Quantum Inf Process
DOI 10.1007/s11128-012-0483-7

An improved formalism for quantum computation based on geometric algebra—case study: Grover's search algorithm

James M. Chappell · Azhar Iqbal · M. A. Lohe · Lorenz von Smekal · Derek Abbott

Received: 23 May 2012 / Accepted: 28 August 2012

Abstract The Grover search algorithm is one of the two key algorithms in the field of quantum computing, and hence it is desirable to represent it in the simplest and most intuitive formalism possible. We show firstly, that Clifford's geometric algebra, provides a significantly simpler representation than the conventional bra-ket notation, and secondly, that the basis defined by the states of maximum and minimum weight in the Grover search space, allows a simple visualization of the Grover search analogous to the precession of a spin-$\frac{1}{2}$ particle. Using this formalism we efficiently solve the exact search problem, as well as easily representing more general search situations. We do not claim the development of an improved algorithm, but show in a tutorial paper that geometric algebra provides extremely compact and elegant expressions with improved clarity for the Grover search algorithm. Being a key algorithm in quantum computing and one of the most studied, it forms an ideal basis for a tutorial on how to elucidate quantum operations in terms of geometric algebra—this is then of interest in extending the applicability of geometric algebra to more complicated problems in fields of quantum computing, quantum decision theory, and quantum information.

Keywords Grover search algorithm · Quantum algorithms · Geometric algebra · Quantum computing

J. M. Chappell (✉) · A. Iqbal · D. Abbott
School of Electrical and Electronic Engineering,
University of Adelaide, Adelaide, SA 5005, Australia
e-mail: james.m.chappell@adelaide.edu.au

M. A. Lohe
School of Chemistry and Physics, University of Adelaide,
Adelaide, SA 5005, Australia

L. von Smekal
Institut für Kernphysik, Technische Universität Darmstadt,
Schlossgartenstraße 9, 64289 Darmstadt, Germany

Published online: 21 September 2012

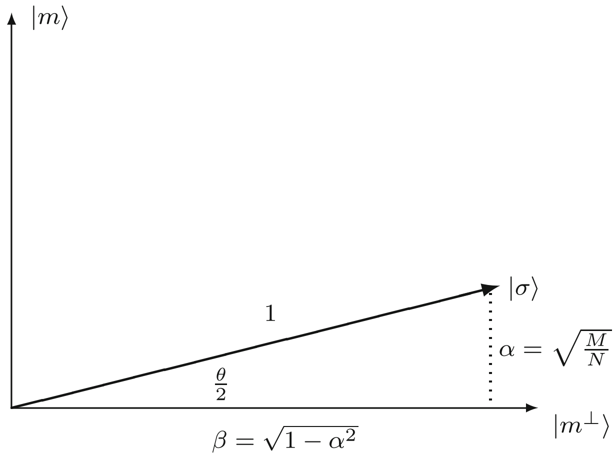

Fig. 1 Geometry of starting state $|\sigma\rangle$ assuming real coefficients on the basis vectors

1 Introduction

The Grover search algorithm [1–3] seeks to evolve a wave function from some starting state $|\sigma\rangle$, into the solution state $|m\rangle$, representing the set of all solutions, which upon measurement will yield one element from this set [4–6]. In order to analyze this evolution, typically an orthonormal basis $|m\rangle$ and $|m^{\perp}\rangle$ is defined, as shown on Fig. 1 upon which the starting state $|\sigma\rangle$ is plotted. However in this paper we use an alternative basis defined by the states of maximum and minimum weight. This allows the initial state $|\sigma\rangle$ and the solution state $|m\rangle$ to be symmetrically positioned in this space, allowing the conceptualizing of the Grover search process, analogous to the precession of a spin-$\frac{1}{2}$ particle in a magnetic field [7]. The particle, in the case of the Grover search, precessing from the direction of the initial state $|\sigma\rangle$ to the solution state $|m\rangle$. This approach is similar to an SO(3) picture that has previously been developed [8], which also plots the path of the state vector during the application of the Grover operator. Clifford algebra has also been applied previously to Grover's algorithm [9–11], however the approach adopted here combines the benefits of an efficient representation as well as an integral geometric visualization. The geometric product of Clifford's geometric algebra can also be used as an alternative to the tensor product notation, hence allowing an alternative description of multi-qubit quantum computation and hence quantum algorithms without the conventional formalism of quantum mechanics [12–18]. Clifford geometric algebra has also been demonstrated to provide a tractable framework for the analysis of N-partite qubit interactions where N is large [19].

1.1 The standard Grover search

Given a search space of N elements, with M of these elements being solutions to a search query as defined by an oracle $f(x)$, where by definition $f(x) = 1$ if x is a solution, and $f(x) = 0$ if x is not a solution. We set up a quantum register with n qubits to index the search space, where we assume for simplicity that $N = 2^n$, and then define the two states

$$|m\rangle = \frac{1}{\sqrt{M}} \sum_{x \in M} |x\rangle, \quad |m^{\perp}\rangle = \frac{1}{\sqrt{N-M}} \sum_{x \notin M} |x\rangle. \tag{1}$$

This allows us to define a uniform superposition starting state [5] in terms of these two states as

$$|\sigma\rangle = \frac{1}{\sqrt{N}} \sum_{x=0}^{N-1} |x\rangle = \sqrt{\frac{N-M}{N}} |m^{\perp}\rangle + \sqrt{\frac{M}{N}} |m\rangle, \tag{2}$$

which is plotted in Fig. 1. It should be remembered that this figure showing a real two-dimensional space does not describe the whole story, in that in general we allow complex coefficients on the basis vectors, thus describing an SU(2) space. In the following section we use the isomorphism so(3) $\cong$ su(2)[1] to describe the search process within a real three-dimensional space.

Grover's solution to the search process [4] involves iteratively applying a unitary operator G defined by

$$G = -G_{\sigma} G_m = -\left(I - 2|\sigma\rangle\langle\sigma|\right)\left(I - 2|m\rangle\langle m|\right). \tag{3}$$

This operator applied to the $n = \log N$ qubits representing the search space, rotates the state vector an angle θ given by

$$\sin\frac{\theta}{2} = \sqrt{\frac{M}{N}} \tag{4}$$

at each application, and after

$$R \leq \left\lceil \frac{\pi}{4} \sqrt{\frac{N}{M}} \right\rceil \tag{5}$$

iterations, the wave function will lie close to the solution state $|m\rangle$.

