_{\text{bad}}\right)e_{\psi}^{-1} = e_{\psi}\left(e_{\text{bad}}e_{\psi}e_{\text{bad}}\right)\frac{e_{\psi}}{\left|e_{\psi}\right|^{2}} = e_{\psi}\left(e_{\text{bad}}e_{\psi}e_{\text{bad}}\right)e_{\psi},\tag{71}$$

where, this time, we have exploited the fact that  $|e_{\psi}|^2 = 1$ . Therefore, from Eq. (71), we uncover that the action of the Grover iterate G on  $e_{\psi}$  yields

$$Ge_{\psi} = e_{\psi}e_{\text{bad}}e_{\psi}e_{\text{bad}}e_{\psi} = (e_{\psi}e_{\text{bad}})e_{\psi}(e_{\text{bad}}e_{\psi}), \tag{72}$$

that is,

$$Ge_{\psi} = ge_{\psi}g^{\dagger},$$
 (73)

where the bivector g is defined as,

$$g \stackrel{\text{def}}{=} e_{\psi} e_{\text{bad}}. \tag{74}$$

The dagger symbol † in Eq. (73) denotes the reversion operation in GA. From Eq. (34), it is clear that

$$e_{\psi} = \sin(\theta) \, e_{\bar{x}} + \cos(\theta) \, e_{\text{bad}}. \tag{75}$$

From Eqs. (74) and (75), we find

$$g = e_{\psi}e_{\text{bad}} = [\sin(\theta) e_{\bar{x}} + \cos(\theta) e_{\text{bad}}] e_{\text{bad}}$$

$$= \cos(\theta) + e_{\bar{x}}e_{\text{bad}}\sin(\theta)$$

$$= \exp[e_{\bar{x}}e_{\text{bad}}\theta], \qquad (76)$$

and,

$$g^{\dagger} = e_{\text{bad}} e_{\psi} = e_{\text{bad}} \left[ \sin \left( \theta \right) e_{\bar{x}} + \cos \left( \theta \right) e_{\text{bad}} \right]$$

$$= \cos \left( \theta \right) + e_{\text{bad}} e_{\bar{x}} \sin \left( \theta \right)$$

$$= \exp \left[ e_{\text{bad}} e_{\bar{x}} \theta \right]. \tag{77}$$

Therefore, using Eqs. (76) and (77), Eq. (73) yields

$$Ge_{\psi} = \exp\left[e_{\bar{x}}e_{\text{bad}}\theta\right]e_{\psi}\exp\left[e_{\text{bad}}e_{\bar{x}}\theta\right]. \tag{78}$$

From the structural analogy with Eq. (56), it becomes evident that the multivector  $ge_{\psi}g^{\dagger}$  describes a rotation by  $2\theta$  of  $e_{\psi}$  in the plane  $e_{\text{bad}}e_{\bar{x}}$ . From Eq. (78), we note that the multivector G can be written as,

$$G = \exp\left[e_{\bar{x}}e_{\text{bad}}\left(2\theta\right)\right] = \cos\left(2\theta\right) + e_{\bar{x}}e_{\text{bad}}\sin\left(2\theta\right). \tag{79}$$

Using the two relations in Eq. (31), it is apparent that

$$\cos(2\theta) = \frac{N-2}{N}, \text{ and } \sin(2\theta) = \frac{2\sqrt{N-1}}{N}.$$
 (80)

Finally, from Eqs. (79) and (80), the multivector G becomes

$$G = \frac{N-2}{N} + \frac{2\sqrt{N-1}}{N} e_{\bar{x}} e_{\text{bad}}.$$
 (81)

Eqs. (73), (78), and (81) are the main GA equations that we use to characterize the Grover iterate. In GA terms, k-iterations of G can be described as follows. From Eq. (73), we obtain

$$G^k e_{\psi} = g^k e_{\psi} \left( g^{\dagger} \right)^k = g^{2k} e_{\psi}. \tag{82}$$

Using Eqs. (75) and (79), the multivector  $G^k e_{\psi}$  in Eq. (82) becomes

$$G^k e_{\psi} = \sin[(2k+1)\theta] e_{\bar{x}} + \cos[(2k+1)\theta] e_{\text{bad}}.$$
 (83)

We observe that  $G^k e_{\psi} = e_{\bar{x}}$  if and only if,

$$\frac{\pi}{2} = (2k+1)\theta \stackrel{N \gg 1}{\approx} \frac{2k+1}{\sqrt{N}},\tag{84}$$

that is, if the number of iterations k = k(N) in the asymptotic limit for N approaching infinity equals

$$k_{\text{Grover}}^{(\text{GA})}(N) \stackrel{N \gg 1}{\approx} \frac{\pi}{4} \sqrt{N}.$$
 (85)

Eq. (85) is the GA analog of Eq. (40) and exhibits the known quadratic speedup relation obtained, this time, from purely GA arguments. Observe that within the GA framework, both quantum states and quantum operators are elements of the same real space  $\left[\mathfrak{cl}^{+}(3)\right]^{n}/E_{n}$ . This is an important conceptual unifying feature that might find some support also from an experimental standpoint as we will briefly argue in what follows. For a detailed GA formulation of logic operations in quantum computing, we refer to our own work presented in [42].

#### D. Geometric algebra and experimental implementations

It is not unusual to employ unphysical concepts in intermediate steps in theoretical physics. However, it is always good to keep in mind that whatever is being described here occurs in a real-world laboratory [72]. For instance, quantum phenomena do not happen in a *complex* Hilbert space. They actually occur in a laboratory where you can only see detectors and emitters (lasers and ion guns, for instance) but no Hermitian operators.

Several experimental proposals for realizing Grover's algorithm have been presented since its theoretical discovery. In [17, 73], Grover's quantum search algorithm was experimentally implemented on NMR quantum computers. For details on nuclear magnetic resonance principles, we refer to [74]. In [75, 76], a quantum optical implementation of Grover's algorithm appeared. For details on linear optical quantum computing, we refer to [77]. In [78], Grover's algorithm was implemented using molecular magnets ( $Fe_8$  and  $Mn_{12}$ ) embedded in a crystal. In [79], Grover's algorithm was implemented using large nuclear spins in semiconductors ( $^{27}Al$ ,  $^{55}Mn$ , and  $^{67}Mn$  with nuclear spin  $I=\frac{5}{2}$ , and  $^{73}Ge$  and  $^{113}In$  with nuclear spin  $I=\frac{9}{2}$ ). It is interesting to note that the implementation of quantum computations using large nuclear spins in GaAs (nuclear spin  $I = \frac{3}{2}$ ) semiconductors is based on a unary representation [80]. This means that once the control over 2I magnetic fields is established and provided that there exists a sufficient signal amplification due to the spin ensemble, quantum computation occurs with a single pulse [80]. As a consequence, nuclear spins can be essentially used either as qubits or as logical gate actions on qubits in these types of experimental settings [79]. This physical implementation of Grover's algorithm seems to support the conceptual unifying feature provided by GA and, in our view, deserves further investigation. For the sake of completeness, we point out that the first application of GA to quantum error correction in liquid NMR quantum computing appeared in [81]. We also emphasize that within the framework of quantum computing with holograms [82, 83], photons are used to realize both qubits and logic gates acting on them. For instance, the CNOT gate can be constructed with a single linear momentum photon in a four-dimensional state space while a qubit can be realized as the polarization state of a photon. In particular, photons are the carriers of quantum information and they interact thanks to the use of interferometers.

To make interferometers more stable against environmental noise, Alsing and collaborators have used holograms of interferometers staked in a photo-thermal refractive piece of glass [83]. Within this theoretical framework, an holographic CNOT gate was realized and its functionality was verified by means of a tomographic analysis in which, due to imperfections of materials, probabilities do not sum to unity resulting in a violation of the unitarity condition. To better understand the connection between physical implementations based on high-dimensional spin systems and the GA language, it may be worthwhile recasting the qudit search problem in GA terms. We leave this line of investigation to future investigations.

### V. THE DIGITAL-TO-ANALOG TRANSITION

From a digital quantum computing viewpoint, Grover's algorithm can be regarded as a definite (discrete-time) sequence of elementary unitary transformations acting on qubits. Specifically, given an initial input state, the output of the algorithm becomes the input state after the action of the sequence of transformations presented in Section III. In digital terms, the length of the algorithm equals the number of unitary transformations that compose the quantum computational software. In [84], an analog version of Grover's algorithm was proposed. The search problem was recast in terms of finding the normalized eigenvector  $|\bar{x}\rangle$  corresponding to the only nonvanishing eigenvalue E of an Hamiltonian  $H_{\bar{x}}$  acting on a complex N-dimensional Hilbert space. The search ends when the system is in the state  $|\bar{x}\rangle$ . More specifically, consider the (continuos-time) quantum mechanical Schrodinger evolution under the time-independent Hamiltonian,

$$H_{\text{Farhi-Gutmann}} = H_{\bar{x}} + H_D,$$
 (86)

where  $H_{\bar{x}}$  and the driving Hamiltonian  $H_D$  are defined as [84],

$$H_{\bar{x}} \stackrel{\text{def}}{=} E |\bar{x}\rangle \langle \bar{x}|, \text{ and } H_D \stackrel{\text{def}}{=} E |\psi\rangle \langle \psi|,$$
 (87)

respectively. The state  $|\psi\rangle$  in Eq. (87) denotes a normalized initial state that does not depend on  $|\bar{x}\rangle$  with  $\langle \bar{x}|\psi\rangle = 1/\sqrt{N} \neq 0$ . Farhi and Gutmann argued that if  $|\bar{x}\rangle$  is chosen from a fixed and known orthonormal basis (or, if  $|\bar{x}\rangle$  is chosen uniformly at random),  $|\bar{x}\rangle$  can be found in a time interval  $\Delta t$  that is proportional to  $\sqrt{N}$  [84],

$$\Delta t \propto \frac{1}{E} \sqrt{N}.$$
 (88)

In particular, they showed that this time interval in Eq. (88) is optimal even if  $H_D = H_D(t)$  in Eq. (86). Despite the same quadratic speedup behavior, Fenner observed that the Hamiltonian in Eq. (86) does not generate the analog

version of the discrete path that characterizes Grover's algorithm in the digital setting [85]. To accomplish this goal, it was proposed in [85] an alternative time-independent search Hamiltonian defined as,

$$H_{\text{Fenner}} \stackrel{\text{def}}{=} \frac{2i_{\mathbb{C}}}{E} \left[ H_{\bar{x}}, H_D \right] = \frac{2i_{\mathbb{C}}E}{\sqrt{N}} \left[ \left| \bar{x} \right\rangle \left\langle \psi \right| - \left| \psi \right\rangle \left\langle \bar{x} \right| \right], \tag{89}$$

where  $i_{\mathbb{C}}$  denotes the *complex* imaginary unit. In particular, it was shown that the time-independent Grover iterate G can be exactly matched on the whole Hilbert space  $\mathcal{H}_2^n$  with  $N \stackrel{\text{def}}{=} 2^n$  by the following time-independent unitary time-evolution operator [85],

$$G_{\text{Fenner}} \stackrel{\text{def}}{=} e^{-\frac{i_{\mathcal{C}}}{\hbar} H_{\text{Fenner}} \bar{t}},\tag{90}$$

where  $\hbar \stackrel{\text{def}}{=} h/2\pi$ , h is the Planck constant ( $h \approx 6.63 \times 10^{-34} \, [\text{MKSA}]$ ), and  $\bar{t}$  approaches  $\pi/4\sqrt{N}$  as N approaches infinity and is formally defined as [85],

$$\bar{t} \stackrel{\text{def}}{=} \frac{\pi - 2\cos^{-1}\left(1/\sqrt{N}\right)}{2} \cdot \frac{N}{\sqrt{N-1}}.$$
(91)

For further details on more general quantum search Hamiltonians, we refer to [86]. In what follows, we set  $\hbar$  equal to one.

### A. Matrix algebra and the Fenner iterate

In what follows, we analyze the Fenner iterate from a matrix algebra viewpoint. Let us assume that  $|\psi\rangle = \alpha |\bar{x}\rangle + \beta |\psi_{\text{bad}}\rangle$  with  $\langle \bar{x}|\psi_{\text{bad}}\rangle = 0$ ,  $\alpha \stackrel{\text{def}}{=} 1/\sqrt{N}$ ,  $\beta \stackrel{\text{def}}{=} \sqrt{(N-1)/N} \in \mathbb{R}_+ \setminus \{0\}$ , and  $\alpha^2 + \beta^2 = 1$ . The matrix representation of  $H_{\text{Fenner}}$  in Eq. (89) on the two-dimensional space spanned by  $|\bar{x}\rangle$  and  $|\psi_{\text{bad}}\rangle$  is given by,

$$[H_{\text{Fenner}}] = \begin{pmatrix} \langle \bar{x} | H_{\text{Fenner}} | \bar{x} \rangle & \langle \bar{x} | H_{\text{Fenner}} | \psi_{\text{bad}} \rangle \\ \langle \psi_{\text{bad}} | H_{\text{Fenner}} | \bar{x} \rangle & \langle \psi_{\text{bad}} | H_{\text{Fenner}} | \psi_{\text{bad}} \rangle \end{pmatrix}$$

$$= \frac{2i_{\mathbb{C}}\beta}{\sqrt{N}} \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}$$

$$= \frac{2i_{\mathbb{C}}\beta}{\sqrt{N}} \sigma_{z}\sigma_{x}, \tag{92}$$

where  $\sigma_x$  and  $\sigma_z$  are Pauli matrices. Observing that  $(\sigma_z \sigma_x)^2 = -I_{2\times 2}$  and  $\{\sigma_x, \sigma_z\} \stackrel{\text{def}}{=} \sigma_x \sigma_z + \sigma_z \sigma_x = 0_{2\times 2}$  (where  $0_{2\times 2}$  denotes the two-by-two null matrix), after some algebra (for further details, see Appendix C), we obtain

$$G(t) = e^{-icH_{\text{Fenner}}t} = e^{\frac{2\beta}{\sqrt{N}}\sigma_z\sigma_x t} = \cos\left(\frac{2\beta}{\sqrt{N}}t\right)I_{2\times 2} + \sin\left(\frac{2\beta}{\sqrt{N}}t\right)\sigma_z\sigma_x,\tag{93}$$

and the properly normalized time-dependent quantum state  $|\psi(t)\rangle$  becomes,

$$|\psi(t)\rangle = G(t)|\psi\rangle$$

$$= \left[\cos\left(\frac{2\beta}{\sqrt{N}}t\right) - \frac{\alpha}{\beta}\sin\left(\frac{2\beta}{\sqrt{N}}t\right)\right]|\psi\rangle + \frac{1}{\beta}\sin\left(\frac{2\beta}{\sqrt{N}}t\right)|\bar{x}\rangle, \tag{94}$$

From Eq. (94), we note that the probability of the amplitude of the target state  $|\bar{x}\rangle$  is given by,

$$\left|\left\langle \bar{x}\left|G\left(t\right)\right|\psi\right\rangle\right|^{2} = \left[\alpha\cos\left(\frac{2\beta}{\sqrt{N}}t\right) + \beta\sin\left(\frac{2\beta}{\sqrt{N}}t\right)\right]^{2}.\tag{95}$$

From Eq. (95), recalling that  $\beta \stackrel{\text{def}}{=} \sqrt{(N-1)/N}$ , we conclude that

$$\left|\left\langle \bar{x}\left|G\left(t\right)\right|\psi\right\rangle\right|^{2} \overset{N\gg1}{\approx} \beta \sin\left(\frac{2\beta}{\sqrt{N}}t\right) = 1 \tag{96}$$

requires

$$t_{\text{Fenner}}(N) = \frac{N}{2\sqrt{N-1}} \sin^{-1}\left(\sqrt{\frac{N}{N-1}}\right) \stackrel{N\gg 1}{\approx} \frac{\pi}{4}\sqrt{N}. \tag{97}$$

Eq. (97) is the Hamiltonian search analog of Eq. (25) obtained in the original digital setting by Grover.

# B. Geometric algebra, the Fenner iterate, and the Grover iterate

In what follows, we analyze the Fenner iterate and its connection to the continuous-time generalization of the Grover iterate from a GA perspective. From Eq. (94), recalling that  $\left[\mathfrak{cl}^+(3)\right]^n/E_n \ni e_\psi = \alpha e_{\bar{x}} + \beta e_{\rm bad}$  and setting  $\theta_{\rm F}(t) \stackrel{\rm def}{=} 2\beta/\sqrt{N}t$ , we obtain

$$e_{\psi(t)} = \{\beta \sin\left[\theta_{\mathrm{F}}(t)\right] + \alpha \cos\left[\theta_{\mathrm{F}}(t)\right]\} e_{\bar{x}} + \{-\alpha \sin\left[\theta_{\mathrm{F}}(t)\right] + \beta \cos\left[\theta_{\mathrm{F}}(t)\right]\} e_{\mathrm{bad}}. \tag{98}$$

From Eq. (98), we observe that

$$[e_{\psi(t)}]_{\{e_{\bar{x}}, e_{\text{bad}}\}} = \begin{pmatrix} \beta & \alpha \\ -\alpha & \beta \end{pmatrix} \begin{pmatrix} \sin \left[\theta_{\text{F}}(t)\right] \\ \cos \left[\theta_{\text{F}}(t)\right] \end{pmatrix},$$
 (99)

that is, the multivector  $e_{\psi(t)}$  expanded in the basis  $\{e_{\bar{x}}, e_{\text{bad}}\}$  has components that can be obtained via a rotation of the components  $\sin [\theta_{\text{F}}(t)]$  and  $\cos [\theta_{\text{F}}(t)]$ . Indeed, the matrix

$$A \stackrel{\text{def}}{=} \begin{pmatrix} \beta & \alpha \\ -\alpha & \beta \end{pmatrix}, \tag{100}$$

is such that  $\det(A) = +1$  and  $AA^t = A^tA = I_{2\times 2}$ . It is therefore, a rotation. We also notice that,

$$e_{\text{Grover}(t)} = \sin \left[\theta_{\text{G}}(t)\right] e_{\bar{x}} + \cos \left[\theta_{\text{G}}(t)\right] e_{\text{bad}}, \tag{101}$$

that is,

$$\left[e_{\text{Grover}(t)}\right]_{\left\{e_{\bar{x}}, e_{\text{bad}}\right\}} = \begin{pmatrix} \sin\left[\theta_{\text{G}}\left(t\right)\right] \\ \cos\left[\theta_{\text{G}}\left(t\right)\right] \end{pmatrix}. \tag{102}$$

To compare Eqs. (99) and (102), let  $\theta_{\rm G}(t) = \theta_{\rm F}(t) = \theta(t)$ . Observe that the temporal linearity of  $\theta_{\rm G}(t)$  arises due to the fact that the Hamiltonian being used for the quantum search is assumed to be time-independent. We wish to uncover a new basis of vectors  $\{e'_{\bar{x}}, e'_{\rm bad}\}$ ,

$$e'_{\bar{x}} = f_1(e_{\bar{x}}, e_{\text{bad}}), \text{ and } e'_{\text{bad}} = f_2(e_{\bar{x}}, e_{\text{bad}}),$$

such that in this new basis, one has

$$\left[e_{\text{Grover}(t)}\right]_{\left\{e_{\bar{x}}',\ e_{\text{bad}}'\right\}} = \begin{pmatrix} \beta & \alpha \\ -\alpha & \beta \end{pmatrix} \begin{pmatrix} \sin\left[\theta_{\text{F}}\left(t\right)\right] \\ \cos\left[\theta_{\text{F}}\left(t\right)\right] \end{pmatrix}. \tag{103}$$

It is straightforward to check that the desired new basis is given by,

$$\begin{pmatrix} e'_{\bar{x}} \\ e'_{\text{bad}} \end{pmatrix} = \begin{pmatrix} \beta & \alpha \\ -\alpha & \beta \end{pmatrix} \begin{pmatrix} e_{\bar{x}} \\ e_{\text{bad}} \end{pmatrix}, \tag{104}$$

that is,

$$\begin{pmatrix} e_{\bar{x}} \\ e_{\text{bad}} \end{pmatrix} = \begin{pmatrix} \beta & -\alpha \\ \alpha & \beta \end{pmatrix} \begin{pmatrix} e'_{\bar{x}} \\ e'_{\text{bad}} \end{pmatrix}. \tag{105}$$

To identify  $e'_{\bar{x}}$  and  $e'_{\text{bad}}$ , we impose,

$$[G_{\text{Grover}}(t)]_{\text{old}} = e^{e_{\bar{x}}e_{\text{bad}}\theta_G(t)} \rightarrow [G_{\text{Grover}}(t)]_{\text{new}} = e^{e'_{\bar{x}}e'_{\text{bad}}\theta_G(t)} = e^{e_3e_1\theta_F(t)} = [G_{\text{Fenner}}(t)]_{\text{old}}, \quad (106)$$

so that,

$$e'_{\bar{x}} = e_3$$
, and  $e'_{\text{bad}} = e_1$ . (107)

We finally obtain,

$$\begin{pmatrix} e_3 \\ e_1 \end{pmatrix} = \begin{pmatrix} \beta & \alpha \\ -\alpha & \beta \end{pmatrix} \begin{pmatrix} e_{\bar{x}} \\ e_{\text{bad}} \end{pmatrix} \text{ and, } \begin{pmatrix} e_{\bar{x}} \\ e_{\text{bad}} \end{pmatrix} = \begin{pmatrix} \beta & -\alpha \\ \alpha & \beta \end{pmatrix} \begin{pmatrix} e_3 \\ e_1 \end{pmatrix}, \tag{108}$$

with  $e'_{\bar{x}}e'_{\text{bad}} = e_{\bar{x}}e_{\text{bad}}$  since,

$$e'_{\bar{x}}e'_{\text{bad}} = e_{3}e_{1}$$

$$= ie_{2}$$

$$= (\beta e_{\bar{x}} + \alpha e_{\text{bad}}) (-\alpha e_{\bar{x}} + \beta e_{\text{bad}})$$

$$= -\alpha \beta + \beta^{2} e_{\bar{x}} e_{\text{bad}} - \alpha^{2} e_{\text{bad}} e_{\bar{x}} + \alpha \beta$$

$$= (\alpha^{2} + \beta^{2}) e_{\bar{x}} e_{\text{bad}}$$

$$= e_{\bar{x}} e_{\text{bad}}.$$
(109)

From Eqs. (106) and (109), we conclude that in GA terms the Fenner iterate can be described in terms of the continuos-time Grover multivector  $e_{Grover(t)}$  which, in turn, is essentially a rotation by  $2\theta$  about the  $e_2$  axis. We conclude that GA methods also have utility in the digital-to-analog transition descriptions of quantum computational software.