1.2 Modified basis vectors for the search space

The Grover search space is known to be isomorphic to an SU(2) space [20], hence we now seek the three generators derived from this two-dimensional complex space shown in Fig. 1. In this case we need to utilize the two non-orthogonal states $|m\rangle$ and $|\sigma\rangle$ as the basis. We therefore have available the four possible operators: $|m\rangle\langle\sigma|$, $|\sigma\rangle\langle m|$, $|m\rangle\langle m|$ and $|\sigma\rangle\langle\sigma|$ from which we define:

[1] The Lie groups are represented by uppercase letters and the same symbols in lowercase for the corresponding Lie algebras.

$$J_1 = \frac{P - |\sigma\rangle\langle\sigma| - |m\rangle\langle m|}{2|\alpha|}, \; J_2 = \frac{-\mathrm{i}\,(\alpha^*|m\rangle\langle\sigma| - \alpha|\sigma\rangle\langle m|)}{2|\alpha|\beta}, \tag{6}$$
$$J_3 = \frac{|\sigma\rangle\langle\sigma| - |m\rangle\langle m|}{2\beta},$$

where $\alpha = \langle\sigma|m\rangle$, $\beta = \sqrt{1-|\alpha|^2}$, and $\mathrm{i} = \sqrt{-1}$ with $P = \frac{(|\sigma\rangle\langle\sigma| - |m\rangle\langle m|)^2}{\beta^2}$. We then find the commutation relations

$$[J_i, J_j] = \mathrm{i}\epsilon_{ijk} J_k\,,\;\; [J_i, J_j]_+ = \delta_{ij}\frac{P}{2}\,,\;\; [P, J_i] = 0, \tag{7}$$

where δ is the Kronecker delta symbol, the $+$ subscript representing the anticommutator and ϵ the Levi–Civita symbol, with the Casimir invariant $C = J_1^2 + J_2^2 + J_3^2 = \frac{3}{4}P$ confirming we have an su(2) algebra. We have the raising and lowering operators

$$J_{\pm} = J_1 \pm \mathrm{i}J_2 \tag{8}$$

and requiring $J_+|\uparrow\rangle = 0$ and $J_-|\downarrow\rangle = 0$, we find the states of highest and lowest weight

$$|\uparrow\rangle = \sec\frac{\theta}{2}\left(\cos\frac{\theta}{4}|\sigma\rangle - \mathrm{e}^{-\mathrm{i}\delta}\sin\frac{\theta}{4}|m\rangle\right), \tag{9}$$
$$|\downarrow\rangle = \sec\frac{\theta}{2}\left(\sin\frac{\theta}{4}|\sigma\rangle - \mathrm{e}^{-\mathrm{i}\delta}\cos\frac{\theta}{4}|m\rangle\right),$$

where $\sin\frac{\theta}{2} = |\alpha|$ and $\alpha = \sin\frac{\theta}{2}\mathrm{e}^{\mathrm{i}\delta}$, and we have ignored a possible complex phase factor. We then find $J_3|\uparrow\rangle = +\frac{1}{2}|\uparrow\rangle$ and $J_3|\downarrow\rangle = -\frac{1}{2}|\downarrow\rangle$, as expected for a spin$-\frac{1}{2}$ system. Hence we can see that the Grover search process, involving the transformation of the starting state $|\sigma\rangle$ to the solution state $|m\rangle$, is essentially a spin-flip operation in an SU(2) space. Writing $|\sigma\rangle$ and $|m\rangle$ in this new basis we obtain

$$|\sigma\rangle = \cos\frac{\theta}{4}|\uparrow\rangle - \sin\frac{\theta}{4}|\downarrow\rangle \tag{10}$$
$$|m\rangle = \mathrm{e}^{\mathrm{i}\delta}\left(\sin\frac{\theta}{4}|\uparrow\rangle - \cos\frac{\theta}{4}|\downarrow\rangle\right).$$

Using these results, we can substitute back into the Grover iteration defined in Eq. (3) to find

$$G = -I + 2\cos^2\frac{\theta}{2}|\uparrow\rangle\langle\uparrow| + \sin\theta|\uparrow\rangle\langle\downarrow| - \sin\theta|\downarrow\rangle\langle\uparrow| + 2\cos^2\frac{\theta}{2}|\downarrow\rangle\langle\downarrow|. \tag{11}$$

This can be immediately written in matrix form as

$$G = \begin{bmatrix} \cos\theta & \sin\theta \\ -\sin\theta & \cos\theta \end{bmatrix}, \tag{12}$$

which shows as expected, that the Grover operation rotates the state vector by an angle θ, where the starting state will be for this basis

$$|\sigma\rangle = \begin{bmatrix} \cos\frac{\theta}{4} \\ -\sin\frac{\theta}{4} \end{bmatrix}. \tag{13}$$

1.3 Clifford's algebra of three-space

Using the orthonormal basis $|\uparrow\rangle, |\downarrow\rangle$, defined in Eq. (9), we now model the search process using the real associative algebra of Clifford's geometric algebra (GA) [21]. We define unit algebraic elements e_1, e_2, e_3, such that $e_1^2 = e_2^2 = e_3^2 = 1$, and for distinct i and j we have the anticommutation rule $e_i e_j = -e_j e_i$. The algebraic elements e_1, e_2, e_3, define a three-dimensional space, and so we can define two vectors $\mathbf{a} = a_1 e_1 + a_2 e_2 + a_3 e_3$ and $\mathbf{b} = b_1 e_1 + b_2 e_2 + b_3 e_3$. It then follows, using the distributive law of multiplication over addition, that

$$\begin{aligned} \mathbf{ab} &= (a_1 e_1 + a_2 e_2 + a_3 e_3)(b_1 e_1 + b_2 e_2 + b_3 e_3) \\ &= a_1 b_1 + a_2 b_2 + a_3 b_3 \\ &\quad + (a_2 b_3 - b_2 a_3) e_2 e_3 + (a_1 b_3 - a_3 b_1) e_1 e_3 + (a_1 b_2 - b_1 a_2) e_1 e_2 \\ &= \mathbf{a} \cdot \mathbf{b} + \iota \mathbf{a} \times \mathbf{b} = \mathbf{a} \cdot \mathbf{b} + \mathbf{a} \wedge \mathbf{b}, \end{aligned} \tag{14}$$

where $\mathbf{a} \cdot \mathbf{b}$ is therefore the conventional dot or inner product and $\mathbf{a} \wedge \mathbf{b}$ is the wedge or outer product. In three dimensions we have the relationship with the conventional vector product that $\mathbf{a} \wedge \mathbf{b} = -\iota \mathbf{a} \times \mathbf{b}$, where we have defined the trivector $\iota = e_1 e_2 e_3$ denoted by the Greek symbol iota, ι, which represents an oriented unit volume. The trivector ι allows the use of the dual representation for bivectors, specifically, $\iota e_1 = e_2 e_3$, $\iota e_2 = e_3 e_1$ and $\iota e_3 = e_1 e_2$.

Using the product defined by Eq. (14), with orthonormal basis elements, we find

$$e_i e_j = e_i . e_j + e_i \wedge e_j = \delta_{ij} + \iota \epsilon_{ijk} e_k, \tag{15}$$

indicating that we have an isomorphism between the basis vectors e_1, e_2, e_3 and the Pauli matrices through the use of the geometric product. We find that $\iota^2 = e_1 e_2 e_3 e_1 e_2 e_3 = -1$ and we also find that ι commutes with all other elements of the algebra and so behaves equivalently to the unit imaginary $\mathrm{i} = \sqrt{-1}$. The bivectors also square to negative one, that is $(e_i e_j)^2 = (e_i e_j)(e_i e_j) = -e_i e_j e_j e_i = -1$, assuming $i \neq j$, which are used to define rotations in the plane of the bivector.

1.3.1 Rotations in 3-space with geometric algebra

The Grover search process involves the incremental rotation of the state vector and in geometric algebra in order to rotate a given vector about an axis defined by a vector **a**, where the length of this vector |**a**| gives the rotation angle, we define a rotor

$$R = \mathrm{e}^{-\iota \mathbf{a}/2} = \cos\left(\frac{|\mathbf{a}|}{2}\right) - \iota \frac{\mathbf{a}}{|\mathbf{a}|} \sin\left(\frac{|\mathbf{a}|}{2}\right). \tag{16}$$

This rotor acts by conjugation to rotate a vector $\mathbf{v} = v_1 e_1 + v_2 e_2 + v_2 e_3$, using

$$\mathbf{v} \xrightarrow{R} \mathbf{v}' = R\mathbf{v}R^\dagger = \mathrm{e}^{-\iota \mathbf{a}/2} \mathbf{v} \mathrm{e}^{\iota \mathbf{a}/2}. \tag{17}$$

The † symbol represents the *reversion* operation, which flips the order of the terms and switches the sign of ι and is used here as it acts analogously to the conventional adjoint † operation that takes the conjugate transpose of a complex matrix.

Either R or $-R$ effects the rotation of the vector $v \to v'$, as Eq. (17) shows, which is simply a statement that the map from the group SU(2) to SO(3) is 2:1. This causes no ambiguity as the rotated vector v' is the same for either map.

1.3.2 Representing quantum states in GA

We can identify a simple 1:1 mapping from complex spinors to the scalars and bivectors of GA as follows [21–23]

$$|\psi\rangle = z_1|\uparrow\rangle + z_2|\downarrow\rangle = \begin{bmatrix} a_0 + \mathrm{i}a_3 \\ -a_2 + \mathrm{i}a_1 \end{bmatrix} \leftrightarrow \psi = a_0 + a_1 \iota e_1 + a_2 \iota e_2 + a_3 \iota e_3. \tag{18}$$

The set of even grade multivectors (the scalars and bivectors of GA in three dimensions) used to represent spinors, is closed under the Clifford product, and itself forms an algebra that is called the even subalgebra.

Converting the complex spinors defined in Eq. (10), we find using Eq. (18)

$$\begin{aligned} |\sigma\rangle &\mapsto \cos\frac{\theta}{4} + \sin\frac{\theta}{4}\iota e_2 = \mathrm{e}^{\iota e_2 \theta/4} \\ |m\rangle &\mapsto \left(\sin\frac{\theta}{4} + \cos\frac{\theta}{4}\iota e_2\right)\mathrm{e}^{\iota\delta e_3} = \mathrm{e}^{\iota e_2(\pi/2 - \theta/4)}\mathrm{e}^{\iota\delta e_3} = \iota e_2 \mathrm{e}^{-\iota e_2 \theta/4}\mathrm{e}^{\iota\delta e_3}. \end{aligned} \tag{19}$$

We can now transform GA type spinors into a real space representation through the transformation

$$S = \psi e_3 \psi^\dagger, \tag{20}$$

which describes an isomorphism between quaternion style rotations and real three-space vectors equivalent to the Bloch sphere representation [8]. This is simply a restatement of the well-known isomorphism so(3) ≅ su(2).

This gives us the three-space vectors

$$\begin{aligned} \sigma &= \mathrm{e}^{\iota e_2\theta/4} e_3 \mathrm{e}^{-\iota e_2\theta/4} = \mathrm{e}^{\iota e_2\theta/2} e_3 = -\sin\frac{\theta}{2}e_1 + \cos\frac{\theta}{2}e_3 \\ m &= \mathrm{e}^{\iota e_2(\pi/2-\theta/4)} \mathrm{e}^{\iota\delta e_3} e_3 \mathrm{e}^{-\iota\delta e_3} \mathrm{e}^{-\iota e_2(\pi/2-\theta/4)} \\ &= -\mathrm{e}^{-\iota e_2\theta/2} e_3 = -\sin\frac{\theta}{2}e_1 - \cos\frac{\theta}{2}e_3. \end{aligned} \tag{21}$$

Analogously we can find $m^{\perp} = \sin\frac{\theta}{2}e_1 + \cos\frac{\theta}{2}e_3$, so that the vectors σ, m and $m^{\perp}$, can now be plotted in real Cartesian space shown in Fig. 2, where the angle θ is measured from e_3, and ϕ is measured from e_1.

2 The Grover search operator in GA

The action of the oracle G_m on $|m\rangle$ is $(I - 2|m\rangle\langle m|)\,|m\rangle = -|m\rangle$, which is to flip the 'm' coordinate about the $|m^{\perp}\rangle$ axis [5]. Reflections are easily handled in GA, through double sided multiplication of the vector representing the axis of reflection, the action of the oracle being therefore

$$m\sigma m. \tag{22}$$

We can see from Fig. 2 that the same axis of reflection is also provided by $-m^{\perp}$. Using the starting state defined in Eq. (21) we find the action of the oracle on the starting state σ as

$$m\sigma m = \mathrm{e}^{-\iota e_2\theta/2} e_3 e_3 \mathrm{e}^{-\iota e_2\theta/2} \mathrm{e}^{-\iota e_2\theta/2} e_3 = \mathrm{e}^{-\iota e_2 3\theta/2} e_3 = \cos\frac{3\theta}{2}e_3 + \sin\frac{3\theta}{2}e_1, \tag{23}$$

which is the required vector (see Fig. 2).