#### VI. INFORMATION GEOMETRY AND THE ANALOG DESCRIPTION

Having performed the transition from the digital to the analog formulation of Grover's algorithm, we are now ready to present an IG-based discussion on quantum computational software suitable for solving search problems on a quantum hardware.

## A. Statistical distinguishability

Before presenting the IG description of Grover's algorithm, several considerations have to be carried out. Information geometry consists of the application of differential geometrical methods to the study of families of probabilities, both classical and quantum, either parametric or nonparametric [20].

In the classical information geometric setting, there is essentially a unique statistical distance that quantifies the distinguishability between two probability distributions  $p_{\theta}(x)$  and  $p_{\theta+d\theta}(x)$ . The quantity x is in the domain of definition  $\mathcal{X}$  of the probability distribution while  $\theta = (\theta^1, ..., \theta^n)$  are the n-real statistical parameters that parametrize  $p_{\theta}(x)$  that belongs to the n-dimensional statistical model (or, statistical manifold)  $\mathcal{M}_s$ ,

$$\mathcal{M}_{s} \stackrel{\text{def}}{=} \left\{ p_{\theta} \left( x \right) = p \left( x | \theta \right) : \theta = \left( \theta^{1}, ..., \theta^{n} \right) \in \Theta \right\}, \tag{110}$$

where  $\Theta \subset \mathbb{R}^n$  is the so-called parameter space. Except for an overall multiplicative constant, there is a unique monotone Riemannian metric with the property of having its line element reduced under stochastic maps known as Markov morphisms [87, 88]. This metric is the so-called Fisher-Rao information metric defined as,

$$g_{ij}^{(FR)}(\theta) \stackrel{\text{def}}{=} \int_{\mathcal{X}} p_{\theta}(x) \,\partial_{i} \log \left[ p_{\theta}(x) \right] \partial_{j} \log \left[ p_{\theta}(x) \right] dx, \tag{111}$$

where  $\partial_i \stackrel{\text{def}}{=} \frac{\partial}{\partial \theta^i}$  with  $1 \leq i \leq n$  and the infinitesimal line element  $ds^2$  on  $\mathcal{M}_s$  becomes,

$$ds^{2} \stackrel{\text{def}}{=} g_{ij}^{(FR)}(\theta) d\theta^{i} d\theta^{j}. \tag{112}$$

It is convenient to note that since,

$$\sqrt{p}\frac{\partial \log p}{\partial \theta} = \frac{1}{\sqrt{p}}\frac{\partial p}{\partial \theta} = 2\frac{\partial \sqrt{p}}{\partial \theta},\tag{113}$$

Eq. (111) can be rewritten as,

$$g_{ij}^{(FR)}(\theta) = 4 \int_{\mathcal{X}} \partial_i \sqrt{p_{\theta}(x)} \partial_j \sqrt{p_{\theta}(x)} dx.$$
 (114)

In the quantum information setting, probability distributions are replaced by density matrices. Quantum statistical distinguishability between density matrices requires that their distance on the space of density matrices must decrease under coarse-graining (that is, stochastic maps). Unlike the classical case, there are infinitely many monotone Riemannian metrics on the space of density matrices that fulfill this requirement [89–91]. Even quantum generalizations of the very same classical Fisher-Rao information metric are not unique. In general, two classically identical expressions in Eqs. (111) and (114) differ when they are extended to a quantum setting. This difference is a manifestation of the non-commutative nature of quantum mechanics and is reminiscent of the idea of quantum discord [92]. Substituting the integral in Eq. (114) with the trace and the probability distributions  $p_{\theta}$  with density operators  $\rho_{\theta}$ , this heuristic quantum generalization of Eq. (114) becomes the so-called quantum Wigner-Yanase metric [93, 94],

$$g_{ij}^{(\text{WY})}\left(\theta\right) \stackrel{\text{def}}{=} 4\text{Tr}\left[\left(\partial_{i}\rho_{\theta}\right)\left(\partial_{j}\rho_{\theta}\right)\right].$$
 (115)

For pure quantum states  $\rho_{\theta} \stackrel{\text{def}}{=} |\psi_{\theta}\rangle \langle \psi_{\theta}|$  with normalized quantum states  $|\psi_{\theta}\rangle$  such that  $\psi_{\theta} = \psi(\theta)$  and  $\rho_{\theta}^2 = \rho_{\theta}$ , after some algebra (for further details, we refer to [44]), it follows that Eq. (115) can be rewritten as

$$g_{ij}^{(WY)}(\theta) = 4 \left[ \text{Re} \left\langle \partial_i \psi_\theta | \partial_j \psi_\theta \right\rangle + \left\langle \partial_i \psi_\theta | \psi_\theta \right\rangle \left\langle \partial_j \psi_\theta | \psi_\theta \right\rangle \right], \tag{116}$$

where  $\text{Re}\left(\cdot\right)$  denotes the *real* part of a *complex* number.

#### B. The metric structure

The metric in Eq. (116) is exactly four times the so-called Fubini-Study metric employed in the standard geometric analysis of quantum evolution [95]. The Fubini-Study metric is a gauge invariant metric on the *complex* projective Hilbert space, the manifold of Hilbert-space rays [96]. If we assume that  $|\psi_{\theta}\rangle$  in Eq. (116) is given by,

$$|\psi_{\theta}\rangle = \sum_{l=1}^{N} \sqrt{p_l(\theta)} e^{i_{\mathbb{C}}\phi_l(\theta)} |l\rangle, \qquad (117)$$

after some straightforward but tedious algebra (for details, we refer to Appendix A in Ref. [44]), we obtain that the infinitesimal Wigner-Yanase line element becomes

$$ds^{2} \stackrel{\text{def}}{=} g_{ij}^{(WY)}(\theta) d\theta^{i} d\theta^{j} = \left\{ \sum_{l=1}^{N} \frac{\dot{p}_{l}^{2}}{p_{l}} + 4 \left[ \sum_{l=1}^{N} p_{l} \dot{\phi}_{l}^{2} - \left( \sum_{l=1}^{N} p_{l} \dot{\phi}_{l} \right)^{2} \right] \right\} d\theta^{2}, \tag{118}$$

where,

$$\dot{p}_l \stackrel{\text{def}}{=} \frac{dp_l(\theta)}{d\theta} \text{ and, } \dot{\phi}_l \stackrel{\text{def}}{=} \frac{d\phi_l(\theta)}{d\theta}.$$
(119)

In what follows, we assume that the density operator  $\rho_{\theta}$  is parametrized by *n*-real parameters  $\theta = (\theta^1, ..., \theta^n)$  and satisfies the standard von Neumann equation,

$$\frac{\partial \rho_{\theta}}{\partial \theta} + \frac{i_{\mathbb{C}}}{\hbar} [T, \, \rho_{\theta}] = 0, \tag{120}$$

where T is the generator of temporal shift such that,

$$\rho_{\text{initial}} \stackrel{\text{def}}{=} \rho_0 \to \rho_{\text{final}} \stackrel{\text{def}}{=} \rho_\theta = e^{-\frac{i_{\mathcal{C}}}{\hbar}\theta T} \rho_0 e^{\frac{i_{\mathcal{C}}}{\hbar}\theta T}. \tag{121}$$

The set of quantum states  $\rho_{\theta}$  in Eq. (121) characterizes the quantum evolution manifold of pure quantum states. Furthermore, the set of parameters  $\theta$  can be viewed as a local coordinate system on such manifold endowed with a metric structure defined by the Wigner-Yanase metric in Eq. (116). Finally, we point out that once the monotone Riemannian metric in Eq. (116) is explicitly known, the other differential geometric quantities such as, for instance, the Christoffel connection coefficients, scalar and sectional curvatures, and the Riemannian curvature tensor can be calculated from it, in principle. For example, assuming  $\theta^{m} = \theta^{m}(\tau)$ , the geodesic equation is given by

$$\frac{d^{2}\theta^{m}\left(\tau\right)}{d\tau^{2}} + \Gamma_{ij}^{m}\left(\theta\right)\frac{d\theta^{i}}{d\tau}\frac{d\theta^{j}}{d\tau} = 0,\tag{122}$$

where the Christoffel connection coefficients  $\Gamma_{ij}^m$  are defined as [20],

$$\Gamma_{ij}^{m} \stackrel{\text{def}}{=} \frac{1}{2} g^{ml} \left( \partial_{i} g_{lj} + \partial_{j} g_{il} - \partial_{l} g_{ij} \right), \tag{123}$$

where, from a classical standpoint,  $g_{ij}$  equals  $g_{ij}^{(FR)}$  in Eq. (111). For further technical details on both classical and quantum aspects of information geometry, we refer to [20]. For a classical derivation of Eq. (122), we refer to Appendix F.

# C. Information geometric description: the dissipationless nature

We are now ready to present an IG description of Grover's algorithm in terms of optimal (dissipationless) geodesic paths. To better emphasize its relevance, a comment on the dissipationless nature of quantum computing is required.

# 1. On the dissipationless nature of quantum computing

A quantum computer obeys the laws of quantum mechanics. Its unique feature is that it can control a superposition of computation paths simultaneously and produce a final state that depends on the interference of these paths. To preserve quantum interferences that form the computation, quantum systems that act as qubits must be sufficiently isolated from external influences. Therefore, a quantum computer is non-dissipative and can operate at low temperatures [97]. As mentioned earlier, the dissipationless nature of quantum computing is due to the fact that, in principle, quantum computation can only occur in systems that are almost completely isolated from the environment. Therefore, despite the extraordinarily difficult practical conditions to satisfy, they must dissipate no energy during the process of computation. In [97], the minimum operable temperature of a quantum computer was assumed to be T = 100mK. Observe that the dissipationless nature of quantum computing and the low temperature operations of the computer imply that, in principle, fluctuations (perturbations) are negligible since they can be kept extremely small. In summary, isolation means unitarity. Unitarity means conservation of probability and invertibility. Invertibility means reversibility. Reversibility means no dissipation. Experimentally, there is a number of factors that can go wrong and we can witness a departure from a unitary and dissipationless scenario. From and experimental standpoint, the fact that measured probabilities are not exactly zero or one is primarily due to imperfect laser-cooling, imperfect state and detector preparation, and decoherence effects. Several sources responsible for decoherence can be identified when considering a physical realization of a quantum computer [98–100]: instabilities in the laser beam power, instabilities in the relative position of the ion with respect to the beams, coupling of internal vibrational modes due to trap imperfections, fluctuating external magnetic fields which can modulate the qubit phases, instabilities in the voltage amplitude, external heating and dissipation of the ion motion [101, 102] and, finally, experimental uncertainties in

interaction times, laser detunings, positions of ions, and phases of lasers. Interestingly, Grover pointed out in [103] that one of the limitations of his quantum search algorithm was the assumption of the absolute absence of fluctuations in the operators U and  $U^{-1}$  during the algorithmic sequence: these operators stay the same at all time steps. In what follows, we shall see the elegance and power of IG methods when applied to the characterization of quantum computational software.

#### 2. Dissipationless information geometric evolution

In its digital representation, Grover's algorithm is essentially a sequence of unitary transformations on a pure state that evolves with discrete k. In the limiting scenario of N approaching infinity, we can replace  $\theta_k = (2k+1)\theta$  with  $\theta(\tau)$ . Then, the output state in Eq. (37) can be approximately described by a quantum mechanical wave-vector  $|\psi_{\theta}\rangle$  given by,

$$|\psi_{\theta}\rangle \stackrel{\text{def}}{=} \sum_{l=0}^{N-1} \sqrt{p_{l}\left(\theta\right)} |l\rangle = \sqrt{p_{0}\left(\theta\right)} |0\rangle + \sum_{l=1}^{N-1} \sqrt{p_{l}\left(\theta\right)} |l\rangle, \tag{124}$$

where  $|\bar{x}\rangle$  and  $|\psi_{\text{bad}}\rangle$  are being replaced with  $|0\rangle$  and the second term in the RHS of Eq. (124), respectively. Furthermore  $p_0(\theta)$  and  $p_l(\theta)$  with  $1 \le l \le N-1$  are defined as,

$$p_0(\theta) \stackrel{\text{def}}{=} \sin^2(\theta)$$
, and  $p_l(\theta) \stackrel{\text{def}}{=} \frac{1}{N-1} \cos^2(\theta)$ , (125)

respectively. At this point, we introduce the so-called Fisher information function  $\mathcal{F}(\theta)$  defined as [104]

$$\mathcal{F}(\theta) \stackrel{\text{def}}{=} \sum_{l=0}^{N-1} p_l \left( \frac{\partial \log p_l}{\partial \theta} \right)^2. \tag{126}$$

It can be shown that  $\mathcal{F}(\theta)$  is invariant under unitary transformations applied to arbitrary normalized quantum states  $|\psi_{\theta}\rangle$  (for further details, see [44]). For further details on the Fisher information function from both information-theoretic and statistical mechanical standpoints, we refer to Appendix D. For the specific case of normalized states in Eq. (124), using Eqs. (118), (124), and (125), the function  $\mathcal{F}(\theta)$  in Eq. (126) becomes

$$\mathcal{F}(\theta) = \sum_{l=0}^{N-1} \frac{\dot{p}_l^2}{p_l} = 4 \sum_{l=0}^{N-1} \left( \frac{\partial \sqrt{p_l}}{\partial \theta} \right)^2 = 4. \tag{127}$$

In the rest of the manuscript, Eq. (127), a peculiarity of Grover's information geometric evolution, shall be referred to as the parametric-independence constraint on the Fisher information function. The relevance of the constancy of the Fisher information function from a quantum information geometric viewpoint can be understood once we observe the connection between  $\mathcal{F}(\theta)$  and the generalized mechanical kinetic energy  $\mathcal{K}(\theta)$  (where  $\theta$  is viewed as a temporal

shift) [105],

$$\mathcal{K}(\theta) \stackrel{\text{def}}{=} \sum_{l=0}^{N-1} \left| \frac{\partial \psi_{\theta}(l)}{\partial \theta} \right|^{2}, \tag{128}$$

where  $\psi_{\theta}(l) = \langle l | \psi_{\theta} \rangle$  and  $p_l(\theta) = |\psi_{\theta}(l)|^2$ . The quantity  $\mathcal{K}(\theta)$  in Eq. (128) can be rewritten as (for further details, we refer to Appendix E),

$$\mathcal{K}(\theta) = \frac{1}{4} \mathcal{F}(\theta) + \sum_{l=0}^{N-1} J_{\theta}^{2}(l) |\psi_{\theta}(l)|^{2},$$
(129)

where  $J_{\theta}(l)$  plays the role of the normalized quantum mechanical current density and is defined as [105],

$$J_{\theta}\left(l\right) \stackrel{\text{def}}{=} \frac{1}{2i_{\mathbb{C}}\left|\psi_{\theta}\left(l\right)\right|^{2}} \left(\frac{\partial\psi_{\theta}\left(l\right)}{\partial\theta}\psi_{\theta}^{*}\left(l\right) - \psi_{\theta}\left(l\right)\frac{\partial\psi_{\theta}^{*}\left(l\right)}{\partial\theta}\right),\tag{130}$$

while  $\mathcal{F}(\theta)$  is the same as in Eq. (127). The symbol \* in Eq. (130) denotes complex conjugation. Assuming,

$$\psi_{\theta}\left(l\right) \stackrel{\text{def}}{=} \sqrt{p_{l}\left(\theta\right)} e^{i\phi_{l}\left(\theta\right)},\tag{131}$$

after some algebra, we obtain

$$\mathcal{K}(\theta) = \left\langle \dot{\psi}_{\theta} \middle| \dot{\psi}_{\theta} \right\rangle, \, \mathcal{F}(\theta) = \sum_{l=0}^{N-1} \frac{\dot{p}_{l}^{2}}{p_{l}} \, \text{and}, \, J_{\theta}(l) = \dot{\phi}_{l}(\theta),$$
(132)

with  $\dot{\psi}_{\theta} \stackrel{\text{def}}{=} \frac{d\psi(\theta)}{d\theta}$ . Using Eq. (132), Eq. (129) becomes

$$\left\langle \dot{\psi}_{\theta} | \dot{\psi}_{\theta} \right\rangle = \frac{1}{4} \sum_{l=0}^{N-1} \frac{\dot{p}_l^2}{p_l} + \sum_{l=0}^{N-1} p_l \dot{\phi}_l^2.$$
 (133)

Since  $\mathcal{F}(\theta) = 4$  and  $J_{\theta}(l) = 0$  for any  $0 \le l \le N - 1$ , from Eq. (133) we arrive at

$$\mathcal{K}(\theta) = \left\langle \dot{\psi}_{\theta} | \dot{\psi}_{\theta} \right\rangle = 1. \tag{134}$$

Finally, we conclude that the constancy of the Fisher information function in Eq. (127) implies that Grover's algorithm is characterized by a constant mechanical kinetic energy in Eq. (134) with the absence of any dissipation of statistical nature. A few considerations of note are as follows. Our information geometric investigation can be linked to other lines of research involving the concept of information, Riemannian geometry, and thermodynamics. Recall that the analog (continuous-time) version of Grover's algorithm as proposed by Farhi and Guttmann required the application of a time-independent Hamiltonian for a time interval  $\Delta t \propto \sqrt{N}$ . In [106], an analog version of Grover's algorithm with a time-dependent Hamiltonian satisfying the adiabaticy condition at all times (that is, locally) by varying the evolution rate of the driving Hamiltonian was proposed. Such local adiabatic evolution of the analog version of Grover's algorithm exhibits the same quadratic speedup as the original version of the algorithm. Furthermore,

exploiting fundamental limits to the minimum time duration (maximum speed) for the dynamical evolution to an orthogonal quantum state [107, 108] (specifically,  $\Delta t \geq \frac{h}{4} \frac{1}{\Delta E}$  with  $\Delta E$  denoting the uncertainty in energy of the system and h being the Planck constant) and establishing a novel time-energy relation, a general upper bound for the evolution speed for driving a quantum state to a target state where the driving Hamiltonian is time-independent was estimated in [109] and, under special conditions, it was shown that this speed reduces to that proposed by Farhi and Guttmann [109]. The relevance of the concept of Fisher information in statistical mechanics was discussed in [110] where it was reported that the Fisher information of a thermodynamic system characterizes the size of fluctuations about equilibrium. Specifically, it was shown that the Fisher information of a probability distribution at thermal equilibrium with respect to the inverse temperature  $\beta \stackrel{\text{def}}{=} (k_B T)^{-1}$  equals the energy fluctuations [110],

$$\mathcal{F}(\beta) = \sigma_E^2 \stackrel{\text{def}}{=} \left\langle \left( E - \left\langle E \right\rangle \right)^2 \right\rangle, \tag{135}$$

where  $k_B$  is the Boltzmann constant with  $k_B \approx 1.38 \times 10^{-23}$  [MKSA]. For more details on the statistical mechanical nature of the Fisher information function, we refer to Appendix D. More recently, inspired by the study of Riemannian geometric aspects of nonequilibrium thermodynamics [111, 112] applied to nanoscale systems [113, 114], the concept of Fisher information together with differential geometric methods have been employed to uncover optimal (minimum dissipation, energy efficient) protocols for designing nonequilibrium nanoscale (stochastic) machines, heat engines, and magnetic refrigerators [115]. Within this Riemannian geometric framework, geodesics represent nonequilibrium control protocols with the lowest achievable dissipation. It would certainly be valuable to investigate the IG description of quantum computational software in the presence of possible energy fluctuations. We leave this topic for future efforts.

# 3. Geodesic paths

Some technical details on the minimization of the action functional in differential geometric terms appear in Appendix F. Here, the geodesic path related to Grover's algorithm can be obtained by minimizing the action functional  $\mathcal{S}[p_l(\theta)]$  defined as,

$$\mathcal{S}\left[p_{l}\left(\theta\right)\right] \stackrel{\text{def}}{=} \int \sqrt{ds_{\text{WY}}^{2}} = \int \mathcal{L}\left(\dot{p}_{l}\left(\theta\right), p_{l}\left(\theta\right)\right) d\theta, \tag{136}$$

with the Lagrangian quantity  $\mathcal{L}\left(\dot{p}_{l}\left(\theta\right),\,p_{l}\left(\theta\right)\right)$  given by,

$$\mathcal{L}\left(\dot{p}_{l}\left(\theta\right), p_{l}\left(\theta\right)\right) \stackrel{\text{def}}{=} \left[\sum_{k=0}^{N-1} \frac{\dot{p}_{l}^{2}\left(\theta\right)}{p_{l}\left(\theta\right)}\right]^{\frac{1}{2}},\tag{137}$$

where the parametric probabilities  $p_l(\theta)$  satisfy the normalization constraint,

$$\sum_{l=0}^{N-1} p_l(\theta) = 1. {(138)}$$

Following [116], we can simplify our analysis by taking into consideration the change of variable  $p_l(\theta) \to q_l^2(\theta)$ . Employing the method of Lagrange multipliers, the new action functional  $S_{new}[q_l(\theta)]$  to be minimized becomes,

$$S_{new}\left[q_l\left(\theta\right)\right] = \int \mathcal{L}_{new}\left(\dot{q}_l\left(\theta\right), \, q_l\left(\theta\right)\right) d\theta = \int \left\{ \left[4\sum_{l=1}^N \dot{q}_l^2\left(\theta\right)\right]^{\frac{1}{2}} - \lambda \left(\sum_{l=1}^N q_l^2\left(\theta\right) - 1\right)\right\} d\theta,\tag{139}$$

where  $\lambda$  is the Lagrange multiplier and  $\mathcal{L}_{new}$  ( $\dot{q}_l(\theta)$ ,  $q_l(\theta)$ ) is the new Lagrangian quantity. The path that minimizes the action functional  $\mathcal{S}_{new}$  [ $q_l(\theta)$ ] satisfies the so-called *actuality constraint*,

$$\frac{\delta S_{new}\left[q_l\left(\theta\right)\right]}{\delta q_l\left(\theta\right)} = 0. \tag{140}$$

After some algebra, it is found that the constraint in Eq. (140) leads to the Euler-Lagrange equation,

$$\frac{d^{2}q_{l}\left(\theta\right)}{d\theta^{2}} - \frac{\dot{\mathcal{L}}\left(\dot{q}_{l}\left(\theta\right), q_{l}\left(\theta\right)\right)}{\mathcal{L}\left(\dot{q}_{l}\left(\theta\right), q_{l}\left(\theta\right)\right)} \frac{dq_{l}\left(\theta\right)}{d\theta} + \frac{\lambda}{2} \mathcal{L}\left(\dot{q}_{l}\left(\theta\right), q_{l}\left(\theta\right)\right) q_{l}\left(\theta\right) = 0,$$
(141)

where  $\dot{\mathcal{L}} = \frac{d\mathcal{L}}{d\theta}$  with  $\mathcal{L}(\dot{q}_l(\theta), q_l(\theta))$  given in Eq. (137) and  $q_l^2(\theta) = p_l(\theta)$ . In the case of Grover's dynamics,  $\mathcal{F}(\theta) = 4$  and, therefore,  $\mathcal{L}(\dot{q}_l(\theta), q_l(\theta)) = 2$  and  $\dot{\mathcal{L}}(\dot{q}_l(\theta), q_l(\theta)) = 0$ . Therefore, setting the Lagrange multiplier  $\lambda = 1$  in order to satisfy Eq. (138), the geodesic Eq. (141) becomes

$$\frac{d^2q_l(\theta)}{d\theta^2} + q_l(\theta) = 0. \tag{142}$$

The solution  $q(\theta)$  of Eq. (142) is given by,

$$q(\theta) = (q_0(\theta), q_1(\theta), ..., q_{N-1}(\theta)),$$
 (143)

with,

$$q_0(\theta) = \sin(\theta)$$
, and  $q_l(\theta) = \frac{1}{\sqrt{N-1}}\cos(\theta)$ , (144)

for any  $1 \leq l \leq N-1$ . Recalling that  $q_l^2(\theta) = p_l(\theta)$ , Eq. (144) leads to the N-dimensional probability vector  $p \stackrel{\text{def}}{=} (p_0(\theta), p_1(\theta), ..., p_{N-1}(\theta))$  with  $p_l(\theta)$  defined in Eq. (125). The quantity p characterizes a geodesic path that satisfies both the parametric-independence and actuality constraints in Eqs. (127) and (140), respectively. It is the path for which the quantum Fisher information action functional  $S_{new}[q_l(\theta)]$  achieves an extremal value.

# D. Information geometric description: the quadratic speedup

We investigate here the IG perspective of the quadratic speedup relation and the superfluity of the Walsh-Hadamard operation in achieving this improvement in a quantum search problem.

### 1. The metric on the complex projective Hilbert space

We recall that the necessity of introducing a metric on the manifold of Hilbert space rays, the so-called *complex* projective Hilbert space  $\mathbb{C}P$ , is due to the non-observability of a phase of a vector in the Hilbert space  $\mathcal{H}$  [96]:  $|\psi(\theta)\rangle$  and  $e^{i_{\mathbb{C}}\alpha(\theta)}|\psi(\theta)\rangle$  with  $\theta$  denoting an n-dimensional parameter define the same point on the manifold of rays. Wootters showed that the absolute statistical distance between two different preparations of the same quantum system equals the angle in Hilbert space between the corresponding rays [116],

$$\cos^2\left(\frac{1}{2}\theta\right) = |\langle\psi|\phi\rangle|^2\,,\tag{145}$$

where the RHS in Eq. (145) denotes the probability of transition from state  $|\psi\rangle$  to state  $|\phi\rangle$ . Up to a constant factor, the only Riemannian metric on the set of rays which is invariant under all possible unitary time evolutions is the angle in Hilbert space. For neighboring pure states  $|\psi\rangle$  and  $|\phi\rangle$ , let us set the statistical distance  $ds_{PS} = \theta$ . Using Eq. (145), we obtain

$$ds_{\rm FS}^2 \stackrel{\text{def}}{=} \frac{1}{4} ds_{\rm PS}^2 = \left\{ \cos^{-1} \left[ |\langle \psi | \phi \rangle| \right] \right\}^2,$$
 (146)

where  $ds_{\rm FS}^2$  denotes the Fubini-Study infinitesimal line element [95, 117]. In the working hypothesis that  $ds_{\rm PS} \ll 1$ , Eq. (145) yields

$$\cos^2\left(\frac{1}{2}ds_{\rm PS}\right) \approx 1 - \frac{1}{4}ds_{\rm PS}^2 = \left|\langle\psi|\phi\rangle\right|^2. \tag{147}$$

Combining Eqs. (146) and (147), we finally obtain the expression of the natural metric on the manifold of Hilbert space rays, the Fubini-Study metric [117],

$$ds_{\text{FS}}^2 = 1 - \left| \langle \psi | \phi \rangle \right|^2. \tag{148}$$

From an information geometric viewpoint, as mentioned earlier, we shall be using the Wigner-Yanase metric which is essentially four times the Fubini-Study metric.

#### 2. Information geometric steps-counting

Within the information geometric setting, the number of steps needed to arrive at the final target state  $|\psi_{\theta_f}\rangle$  from the initial state  $|\psi_{\theta_i}\rangle$  can be estimated as follows.

First, we note that the distance covered in a single step leading to  $|\psi_{\theta_{i+1}}\rangle \stackrel{\text{def}}{=} G |\psi_{\theta_i}\rangle$  from  $|\psi_{\theta_i}\rangle$  where G is the Grover iterate can be computed in an explicit manner using the Wigner-Yanase metric once we find  $|\psi_{\theta_{i+1}}\rangle$ . Recall

that the Grover iterate can be written as  $G \stackrel{\text{def}}{=} -I_i U^{-1} I_f U$  where U is a unitary operator while  $I_i$  and  $I_f$  are defined as,

$$I_i \stackrel{\text{def}}{=} 1 - 2 |\psi_{\theta_i}\rangle \langle \psi_{\theta_i}|, \text{ and } I_f \stackrel{\text{def}}{=} 1 - 2 |\psi_{\theta_f}\rangle \langle \psi_{\theta_f}|,$$
 (149)

respectively. We emphasize that the unitary operator U was originally represented by the Walsh-Hadamard operation in Grover's quantum search algorithm. However, Grover showed later that any unitary operation can be used in his algorithm to arrive at the same quadratic speedup [103]. Using Eq. (149) and recalling that

$$U_{if} \stackrel{\text{def}}{=} \left\langle \psi_{\theta_i} \left| U \right| \psi_{\theta_f} \right\rangle, U_{if}^* \stackrel{\text{def}}{=} \left\langle \psi_{\theta_f} \left| U^{-1} \right| \psi_{\theta_i} \right\rangle, \text{ and } \left| U_{if} \right|^2 \stackrel{\text{def}}{=} U_{if} U_{if}^*, \tag{150}$$

after some algebra, we obtain

$$\left|\psi_{\theta_{i+1}}\right\rangle = G\left|\psi_{\theta_{i}}\right\rangle$$

$$= -I_{i}U^{-1}I_{f}U\left|\psi_{\theta_{i}}\right\rangle$$

$$= \left(1 - 4\left|U_{fi}\right|^{2}\right)\left|\psi_{\theta_{i}}\right\rangle + 2U_{fi}U^{-1}\left|\psi_{\theta_{f}}\right\rangle, \tag{151}$$

that is,

$$\left|\psi_{\theta_{i+1}}\right\rangle = \left(1 - 4\left|U_{fi}\right|^{2}\right)\left|\psi_{\theta_{i}}\right\rangle + 2U_{fi}U^{-1}\left|\psi_{\theta_{f}}\right\rangle. \tag{152}$$

The Wigner-Yanase line element between  $|\psi_{\theta_i}\rangle$  and  $|\psi_{\theta_{i+1}}\rangle$  is given by,

$$\left[ds_{\text{WY}}^2\right]_{i\to i+1} = 4\left[1 - \left|\left\langle\psi_{\theta_i}|\psi_{\theta_{i+1}}\right\rangle\right|^2\right]. \tag{153}$$

Substituting Eq. (152) into Eq. (153), we find

$$\left[ds_{\text{WY}}^{2}\right]_{i\to i+1} = 16 \left|U_{fi}\right|^{2} \left[1 - \left|U_{fi}\right|^{2}\right]. \tag{154}$$

Second, assume that  $|\psi_{\theta_f}\rangle$  is reached through a succession of a countable set of intermediate steps. Specifically,  $|\psi_{\theta_f}\rangle$  can be reached as follows. First, we transition in  $\mathcal{N}_s$  steps from  $|\psi_{\theta_i}\rangle$  to  $|\tilde{\psi}_{\theta_f}\rangle$ ,

$$\left|\tilde{\psi}_{\theta_f}\right\rangle \stackrel{\text{def}}{=} U^{-1} \left|\psi_{\theta_f}\right\rangle. \tag{155}$$

Then, with a single application of the unitary operator U, the target state  $|\psi_{\theta_f}\rangle$  is reached. Observe that G preserves the two-dimensional space spanned by  $|\psi_{\theta_i}\rangle$  and  $|\tilde{\psi}_{\theta_f}\rangle$  because of Eq. (152) and since

$$G\left|\tilde{\psi}_{\theta_f}\right\rangle = \left|\tilde{\psi}_{\theta_f}\right\rangle - 2\left\langle\psi_{\theta_i}|\tilde{\psi}_{\theta_f}\right\rangle|\psi_{\theta_i}\rangle. \tag{156}$$

We point out that in the original digital description of Grover's work, the evolution of the algorithm occurs with a discrete number of iterations. In the analog description, the evolution becomes approximately continuous in the limiting case in which the dimensionality  $N \stackrel{\text{def}}{=} 2^n$  of the Hilbert space approaches infinity. For this reason, it is reasonable to assume that the number of iterations remains countable also in the analog case. A simple calculation shows that the Wigner-Yanase line element between  $|\psi_{\theta_i}\rangle$  and  $|\tilde{\psi}_{\theta_f}\rangle \stackrel{\text{def}}{=} U^{-1} |\psi_{\theta_f}\rangle$  is given by,

$$\left[ds_{\text{WY}}^{2}\right]_{i\to f} = 4\left[1 - \left|\left\langle\psi_{\theta_{i}}|\tilde{\psi}_{\theta_{f}}\right\rangle\right|^{2}\right] = 4\left[1 - \left|U_{fi}\right|^{2}\right]. \tag{157}$$

Assuming that  $|U_{fi}| \ll 1$  (for further details, see Appendix G), it happens that

$$[ds_{WY}^2]_{i \to i+1} = [ds_{WY}^2]_{i+1 \to i+2} = \dots = [ds_{WY}^2]_{i+l-2 \to i+l-1} = [ds_{WY}^2]_{i+l-1 \to i+l},$$
(158)

where  $l \in \mathbb{R}$  and  $|\psi_{\theta_{i+l}}\rangle \stackrel{\text{def}}{=} G^l |\psi_{\theta_i}\rangle$  is equal to

$$|\psi_{\theta_{i+l}}\rangle = (1 - 4|U_{fi}|^2) |\psi_{\theta_{i+l-1}}\rangle + 2U_{fi}G^{l-1}U^{-1} |\psi_{\theta_f}\rangle.$$
 (159)

At this point, the number of equal-length steps  $\mathcal{N}_s$  needed to navigate a distance  $[ds_{\mathrm{WY}}]_{i \to f}$  becomes

$$\mathcal{N}_s \stackrel{\text{def}}{=} \left( \frac{\left[ ds_{\text{WY}}^2 \right]_{i \to f}}{\left[ ds_{\text{WY}}^2 \right]_{i \to i+1}} \right)^{\frac{1}{2}}. \tag{160}$$

Using Eqs. (154) and (157), in the working hypothesis that  $|U_{fi}| \ll 1$ , we obtain

$$\mathcal{N}_s \propto \frac{1}{\sqrt{|U_{fi}|^2}}.\tag{161}$$

Observe that when  $|U_{fi}| \ll 1$ , the quantum states  $|\psi_{\theta_i}\rangle$  and  $|\tilde{\psi}_{\theta_f}\rangle$  are approximately orthogonal. Eq. (161) implies that the number of steps needed to arrive at the final target state from the initial state is inversely proportional to the square root of the probability of transition from the *i*-th state to the *f*-th state under the unitary evolution operator U. Eq. (161) is the quantum information geometric analog of what Grover and Pati obtained by means of matrix algebra arguments and geometric quantum mechanical methods in Refs. [39] and [103], respectively. Note that  $U_{fi}$  denotes the amplitude of arriving at state  $|\psi_{\theta_f}\rangle$  by applying U to  $|\psi_{\theta_i}\rangle$ . At this point, if we perform an experiment and observe the system,  $|U_{fi}|^2$  becomes the probability of arriving at the target state  $|\psi_{\theta_f}\rangle$  by starting from the initial basis state  $|\psi_{\theta_i}\rangle$ . According to this line of reasoning, in order to achieve a single success one needs to perform this experiment at least  $\mathcal{O}\left(1/|U_{fi}|^2\right)$  number of times. If  $|U_{fi}| \ll 1$ , from Eq. (161) we conclude that the number of steps (repetition of this experiment) reduces to  $\mathcal{O}\left(1/|U_{fi}|\right)$ . This is a remarkable improvement achievable with any unitary U. As a final side remark, we point out that assuming  $N \stackrel{\text{def}}{=} 2^n$  is needed if U equals the Walsh-Hadamard

operation since this is the only case in which this operator is well-defined. However, since the Grover iterate G can be constructed with arbitrary unitary operations U, this assumption can be removed [118]. Our analysis based on quantum IG confirms this fact.

# VII. ON GROVER'S FIXED-POINT QUANTUM SEARCH ALGORITHM

In this Section, we present a qualitative discussion concerning Grover's fixed point phase- $\frac{\pi}{3}$  quantum search algorithm [46, 47] from both a geometric algebra and information geometry perspectives.

#### A. Preliminaries

Grover's original quantum search is characterized by an iterative procedure that, in the asymptotic limit of a very large number N of unsorted items, allows us to identify with certainty one of the  $N_m$  marked items in approximately kiterations with  $k \approx \frac{\pi}{4} \sqrt{N/N_m}$ . We recall that Grover's original quantum search algorithm is constructed by iteratively applying to  $|0\rangle^{\otimes n} \in \mathcal{H}_2^n$  the operator G,

$$G \stackrel{\text{def}}{=} -R_{\psi}^{(\pi)} U^{\dagger} R_{\bar{x}}^{(\pi)} U, \tag{162}$$

where the unitary U is the Walsh-Hadamard transformation while  $R_{\psi}^{(\pi)}$  and  $R_{\bar{x}}^{(\pi)}$  are the selective inversion operators of the states  $|\psi\rangle$  and  $|\bar{x}\rangle$ , respectively. They are given by,

$$R_{sb}^{(\pi)} \stackrel{\text{def}}{=} I - 2 |\psi\rangle\langle\psi| \text{ and } R_{\bar{x}}^{(\pi)} \stackrel{\text{def}}{=} I - 2 |\bar{x}\rangle\langle\bar{x}|,$$
 (163)

respectively. The failure probability after k-iterations of Grover's original search algorithm is given by,

$$P_{\text{failure}}^{(k\text{-iterations})}(k) = 1 - \left| \left\langle \bar{x} | G^k | \psi \right\rangle \right|^2 = 1 - \sin^2 \left[ (2k+1) \theta \right], \tag{164}$$

where  $P_{\text{failure}}^{(k\text{-iterations})}(k) = P_{\text{failure}}^{(k\text{-iterations})}(k+T)$  with  $T \stackrel{\text{def}}{=} \pi/(2\theta)$ . A limitation of this search scheme is that success can be achieved only when the number  $N_m$  of marked items is known beforehand so that the number k of iterations landing the initial state closest to the marked state can be predicted [119]. For instance, since the iterative procedure is essentially a rotation, once the target is reached, further iterations will drive the system away from the target state. As a consequence, the success probability rapidly decreases and drops to zero. In summary, to know when to terminate the algorithm, the fraction  $N/N_m$  of marked items must be known precisely. To undertake a quantum search when the number  $N_m$  of marked items is not known ahead of time, Grover proposed a different kind of search method based

upon a recursive procedure known as fixed-point quantum search [46, 47]. In this different kind of quantum search, the system is always moved towards the target state with the consequence that the success probability is continuously amplified in a monotonic fashion. In other towards, there is a monotonic convergence toward the solution.