The action of the other half of the Grover operator $G_\sigma = I - 2|\sigma\rangle\langle\sigma|$ also produces a reflection, but this time about the σ vector. This therefore implies a full Grover iteration of the starting state will be $\sigma(m\sigma m)\sigma = (\sigma m)\sigma(m\sigma) = G\sigma G^{\dagger}$, where we have used the associativity of GA. This then gives the combined Grover operator as

$$G = -\sigma m = \mathrm{e}^{\iota e_2\theta/2} e_3 e_3 \mathrm{e}^{\iota e_2\theta/2} = \mathrm{e}^{\iota e_2\theta}, \tag{24}$$

a significantly more compact form for the standard Grover operator, in comparison to Eq. (3). We can see by inspection, that the Grover operator represents a rotation of 2θ about the e_2 axis, which will clearly rotate the vector σ onto m, after an appropriate number of operations, as shown in Fig. 2. Clearly this formula provides a minimalist algebraic expression for the Grover search, consisting simply of the exponential of an angle θ, and a rotation plane ιe_2. This expression is also easily generalized to describe the general Grover search by simply replacing the rotation plane ιe_2 with a more general rotation plane in three dimensions as shown in Eq. (33).

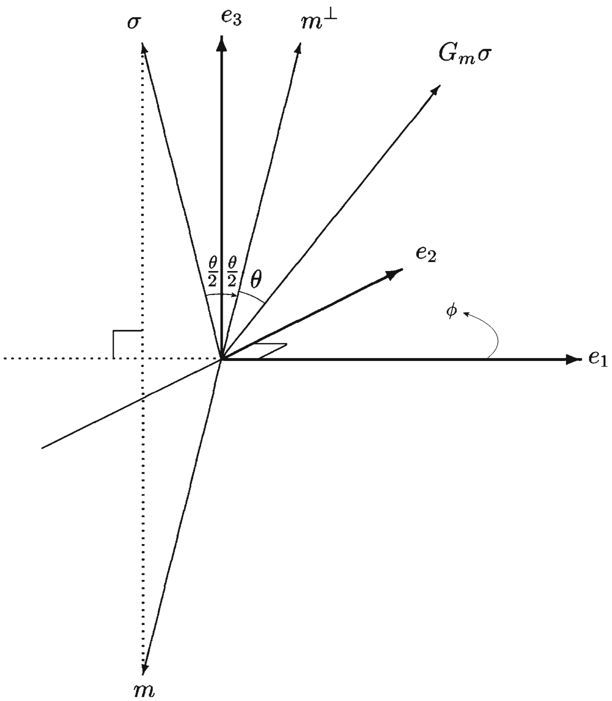

Fig. 2 Grover search in three-space based on states of maximum and minimum weight. The two possible precession axes are now simply e_1 and e_2, which will rotate σ onto m and hence solve the search problem. The starting state σ lies at an angle of $\frac{\theta}{2}$ to the e_3 axis and the action of the oracle G_m on σ, will flip this state about the m axis to $G_m\sigma$ as shown. The angle ϕ is measured in the plane of e_1 and e_2 as shown

Hence, after k iterations we require the Grover operator G to rotate the vector σ, defined in Eq. (21), onto the solution vector m, and so we require

$$G^k \sigma G^{\dagger k} = \mathrm{e}^{\iota k e_2 \theta} \mathrm{e}^{\iota e_2 \theta/2} e_3 \mathrm{e}^{-\iota k e_2 \theta} = \mathrm{e}^{\iota e_2 (2k\theta + \theta/2)} e_3 = m, \tag{25}$$

using $\left(\mathrm{e}^{\iota e_2 \theta}\right)^k = \mathrm{e}^{\iota k e_2 \theta}$, with m defined in Eq. (21). We therefore require

$$\mathrm{e}^{\iota e_2 (2k\theta + \theta/2)} e_3 = \mathrm{e}^{\iota e_2 (\pi - \theta/2)} e_3. \tag{26}$$

Now, by equating exponents, ignoring rotations modulo 2π, we find the condition

$$k = \frac{\pi}{2\theta} - \frac{1}{2}, \tag{27}$$

and using $\theta = 2\arcsin\sqrt{\frac{M}{N}}$ for a database with M solutions, we find

$$k = \frac{\pi}{4\arcsin\sqrt{\frac{M}{N}}} - \frac{1}{2} \approx \frac{\pi}{4}\sqrt{\frac{N}{M}}, \tag{28}$$

the well known result for the standard Grover search. However, clearly, there is no guarantee that the formula will return k as an integer, and because it will need to be rounded to the nearest integer describing the number of Grover operations, we will not always return exactly the solution space upon measurement. However we can modify the search slightly, in order to guarantee that k will be an integer, and hence reliably return the solution state $|m\rangle$.

2.1 Exact Grover search

The Grover operator, defined in Eq. (3), can be modified so that it rotates the starting state $|\sigma\rangle$ exactly onto the solution states $|m\rangle$, thus finding a solution with certainty [20,24]. In order to create the exact Grover search, the Grover operator is typically generalized to

$$G = -\left(I - (1 - \mathrm{e}^{\mathrm{i}\phi_1})|\sigma\rangle\langle\sigma|\right)\left(I - (1 - \mathrm{e}^{\mathrm{i}\phi_2})|m\rangle\langle m|\right), \tag{29}$$

so that when the oracle identifies a solution it applies a complex phase $\mathrm{e}^{\mathrm{i}\phi_2}$ to the wave function and not just the scalar negative one [20]. This has the effect of slightly slowing down the search process allowing the solution state $|m\rangle$ to be reached exactly using an integral number of iterations.

A reflection can be viewed as a rotation by π in one higher dimension, so if we rotate by an angle ϕ_2 about the m axis, which will be clockwise as viewed from above the e_3 axis, we obtain the oracle

$$G_m = \mathrm{e}^{\iota\frac{\phi_2}{2}(\sin(\theta/2)e_1 + \cos(\theta/2)e_3)}. \tag{30}$$