Since its introduction, Grover's fixed-point quantum search algorithm has been implemented under a variety of different schemes. In [120], it was implemented on a two-qubit NMR quantum computer. The two qubits were described in terms of the  $^{1}H$  (protium) and the  $^{13}C$  (carbon-13) nuclei. The quantum search was performed in the case of N=4 unsorted items and either  $N_{m}=1$  or  $N_{m}=2$  marked items. In [121], an improved version of Grover's fixed-point quantum search algorithm exhibiting quadratic speedup proposed by Yoder and collaborators in [122] was implemented on a three-qubit quantum computer by using the bang-bang control technique. The three qubits were described in terms of the  $^{1}H$  (protium), the  $^{13}C$  (carbon-13), and the  $^{19}F$  (fluorine-19) nuclei. The quantum search was performed in the case of N=4 unsorted items and  $N_{m}=1$  marked items.

Grover noticed that the achievement of the monotonic convergence toward the solution (the fixed point) could not have been achieved via iterations of the same unitary transformation since unitary transformations are characterized by eigenvalues of magnitude one. Therefore, any iteration is inherently periodic. To solve this issue, Grover proposed a clever recursive scheme defined in terms of suitably designed distinct unitary operations performed at successive iterations. Specifically, the recursive scheme proposed by Grover is given by,

$$U_{k+1} \stackrel{\text{def}}{=} U_k R_{sh}^{(\pi/3)} U_k^{\dagger} R_{\bar{x}}^{(\pi/3)} U_k, \tag{165}$$

where  $U_0 = U$ , U is some unitary operator while  $R_{\psi}^{(\pi/3)}$  and  $R_{\bar{x}}^{(\pi/3)}$  are the selective  $\pi/3$ -phase shift operators of the initial (source) and final (target) states, respectively. They are defined as,

$$R_{\psi}^{(\pi/3)} \stackrel{\text{def}}{=} I - \left[1 - e^{ic\frac{\pi}{3}}\right] |\psi\rangle\langle\psi| \text{ and } R_{\bar{x}}^{(\pi/3)} \stackrel{\text{def}}{=} I - \left[1 - e^{ic\frac{\pi}{3}}\right] |\bar{x}\rangle\langle\bar{x}|, \tag{166}$$

respectively. The failure probability after k-recursive steps of Grover's fixed-point search algorithm is given by,

$$P_{\text{failure}}^{(k\text{-recursive steps})}(k) = 1 - |\langle \bar{x}|U_k|\psi\rangle|^2 = \epsilon^{3^k},$$
 (167)

where  $\epsilon \stackrel{\text{def}}{=} 1 - |\langle \bar{x} | U_0 | \psi \rangle|^2 \ll 1$  denotes the probability of failure after no-recursive step. For the sake of later convenience, let us introduce the generalized Grover iterate  $G(\alpha, \beta) \stackrel{\text{def}}{=} -R_{\psi}^{(\alpha)} R_{\bar{x}}^{(\beta)}$  defined as the product of two generalized reflection operators with  $\alpha, \beta \in \mathbb{R}$ . The two dimensional matrix representation of  $G(\alpha, \beta)$  with respect

to  $\{|\psi_{\rm bad}\rangle, |\bar{x}\rangle\}$  is given by,

$$[G(\alpha, \beta)] = \begin{pmatrix} \langle \psi_{\text{bad}} | G(\alpha, \beta) | \psi_{\text{bad}} \rangle & \langle \psi_{\text{bad}} | G(\alpha, \beta) | \bar{x} \rangle \\ \langle \bar{x} | G(\alpha, \beta) | \psi_{\text{bad}} \rangle & \langle \bar{x} | G(\alpha, \beta) | \bar{x} \rangle \end{pmatrix}$$

$$= \begin{pmatrix} (1 - e^{i_{\mathbb{C}}\alpha})\cos^{2}(\theta) - 1 & e^{i_{\mathbb{C}}\beta}(1 - e^{i_{\mathbb{C}}\alpha})\sin(\theta)\cos(\theta) \\ (1 - e^{i_{\mathbb{C}}\alpha})\sin(\theta)\cos(\theta) & e^{i_{\mathbb{C}}\beta}[(1 - e^{i_{\mathbb{C}}\alpha})\sin^{2}(\theta) - 1] \end{pmatrix},$$
(168)

with  $\sin(\theta) \stackrel{\text{def}}{=} \langle \bar{x} | \psi \rangle$  and  $\cos(\theta) \stackrel{\text{def}}{=} \langle \psi_{\text{bad}} | \psi \rangle$ . We observe that for  $\alpha = \beta = \pi$  we recover the matrix representation of the original Grover iterate (see Eq. (43) in Section III).

#### B. Insights from geometric algebra

We present a few remarks in order to make a parallel comparison between the original Grover algorithm and the fixed-point search algorithm using GA. The original Grover algorithm generates a sequence of quantum states  $\{|\psi_k\rangle\}$  such that,

$$|\psi_{k+1}\rangle = G|\psi_k\rangle = G^2|\psi_{k-1}\rangle = \dots = G^{k-1}|\psi_2\rangle = G^k|\psi_1\rangle \equiv G^k|\psi\rangle, \qquad (169)$$

where we assume that the operator G in Eq. (169) is given by  $G \stackrel{\text{def}}{=} -R_{\psi}^{(\pi)} \circ R_{\bar{x}}^{(\pi)}$ . Using the GA language introduced in Section III, the quantum state  $|\psi_{k+1}\rangle$  expressed as the action of  $G^k$  onto  $|\psi\rangle$  becomes the nonhomogeneous multivector expressed as

$$|\psi_{k+1}\rangle = G^k |\psi\rangle \xrightarrow{GA} g^k e_{\psi} (g^{\dagger})^k,$$
 (170)

where the bivector  $g \stackrel{\text{def}}{=} e_{\psi}e_{\text{bad}} = \exp\left(e_{\bar{x}}e_{\text{bad}}\theta\right)$  with  $e_{\psi}$ ,  $e_{\text{bad}}$ , and  $e_{\bar{x}} \in \left[cl^{+}\left(3\right)\right]^{n}/E_{n}$ . The fixed-search quantum search algorithm generates a sequence of quantum states  $\{|\psi_{k}\rangle\}$  such that,

$$|\psi_{k+1}\rangle = \mathcal{G}_k |\psi_k\rangle = \mathcal{G}_k \mathcal{G}_{k-1} |\psi_{k-1}\rangle = \dots = \mathcal{G}_k \mathcal{G}_{k-1} \dots \mathcal{G}_2 \mathcal{G}_1 |\psi_1\rangle \equiv \mathcal{G}_k \mathcal{G}_{k-1} \dots \mathcal{G}_2 \mathcal{G}_1 |\psi\rangle, \tag{171}$$

where we consider that the operator  $\mathcal{G}_k$  in Eq. (171) is defined as  $\mathcal{G}_k \stackrel{\text{def}}{=} R_{\psi_k}^{(\pi/3)} \circ R_{\bar{x}}^{(\pi/3)}$ . More specifically, following the analysis in Ref. [123], we obtain

$$|\psi_k\rangle = \sqrt{1 - |\langle \bar{x}|\psi_k\rangle|^2} |\psi_{\text{bad},k}\rangle + \langle \bar{x}|\psi_k\rangle |\bar{x}\rangle, \qquad (172)$$

where,

$$c_{k+1} = \langle \bar{x} | \psi_{k+1} \rangle \stackrel{\text{def}}{=} e^{i_{\mathbb{C}} \frac{\pi}{3}} \left( e^{i_{\mathbb{C}} \frac{\pi}{3}} + \epsilon_k \right) c_k, \tag{173}$$

 $\epsilon_{k+1} = \epsilon_k^3, \ \epsilon_k \stackrel{\text{def}}{=} 1 - |c_k|^2 = \epsilon^{3^{k-1}}, \ \text{and}$ 

$$|\psi_{\text{bad}, k+1}\rangle \stackrel{\text{def}}{=} e^{ic\frac{\pi}{3}} |\psi_{\text{bad}, k}\rangle.$$
 (174)

Using Eqs. (172) and (174),  $|\psi_k\rangle = \mathcal{G}_{k-1} |\psi_{k-1}\rangle$  becomes

$$|\psi_k\rangle = c_k |\bar{x}\rangle + \sqrt{\epsilon_k} e^{ic\frac{\pi}{3}(k-1)} |\psi_{\text{bad}, 1}\rangle.$$
 (175)

Using the GA language introduced in Section III, the quantum state  $|\psi_{k+1}\rangle$  expressed as the action of  $\mathcal{G}_k\mathcal{G}_{k-1}...\mathcal{G}_2\mathcal{G}_1$  onto  $|\psi\rangle$  becomes the nonhomogeneous multivector expressed as

$$|\psi_{k+1}\rangle = \mathcal{G}_k \mathcal{G}_{k-1} \dots \mathcal{G}_2 \mathcal{G}_1 |\psi\rangle \xrightarrow{GA} (g_k g_{k-1} \dots g_2 g_1) e_\psi (g_k g_{k-1} \dots g_2 g_1)^{\dagger}, \qquad (176)$$

where the bivector  $g_m \stackrel{\text{def}}{=} e_{\psi} e_{\text{bad, }m}$ . Eq. (176) is the analog of Eq. (82) in Section IV. Observe that the sequence of nested rotations  $\mathcal{G}$  is expressed in the GA language in terms of a so-called sandwiching product [124].

### C. Insights from information geometry

We recall that the convergence toward a fixed point is achieved by means of unitary transformations in Grover's fixed-point quantum algorithm. However, such a convergence can also be obtained by introducing irreversible damping by projective measurement operations in the quantum algorithm [125]. Damping can be produced by coupling the system to a bath or, more artificially, by employing a single ancilla spin that is measured after undergoing a unitary evolution with the quantum system [126].

# 1. Monotonic decrease of the Fisher information

From Eq. (175), noticing that  $\sqrt{\epsilon_k} = \exp\left[\frac{1}{2}3^{k-1}\ln\left(\epsilon\right)\right]$  with  $\ln\left(\epsilon\right) \leq 0$  since  $0 \leq \epsilon \ll 1$ , the output state of Grover's fixed-point quantum search algorithm can be formally rewritten in terms of a quantum mechanical wave-vector  $|\psi_\theta\rangle$  given by,

$$|\psi_{\theta}\rangle \stackrel{\text{def}}{=} \sum_{l=0}^{N-1} \sqrt{p_{l}\left(\theta\right)} e^{i_{\mathbb{C}}\phi_{l}\left(\theta\right)} |l\rangle = \sqrt{p_{0}\left(\theta\right)} e^{i_{\mathbb{C}}\phi_{0}\left(\theta\right)} |0\rangle + \sum_{l=1}^{N-1} \sqrt{p_{l}\left(\theta\right)} e^{i_{\mathbb{C}}\phi_{l}\left(\theta\right)} |l\rangle, \tag{177}$$

where  $|\bar{x}\rangle$  and  $|\psi_{\text{bad}}\rangle$  are being replaced with  $|0\rangle$  and the second term in the RHS of Eq. (177), respectively. For the sake of clarity, we limit our discussion to N=2. In this case, probabilities  $p_0(\theta)$  and  $p_1(\theta)$  in Eq. (177) can be parametrized as follows,

$$p_0(\theta) \stackrel{\text{def}}{=} 1 - \xi(\theta) e^{-\theta}$$
, and  $p_1(\theta) \stackrel{\text{def}}{=} \xi(\theta) e^{-\theta}$ , (178)

respectively. The function  $\xi(\theta)$  is assumed to be some differentiable function with values in the interval ]0,1] so that the leading asymptotic behavior of the Fisher information  $\mathcal{F}(\theta)$  is determined by the exponentially decaying term  $e^{-\theta}$  with  $\theta$  being the temporal shift. Indeed,  $\mathcal{F}(\theta)$  is defined in terms of  $p_0(\theta)$  and  $p_1(\theta)$  in Eq. (178) and becomes

$$\mathcal{F}(\theta) = \left\{ \frac{\left[\dot{\xi}(\theta) - \xi(\theta)\right]^2}{\xi(\theta)\left[1 - \xi(\theta)e^{-\theta}\right]} \right\} e^{-\theta},\tag{179}$$

where  $\dot{\xi} = \frac{d\xi}{d\theta}$ . Note that unlike the case of Grover's original quantum search scheme, the Fisher information corresponding to Grover's fixed-point quantum algorithm is not constant. Furthermore, although the Fisher information does not depend on the presence of complex phase factors in quantum states, such phase information becomes important when linking the Fisher information to the generalized mechanical kinetic energy  $\mathcal{K}(\theta)$ . In particular, the presence of non-constant phases  $\phi_l = \phi_l(\theta)$  with  $\dot{\phi}_l(\theta) \neq 0$  implies the emergence of normalized quantum mechanical current densities  $J_{\theta}(l) = \dot{\phi}_l(\theta)$ . In what follows, as a simplifying working assumption, we consider that  $\phi_l(\theta) = \phi_l$  are nonzero but constant phases. We leave a more rigorous investigation of this nontrivial issue concerning a quantum information geometric characterization of the effect of time-varying phases to future scientific efforts [127, 128]. Within our working hypothesis, the generalized mechanical kinetic energy  $\mathcal{K}(\theta)$  becomes

$$\mathcal{K}(\theta) = \frac{1}{4} \left\{ \frac{\left[\dot{\xi}(\theta) - \xi(\theta)\right]^2}{\xi(\theta)\left[1 - \xi(\theta)e^{-\theta}\right]} \right\} e^{-\theta}.$$
 (180)

We remark that due to the polynomial nature of  $\xi(\theta)$ ,  $K(\theta)$  in Eq. (180) exhibits a non-increasing behavior in the asymptotic limit of very large  $\theta$  values. It is interesting to observe that the monotonic decreasing behavior of the Fisher information appears naturally in dissipative kinetic models where energy is non-increasing. For instance, the energy in the Boltzmann equation is decreasing when the binary collisions are dissipative and the Fisher information decreases along the solutions of either the Boltzmann [129] or the Landau [130] equation of Maxwellian molecules. In the language of thermodynamics, our approximate information geometric analysis of Grover's fixed-point quantum search algorithm seems to lead to the conclusion that the size of the energy fluctuations about equilibrium represented by the Fisher information decreases during the geometric evolution of the system towards the target item.

# 2. Quantum search with damping

Following the line of reasoning outlined in the case of Grover's original quantum search algorithm, the geodesic path related to Grover's fixed-point quantum search algorithm can be obtained by minimizing the action functional

 $\mathcal{S}[p_l(\theta)]$  defined as,

$$\mathcal{S}\left[p_l\left(\theta\right)\right] \stackrel{\text{def}}{=} \int \sqrt{ds_{\text{WY}}^2}.\tag{181}$$

It follows that the geodesic paths  $q_l = q_l(\theta)$  with  $p_l(\theta) \stackrel{\text{def}}{=} q_l^2(\theta)$  satisfy the relation,

$$\frac{d^{2}q_{l}\left(\theta\right)}{d\theta^{2}} - \frac{\dot{\mathcal{L}}\left(\dot{q}_{l}\left(\theta\right), q_{l}\left(\theta\right)\right)}{\mathcal{L}\left(\dot{q}_{l}\left(\theta\right), q_{l}\left(\theta\right)\right)} \frac{dq_{l}\left(\theta\right)}{d\theta} + \frac{1}{2}\mathcal{L}\left(\dot{q}_{l}\left(\theta\right), q_{l}\left(\theta\right)\right) q_{l}\left(\theta\right) = 0,$$
(182)

where  $\mathcal{L}(\theta) \stackrel{\text{def}}{=} \mathcal{L}(\dot{q}_l(\theta), q_l(\theta))$  denotes the Lagrangian of the system under investigation with  $\mathcal{L}(\dot{p}_l(\theta), p_l(\theta)) \stackrel{\text{def}}{=} \sqrt{\mathcal{F}(\theta)}$ . We observe that while Eq. (182) reduces to a simple harmonic oscillator equation in the case of Grover's original algorithm (see Eq. (142) in Section VI), it now becomes a slightly more complicated version of the standard damped harmonic oscillator equation,

$$\ddot{x} + b\dot{x} + kx = 0, (183)$$

where b denotes the damping factor, k is the spring constant, and  $\dot{x} = \frac{dx}{dt}$ . The general solution of Eq. (183) is given by,

$$x(t) = Ae^{-\frac{b}{2}t}\sin\left(\frac{\sqrt{4k - b^2}}{2}t + \varphi\right),\tag{184}$$

where A and  $\varphi$  are two real integration constants. We shall omit here the detailed investigation of geodesic paths in the case of the fixed-point quantum algorithm. However, to better grasp the complications that can arise when departing from the standard damped harmonic oscillator motion and to get a bit closer to the actual quantum scenario, in what follows we take into consideration the case in which  $\dot{\mathcal{L}}/\mathcal{L}$  is kept constant while  $\mathcal{L}$  is not constant. Specifically, we assume  $\mathcal{L}(\theta) = \mathcal{L}_0 e^{-\gamma \theta}$  with  $\mathcal{L}_0$  and  $\gamma$  constant quantities in  $\mathbb{R}_+ \setminus \{0\}$ . In this case, omitting the index l in  $q_l(\theta)$ , Eq. (182) becomes

$$\frac{d^{2}q\left(\theta\right)}{d\theta^{2}} + \gamma \frac{dq\left(\theta\right)}{d\theta} + \frac{1}{2}\mathcal{L}_{0}e^{-\gamma\theta}q\left(\theta\right) = 0. \tag{185}$$

The general solution of Eq. (185) can be formally written in closed form as,

$$q(\theta) = \sqrt{\frac{\mathcal{L}_0}{2\gamma^2}} e^{-\frac{\gamma}{2}\theta} \left[ A\mathcal{J}_1 \left( \sqrt{\frac{2\mathcal{L}_0}{\gamma^2}} e^{-\frac{\gamma}{2}\theta} \right) + B\mathcal{Y}_1 \left( \sqrt{\frac{2\mathcal{L}_0}{\gamma^2}} e^{-\frac{\gamma}{2}\theta} \right) \right], \tag{186}$$

where A and B are suitable integration constants while  $\mathcal{J}_{\nu}(x)$  and  $\mathcal{Y}_{\nu}(x)$  with integer order  $\nu = +1$  are Bessel functions of the first and the second kind [131], respectively. We recall that the limiting form of the Bessel function  $\mathcal{J}_{\nu}(x)$  for small arguments in the case in which  $\nu$  is fixed and x approaches zero is given by [131],

$$\mathcal{J}_{\nu}\left(x\right) \approx \left(\frac{1}{2}x\right)^{\nu} \frac{1}{\Gamma\left(\nu+1\right)},$$
(187)

where  $\Gamma$  is the Euler Gamma function with  $\Gamma(\nu+1) \stackrel{\text{def}}{=} \nu!$ . If we set  $\mathcal{L}_0 = 2$  and  $\gamma = 1$ , recalling that  $p_l(\theta) \stackrel{\text{def}}{=} q_l^2(\theta)$  and assuming N = 2, we obtain from Eqs. (186) and (187) the following asymptotic expansions of the probabilities  $p_0(\theta)$  and  $p_1(\theta)$ ,

$$p_0(\theta) \approx 1 - \xi_A(\theta) e^{-\theta}$$
, and  $p_1(\theta) \approx \xi_A(\theta) e^{-\theta}$  (188)

respectively, for some constant  $\mathcal{A}\in\left]0,1\right]$  and  $\xi_{\mathcal{A}}\left(\theta\right)\approx\mathcal{A}e^{-\theta}$ . Note that the functional form of the probabilities in Eq. (188) obtained from our approximate information geometric analysis based upon the integration of the geodesic equation is consistent with that proposed in Eq. (178). Such probabilities seem to suggest a kind of critically damped quantum search and, in terms of the standard damped harmonic oscillator solution in Eq. (184), they would be linked to the case  $b^2 = 4k$  (critically damped motion). This is a quite intriguing finding that would deserve further investigation. Indeed, observe that it is known that dissipation can be used in a constructive manner in quantum search problems [126, 132]. For instance, in Ref. [126] it was shown that introducing dissipation into Grover's original quantum search algorithm has positive effects because it leads to a more robust search where the results oscillating between target and non-target items can be damped out. This is exactly what our approximate analysis seems to suggest. At this juncture, we remark in earnest that there are several aspects of our investigation in need of deeper understanding. For instance, take into consideration the phase factor  $e^{ic\phi(x)}$  that characterizes the wave function  $\psi(x) \stackrel{\text{def}}{=} \sqrt{p(x)}e^{ic\phi(x)}$  of a quantum state with  $p(x) \stackrel{\text{def}}{=} |\psi(x)|^2$  being a well-defined probability distribution. The role played by this factor in the differential geometric formulation of the quantum mechanical evolution of pure states needs to be further clarified since, for instance, the phase appears in the Fubini-Study metric. A full understanding based upon a more rigorous analysis of the role of the phase factor together with the monotonic decreasing behavior of dissipative quantum mechanical systems within their information geometric characterization requires further study and we leave it to future investigations. Once this analysis is completed, it will be interesting to investigate the manner in which different types of search algorithms manifest themselves from a fully quantum information geometric standpoint. This last consideration seems to be especially relevant due to the fact that, within the adiabatic quantum search framework [133], there exist algorithms that are fixed-point but lack the Grover-like scaling, some are not fixed-point but exhibit the Grover-like scaling, and some possess both features.

#### VIII. FINAL REMARKS

In this article, we used methods of geometric algebra and information geometry to enhance the algebraic efficiency and the geometrical significance of the digital and analog representations of Grover's algorithm, respectively. A summary of our main findings is presented below.

## A. Summary of results

- Our analysis seems to confirm that the mathematical methods of GA and IG cannot replace the physical intuition of the quantum algorithm developer. However, GA is an excellent tool for assisting in the comprehension of the algorithmic steps by mimicking them once these have been already uncovered somehow (this is the real piece of art) by the developer. IG, in turn, seems to yield very interesting insights. It provides fresh perspectives (its action is not limited to mimicking) and does provide alternative intermediate algorithmic steps that can lead to improvements with respect to the original algorithm. Finally, its statistical nature, leads naturally to considerations of thermodynamical nature which are essential in actual physical implementations of any quantum computational software running on quantum hardware.
- In reexamining the standard mathematical steps that specify Grover's algorithm, we uncovered and fixed a typographical error that appears in [54] that concerns the inversion about the mean operator. This result appears in Eq. (21) and it is derived in detail in Eq. (A5) located in Appendix A.
- Using the GA language, we presented an elegant characterization of the Grover iterate in terms of a multivector in the reduced even subalgebra  $\left[\mathfrak{cl}^+(3)\right]^n/E_n$ . In particular, the power of GA in handling reflections and rotations was emphasized. These results are reported in Eqs. (73), (78), and (81). In addition, the quadratic speedup relation was recovered in simple GA terms and appears in Eq. (85). Details on the GA of physical space, spacetime, quantum states and quantum operators are featured in Appendix B.
- Quantum phenomena are generally observed only in carefully prepared experiments in a very refined laboratory, not in a *complex* Hilbert space. Within GA, quantum states and quantum operators become united being elements of the same real space  $\left[\mathfrak{cl}^+(3)\right]^n/E_n$ . This is an important conceptual unifying feature of GA that, we argued, finds some support also in some experimental settings: *unary* representation of the implementation of Grover's algorithm with large nuclear spins in semiconductors [79, 80], and quantum computing with holograms

[82, 83].

- We showed that GA helps to clarify the digital-to-analog transition descriptions of quantum computational software. Specifically, we demonstrated that from a GA perspective, the Fenner iterate can be described in terms of the continuos-time Grover multivector in  $\left[\mathfrak{cl}^+(3)\right]^n/E_n$  which, in turn, is essentially a rotation by  $2\theta$  about the  $e_2$  axis. This finding is reported in Eqs. (106) and (109). For the sake of clarity, we recall that the angle  $\theta$  equals  $\sin^{-1}\left[\langle \bar{x}|\psi\rangle\right] = \sin^{-1}\left[N^{-1/2}\right]$ , while  $e_2$  is a grade-1 multivector (that is, a vector) that belongs to the Pauli algebra  $\mathfrak{cl}(3)$  (for further details, see Appendix B).
- Considering the continuous-time description of Grover's algorithm, we showed that the quantum search problem reduces to finding optimal geodesic paths that minimize lengths on a manifold of pure density matrices with a metric structure defined by the Wigner-Yanase metric tensor in Eq. (115). This result is reported in Eq. (141).
- We discussed the dissipationless nature of Grover's quantum search algorithm from an IG perspective. Specifically, we computed the Fisher information function and uncovered that it is constant (see Eq. (127)). Then, discussing the role of the Fisher information function in statistical mechanics (see Eq. (135)) and showing its connection to a generalized version of mechanical kinetic energy (see Eq. (129)), we concluded that the transport along selected geodesic paths from the initial state toward the target state occurs without heat-like generation. Further details on the Fisher information function and the mechanical kinetic energy were confined to Appendix D and Appendix E.
- The quadratic speedup behavior was recovered in pure information geometric terms and with an arbitrary unitary operation replacing the Walsh-Hadamard operation that appears in the original digital version of the quantum search problem as discussed by Grover in [11]. This finding is reported in Eq. (161).
- A GA description of the sequence of nested rotations defined in terms of generalized reflection operators that appear in Grover's fixed-point quantum search algorithm was presented. This finding appears in Eq. (176). We also provided an approximate IG characterization of the dissipative nature of the fixed-point quantum search. In particular, we have shown that the algorithm seems to be characterized by probabilities evolving according to a damped-like harmonic oscillator type of motion. Finally, the monotonic convergence behavior toward the target item as a consequence of the monotonic decrease of the Fisher information is briefly addressed. Eqs. (185) and (188) summarize such insights in a more quantitative fashion.

## B. Limitations, improvements, and future investigations

It is certainly a nontrivial task to cover in a satisfactory manner so many different fields (quantum computing, geometric algebra, information geometry), provide a unifying picture of a specific problem (quantum computational software), and try to maintain some minimum link with physical implementations occurring in laboratories. This article has been written so as to reach as many readers (applied mathematicians, computer scientists, geometers, quantum information theorists, statistical physicists) as possible. However, despite the massive effort on the author's part, this work still remains preliminary in nature. In any case, we think the relevance of this analysis is twofold. First, there is a tutorial component. We presented a novel joint application of special mathematical methods in the field of quantum computing. This may inspire experts in geometric algebra and information geometry to seek new applications for their theoretical methods within the field of quantum information science. Second, there is research component. The effort of recasting and analyzing in detail a known algorithm using mathematical methods that emphasize its interpretation (geometry) and power (algebra) will hopefully assist scientists in searching for new quantum algorithms. We think that our hybrid geometrization of Grover's search algorithm does enhance our intuition and visualization of the art of quantum algorithm design. This, in turn, might help mitigating the non-triviality of designing quantum algorithms. After all, this was also one of the hopes expressed by Nielsen and collaborators [8]. Possible future investigations can be outlined as follows.

- First, it might be interesting to use GA and IG to explore departures from the original set of working hypotheses that characterize Grover's quantum search algorithm: from a unique to multiple targets, from a uniform to an arbitrary initial amplitude distribution, from a flat superposition to an entangled superposition for the initial state, from a power of two to an arbitrary dimensionality of the search space. Given the enhanced algebraic efficiency and the strengthened geometrical intuition provided by GA and IG, this type of work would be useful for checking in a faster manner the consequences of various modifications to the algorithm. Furthermore, since GA and IG provide different mathematical structures, they may suggest different types of variations that may lead unexpectedly to searching for new and yet unknown quantum algorithms. We leave such a psychological excitement to future investigations.
- Second, inspired in part by our works on quantum error correction with both qubits and qudits [4–6], we hope that the work presented here paves the way to a new application of GA extended to quantum search with qudits (higher-dimensional spin systems) [134]. In addition to pure theoretical motivations, we expect this line

of research to be especially relevant for enhancing our comprehension of the connection between theory and experiment and, more specifically, the connection between different experimental implementations of quantum search algorithms with ordinary two-dimensional spin systems and higher-dimensional spin systems [79].

- Third, motivated by our thermodynamical analysis of information transfer in complex systems [135] and by our works on entropic investigations of quantum error correction in the presence of imperfections [136, 137], we hope that the work presented here paves the way to a thorough thermodynamic analysis of information geometric nature applied to computational software used for search problems in quantum computing. We expect this type of work to be especially important for finding optimal algorithms where the thermodynamically-based concept of optimality has a physical meaning directly related to the actual experimental realization of the algorithm itself. As mentioned earlier, we are confident that this line of research will further advance our understanding of the nontrivial connection between experiment and theory in quantum computing.
- Fourth, given the highly debated role of entanglement in quantum search [50–53, 138] and following the previously proposed (experimentally testable) measure of entanglement between two quantum states described by density matrices from a statistical point of view [139, 140], it would be intriguing to investigate the role of entanglement in the quantum search problem recast into information geometric terms.

In conclusion, we hope that our work will have the attention of other scientists with cross-disciplinary interests and will lead to both technologically feasible and experimentally testable new significant advances in quantum computing guided by physical intuition combined with powerful mathematical tools.

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## Appendix A: Inversion about the mean operator

In this Appendix, we wish to show that the action of the operator  $2|\psi\rangle\langle\psi|-I_{\mathcal{H}_2^n}$  that appears in Eq. (18) on an arbitrary vector  $|\phi\rangle$  in  $\mathcal{H}_2^n$ ,

$$|\phi\rangle = \sum_{x=0}^{N-1} \alpha_x |x\rangle, \tag{A1}$$

with  $\alpha_x \in \mathbb{C}$  for any  $x \in \mathcal{X}$  is given by,

$$(2|\psi\rangle\langle\psi| - I_{\mathcal{H}_2^n})|\phi\rangle = \sum_{x=0}^{N-1} (2\mu_\alpha - \alpha_x)|x\rangle, \tag{A2}$$

where  $\mu_{\alpha}$  is the mean of the amplitudes defined as,

$$\mu_{\alpha} \stackrel{\text{def}}{=} \frac{1}{N} \sum_{x=0}^{N-1} \alpha_x. \tag{A3}$$

Recall that  $2\left|\psi\right\rangle\left\langle\psi\right|-I_{\mathcal{H}_{2}^{n}}=H^{\otimes n}U_{\bar{x}=0}H^{\otimes n},$  therefore

$$(2 |\psi\rangle \langle \psi| - I_{\mathcal{H}_{2}^{n}}) |\phi\rangle = (H^{\otimes n}U_{\bar{x}=0}H^{\otimes n}) \left( \sum_{x=0}^{N-1} \alpha_{x} |x\rangle \right)$$

$$= H^{\otimes n}U_{\bar{x}=0} \left( \frac{1}{\sqrt{N}} \sum_{x=0}^{N-1} \alpha_{x} \sum_{y=0}^{N-1} (-1)^{xy} |y\rangle \right)$$

$$= \frac{1}{\sqrt{N}} H^{\otimes n} \left( \sum_{x,y=0}^{N-1} (-1)^{xy} \alpha_{x} U_{\bar{x}=0} |y\rangle \right)$$

$$= \frac{1}{\sqrt{N}} H^{\otimes n} \left[ \sum_{x=0}^{N-1} \alpha_{x} \sum_{y=0} (-1)^{xy} U_{\bar{x}=0} |y\rangle + \sum_{x=0}^{N-1} \alpha_{x} \sum_{y=1}^{N-1} (-1)^{xy} U_{\bar{x}=0} |y\rangle \right]$$

$$= \frac{1}{\sqrt{N}} H^{\otimes n} \left[ \sum_{x=0}^{N-1} \alpha_{x} |0\rangle - \sum_{x=0}^{N-1} \sum_{y=1}^{N-1} (-1)^{xy} \alpha_{x} |y\rangle \right]$$

$$= \frac{1}{\sqrt{N}} \sum_{x=0}^{N-1} \alpha_{x} H^{\otimes n} |0\rangle - \frac{1}{\sqrt{N}} \sum_{x=0}^{N-1} \sum_{y=1}^{N-1} (-1)^{xy} \alpha_{x} H^{\otimes n} |y\rangle$$

$$= \frac{1}{\sqrt{N}} \sum_{x=0}^{N-1} \alpha_{x} H^{\otimes n} |0\rangle - \frac{1}{\sqrt{N}} \sum_{x=0}^{N-1} \sum_{y=1}^{N-1} (-1)^{xy} \alpha_{x} H^{\otimes n} |y\rangle$$

$$= \sum_{x=0}^{N-1} \mu_{\alpha} |x\rangle - \frac{1}{\sqrt{N}} \left[ \sqrt{N} \sum_{x=0}^{N-1} \alpha_{x} |x\rangle - \left( \sum_{x=0}^{N-1} \alpha_{x} \right) (H |0\rangle) \right]$$

$$= \sum_{x=0}^{N-1} \mu_{\alpha} |x\rangle + \frac{1}{\sqrt{N}} \sum_{x=0}^{N-1} \alpha_{x} H |0\rangle - \sum_{x=0}^{N-1} \alpha_{x} |x\rangle$$

$$= \sum_{x=0}^{N-1} \mu_{\alpha} |x\rangle + \sum_{x=0}^{N-1} \mu_{\alpha} |x\rangle - \sum_{x=0}^{N-1} \alpha_{x} |x\rangle$$

$$= \sum_{x=0}^{N-1} \mu_{\alpha} |x\rangle + \sum_{x=0}^{N-1} \mu_{\alpha} |x\rangle - \sum_{x=0}^{N-1} \alpha_{x} |x\rangle$$

$$= \sum_{x=0}^{N-1} \mu_{\alpha} |x\rangle + \sum_{x=0}^{N-1} \mu_{\alpha} |x\rangle - \sum_{x=0}^{N-1} \alpha_{x} |x\rangle$$

$$= \sum_{x=0}^{N-1} \mu_{\alpha} |x\rangle + \sum_{x=0}^{N-1} \mu_{\alpha} |x\rangle - \sum_{x=0}^{N-1} \alpha_{x} |x\rangle$$

$$= \sum_{x=0}^{N-1} \mu_{\alpha} |x\rangle + \sum_{x=0}^{N-1} \mu_{\alpha} |x\rangle - \sum_{x=0}^{N-1} \alpha_{x} |x\rangle$$

$$= \sum_{x=0}^{N-1} (2\mu_{\alpha} - \alpha_{x}) |x\rangle, \tag{A4}$$

that is,

$$(2|\psi\rangle\langle\psi| - I_{\mathcal{H}_2^n})|\phi\rangle = \sum_{x=0}^{N-1} (2\mu_\alpha - \alpha_x)|x\rangle.$$
(A5)

Note that the expression xy in Eq. (A4) with x and y in  $\{0,1\}^n$  denotes the bitwise inner product of x and y, modulo 2. The possibility of reducing to modulo 2 is due to the fact that  $(-1)^2 = 1$ . Furthermore, for the sake of clarity, we point out that for n = 2 and N = 4 we have that  $\mathcal{X} \stackrel{\text{def}}{=} \{0, 1, 2, 3\}$  with  $x = 0 \leftrightarrow 00$ ,  $x = 1 \leftrightarrow 01$ ,  $x = 2 \leftrightarrow 10$ , and  $x = 3 \leftrightarrow 11$ .

## Appendix B: Elements of geometric algebra

In this Appendix, we introduce basic elements of GA of physical space and spacetime [19]. These two geometric algebras shall be denoted as  $\mathfrak{cl}(3)$  and  $\mathfrak{cl}(1,3)$ , respectively. Finally, we briefly present the GA formalism for quantum states and quantum operators.

### 1. Physical space

The key idea in GA is that of uniting the inner and outer products into a single product, namely the *geometric* product. This product is associative and invertible. Consider two three-dimensional vectors a and b. The geometric product between them is defined as,

$$ab \stackrel{\text{def}}{=} a \cdot b + a \wedge b, \tag{B1}$$

where  $a \cdot b$  is a scalar (a 0-grade multivector), while  $a \wedge b = i(a \times b)$  is a bivector (a grade-2 multivector). The quantity i is not the imaginary unit  $i_{\mathbb{C}}$  usually employed in physics and is known as the unit pseudoscalar. Classical physics takes places in the three-dimensional Euclidean space  $\mathbb{R}^3$ . Adding and multiplying vectors generate a geometric algebra denoted  $\mathfrak{cl}(3)$ . The whole algebra can be generated by a right-handed set of orthonormal vectors  $\{e_1, e_2, e_3\}$  fulfilling the relation,

$$e_l e_m = e_l \cdot e_m + e_l \wedge e_m = \delta_{lm} + \varepsilon_{lmk} i e_k, \tag{B2}$$

where i is the above-mentioned unit three-dimensional pseudoscalar,

$$i \equiv i_{\mathfrak{cl}(3)} \stackrel{\text{def}}{=} e_1 e_2 e_3.$$
 (B3)

We point out that Eq. (B2) exhibits the same algebraic relations as Pauli's  $\sigma$ -matrices. Indeed, the Pauli matrices constitute a representation of the Clifford algebra  $\mathfrak{cl}(3)$ , also called the Pauli algebra. The GA of physical space  $\mathfrak{cl}(3)$  is generated by a scalar, three vectors, three bivectors (area elements) and a trivector (volume element). Therefore,  $\mathfrak{cl}(3)$  is a eight-dimensional linear space,

$$\dim_{\mathbb{R}} \left[ \mathfrak{cl}(3) \right] = \sum_{k=0}^{3} \dim \left[ \mathfrak{cl}^{(k)}(3) \right] = \sum_{k=0}^{3} \binom{3}{k} = 2^{3} = 8$$
 (B4)

where  $\mathfrak{cl}^{(k)}(3)$  are the  $\binom{3}{k}$ -dimensional subspaces of  $\mathfrak{cl}(3)$  spanned by the grade-k multivectors in the algebra. A basis set  $\mathcal{B}_{\mathfrak{cl}(3)}$  of  $\mathfrak{cl}(3)$  is,

$$\mathcal{B}_{\mathfrak{cl}(3)} \stackrel{\text{def}}{=} \{1; e_1, e_2, e_3; e_1e_2, e_2e_3, e_3e_1; e_1e_2e_3\}.$$
 (B5)

An arbitrary multivector  $M \in \mathfrak{cl}(3)$  can be decomposed as,

$$M = \sum_{k=0}^{3} \langle M \rangle_k = \langle M \rangle_0 + \langle M \rangle_1 + \langle M \rangle_2 + \langle M \rangle_3$$
$$= \alpha + a + ib + i\beta = \text{scalar} + \text{vector} + \text{bivector} + \text{trivector}. \tag{B6}$$

The quantities  $\alpha$  and  $\beta$  in Eq. (B6) are real scalars while  $a = a \cdot e^k e_k$  and  $b = b \cdot e^k e_k$  are vectors. The quantity  $\langle M \rangle_k$  is the grade-k multivectorial part of the nonhomogeneous multivector  $M \in \mathfrak{cl}(3)$ . The unit pseudoscalar i is uniquely generated by the frame  $\{e_1, e_2, e_3\}$  and it represents an oriented unit volume. Furthermore, it is such that

$$i^2 = -1$$
,  $iM = Mi \quad \forall M \in \mathfrak{cl}(3)$ , and  $i^{\dagger} = -i$ . (B7)

The symbol  $\dagger$  in Eq. (B7) is called *reversion or Hermitian adjoint*. Within the Pauli algebra the operation of reversion plays the role of complex conjugation in  $\mathbb{C}$ . For further details, we refer to [19].