For $\phi_2 = \pi$ we find $G_m = \iota(\sin(\theta/2)e_1 + \cos(\theta/2)e_3) = \iota m$, so that the action of the oracle

$$G_m\sigma G_m^\dagger = \iota m\sigma(-\iota m) = m\sigma m, \tag{31}$$

gives the same result as the standard Grover oracle found previously in Eq. (22). Similarly

$$G_\sigma = \mathrm{e}^{-\iota\frac{\phi_1}{2}(-\sin(\theta/2)e_1 + \cos(\theta/2)e_3)} \tag{32}$$

will be a rotation about the σ axis. Hence the Grover operator for the exact search will be

$$\begin{aligned} G &= -G_\sigma G_m \\ &= -\mathrm{e}^{-\iota\frac{\phi_1}{2}(-\sin(\theta/2)e_1+\cos(\theta/2)e_3)}\mathrm{e}^{\iota\frac{\phi_2}{2}(\sin(\theta/2)e_1+\cos(\theta/2)e_3)} \\ &= -\mathrm{e}^{\iota\beta\hat{v}}, \end{aligned} \tag{33}$$

where we have written the Grover operator in terms of a unit three-vector $\hat{v}$ describing a precession axis, and β a rotation angle about this axis. Clearly this is a significantly more compact form than the conventional operator shown in Eq. (29). Expanding the second line of Eq. (33) above we find

$$\begin{aligned} G = \cos\frac{\phi_1}{2}\cos\frac{\phi_2}{2} + \cos\theta\sin\frac{\phi_1}{2}\sin\frac{\phi_2}{2} + \sin\frac{\phi_1+\phi_2}{2}\sin\frac{\theta}{2}\iota e_1 \\ + \sin\frac{\phi_1}{2}\sin\frac{\phi_2}{2}\sin\theta\iota e_2 - \cos\frac{\theta}{2}\sin\frac{\phi_1-\phi_2}{2}\iota e_3, \end{aligned} \tag{34}$$

giving a detailed expression for the general Grover operator. Eq. (33) can be written as $G = -\cos\beta - \iota\hat{v}\sin\beta$, which when compared with Eq. (34) allows β and $\mathbf{v}$ to be easily calculated. This result, however, is not required in what follows and so for brevity, the relation is not included.

2.1.1 Phase matching

We can see from Fig. 2, which uses the alternate orthonormal basis $|\uparrow\rangle$ and $|\downarrow\rangle$, that σ and m now lie in the plane of e_1 and e_3, and hence using a geometric argument the Grover precession axis must therefore lie in the plane of e_1 and e_2 in order for the σ vector to be able to be rotated precisely onto the m vector. Hence we need to eliminate the e_3 component in the precession axis, and so, by inspection of Eq. (34), we require $\phi_1 = \phi_2$, which is the well known phase matching condition [24,25]. Hence the exact search will be in the form

$$G = -\mathrm{e}^{\iota\beta(\sin\alpha e_1+\cos\alpha e_2)}, \tag{35}$$

where we find

$$\begin{aligned} \sin\frac{\beta}{2} &= \sin\frac{\theta}{2}\sin\frac{\phi}{2} \\ \cot\alpha &= \cos\frac{\theta}{2}\tan\frac{\phi}{2}, \end{aligned} \tag{36}$$

which can be re-expressed assuming a normalization factor Z as

$$G = \mathrm{e}^{\iota\beta(\cos\frac{\phi}{2}e_1+\cos\frac{\theta}{2}\sin\frac{\phi}{2}e_2)/Z}. \tag{37}$$

This equation clearly shows the precession plane perpendicular to the vector $\cos\frac{\phi}{2}e_1 + \cos\frac{\theta}{2}\sin\frac{\phi}{2}e_2$, and if we select $\phi = \pi$, we recover the standard Grover search operation.

To calculate ϕ for the exact search we, once again, have the vector equation given by Eq. (25). Substituting our modified Grover operator, along with Eq. (21), we find

$$\mathrm{e}^{\iota k\beta(\sin\alpha e_1+\cos\alpha e_2)}\mathrm{e}^{\iota e_2\theta/2}e_3\mathrm{e}^{-\iota k\beta(\sin\alpha e_1+\cos\alpha e_2)} = -\mathrm{e}^{-\iota e_2\theta/2}e_3, \tag{38}$$

which can be rearranged to

$$\mathrm{e}^{\iota k\beta(\sin\alpha e_1+\cos\alpha e_2)}\mathrm{e}^{\iota e_2\theta/2}\mathrm{e}^{\iota k\beta(\sin\alpha e_1+\cos\alpha e_2)}\mathrm{e}^{\iota e_2\theta/2} = -1 \tag{39}$$

or

$$(\mathrm{e}^{\iota k\beta(\sin\alpha e_1+\cos\alpha e_2)}\mathrm{e}^{\iota e_2\theta/2})^2 = -1. \tag{40}$$

Now, because we can always replace two consecutive precessions, with a single precession operation, we can write

$$\mathrm{e}^{\iota k\beta(\sin\alpha e_1+\cos\alpha e_2)}\mathrm{e}^{\iota e_2\theta/2} = \mathrm{e}^{\iota\kappa\hat{\mathbf{v}}} = \cos\kappa + \iota\hat{\mathbf{v}}\sin\kappa, \tag{41}$$

for some unit vector $\hat{\mathbf{v}}$. Thus, from Eq. (40), we need to solve

$$(\mathrm{e}^{\iota\kappa\hat{\mathbf{v}}})^2 = \mathrm{e}^{2\iota\kappa\hat{\mathbf{v}}} = \cos 2\kappa + \iota\hat{\mathbf{v}}\sin 2\kappa = -1 \tag{42}$$

and so clearly $\kappa = \frac{\pi}{2}$. Thus the right hand side of Eq. (41), is equal to $\iota\hat{\mathbf{v}}$, implying that the scalar part is zero. Expanding the L.H.S. of Eq. (41), and setting the scalar part to zero, we find

$$\left\langle(\cos k\beta + \iota\sin k\beta(\sin\alpha e_1 + \cos\alpha e_2))\left(\cos\frac{\theta}{2} + \iota\sin\frac{\theta}{2}e_2\right)\right\rangle_0 \tag{43}$$
$$= \cos k\beta\cos\frac{\theta}{2} - \sin k\beta\sin\frac{\theta}{2}\cos\alpha = 0.$$

Re-arranging this equation we find

$$\cot k\beta = \tan\frac{\theta}{2}\cos\alpha = \frac{\sin\frac{\theta}{2}}{\sqrt{\cos^2\frac{\theta}{2} + \cot^2\frac{\phi}{2}}}. \tag{44}$$

Isolating k, we find

$$k = \frac{\operatorname{arccot}\left(\frac{\sin\frac{\theta}{2}}{\sqrt{\cos^2\frac{\theta}{2}+\cot^2\frac{\phi}{2}}}\right)}{2\arcsin(\sin\frac{\theta}{2}\sin\frac{\phi}{2})}. \tag{45}$$