#### 2. Spacetime

The spacetime algebra  $\mathfrak{cl}(1,3)$  is the GA of Minkowski spacetime. It is generated by four orthogonal basis vectors  $\{\gamma_{\mu}\}_{\mu=0,1,2,3}$  satisfying the relations

$$\gamma_{\mu} \cdot \gamma_{\nu} = \frac{1}{2} \left( \gamma_{\mu} \gamma_{\nu} + \gamma_{\nu} \gamma_{\mu} \right) = \operatorname{diag}(+ - - -), \tag{B8}$$

and,

$$\gamma_{\mu} \wedge \gamma_{\nu} = \frac{1}{2} \left( \gamma_{\mu} \gamma_{\nu} - \gamma_{\nu} \gamma_{\mu} \right), \tag{B9}$$

with  $\mu$ ,  $\nu \in \{0, 1, 2, 3\}$ . We note that Eqs. (B8) and (B9) exhibit the same algebraic relations as Dirac's  $\gamma$ -matrices. Indeed, the Dirac matrices constitute a representation of the spacetime algebra  $\mathfrak{cl}(1,3)$ . From Eqs. (B8) and (B9), it is straightforward to verify that

$$\gamma_0^2 = 1, \, \gamma_0 \cdot \gamma_i = 0, \, \text{and} \, \gamma_i \cdot \gamma_j = -\delta_{ij},$$
(B10)

with  $i, j \in \{1, 2, 3\}$ . The spacetime Clifford algebra  $\mathfrak{cl}(1, 3)$  is a sixteen-dimensional linear space and a suitable basis  $\mathcal{B}_{\mathfrak{cl}(1,3)}$  is given by,

$$\mathcal{B}_{\mathfrak{cl}(1,3)} \stackrel{\text{def}}{=} \{1, \gamma_{\mu}, \gamma_{\mu} \wedge \gamma_{\nu}, i\gamma_{\mu}, i\},$$
(B11)

whose elements represent scalars, vectors, bivectors, trivectors and pseudoscalars, respectively. A general multivector  $M \in \mathfrak{cl}(1,3)$  can be decomposed as

$$M = \sum_{k=0}^{4} \langle M \rangle_k = \alpha + a + B + ib + i\beta, \tag{B12}$$

where  $\alpha$  and  $\beta$  are real scalars, a and b are real spacetime vectors and B is a bivector. A general spacetime vector  $a \in \mathfrak{cl}(1,3)$  can be written as

$$a = a^{\mu} \gamma_{\mu}, \tag{B13}$$

with  $\mu \in \{0, 1, 2, 3\}$ . By selecting  $\gamma_0$  as the future-pointing timelike unit vector, the  $\gamma_0$ -vector determines a map between spacetime vectors a and the even subalgebra  $\mathfrak{cl}^+(1,3)$  of the full spacetime algebra  $\mathfrak{cl}(1,3)$  via the relation

$$a\gamma_0 = a_0 + \mathbf{a},\tag{B14}$$

where  $a_0 \stackrel{\text{def}}{=} a \cdot \gamma_0$  and  $\mathbf{a} \stackrel{\text{def}}{=} a \wedge \gamma_0$ . Observe that the ordinary three-dimensional vector  $\mathbf{a} \in \mathfrak{cl}(3)$  becomes a spacetime bivector  $a \wedge \gamma_0$  in  $\mathfrak{cl}(1,3)$ . We remark that the metric structure of the space whose GA is being built reflects the properties of the unit pseudoscalar of the algebra. Indeed, the existence of a pseudoscalar is equivalent to the existence of a metric. In  $\mathfrak{cl}(1,3)$  the unit pseudoscalar is the highest-grade element,

$$i \equiv i_{\mathfrak{cl}(1,3)} \stackrel{\text{def}}{=} \gamma_0 \gamma_1 \gamma_2 \gamma_3,$$
 (B15)

and it represents an oriented unit four-dimensional volume element. Since i in Eq. (B15) can be constructed from a right-handed vector basis by the oriented product  $\gamma_0\gamma_1\gamma_2\gamma_3$ , the corresponding volume element is said to be right-handed. The volume element i has magnitude  $|i| = \langle i^{\dagger}i \rangle_0^{\frac{1}{2}} = 1$ , where  $\langle M \rangle_0$  denotes the 0-grade component of the multivector  $M \in \mathfrak{cl}(1,3)$ . The dagger  $\dagger$  is the reverse or the Hermitian adjoint. For example, given a multivector

 $M=\gamma_2\gamma_3,\ M^\dagger$  is obtained by reversing the order of vectors in the product. That is,  $M^\dagger=\gamma_3\gamma_2=-\gamma_2\gamma_3$ . It is commonly said that i specifies an orientation for spacetime. The pseudoscalar in Eq. (B15) satisfies  $i^2=\pm 1$  with the sign depending on the dimension and the signature of the space whose GA is being taken into consideration. For instance, in spaces of positive definite metric, the pseudoscalar has magnitude |i|=1 while the value of  $i^2$  depends only on the dimension n of space as  $i^2=(-1)^{n(n-1)/2}$ . Therefore in a space of even dimension (like the Minkowski spacetime considered here, n=4), i anticommutes with odd-grade multivectors and commutes with even-grade elements of the algebra,

$$iM = \pm Mi \tag{B16}$$

where the multivector M is even for (+) and odd for (-). For further details, we refer to [19].

## 3. Quantum states and quantum operators

## a. Conceptual ideas

In what follows, we describe the minimum amount of tools necessary to follow our investigation in Sections III, IV, and V. The multiparticle spacetime algebra (MSTA) is the GA of a relativistic configuration space and it is used in geometric algebra to describe states and operators acting upon them. Within this language, complex Hilbert spaces and the imaginary unit  $i_{\mathbb{C}}$  in ordinary quantum mechanics are no longer fundamental. In addition, the ordinary quantum mechanical tensor product which is used to construct both multiparticle states and operators acting upon them and, in addition, to isolate the Hilbert space of different particles, is replaced by the geometric product within the GA language. The unique feature of the MSTA is that it implies a separate copy of the three spatial dimensions for each particle, as well as the time dimension. Specifically, MSTA is the GA of n-particle configuration space which, for relativistic systems, consists of n copies (each copy is a 1-particle space) of Minkowski spacetime. A convenient basis for the MSTA is given by the set  $\{\gamma_{\mu}^a\}$ , where  $\mu \in \{0,1,2,3\}$  labels the spacetime vector and  $a \in \{1,...,n\}$  labels the particle space. These basis vectors  $\gamma_{\mu}^a$  fulfill the orthogonality conditions  $\gamma_{\mu}^a \cdot \gamma_{\nu}^b = \delta^{ab} \eta_{\mu\nu}$  with  $\eta_{\mu\nu} \stackrel{\text{def}}{=} \text{diag}(+, -, -, -)$ . Because of their orthogonality, vectors from different particle spaces anticommute. Recall that,

$$\dim_{\mathbb{R}} \left[ \mathfrak{cl} \left( 1, 3 \right) \right] = 16, \ \dim_{\mathbb{R}} \left[ \mathfrak{cl} \left( 3 \right) \right] = 8, \ \text{and} \ \dim_{\mathbb{R}} \left[ \mathfrak{cl}^+ \left( 3 \right) \right] = 4, \tag{B17}$$

where  $\mathfrak{cl}^+(3)$  is the even subalgebra of  $\mathfrak{cl}(3)$ . A basis for the entire MSTA has  $2^{4n}$  degrees of freedom, that is

$$\dim_{\mathbb{R}} \left[ \mathfrak{cl} \left( 1, 3 \right) \right]^n = 2^{4n}. \tag{B18}$$

In the GA version of nonrelativistic quantum mechanics, a single absolute time identifies all of the individual time coordinates. For each a, this vector is chosen to be  $\gamma_0^a$ . In such a spacetime split, bivectors are used for modelling spatial vectors relative to these timelike vectors. A basis set of relative vectors is then defined by  $e_k^a \stackrel{\text{def}}{=} \gamma_k^a \gamma_0^a$ , with  $k \in \{1, 2, 3\}$  and  $a \in \{1, ..., n\}$ . The set  $\{\sigma_k^a\}$  spans the GA of relative space  $\mathfrak{cl}(3) \cong \mathfrak{cl}^+(1, 3)$  for each particle space. Therefore, each particle space has a basis given by,

$$1, \{e_k\}, \{ie_k\}, i,$$
 (B19)

where, suppressing the particle space indices, the pseudoscalar i is defined as  $i \stackrel{\text{def}}{=} e_1 e_2 e_3$ . Observe that the basis in Eq. (B19) defines the Pauli algebra, that is to say the GA of the three-dimensional physical (Euclidean) space. However, the ordinary three Pauli  $\sigma_k$  are no longer regarded in GA as three matrix-valued components of a single isospace vector, but as three independent basis vectors  $e_k$  for real space. Unlike spacetime basis vectors, relative vectors  $\{e_k^a\}$  from separate particle spaces commute,

$$e_k^a e_j^b = e_j^b e_k^a, \forall a \neq b. \tag{B20}$$

The direct product space of n copies of  $\mathfrak{cl}(3)$  denoted as,

$$[\mathfrak{cl}(3)]^n \stackrel{\text{def}}{=} \mathfrak{cl}(3) \otimes \dots \otimes \mathfrak{cl}(3), \tag{B21}$$

is generated by  $\{e_k^a\}$  with  $k \in \{1, 2, 3\}$  and  $a \in \{1, ..., n\}$ . Within the MSTA setting, 1-particle Pauli spinors are represented as elements of  $\mathfrak{cl}^+(3)$ , the even subalgebra of the Pauli algebra  $\mathfrak{cl}(3)$  spanned by  $\{1, ie_k\}$ . We have,

$$\dim_{\mathbb{R}} \left[ \mathcal{H}_2^1 \right] = 4 = \dim_{\mathbb{R}} \left[ \mathfrak{cl}^+(3) \right]. \tag{B22}$$

We point out that within MSTA, the right multiplication by  $ie_3$  plays the role of the *complex* imaginary unit  $i_{\mathbb{C}}$  in conventional quantum theory. However, in the *n*-particle algebra there are *n*-copies of  $ie_3$ , namely  $ie_3^a$  with  $a \in \{1, ..., n\}$ . Therefore, in order to faithfully reproduce ordinary quantum mechanics, the right-multiplication by all of these  $ie_3^a$  must lead to the same result. This constraint requires that the *n*-particle multivector  $\psi$  must satisfy,

$$\psi i e_3^1 = \psi i e_3^2 = \dots = \psi i e_3^{n-1} = \psi i e_3^n. \tag{B23}$$

The constraint conditions in Eq. (B23) are obtained by introducing the n-particle correlator  $E_n$  defined as,

$$E_n \stackrel{\text{def}}{=} \prod_{b=2}^{n} \frac{1}{2} \left( 1 - ie_3^1 i e_3^b \right), \tag{B24}$$

such that,

$$E_n i e_3^a = E_n i e_3^b = J_n, \, \forall a, b \in \{1, ..., n\}.$$
 (B25)

We remark that despite the fact that  $E_n$  in Eq. (B24) has been defined by correlating all the spaces to the space with a=1, the value of  $E_n$  does not depend on this choice. The quantity  $J_n$  in Eq. (B25) defines the complex structure and is such that  $J_n^2 = -E_n$ . The number of real degrees of freedom is reduced from  $4^n = \dim_{\mathbb{R}} \left[\mathfrak{cl}^+(3)\right]^n$  to the expected  $2^{n+1} = \dim_{\mathbb{R}} \mathcal{H}_2^n$  via right-multiplication by the quantum correlator  $E_n$  which can be regarded as a projection operation. From a physical standpoint, this projection can be interpreted as locking the phases of the various particles together. The reduced even subalgebra space will be denoted by  $\left[\mathfrak{cl}^+(3)\right]^n/E_n$  and is such that,

$$\dim_{\mathbb{R}} \left[ \mathcal{H}_2^n \right] = 2^{n+1} = \dim_{\mathbb{R}} \left\{ \left[ \mathfrak{cl}^+(3) \right]^n / E_n \right\}. \tag{B26}$$

As elements of  $\mathfrak{cl}^+(3)$  represent 1-particle spinors (or, single-qubit states in  $\mathcal{H}_2^1$ ), multivectors belonging to  $\left[\mathfrak{cl}^+(3)\right]^n/E_n$  can be regarded as *n*-particle spinors (or, *n*-qubit states in  $\mathcal{H}_2^n$ ). For further details, we refer to [19, 69].

### b. Practical rules

In what follows, we outline the minimum amount of translation rules from elements of *complex* Hilbert spaces to elements of *real* geometric Clifford algebras needed to follow our investigation. First, the GA analog of a qubit  $|\psi\rangle \in \mathcal{H}_2^1$  is given by,

$$|\psi\rangle = \begin{pmatrix} a^0 + i_{\mathbb{C}}a^3 \\ -a^2 + i_{\mathbb{C}}a^1 \end{pmatrix} \leftrightarrow \psi = a^0 + a^1 i e_1 + a^2 i e_2 + a^3 i e_3,$$
 (B27)

where  $a^0$ ,  $a^1$ ,  $a^2$ , and  $a^3$  are real constants and the multivector  $\psi \in \mathfrak{cl}^+(3)$ . For example,  $|\psi\rangle = \binom{1}{-1}$  becomes  $1 + ie_2$ . For any k = 1, 2, 3, the action of a Pauli operator  $\sigma_k$  on a qubit  $|\psi\rangle$  becomes,

$$\sigma_k |\psi\rangle \leftrightarrow e_k \psi e_3.$$
 (B28)

The multiplication of a qubit  $|\psi\rangle$  by the *complex* imaginary unit  $i_{\mathbb{C}}$  is given by,

$$i_{\mathbb{C}} |\psi\rangle \leftrightarrow \psi i e_3.$$
 (B29)

The complex conjugation  $|\psi\rangle^*$  of a qubit  $|\psi\rangle$  becomes

$$|\psi\rangle^* \leftrightarrow e_2 \psi e_2.$$
 (B30)

The inner product between a qubit  $|\psi\rangle$  and itself is given by,

$$\langle \psi | \psi \rangle \leftrightarrow \langle \psi^{\dagger} \psi \rangle_{0 \text{-grade}} = (a^0)^2 + (a^k)^2.$$
 (B31)

The inner product  $\langle \psi | \phi \rangle$  between two qubits  $| \phi \rangle$  and  $| \psi \rangle$  becomes,

$$\langle \psi | \phi \rangle \leftrightarrow \langle \psi^{\dagger} \phi \rangle_{0\text{-grade}} - \langle \psi^{\dagger} \phi i e_3 \rangle_{0\text{-grade}} i e_3.$$
 (B32)

For example, if  $|\psi\rangle = \binom{1}{i}$  and  $|\phi\rangle = \binom{1}{1}$ , then  $\langle\psi|\phi\rangle = 1 - i_{\mathbb{C}}$  becomes  $1 - ie_3$ . The GA analog of a pure-state density matrix  $\rho_{\text{pure, single-qubit}} = |\psi\rangle\langle\psi|$  with  $|\psi\rangle \in \mathcal{H}_2^1$  is given by,

$$\begin{split} |\psi\rangle \left\langle \psi \right| &\leftrightarrow \rho_{\text{pure, single-qubit}}^{\text{(GA)}} = \psi E_{+}^{1} \psi^{\dagger} \\ &= \psi \frac{1}{2} \left( 1 + e_{3}^{1} \right) \psi^{\dagger} \\ &= \frac{1}{2} \left( 1 + \psi e_{3}^{1} \psi^{\dagger} \right) \\ &= \frac{1}{2} \left( 1 + s \right), \end{split} \tag{B33}$$

where multivectors  $E^1_+$  and s are defined as,

$$E_{+}^{1} \stackrel{\text{def}}{=} \frac{1}{2} \left( 1 + e_{3}^{1} \right) \text{ and, } s \stackrel{\text{def}}{=} \psi e_{3}^{1} \psi^{\dagger},$$
 (B34)

respectively. For example, if  $|\psi\rangle = \binom{1}{-1}$ ,  $|\psi\rangle\langle\psi|$  becomes  $1 - e_1$ . The GA analog of a mixed-state density matrix,

$$\rho_{\text{mixed, single-qubit}} = \sum_{i=1}^{n} p_i |\psi_i\rangle \langle \psi_i|,$$
(B35)

where  $|\psi_i\rangle$  is a normalized single-qubit state, is given by

$$\sum_{i=1}^{n} p_i |\psi_i\rangle \langle \psi_i| \leftrightarrow \rho_{\text{mixed, single-qubit}}^{\text{(GA)}} = \sum_{i=1}^{n} p_i \psi_i E_+^1 \psi_i^{\dagger}, \tag{B36}$$

that is,

$$\rho_{\text{mixed, single-qubit}}^{(GA)} = \sum_{i=1}^{n} p_i \psi_i E_+^1 \psi_i^{\dagger}$$

$$= \sum_{i=1}^{n} p_i \psi_i \left[ \frac{1}{2} \left( 1 + e_3^1 \right) \right] \psi_i^{\dagger}$$

$$= \frac{1}{2} \sum_{i=1}^{n} \left[ \left( p_i + p_i \psi_i e_3^1 \psi_i^{\dagger} \right) \right]$$

$$= \frac{1}{2} \left( 1 + \sum_{i=1}^{n} p_i s_i \right)$$

$$= \frac{1}{2} (1 + S), \tag{B37}$$

where multivectors S and  $s_i$  are defined as,

$$S \stackrel{\text{def}}{=} \sum_{i=1}^{n} p_i s_i \text{ and, } s_i \stackrel{\text{def}}{=} \psi_i e_3^1 \psi_i^{\dagger}, \tag{B38}$$

respectively. For example, if  $p_1 = \frac{1}{4}$ ,  $p_2 = \frac{3}{4}$ ,  $|\psi_1\rangle = \binom{1}{0}$ , and  $|\psi_2\rangle = \binom{0}{1}$ , then  $p_1 |\psi_1\rangle \langle \psi_1| + p_2 |\psi_2\rangle \langle \psi_2|$  becomes  $\frac{1}{2} \left(1 - \frac{1}{2}e_3\right)$ . The GA analog of a mixed-state density matrix,

$$\rho_{\text{mixed, multi-qubit}} = \sum_{i=1}^{n} p_i |\psi_i\rangle \langle \psi_i|, \qquad (B39)$$

where  $|\psi_i\rangle$  is a normalized multi-qubit state, is given by

$$\sum_{i=1}^{n} p_{i} |\psi_{i}\rangle \langle \psi_{i}| \leftrightarrow \rho_{\text{mixed, multi-qubit}}^{\text{(GA)}} = \overline{(\psi E_{n}) E_{+} (\psi E_{n})^{\sim}}, \tag{B40}$$

that is,

$$\rho_{\text{mixed, multi-qubit}}^{(GA)} = \overline{(\psi E_n) E_+ (\psi E_n)^{\sim}} = \sum_{i=1}^n p_i (\psi_i E_n) E_+ (\psi_i E_n)^{\sim}, \tag{B41}$$

where,

$$E_n \stackrel{\text{def}}{=} \prod_{k=2}^n \frac{1}{2} \left( 1 - ie_3^1 i e_3^k \right) \text{ and, } E_+ \stackrel{\text{def}}{=} E_+^1 \dots E_+^n.$$
 (B42)

For any  $l \in \{1, ..., n\}$ ,

$$E_{+}^{l} \stackrel{\text{def}}{=} \frac{1}{2} \left( 1 + e_{3}^{l} \right). \tag{B43}$$

In Eq. (B41), the over-line and tilde symbols denote the ensemble-average and the space-time reversion, respectively. In addition,  $E_n$  is the *n*-particle correlator while  $E_+$  is the geometric product of *n*-idempotents. Finally, consider a quantum state given by,

$$|\psi\rangle \stackrel{\text{def}}{=} |\psi_{i_1}, ..., \psi_{i_n}\rangle \in \mathcal{H}_2^n.$$
 (B44)

The corresponding GA element is given by,

$$\psi \stackrel{\text{def}}{=} \psi_{i_1}^1 \dots \psi_{i_n}^n E_n \in \left[ \mathfrak{cl}^+(3) \right]^n / E_n, \tag{B45}$$

where  $E_n$  is the *n*-particle correlator in Eq. (B42). The superscripts denote which space the multivector belongs to. Observe that vectors from different spaces anticommute since they are orthogonal. Furthermore, bivectors from different spaces commute. We also point out that  $i_{\mathbb{C}} | \psi \rangle \leftrightarrow \psi J_n$ , where  $J_n \stackrel{\text{def}}{=} E_n i e_3^a$ . The index a can be any index in  $\{1,...,n\}$  with  $J_n^2 = -E_n$ ,  $J_n = J_n E_n = E_n J_n$ , and  $E_n^2 = E_n$ . The (non-simple) bivector  $J_n$  defines the *complex* structure in the MSTA. For further technical details, we refer to [19, 66–70].

## Appendix C: The unitary time-evolution operator

In this Appendix, we show the computational steps needed to recover Eqs. (93) and (94). In what follows, we set  $\hbar = 1$ . Observe that,

$$G(t) = e^{-icH_{\text{Fenner}}t}$$

$$= e^{\frac{2\beta}{\sqrt{N}}\sigma_z\sigma_x t}$$

$$= \sum_{k=0}^{+\infty} \frac{1}{k!} \left(\frac{2\beta}{\sqrt{N}}\sigma_z\sigma_x t\right)^k$$

$$= I + \frac{2\beta}{\sqrt{N}}\sigma_z\sigma_x t + \left(\frac{2\beta}{\sqrt{N}}\sigma_z\sigma_x\right)^2 \frac{t^2}{2!} + \left(\frac{2\beta}{\sqrt{N}}\sigma_z\sigma_x\right)^3 \frac{t^3}{3!}$$

$$+ \left(\frac{2\beta}{\sqrt{N}}\sigma_z\sigma_x\right)^4 \frac{t^4}{4!} + \left(\frac{2\beta}{\sqrt{N}}\sigma_z\sigma_x\right)^5 \frac{t^5}{5!} + \dots$$

$$= I + \frac{2\beta}{\sqrt{N}} (\sigma_z\sigma_x)t + \left(\frac{2\beta}{\sqrt{N}}\right)^2 (\sigma_z\sigma_x)^2 \frac{t^2}{2!} + \left(\frac{2\beta}{\sqrt{N}}\right)^3 (\sigma_z\sigma_x)^3 \frac{t^3}{3!}$$

$$+ \left(\frac{2\beta}{\sqrt{N}}\right)^4 (\sigma_z\sigma_x)^4 \frac{t^4}{4!} + \left(\frac{2\beta}{\sqrt{N}}\right)^5 (\sigma_z\sigma_x)^5 \frac{t^5}{5!} + \dots$$

$$= I + \frac{2\beta}{\sqrt{N}} (\sigma_z\sigma_x)t - \left(\frac{2\beta}{\sqrt{N}}\right)^2 \frac{t^2}{2!} - \left(\frac{2\beta}{\sqrt{N}}\right)^3 (\sigma_z\sigma_x) \frac{t^3}{3!}$$

$$+ \left(\frac{2\beta}{\sqrt{N}}\right)^4 \frac{t^4}{4!} + \left(\frac{2\beta}{\sqrt{N}}\right)^5 (\sigma_z\sigma_x) \frac{t^5}{5!} + \dots$$

$$= \left[1 - \left(\frac{2\beta}{\sqrt{N}}\right)^2 \frac{t^2}{2!} + \left(\frac{2\beta}{\sqrt{N}}\right)^4 \frac{t^4}{4!} + \dots\right] I_{2\times 2}$$

$$+ \left[\frac{2\beta}{\sqrt{N}}t - \left(\frac{2\beta}{\sqrt{N}}\right)^3 \frac{t^3}{3!} + \left(\frac{2\beta}{\sqrt{N}}\right)^5 \frac{t^5}{5!} + \dots\right] \sigma_z\sigma_x$$

$$= \cos\left(\frac{2\beta}{\sqrt{N}}t\right) I_{2\times 2} + \sin\left(\frac{2\beta}{\sqrt{N}}t\right) \sigma_z\sigma_x, \tag{C1}$$

that is, finally

$$G(t) = e^{-i_{\mathbb{C}}H_{\text{Fenner}}t} = \cos\left(\frac{2\beta}{\sqrt{N}}t\right)I_{2\times 2} + \sin\left(\frac{2\beta}{\sqrt{N}}t\right)\sigma_z\sigma_x. \tag{C2}$$

Eq. (C2) is equivalent to Eq. (93). Furthermore, the time-dependent quantum state  $|\psi(t)\rangle \stackrel{\text{def}}{=} G(t) |\psi\rangle$  becomes,

$$|\psi(t)\rangle = G(t) |\psi\rangle$$

$$= \cos\left(\frac{2\beta}{\sqrt{N}}t\right) |\psi\rangle + \sin\left(\frac{2\beta}{\sqrt{N}}t\right) \sigma_{z}\sigma_{x} |\psi\rangle$$

$$= \cos\left(\frac{2\beta}{\sqrt{N}}t\right) |\psi\rangle + \sin\left(\frac{2\beta}{\sqrt{N}}t\right) \sigma_{z}\sigma_{x} (\alpha |\bar{x}\rangle + \beta |\psi_{\text{bad}}\rangle)$$

$$= \cos\left(\frac{2\beta}{\sqrt{N}}t\right) |\psi\rangle + \sin\left(\frac{2\beta}{\sqrt{N}}t\right) (\beta |\bar{x}\rangle - \alpha |\psi_{\text{bad}}\rangle)$$

$$= \cos\left(\frac{2\beta}{\sqrt{N}}t\right) |\psi\rangle + \sin\left(\frac{2\beta}{\sqrt{N}}t\right) \left\{\beta |\bar{x}\rangle - \alpha \left[\frac{1}{\beta} (|\psi\rangle - \alpha |\bar{x}\rangle)\right]\right\}$$

$$= \cos\left(\frac{2\beta}{\sqrt{N}}t\right) |\psi\rangle + \beta \sin\left(\frac{2\beta}{\sqrt{N}}t\right) |\bar{x}\rangle - \frac{\alpha}{\beta} \sin\left(\frac{2\beta}{\sqrt{N}}t\right) |\psi\rangle + \frac{\alpha^{2}}{\beta} \sin\left(\frac{2\beta}{\sqrt{N}}t\right) |\bar{x}\rangle$$

$$= \left[\cos\left(\frac{2\beta}{\sqrt{N}}t\right) - \frac{\alpha}{\beta} \sin\left(\frac{2\beta}{\sqrt{N}}t\right)\right] |\psi\rangle + \frac{1}{\beta} \sin\left(\frac{2\beta}{\sqrt{N}}t\right) |\bar{x}\rangle, \tag{C3}$$

that is,

$$|\psi(t)\rangle = \left[\cos\left(\frac{2\beta}{\sqrt{N}}t\right) - \frac{\alpha}{\beta}\sin\left(\frac{2\beta}{\sqrt{N}}t\right)\right]|\psi\rangle + \frac{1}{\beta}\sin\left(\frac{2\beta}{\sqrt{N}}t\right)|\bar{x}\rangle.$$
 (C4)

Eq. (C4) is equivalent to Eq. (94). As a consistency check, note that

$$\langle \psi(t) | \psi(t) \rangle = \left[ \cos(x) - \frac{\alpha}{\beta} \sin(x) \right]^2 + \left[ \frac{1}{\beta} \sin(x) \right]^2 + \frac{2\alpha}{\beta} \sin(x) \left[ \cos(x) - \frac{\alpha}{\beta} \sin(x) \right] = 1, \tag{C5}$$

where  $x \stackrel{\text{def}}{=} \frac{2\beta}{\sqrt{N}} t$ , and  $\alpha = \langle \bar{x} | \psi \rangle = \langle \psi | \bar{x} \rangle$ .

# Appendix D: On the Fisher information

In this Appendix, we discuss the meaning of the Fisher information function from both an information-theoretical and statistical mechanical standpoints.

# 1. Information Theory

Let us recall that the Fisher information  $\mathcal{F}(\theta)$  is a measure of the amount of information that an observable random variable X carries about an unknown parameter  $\theta$  upon which the probability  $p(x|\theta) = p_{\theta}(x)$  depends and is defined as,

$$\mathcal{F}(\theta) \stackrel{\text{def}}{=} \left\langle \left( \frac{\partial \log p(x|\theta)}{\partial \theta} \right)^2 \right\rangle = \int p(x|\theta) \left( \frac{\partial \log p(x|\theta)}{\partial \theta} \right)^2 dx. \tag{D1}$$

In what follows, we assume to consider continuous random variables. The probability  $p(x|\theta)$  is known as the likelihood function while the quantity  $\partial_{\theta} \log p(x|\theta)$  with  $\partial_{\theta} \stackrel{\text{def}}{=} \frac{\partial}{\partial \theta}$  is known as the score. Observe that the expectation value of the score is zero. Indeed, from the normalization condition

$$\int p(x|\theta) dx = 1, \tag{D2}$$

it follows that,

$$\frac{\partial}{\partial \theta} \left( \int p(x|\theta) \, dx \right) = 0. \tag{D3}$$

After some simple algebra, we find

$$\frac{\partial \log p(x|\theta)}{\partial \theta} = \frac{1}{p(x|\theta)} \frac{\partial p(x|\theta)}{\partial \theta}.$$
 (D4)

Using Eqs. (D3) and (D4), in the working hypothesis that differentiation and integration can be interchanged, we obtain

$$\langle \partial_{\theta} \log p(x|\theta) \rangle = 0. \tag{D5}$$

Therefore, from Eqs. (D1) and (D5), we conclude that the Fisher information  $\mathcal{F}(\theta)$  can be regarded as the variance of the score function. From an information-theoretic standpoint it is convenient to observe that the Fisher information can also be viewed as the negative of the expectation value of the second derivative with respect to  $\theta$  of  $\log p(x|\theta)$ ,

$$\mathcal{F}(\theta) = -\left\langle \frac{\partial^2 \log p(x|\theta)}{\partial \theta^2} \right\rangle. \tag{D6}$$

Indeed, note that

$$-\left\langle \frac{\partial^{2} \log p(x|\theta)}{\partial \theta^{2}} \right\rangle = -\int p(x|\theta) \frac{\partial^{2} \log p(x|\theta)}{\partial \theta} dx$$

$$= -\int p(x|\theta) \frac{\partial}{\partial \theta} \left[ \frac{\partial \log p(x|\theta)}{\partial \theta} \right] dx$$

$$= -\int p(x|\theta) \frac{\partial}{\partial \theta} \left[ \frac{1}{p(x|\theta)} \frac{\partial p(x|\theta)}{\partial \theta} \right] dx$$

$$= -\int p(x|\theta) \left[ \frac{\partial}{\partial \theta} \left( \frac{1}{p(x|\theta)} \right) \frac{\partial p(x|\theta)}{\partial \theta} + \frac{1}{p(x|\theta)} \frac{\partial^{2} p(x|\theta)}{\partial \theta^{2}} \right] dx$$

$$= -\int p(x|\theta) \left[ -\frac{1}{p^{2}(x|\theta)} \left( \frac{\partial p(x|\theta)}{\partial \theta} \right)^{2} + \frac{1}{p(x|\theta)} \frac{\partial^{2} p(x|\theta)}{\partial \theta^{2}} \right] dx$$

$$= \int \frac{1}{p(x|\theta)} \left( \frac{\partial p(x|\theta)}{\partial \theta} \right)^{2} dx - \int \frac{\partial^{2} p(x|\theta)}{\partial \theta^{2}} dx$$

$$= \int \frac{1}{p(x|\theta)} p^{2}(x|\theta) \left( \frac{\partial \log p(x|\theta)}{\partial \theta} \right)^{2} dx - \frac{\partial^{2}}{\partial \theta^{2}} \int p(x|\theta) dx$$

$$= \int p(x|\theta) \left( \frac{\partial \log p(x|\theta)}{\partial \theta} \right)^{2} dx$$

$$= \mathcal{F}(\theta). \tag{D7}$$

This concludes the explicit verification.

## 2. Statistical Mechanics

Let us evaluate the Fisher information  $\mathcal{F}(\theta)$  for a thermodynamical system at equilibrium with probability  $p(x|\theta)$  given by,

$$p(x|\theta) = \frac{e^{-\beta E(x,\theta)}}{\mathcal{Z}(\theta)},\tag{D8}$$

where  $\beta \stackrel{\text{def}}{=} \left(k_B T\right)^{-1}$  and  $\mathcal{Z}\left(\theta\right)$  denotes the partition function of the system defined as,

$$\mathcal{Z}(\theta) \stackrel{\text{def}}{=} \int e^{-\beta E(x,\theta)} dx. \tag{D9}$$

In terms of the free energy  $F(\theta)$ , the partition function  $\mathcal{Z}(\theta)$  becomes

$$\mathcal{Z}(\theta) = e^{-\beta F(\theta)},\tag{D10}$$

that is,

$$F(\theta) \stackrel{\text{def}}{=} -k_B T \log \left[ \mathcal{Z}(\theta) \right] \tag{D11}$$

Using Eqs. (D8) and (D11), the probability  $p(x|\theta)$  can be rewritten as

$$p(x|\theta) = e^{\beta F(\theta) - \beta E(x,\theta)}.$$
 (D12)

Substituting Eq. (D12) into Eq. (D1), after some algebra, the Fisher information function becomes

$$\mathcal{F}(\theta) = \beta^2 \left\langle \left( \frac{\partial F}{\partial \theta} - \frac{\partial E}{\partial \theta} \right)^2 \right\rangle. \tag{D13}$$

To further simplify Eq. (D13), let us rewrite  $\partial F/\partial \theta$  in a convenient manner. From Eqs. (D9) and (D11), we obtain

$$\frac{\partial F}{\partial \theta} = -k_B T \frac{\partial}{\partial \theta} \left\{ \log \left[ \int e^{-\beta E(x,\theta)} dx \right] \right\} 
= -k_B T \frac{\partial}{\partial \theta} \left[ \int e^{-\beta E(x,\theta)} dx \right] 
\int e^{-\beta E(x,\theta)} dx 
= -k_B T \frac{\int \left( -\beta \frac{\partial E}{\partial \theta} \right) e^{-\beta E(x,\theta)} dx}{\int e^{-\beta E(x,\theta)} dx} 
= \int \frac{\partial E}{\partial \theta} \left( \frac{e^{-\beta E(x,\theta)}}{\int e^{-\beta E(x,\theta)} dx} \right) dx 
= \int \frac{\partial E}{\partial \theta} p(x|\theta) dx 
= \left\langle \frac{\partial E}{\partial \theta} \right\rangle, \tag{D14}$$

that is,

$$\frac{\partial F}{\partial \theta} = \left\langle \frac{\partial E}{\partial \theta} \right\rangle. \tag{D15}$$

Combining Eqs. (D13) and (D15), the Fisher information  $\mathcal{F}(\theta)$  becomes

$$\mathcal{F}(\theta) = \beta^2 \left\langle \left( \left\langle \frac{\partial E}{\partial \theta} \right\rangle - \frac{\partial E}{\partial \theta} \right)^2 \right\rangle. \tag{D16}$$

Eq. (D16) implies that the Fisher information of a system at thermal equilibrium whose energy is controlled by a parameter  $\theta$  is proportional to the variance of the infinitesimal change in energy with respect to a change in the control parameter. In the working hypothesis that the control parameter  $\theta$  equals  $\beta$  with  $E = E(\beta)$ ,

$$E(\beta) = \langle E \rangle + \beta \left( \frac{\partial E}{\partial \beta} - \left\langle \frac{\partial E}{\partial \beta} \right\rangle \right) + \mathcal{O}(\beta^2), \qquad (D17)$$

it follows that the Fisher information  $\mathcal{F}(\theta)$  describes the size of energy fluctuations about equilibrium,

$$\mathcal{F}(\theta) = \sigma_E^2 \stackrel{\text{def}}{=} \left\langle \left( \langle E \rangle - E \right)^2 \right\rangle. \tag{D18}$$

## Appendix E: On the mechanical kinetic energy

In this Appendix, we clarify the relation between the Fisher information function and the mechanical kinetic energy. We recall that the mechanical kinetic energy with respect to the parameter  $\theta$  is defined as,

$$\mathcal{K}\left(\theta\right) \stackrel{\text{def}}{=} \sum_{m=0}^{N-1} \left| \frac{\partial \psi_{\theta}\left(m\right)}{\partial \theta} \right|^{2} = \sum_{m=0}^{N-1} \left| \dot{\psi}_{\theta}\left(m\right) \right|^{2}, \tag{E1}$$

with  $\dot{\psi}_{\theta}\left(m\right)\stackrel{\mathrm{def}}{=}\partial_{\theta}\left[\psi_{\theta}\left(m\right)\right]$ . The wavefunction  $\psi_{\theta}\left(m\right)$  is a probability amplitude defined as,

$$\psi_{\theta}\left(m\right) \stackrel{\text{def}}{=} \left\langle m|\psi\left(\theta\right)\right\rangle,\tag{E2}$$

with  $\langle m|l\rangle = \delta_{ml}$  and the state  $|\psi(\theta)\rangle$  is given by,

$$|\psi(\theta)\rangle = \sum_{m=0}^{N-1} \sqrt{p_m(\theta)} e^{i_{\mathbb{C}}\phi_m(\theta)} |m\rangle, \qquad (E3)$$

where  $p_m(\theta) \stackrel{\text{def}}{=} |\psi_{\theta}(m)|^2$ . Using the polar decomposition of the wavefunction  $\psi_{\theta}(m)$ ,

$$\psi_{\theta}(m) = r_{\theta}(m) e^{i_{\mathbb{C}}\phi_{\theta}(m)}, \tag{E4}$$

after some algebra, it follows from Eqs. (E1) and (E4) that

$$\mathcal{K}(\theta) = \sum_{m=0}^{N-1} \left\{ \left( \frac{\partial r_{\theta}(m)}{\partial \theta} \right)^{2} + \left[ r_{\theta}(m) \frac{\partial \phi_{\theta}(m)}{\partial \theta} \right]^{2} \right\}.$$
 (E5)

At this point we make two observations. First, since  $p_m\left(\theta\right) = \left|\psi_\theta\left(m\right)\right|^2$ , the Fisher information

$$\mathcal{F}(\theta) \stackrel{\text{def}}{=} \sum_{m=0}^{N-1} p_m(\theta) \left( \frac{\partial \log p_m(\theta)}{\partial \theta} \right)^2, \tag{E6}$$

becomes

$$\mathcal{F}(\theta) = 4 \sum_{m=0}^{N-1} \left( \frac{\partial r_{\theta}(m)}{\partial \theta} \right)^{2}.$$
 (E7)

Second, recalling that the quantum mechanical current density with respect to the parameter  $\theta$  is defined as,

$$J_{\theta}\left(m\right) \stackrel{\text{def}}{=} \frac{1}{2i_{\mathbb{C}} \left|\psi_{\theta}\left(m\right)\right|^{2}} \left(\frac{\partial \psi_{\theta}\left(m\right)}{\partial \theta} \psi_{\theta}^{*}\left(m\right) - \psi_{\theta}\left(m\right) \frac{\partial \psi_{\theta}^{*}\left(m\right)}{\partial \theta}\right), \tag{E8}$$

inserting Eq. (E4) into Eq. (E8), we obtain  $J_{\theta}\left(m\right)=\partial_{\theta}\left[\phi_{\theta}\left(m\right)\right]$  and

$$\sum_{m=0}^{N-1} J_{\theta}^{2}(m) \left| \psi_{\theta}(m) \right|^{2} = \sum_{m=0}^{N-1} \left[ r_{\theta}(m) \frac{\partial \phi_{\theta}(m)}{\partial \theta} \right]^{2}.$$
 (E9)

Finally, from Eqs. (E7) and (E9), we conclude that the quantum mechanical kinetic energy  $\mathcal{K}(\theta)$  in Eq. (E5) can be written as

$$\mathcal{K}(\theta) = \frac{1}{4} \mathcal{F}(\theta) + \sum_{m=0}^{N-1} J_{\theta}^{2}(m) |\psi_{\theta}(m)|^{2}.$$
 (E10)

Observe that in the case of the IG formulation of the quantum search problem,  $\mathcal{F}(\theta) = 4$ ,  $J_{\theta}(m) = 0$  for any  $0 \le m \le N - 1$ , and  $\mathcal{K}(\theta)$  is constantly equal to one.

# Appendix F: Optimal paths

In this Appendix, we consider optimal paths as trajectories that minimize the length, that is, the geodesic paths satisfying Eq. (122). The following computation follows standard methods of Einstein's general relativity [141].