Using calculus we can find the minimum at $\phi = \pi$, which thus returns the number of iterations for the standard Grover search given by Eq. (27), which shows that this modification fails to speed up the search [26–31]. However we are able now to set ϕ in Eq. (45), so as to make k an integer, which will therefore be the fastest exact search possible. Hence the minimum integer iterations will be

$$k_m = \left\lceil \frac{\pi}{2\theta} - \frac{1}{2} \right\rceil. \tag{46}$$

Substituting back into Eq. (45) and re-arranging we then find an expression for ϕ

$$2k_m \arcsin\left(\sin\frac{\theta}{2}\sin\frac{\phi}{2}\right) = \operatorname{arccot}\left(\frac{\sin\frac{\theta}{2}}{\sqrt{\cos^2\frac{\theta}{2} + \cot^2\frac{\phi}{2}}}\right), \tag{47}$$

which we can simplify to give explicitly

$$\sin\frac{\phi}{2} = \sin\frac{\pi}{4k_m + 2}\csc\frac{\theta}{2}. \tag{48}$$

We have ϕ now determined directly from the known θ and k_m defined in Eqs. (4) and (46) respectively, thus solving the exact search using the Grover operator defined in Eq. (35).

An example using this formula for the exact search is given in the "Appendix", which shows how the starting polarization vector now rotates exactly onto the solution states, as required.

2.2 General exact Grover search

Most generally we can write the Grover operator as

$$G = -UI_\gamma U^{-1}G_m = -G'_\sigma G_m \tag{49}$$

where $G'_\sigma = UI_\gamma U^{-1}$ and $I_\gamma = I + (\mathrm{e}^{\mathrm{i}\phi_1} - 1)|\gamma\rangle\langle\gamma|$ where we normally choose $\gamma = |0\rangle = |0\ldots0\rangle$ [2,32,33]. For $U = H$ we have

$$G'_\sigma = -UI_\gamma U^{-1} = I + (\mathrm{e}^{\mathrm{i}\phi_1} - 1)H|\gamma\rangle\langle\gamma|H = I + (\mathrm{e}^{\mathrm{i}\phi_1} - 1)|\sigma\rangle\langle\sigma| = G_\sigma.$$

So with this modified operator we effectively use a modified vector to σ, namely the vector $\gamma = U|0\rangle$, giving

$$|\gamma\rangle = -\mathrm{e}^{-\mathrm{i}\phi/2}\cos\frac{\theta_0}{4}|\uparrow\rangle + \mathrm{e}^{\mathrm{i}\phi/2}\sin\frac{\theta_0}{4}|\downarrow\rangle,$$

equivalent to a starting polarization vector

$$\gamma = -\sin\frac{\theta_0}{2}\cos\phi_0 e_1 - \sin\frac{\theta_0}{2}\sin\phi_0 e_2 + \cos\frac{\theta_0}{2}e_3. \tag{50}$$

Comparing this with the polarization vector for the standard Grover search $\sigma = -\sin\frac{\theta}{2}e_1 + \cos\frac{\theta}{2}e_3$, as shown on Fig. 2, we see that we have changed the projection in the e_3 direction by changing θ to θ_0, and hence rotated the vector in the e_{12} plane given by the angle ϕ_0. If $\phi_0 = 0$, then we recover the standard exact Grover search. As the starting polarization vector in Eq. (50) is a unit vector, we simply adapt G_σ to rotate about this new vector, that is we have

$$G_\gamma = \mathrm{e}^{-\iota\gamma\phi_1/2} = \mathrm{e}^{-\iota\frac{\phi_1}{2}(-\sin\frac{\theta_0}{2}\cos\phi_0 e_1 - \sin\frac{\theta_0}{2}\sin\phi_0 e_2 + \cos\frac{\theta_0}{2}e_3)} \tag{51}$$

and hence for the general exact search, given by $G = -G_\gamma G_m$, we have

$$G = \mathrm{e}^{-\iota\frac{\phi_1}{2}(-\sin\frac{\theta_0}{2}\cos\phi_0 e_1 - \sin\frac{\theta_0}{2}\sin\phi_0 e_2 + \cos\frac{\theta_0}{2}e_3)}\mathrm{e}^{\iota\phi_2/2(\sin(\theta/2)e_1 + \cos(\theta/2)e_3)}. \tag{52}$$

However this equation is clearly fairly cumbersome. As a more elegant alternative, we can simply adjust our basis states, given by Eq. (9), and then the exact solution, given by Eq. (35), immediately applies.

3 Summary

The two main strengths of geometric algebra are its method of handling rotations and its integral geometric representation, and hence its perfect suitability in describing the Grover search. We find Clifford's geometric algebra provides a simplified representation for the Grover operator shown in Eq. (24) compared with Eq. (3) and also provides a clear geometric picture of the search process. Using the states of maximum and minimum weight, we find that we can interpret the search process as the precession of a spin-$\frac{1}{2}$ particle, thus providing a simple visual picture, as shown in Fig. 2. This is not possible with the standard formalism as it requires two complex axes, forming a four-dimensional space, and hence is difficult to visualize. We also find that the exact Grover search Eq. (35) has an efficient algebraic solution, as shown in Eq. (48). Improved intuition obtained via the use of Clifford's geometric algebra may possibly assist the search for new quantum algorithms.

This tutorial has been based on the standard Grover search algorithm [4] but an interesting extension would be to apply the GA formalism to the partial search process, which is also describable within an SU(2) space [34] and to the fixed point search [35].

Acknowledgments We are grateful to Sam Braunstein for drawing our attention to the potential applicability of our approach to the partial search process.

4 Appendix

4.1 Example of an exact search over 16 elements

After k iterations we have the polarization vector

$$\begin{aligned} P &= G^k \sigma G^{\dagger k} \\ &= \mathrm{e}^{\iota k\beta(\sin\alpha e_1+\cos\alpha e_2)} \mathrm{e}^{\iota e_2\theta/2} e_3 \mathrm{e}^{-\iota k\beta(\sin\alpha e_1+\cos\alpha e_2)} \\ &= -\left(\sin^2\alpha \sin\frac{\theta}{2} + \sin\frac{\theta}{2}\cos^2\alpha\cos 2\beta k + \cos\alpha\cos\frac{\theta}{2}\sin 2\beta k\right) e_1 \\ &\quad + \left(-\frac{1}{2}\sin\frac{\theta}{2}\sin 2\alpha + \frac{1}{2}\sin 2\alpha \sin\frac{\theta}{2}\cos 2\beta k + \cos\frac{\theta}{2}\sin\alpha\sin 2\beta k\right) e_2 \\ &\quad + \left(\cos\frac{\theta}{2}\cos 2\beta k - \cos\alpha\sin\frac{\theta}{2}\sin 2\beta k\right) e_3. \end{aligned} \tag{53}$$

For 16 elements we find from Eq. (46) $k_m = 3$, and we then find ϕ from Eq. (48) for an exact search of $\phi = 2.19506$. This gives the polarization vector after k iterations

$$\begin{aligned} P = &-(0.0546434 + 0.195357\cos 2\beta k + 0.855913\sin 2\beta k)e_1 \\ &+(-0.10332 + 0.10332\cos 2\beta k + 0.452673\sin 2\beta k)e_2 \\ &+(0.968246\cos 2\beta k - 0.220996\sin 2\beta k)e_3. \end{aligned} \tag{54}$$

Using α and β defined in Eq. (36), beginning from a starting vector $\sigma = (-0.25, 0, 0.9682)$, with a required solution vector $m = (-0.25, 0, -0.9682)$, we generate a polarization vector P as

$$\begin{aligned} \sigma &= (-0.25, 0, 0.9682) \\ G\sigma &= (-0.8456, 0.315, 0.4309) \\ G^2\sigma &= (-0.8456, 0.315, -0.4309) \\ G^3\sigma &= (-0.25, 0, -0.9682) \end{aligned} \tag{55}$$

thus producing the exact solution m after $k_m = 3$ iterations as required.

4.2 Description of the Grover su(2) algebra

We found previously

$$P = \frac{(|\sigma\rangle\langle\sigma| - |m\rangle\langle m|)^2}{\beta^2} = \frac{|\sigma\rangle\langle\sigma| - \alpha|\sigma\rangle\langle m| - \alpha^*|m\rangle\langle\sigma| + |m\rangle\langle m|}{1-|\alpha|^2}, \tag{56}$$

so that

$$P^2 = \frac{|\sigma\rangle\langle\sigma| - \alpha|\sigma\rangle\langle m| - \alpha^*|m\rangle\langle\sigma| + |m\rangle\langle m|}{1-|\alpha|^2} = P. \tag{57}$$

We also find

$$P|\sigma\rangle = \frac{|\sigma\rangle\langle\sigma| - \alpha|\sigma\rangle\langle m| - \alpha^*|m\rangle\langle\sigma| + |m\rangle\langle m|}{1-|\alpha|^2}|\sigma\rangle = |\sigma\rangle$$
$$P|m\rangle = \frac{|\sigma\rangle\langle\sigma| - \alpha|\sigma\rangle\langle m| - \alpha^*|m\rangle\langle\sigma| + |m\rangle\langle m|}{1-|\alpha|^2}|m\rangle = |m\rangle. \tag{58}$$

We can calculate

$$\begin{aligned}
J_1 J_2 &= \frac{\mathrm{i}\,(|\sigma\rangle\langle\sigma| - |m\rangle\langle m|)}{4\beta} = \frac{1}{2}\mathrm{i}J_3 \\
J_2 J_1 &= -\frac{\mathrm{i}\,(|\sigma\rangle\langle\sigma| - |m\rangle\langle m|)}{4\beta} = -\frac{1}{2}\mathrm{i}J_3 \\
J_2 J_3 &= \frac{\mathrm{i}\left(|\alpha|^2|\sigma\rangle\langle\sigma| + |\alpha|^2|m\rangle\langle m| - \alpha|\sigma\rangle\langle m| - \alpha^*|m\rangle\langle\sigma|\right)}{4|\alpha|(1-|\alpha|^2)} = \frac{1}{2}\mathrm{i}J_1 \\
J_3 J_2 &= \frac{\mathrm{i}\left(-|\alpha|^2|\sigma\rangle\langle\sigma| - |\alpha|^2|m\rangle\langle m| + \alpha|\sigma\rangle\langle m| + \alpha^*|m\rangle\langle\sigma|\right)}{4|\alpha|(1-|\alpha|^2)} = -\frac{1}{2}\mathrm{i}J_1 \\
J_3 J_1 &= \frac{\alpha^*|m\rangle\langle\sigma| - \alpha|\sigma\rangle\langle m|}{4|\alpha|\beta} = \frac{1}{2}\mathrm{i}J_2 \\
J_1 J_3 &= \frac{-\alpha^*|m\rangle\langle\sigma| + \alpha|\sigma\rangle\langle m|}{4|\alpha|\beta} = -\frac{1}{2}\mathrm{i}J_2
\end{aligned} \tag{59}$$

and noting that P commutes with J_1, J_2 and J_3, we have demonstrated the commutator relations shown in Eq. (7).

We have raising and lowering operators $J_\pm = J_1 \pm \mathrm{i}J_2$ from which we define the states of highest and lowest weight, requiring

$$\begin{aligned}
J_+(d_1|m\rangle + d_2|\sigma\rangle) &= 0 \\
J_-(d_3|m\rangle + d_4|\sigma\rangle) &= 0.
\end{aligned} \tag{60}$$

We firstly note that

$$\begin{aligned}
J_1|\sigma\rangle &= \frac{-\alpha^*}{2|\alpha|}|m\rangle \\
J_1|m\rangle &= \frac{-\alpha}{2|\alpha|}|\sigma\rangle \\
J_2|\sigma\rangle &= \frac{-\mathrm{i}\alpha^*}{2|\alpha|\sqrt{1-|\alpha|^2}}|m\rangle + \frac{\mathrm{i}|\alpha|}{2\sqrt{1-|\alpha|^2}}|\sigma\rangle \\
J_2|m\rangle &= \frac{-\mathrm{i}|\alpha|}{2\sqrt{1-|\alpha|^2}}|m\rangle + \frac{\mathrm{i}\alpha}{2|\alpha|\sqrt{1-|\alpha|^2}}|\sigma\rangle \\
J_3|\sigma\rangle &= \frac{1}{2\sqrt{1-|\alpha|^2}}(|\sigma\rangle - \alpha^*|m\rangle)
\end{aligned} \tag{61}$$

$$J_3|m\rangle = \frac{1}{2\sqrt{1-|\alpha|^2}}(\alpha|\sigma\rangle - |m\rangle).$$

From Eq. (60) we then find

$$d_1 = -d_2\frac{\alpha^*(1-\beta)}{|\alpha|^2}\,,\; d_3 = -d_4\frac{\alpha^*(1+\beta)}{|\alpha|^2}, \tag{62}$$

which gives the states of maximum and minimum weight

$$\begin{aligned} |\uparrow\rangle &= d_2\left(-\frac{\alpha^*(1-\beta)}{|\alpha|^2}|m\rangle + |\sigma\rangle\right) = k_1\left(-\mathrm{e}^{-\mathrm{i}\delta}\sin\frac{\theta}{4}|m\rangle + \cos\frac{\theta}{4}|\sigma\rangle\right) \\ |\downarrow\rangle &= d_4\left(-\frac{\alpha^*(1+\beta)}{|\alpha|^2}|m\rangle + |\sigma\rangle\right) = k_2\left(-\mathrm{e}^{-\mathrm{i}\delta}\cos\frac{\theta}{4}|m\rangle + \sin\frac{\theta}{4}|\sigma\rangle\right) \end{aligned} \tag{63}$$

and with the normalization $\langle\uparrow|\uparrow\rangle = \langle\downarrow|\downarrow\rangle = 1$ we find $|k_1| = |k_2| = \sec\frac{\theta}{2}$, and ignoring a global phase we therefore have the results shown in Eq. (9).