The action functional to minimize is given by,

$$S \stackrel{\text{def}}{=} \int dS = \int \sqrt{dS^2} = \int \sqrt{g_{\mu\nu}(\theta) d\theta^{\mu} d\theta^{\nu}}, \tag{F1}$$

where the classical Fisher-Rao information metric  $g_{\mu\nu}\left(\theta\right)$  is defined as,

$$g_{\mu\nu}\left(\theta\right) \stackrel{\text{def}}{=} \int dx p\left(x|\theta\right) \frac{\partial \log p\left(x|\theta\right)}{\partial \theta^{\mu}} \frac{\partial \log p\left(x|\theta\right)}{\partial \theta^{\nu}} = \int dx \frac{1}{p\left(x|\theta\right)} \frac{\partial p\left(x|\theta\right)}{\partial \theta^{\mu}} \frac{\partial p\left(x|\theta\right)}{\partial \theta^{\nu}} = 4 \int dx \frac{\partial \sqrt{p\left(x|\theta\right)}}{\partial \theta^{\mu}} \frac{\partial \sqrt{p\left(x|\theta\right)}}{\partial \theta^{\nu}}.$$
 (F2)

We want to compute  $\delta S$ , that is

$$\delta S = \delta \left( \int dS \right) = \int \delta (dS). \tag{F3}$$

Let us notice that,

$$\delta(dS) = \frac{\delta(dS^2)}{2dS}.$$
 (F4)

Thus, substituting Eq. (F4) into Eq. (F3), we obtain

$$\delta S = \int \frac{\delta \left( dS^2 \right)}{2dS}.$$
 (F5)

Let us notice that  $\delta(dS^2)$  in Eq. (F5) may be rewritten as,

$$\delta (dS^2) = d\theta^{\mu} d\theta^{\nu} \frac{\partial g_{\mu\nu}}{\partial \theta^{\rho}} \delta \theta^{\rho} + 2g_{\mu\nu} d\theta^{\mu} d\delta \theta^{\nu}.$$
 (F6)

Substituting Eq. (F6) into Eq. (F5), the variation  $\delta S$  becomes

$$\delta S = \int \left( \frac{1}{2} \frac{d\theta^{\mu}}{dS} \frac{d\theta^{\nu}}{dS} \frac{\partial g_{\mu\nu}}{\partial \theta^{\rho}} \delta \theta^{\rho} + g_{\mu\nu} \frac{d\theta^{\mu}}{dS} \frac{d\delta \theta^{\nu}}{dS} \right) dS.$$
 (F7)

Note that integrating by parts and imposing that  $\delta\theta^{\nu} = 0$  at the extremum, it happens that the second term in the integrand of Eq. (F7) may be rewritten as,

$$\int g_{\mu\nu} \frac{d\theta^{\mu}}{dS} \frac{d\delta\theta^{\nu}}{dS} dS = g_{\mu\nu} \frac{d\theta^{\mu}}{dS} \delta\theta^{\nu} - \int \frac{d}{dS} \left( g_{\mu\nu} \frac{d\theta^{\mu}}{dS} \right) \delta\theta^{\nu} dS = -\int \frac{d}{dS} \left( g_{\mu\nu} \frac{d\theta^{\mu}}{dS} \right) \delta\theta^{\nu} dS.$$
 (F8)

Thus, substituting Eq. (F8) into Eq. (F7), the variation  $\delta S$  becomes

$$\delta S = \int \left[ \frac{1}{2} \frac{d\theta^{\mu}}{dS} \frac{d\theta^{\nu}}{dS} \frac{\partial g_{\mu\nu}}{\partial \theta^{\rho}} \delta \theta^{\rho} - \frac{d}{dS} \left( g_{\mu\nu} \frac{d\theta^{\mu}}{dS} \right) \delta \theta^{\nu} \right] dS, \tag{F9}$$

that is,

$$\delta S = \int \left[ \frac{1}{2} \frac{d\theta^{\mu}}{dS} \frac{d\theta^{\nu}}{dS} \frac{\partial g_{\mu\nu}}{\partial \theta^{\rho}} - \frac{d}{dS} \left( g_{\mu\rho} \frac{d\theta^{\mu}}{dS} \right) \right] \delta \theta^{\rho} dS. \tag{F10}$$

Imposing  $\delta S = 0$  for any  $\delta \theta^{\rho}$  yields,

$$\frac{1}{2}\frac{d\theta^{\mu}}{dS}\frac{d\theta^{\nu}}{dS}\frac{\partial g_{\mu\nu}}{\partial \theta^{\rho}} - \frac{d}{dS}\left(g_{\mu\rho}\frac{d\theta^{\mu}}{dS}\right) = 0.$$
 (F11)

Let us observe that,

$$\frac{1}{2}\frac{d\theta^{\mu}}{dS}\frac{d\theta^{\nu}}{dS}\frac{\partial g_{\mu\nu}}{\partial \theta^{\rho}} - \frac{d}{dS}\left(g_{\mu\rho}\frac{d\theta^{\mu}}{dS}\right) = \frac{1}{2}\frac{d\theta^{\mu}}{dS}\frac{d\theta^{\nu}}{dS}\frac{\partial g_{\mu\nu}}{\partial \theta^{\rho}} - \frac{\partial g_{\mu\rho}}{\partial \theta^{\nu}}\frac{d\theta^{\nu}}{dS}\frac{d\theta^{\mu}}{dS} - g_{\mu\rho}\frac{d^{2}\theta^{\mu}}{dS^{2}}.$$
 (F12)

Furthermore, note that

$$\frac{\partial g_{\mu\rho}}{\partial \theta^{\nu}} \frac{d\theta^{\nu}}{dS} \frac{d\theta^{\mu}}{dS} = \frac{1}{2} \left( \frac{\partial g_{\mu\rho}}{\partial \theta^{\nu}} + \frac{\partial g_{\nu\rho}}{\partial \theta^{\mu}} \right) \frac{d\theta^{\nu}}{dS} \frac{d\theta^{\mu}}{dS}. \tag{F13}$$

Thus, substituting Eqs. (F13) and (F12) into Eq. (F11), we obtain

$$g_{\mu\rho}\frac{d^2\theta^{\mu}}{dS^2} + \frac{1}{2}\left(-\frac{\partial g_{\mu\nu}}{\partial\theta^{\rho}} + \frac{\partial g_{\mu\rho}}{\partial\theta^{\nu}} + \frac{\partial g_{\nu\rho}}{\partial\theta^{\mu}}\right)\frac{d\theta^{\mu}}{dS}\frac{d\theta^{\nu}}{dS} = 0.$$
 (F14)

However, recall that [141],

$$\Gamma_{\rho, \ \mu\nu} \stackrel{\text{def}}{=} \frac{1}{2} \left( \frac{\partial g_{\rho\mu}}{\partial \theta^{\nu}} + \frac{\partial g_{\rho\nu}}{\partial \theta^{\mu}} - \frac{\partial g_{\mu\nu}}{\partial \theta^{\rho}} \right). \tag{F15}$$

Therefore substituting Eq. (F15) into Eq. (F14), we find

$$g_{\mu\rho}\frac{d^2\theta^{\mu}}{dS^2} + \Gamma_{\rho,\ \mu\nu}\frac{d\theta^{\mu}}{dS}\frac{d\theta^{\nu}}{dS} = 0,\tag{F16}$$

that is,

$$g^{\rho\rho}g_{\mu\rho}\frac{d^2\theta^{\mu}}{dS^2} + g^{\rho\rho}\Gamma_{\rho,\ \mu\nu}\frac{d\theta^{\mu}}{dS}\frac{d\theta^{\nu}}{dS} = 0.$$
 (F17)

In conclusion, we obtain that the minimization of the action functional S leads to the following geodesic equation,

$$\frac{d^2\theta^{\rho}}{dS^2} + \Gamma^{\rho}_{\mu\nu} \frac{d\theta^{\mu}}{dS} \frac{d\theta^{\nu}}{dS} = 0, \tag{F18}$$

where  $\Gamma^{\rho}_{\mu\nu}$  are the usual Christoffel connection coefficients of the second type [141].

# Appendix G: Walking on information geometric paths

In this Appendix, we briefly describe the steps on information geometric paths together with their size and normalization. The approximate unitarity of the Grover operator restricted to the two-dimensional space spanned by  $|\psi_{\theta_i}\rangle$  and  $U^{-1}|\psi_{\theta_f}\rangle$  is addressed.

## 1. The steps

Observe that,

$$\left|\psi_{\theta_{i+1}}\right\rangle = G\left|\psi_{\theta_{i}}\right\rangle$$

$$= \left(1 - 4\left|U_{fi}\right|^{2}\right)\left|\psi_{\theta_{i}}\right\rangle + 2U_{fi}U^{-1}\left|\psi_{\theta_{f}}\right\rangle. \tag{G1}$$

To be explicit, we have

$$\begin{aligned} \left| \psi_{\theta_{i+1}} \right\rangle &= G \left| \psi_{\theta_{i}} \right\rangle \\ &= - \left( 1 - 2 \left| \psi_{\theta_{i}} \right\rangle \left\langle \psi_{\theta_{i}} \right| \right) U^{-1} \left( 1 - 2 \left| \psi_{\theta_{f}} \right\rangle \left\langle \psi_{\theta_{f}} \right| \right) U \left| \psi_{\theta_{i}} \right\rangle \\ &= - \left( 1 - 2 \left| \psi_{\theta_{i}} \right\rangle \left\langle \psi_{\theta_{i}} \right| \right) U^{-1} \left[ U \left| \psi_{\theta_{i}} \right\rangle - 2 \left\langle \psi_{\theta_{f}} \left| U \right| \psi_{\theta_{i}} \right\rangle \left| \psi_{\theta_{f}} \right\rangle \right] \\ &= - \left( 1 - 2 \left| \psi_{\theta_{i}} \right\rangle \left\langle \psi_{\theta_{i}} \right| \right) \left[ \left| \psi_{\theta_{i}} \right\rangle - 2 \left\langle \psi_{\theta_{f}} \left| U \right| \psi_{\theta_{i}} \right\rangle \right] U^{-1} \left| \psi_{\theta_{f}} \right\rangle \\ &= - \left| \psi_{\theta_{i}} \right\rangle + 2 \left| \psi_{\theta_{i}} \right\rangle + 2 \left\langle \psi_{\theta_{f}} \left| U \right| \psi_{\theta_{i}} \right\rangle \left( 1 - 2 \left| \psi_{\theta_{i}} \right\rangle \left\langle \psi_{\theta_{i}} \right| \right) U^{-1} \left| \psi_{\theta_{f}} \right\rangle \\ &= \left| \psi_{\theta_{i}} \right\rangle + 2 U_{fi} U^{-1} \left| \psi_{\theta_{f}} \right\rangle - 4 U_{fi} \left\langle \psi_{\theta_{i}} \left| U^{-1} \right| \psi_{\theta_{f}} \right\rangle \left| \psi_{\theta_{i}} \right\rangle \\ &= \left| \psi_{\theta_{i}} \right\rangle + 2 U_{fi} U^{-1} \left| \psi_{\theta_{f}} \right\rangle - 4 U_{fi} U_{fi}^{*} \left| \psi_{\theta_{i}} \right\rangle \\ &= \left( 1 - 4 \left| U_{fi} \right|^{2} \right) \left| \psi_{\theta_{i}} \right\rangle + 2 U_{fi} U^{-1} \left| \psi_{\theta_{f}} \right\rangle. \end{aligned} \tag{G2}$$

Note also that,

$$\left|\psi_{\theta_{i+2}}\right\rangle = G^{2} \left|\psi_{\theta_{i}}\right\rangle = G \left|\psi_{\theta_{i+1}}\right\rangle$$

$$= \left(1 - 4 \left|U_{fi}\right|^{2}\right) \left|\psi_{\theta_{i+1}}\right\rangle + 2U_{fi}GU^{-1} \left|\psi_{\theta_{f}}\right\rangle. \tag{G3}$$

Furthermore, we find

$$\left|\psi_{\theta_{i+3}}\right\rangle = G^{3} \left|\psi_{\theta_{i}}\right\rangle = G^{2} \left|\psi_{\theta_{i+1}}\right\rangle = G \left|\psi_{\theta_{i+2}}\right\rangle$$
$$= \left(1 - 4 \left|U_{fi}\right|^{2}\right) \left|\psi_{\theta_{i+2}}\right\rangle + 2U_{fi}G^{2}U^{-1} \left|\psi_{\theta_{f}}\right\rangle. \tag{G4}$$

Following this line of computation, we obtain

$$\left|\psi_{\theta_{i+l}}\right\rangle = G^{l} \left|\psi_{\theta_{i}}\right\rangle = G^{l-1} \left|\psi_{\theta_{i+1}}\right\rangle = \dots = G \left|\psi_{\theta_{i+l-1}}\right\rangle$$

$$= \left(1 - 4 \left|U_{fi}\right|^{2}\right) \left|\psi_{\theta_{i+l-1}}\right\rangle + 2U_{fi}G^{l-1}U^{-1} \left|\psi_{\theta_{f}}\right\rangle, \tag{G5}$$

for any  $1 \le l \le \mathcal{N}_s$  with  $i + \mathcal{N}_s \equiv f$ .

# 2. The size of the steps

Observe that,

$$\langle \psi_{\theta_i} | G | \psi_{\theta_i} \rangle = \langle \psi_{\theta_{i+l}} | G | \psi_{\theta_{i+l}} \rangle \Leftrightarrow \langle \psi_{\theta_i} | \psi_{\theta_{i+1}} \rangle = \langle \psi_{\theta_{i+l}} | \psi_{\theta_{i+l+1}} \rangle, \tag{G6}$$

for any  $1 \leq l \leq \mathcal{N}_s$  with  $i + \mathcal{N}_s \equiv f$ . If  $\langle \psi_{\theta_i} | G | \psi_{\theta_i} \rangle = \langle \psi_{\theta_{i+l}} | G | \psi_{\theta_{i+l}} \rangle$ , then

$$\left[ds_{\text{WY}}^{2}\right]_{i\to i+1} = \left[ds_{\text{WY}}^{2}\right]_{i+l\to i+l+1} \stackrel{\text{def}}{=} 4 \left[1 - \left|\left\langle \psi_{\theta_{i+l}} | \psi_{\theta_{i+l+1}} \right\rangle \right|^{2}\right],\tag{G7}$$

for any  $1 \leq l \leq \mathcal{N}_s$ . Let us verify that  $\langle \psi_{\theta_i} | G | \psi_{\theta_i} \rangle = \langle \psi_{\theta_{i+l}} | G | \psi_{\theta_{i+l}} \rangle$ . Note that

$$G^{l} |\psi_{\theta_{i}}\rangle = |\psi_{\theta_{i+1}}\rangle,$$
 (G8)

implies

$$\langle \psi_{\theta_{i+l}} | = \langle \psi_{\theta_i} | \left( G^l \right)^{\dagger} = \langle \psi_{\theta_i} | \left( G^l \right)^{-1} = \langle \psi_{\theta_i} | \left( G^{-1} \right)^l = \langle \psi_{\theta_i} | G^{-l}. \tag{G9}$$

Therefore,

$$\langle \psi_{\theta_{i+l}} | G | \psi_{\theta_{i+l}} \rangle = \langle \psi_{\theta_i} | G^{-l} G | \psi_{\theta_{i+l}} \rangle = \langle \psi_{\theta_i} | G G^{-l} | \psi_{\theta_{i+l}} \rangle = \langle \psi_{\theta_i} | G | \psi_{\theta_i} \rangle. \tag{G10}$$

From Eq. (G6) and the definition of the infinitesimal line element in Eq. (G7), we conclude that Eq. (G10) implies that the steps are equally spaced. We remark that while G is a unitary operator when acting on  $\mathcal{H}_2^n$ , it is only approximately unitary when restricted to the two-dimensional space spanned by  $|\psi_{\theta_i}\rangle$  and  $U^{-1}|\psi_{\theta_f}\rangle$ . Indeed, recalling that

$$G \left| \psi_{\theta_i} \right\rangle = \left[ 1 - 4 \left| U_{fi} \right|^2 \right] \left| \psi_{\theta_i} \right\rangle + 2U_{fi}U^{-1} \left| \psi_{\theta_f} \right\rangle, \tag{G11}$$

and,

$$GU^{-1} \left| \psi_{\theta_f} \right\rangle = -2U_{fi}^* \left| \psi_{\theta_i} \right\rangle + U^{-1} \left| \psi_{\theta_f} \right\rangle, \tag{G12}$$

after some algebra, we find

$$[G]_{\operatorname{Span}\{|\psi_{\theta_{i}}\rangle, \ U^{-1}|\psi_{\theta_{f}}\rangle\}} \stackrel{\operatorname{def}}{=} \begin{pmatrix} \langle \psi_{\theta_{i}}|G|\psi_{\theta_{i}}\rangle & \langle \psi_{\theta_{i}}|GU^{-1}|\psi_{\theta_{f}}\rangle \\ \langle \psi_{\theta_{f}}|UG|\psi_{\theta_{i}}\rangle & \langle \psi_{\theta_{f}}|UGU^{-1}|\psi_{\theta_{f}}\rangle \end{pmatrix}, \tag{G13}$$

that is,

$$[G]_{\text{Span}\{|\psi_{\theta_{i}}\rangle, U^{-1}|\psi_{\theta_{f}}\rangle\}} = \begin{pmatrix} 1 - 2|U_{fi}|^{2} & -U_{fi}^{*} \\ U_{fi}\left[1 - 4|U_{fi}|^{2}\right] + 2U_{fi} & 1 - 2|U_{fi}|^{2} \end{pmatrix}.$$
(G14)

Observe that it is necessary to impose  $|U_{fi}| \ll 1$  in order to preserve the nature of the rotation operator of G,

$$\det \left\{ [G]_{\text{Span} \left\{ |\psi_{\theta_i}\rangle, \ U^{-1} | \psi_{\theta_f}\rangle \right\}} \right\} = 1 - |U_{fi}|^2 \stackrel{|U_{fi}| \ll 1}{\approx} 1. \tag{G15}$$

# 3. The normalization of the steps

Recall that,

$$|\psi_{\theta_{i+l}}\rangle = (1 - 4|U_{fi}|^2) |\psi_{\theta_{i+l-1}}\rangle + 2U_{fi}G^{l-1}U^{-1} |\psi_{\theta_f}\rangle.$$
 (G16)

Let us verify that  $\langle \psi_{\theta_{i+l}} | \psi_{\theta_{i+l}} \rangle = 1$ , for any  $1 \leq l \leq \mathcal{N}_s$  with  $i + \mathcal{N}_s \equiv f$ . From Eq. (G16), we find

$$\langle \psi_{\theta_{i+l}} | \psi_{\theta_{i+l}} \rangle = \left[ 1 - 4 |U_{fi}|^{2} \right]^{2} + 2U_{fi} \left[ 1 - 4 |U_{fi}|^{2} \right] \langle \psi_{\theta_{i+l-1}} | G^{l-1}U^{-1} | \psi_{\theta_{f}} \rangle$$

$$+ 2U_{fi}^{*} \left[ 1 - 4 |U_{fi}|^{2} \right] \langle \psi_{\theta_{f}} | UG^{1-l} | \psi_{\theta_{i+l-1}} \rangle + 4 |U_{fi}|^{2} \langle \psi_{\theta_{f}} | UG^{1-l}G^{l-1}U^{-1} | \psi_{\theta_{f}} \rangle$$

$$= \left[ 1 - 4 |U_{fi}|^{2} \right]^{2} + 2U_{fi} \left[ 1 - 4 |U_{fi}|^{2} \right] \langle \psi_{\theta_{i}} | U^{-1} | \psi_{\theta_{f}} \rangle$$

$$+ 2U_{fi}^{*} \left[ 1 - 4 |U_{fi}|^{2} \right] \langle \psi_{\theta_{f}} | U | \psi_{\theta_{i}} \rangle + 4 |U_{fi}|^{2}$$

$$= \left[ 1 - 4 |U_{fi}|^{2} \right]^{2} + 2U_{fi}U_{fi}^{*} \left[ 1 - 4 |U_{fi}|^{2} \right] + 2U_{fi}^{*}U_{fi} \left[ 1 - 4 |U_{fi}|^{2} \right] + 4 |U_{fi}|^{2}$$

$$= 1 + 16 |U_{fi}|^{4} - 8 |U_{fi}|^{2} + 2 |U_{fi}|^{2} - 8 |U_{fi}|^{4} + 2 |U_{fi}|^{2} \left[ 1 - 4 |U_{fi}|^{2} \right] + 4 |U_{fi}|^{2}$$

$$= 1 + 16 |U_{fi}|^{4} - 8 |U_{fi}|^{2} + 2 |U_{fi}|^{2} - 8 |U_{fi}|^{4} + 2 |U_{fi}|^{2} - 8 |U_{fi}|^{4} + 4 |U_{fi}|^{2}$$

$$= 1 - 8 |U_{fi}|^{2} + 4 |U_{fi}|^{2} + 4 |U_{fi}|^{2}$$

$$= 1, \tag{G17}$$

that is,

$$\left\langle \psi_{\theta_{i+l}} | \psi_{\theta_{i+l}} \right\rangle = 1. \tag{G18}$$

Eq. (G18) implies that states  $|\psi_{\theta_{i+l}}\rangle$  with  $1 \leq l \leq \mathcal{N}_s$  are properly normalized.