References

1. Grover, L.: A framework for fast quantum mechanical algorithms. In: Proceedings of the Thirtieth Annual ACM Symposium on Theory of Computing, ACM, pp. 53–62 (1998)
2. Grover, L.: Quantum computers can search rapidly by using almost any transformation. Phys. Rev. Lett. **80**(19), 4329–4332 (1998)
3. Grover, L.: From schrödingers equation to the quantum search algorithm. Am. J. Phys. **69**(7), 769–777 (2001)
4. Grover, L.: Quantum mechanics helps in searching for a needle in a haystack. Phys. Rev. Lett. **79**(2), 325–328 (1997)
5. Nielsen, M., Chuang, I.: Quantum Computation and Quantum Information, 1st edn. Addison-Wesley, Cambridge (2002)
6. Ng, J., Abbott, D.: Introduction to solid-state quantum computation for engineers. Microelectron. J. **33**(1–2), 171–177 (2002)
7. Chappell, J., Iqbal, A., Lohe, M., Von Smekal, L.: An analysis of the quantum penny flip game using geometric algebra. J. Phys. Soc. Jpn. **78**(5), 54801–54804 (2009)
8. Long, G., Tu, C., Li, Y., Zhang, W., Yan, H.: An SO(3) picture for quantum searching. J. Phys. A Math. Gen. **34**(4), 861–866 (2001)
9. Alves, R., Lavor, C.: Clifford algebra applied to Grover's algorithm. Adv. Appl. Clifford Algebras **20**, 477–488 (2010)
10. Somaroo, S., Cory, D., Havel, T.: Expressing the operations of quantum computing in multiparticle geometric algebra. Phys. Lett. A **240**(1–2), 1–7 (1998)
11. Gregorič, M., Mankoč Borštnik, N.: Quantum gates and quantum algorithms with clifford algebra techniques. Int. J. Theor. Phys. **48**(2), 507–515 (2009)
12. Hestenes, D., Sobczyk, G.: Clifford Algebra to Geometric Calculus: A Unified Language for Mathematics and Physics, vol. 5. Springer, Berlin (1984)
13. Hestenes, D.: Clifford Algebras and Their Applications in Mathematical Physics (Reidel, Dordrecht/Boston, 1986), chap. Clifford Algebra and the interpretation of quantum mechanics (1986)
14. Aerts, D., Czachor, M.: Cartoon computation: quantum-like computing without quantum mechanics. J. Phys. A Math. Theor. **40**(13), F259 (2007)
15. Aerts, D., Czachor, M.: Tensor-product versus geometric-product coding. Phys. Rev. A **77**, 012316 (2008)

16. Aerts, D., Czachor, M., Orlowski, L.: Teleportation of geometric structures in 3D. J. Phys. A Math. Theor. **42**(13), 135307 (2009)
17. Vlasov, A.Y.: eprint arXiv:quant-ph/9907079 (1999)
18. Vlasov, A.Y.: Clifford algebras and universal sets of quantum gates. Phys. Rev. A **63**, 054302 (2001)
19. Chappell, J.M., Iqbal, A., Abbott, D.: N-player quantum games in an EPR setting. PLoS ONE **7**(5), e36404 (2012)
20. Hsieh, J., Li, C.: General su(2) formulation for quantum searching with certainty. Phys. Rev. A **65**, 052322 (2002)
21. Doran, C., Lasenby, A.: Geometric Algebra for Physicists. Cambridge University Press, Cambridge (2003)
22. De Sabbata, V., Datta, B.: Geometric Algebra and Applications to Physics. Taylor & Francis Group, London (2007)
23. Parker, R., Doran, C.: Analysis of One and Two Particle Quantum Systems Using Geometric Algebra. pp. 213–226. Birkhäuser, Boston, MA (2002)
24. Li, C., Hwang, C., Hsieh, J., Wang, K.: General phase-matching condition for a quantum searching algorithm. Phys. Rev. A **65**(3), 034305 (2002)
25. Long, G., Li, Y., Zhang, W., Niu, L.: Phase matching in quantum searching. Phys. Lett. A **262**(1), 27–34 (1999)
26. Zalka, C.: Grover's quantum searching algorithm is optimal. Phys. Rev. A **60**, 2746–2751 (1999)
27. Boyer, M., Brassard, G., Høyer, P., Tappa, A.: Tight bounds on quantum searching. Fortsch. Phys. **46/49**, 493–506 (1998)
28. Shapira, D., Shimoni, Y., Biham, O.: Algebraic analysis of quantum search with pure and mixed states. Phys. Rev. A **71**, 042320 (2005)
29. Biham, E., Biham, O., Biron, D., Grassl, M., Lidar, D.A., Shapira, D.: Analysis of generalized Grover quantum search algorithms using recursion equations. Phys. Rev. A **63**, 012310 (2000)
30. Høyer, P.: Arbitrary phases in quantum amplitude amplification. Phys. Rev. A **62**(5), 052304–052309 (2000)
31. Brassard, G., Hoyer, P.: An exact quantum polynomial-time algorithm for simon's problem. In: Proceedings of the 5th Israeli Symposium on Theory of Computing and Systems ISTCS, pp. 12–23 (1997)
32. Biham, E., Biham, O., Biron, D., Grassl, M., Lidar, D.: Grover's quantum search algorithm for an arbitrary initial amplitude distribution. Phys. Rev. A **60**(4), 2742 (1999)
33. Biham, E., Kenigsberg, D.: Grover's quantum search algorithm for an arbitrary initial mixed state. Phys. Rev. A **66**, 062301 (2002)
34. Korepin, V.E., Vallilo, B.C.: Group theoretical formulation of a quantum partial search algorithm. Prog. Theor. Phys. **116**, 783–793 (2006)
35. Grover, L.K.: Fixed-point quantum search. Phys. Rev. Lett. **95**, 150501–150504 (2005)