Quantum Algorithms: Database Search and its Variations

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Abstract

The driving force in the pursuit for quantum computation is the exciting possibility that quantum algorithms can be more efficient than their classical analogues. Research on the subject has unraveled several aspects of how that can happen. Clever quantum algorithms have been discovered in recent years, although not systematically, and the field remains under active investigation. This article is an introduction to the quantum database search algorithm. Its extension to the quantum spatial search algorithm is also described.

1 Quantum Computation

Any physical system—with some initial state, some final state, and some interaction in between—is a candidate for an information processing device, i.e., a computer. One only needs to construct a suitable map between the physical properties of the system and the desired abstract mathematical variables. The initial state becomes the input, the final state becomes the output, and the interaction provides appropriate logic operations. Most of the development in theoretical computer science has been in the framework of “particle-like” discrete digital systems. The growth in semiconductor technology has been so explosive—doubling the number of transistors on a chip every 18-24 months according to Moore’s law—that many choices made in constructing the theoretical framework of computer science (see for example, Ref.[1]) were almost forgotten. Computer architecture became essentially synonymous with digital electronic circuits implementing Boolean operations, pushing aside other competing models. It is known that “wave-like” analogue computation can also be carried out (e.g., using RLC circuits), but that has not been explored as intensively. Even though a specific operation may be easier to implement in digital mode than in analogue mode, or vice versa, considerations of computational complexity are essentially the same for digital and analogue algorithms. The choice between the two is therefore left to criteria for hardware stability. Discrete variables are then a clear favourite—they allow a degree of precision, by implementation of error correction procedures, that continuous variables cannot provide.

The situation has changed with the advent of quantum computation. First came the realisation that with shrinking size of its elementary components, sooner or later, the computer technology will inevitably encounter the dynamics of the atomic scale [2]. The laws that apply at the atomic scale are those of quantum mechanics and not those of electrical circuits. The computational framework needs reanalysis, because quantum objects display both “particle-like” and “wave-like” behaviour—the discrete eigenstates that form the Hilbert space basis as well as the superposition principle that allows for simultaneous existence of multiple components. In what way would this combination alter the axioms of the classical information theory? Is there much more to information theory than just Boolean logic? Many investigations in quantum information theory are addressed to such questions.

The next step was automatic. Clearly, with both “particle-like” and “wave-like” behaviour at their disposal, quantum algorithms can only improve up on their classical counterparts. Note that the inputs and the outputs of all the computational problems we investigate are always classical (or are uniquely mapped to classical states); at the most a quantum computer may solve a problem by a simpler non-classical algorithmic route compared to the classical one. We clearly understand that the concept of what is computable and what is not does not change in going from classical to quantum computation. The scaling rules characterising how efficiently a problem can be solved are altered, however, and the important question is by how much. Explorations using several toy examples have demonstrated that the improvement provided by a quantum solution, relative to the corresponding Boolean logic solution, depends on the problem. The extraordinary feature is that in certain cases the difference is large enough to challenge the conventional complexity classification of computational problems.

The key ingredient for the superiority of quantum algorithms over the Boolean ones happens to be the parallelism provided by the superposition of quantum states. A typical quantum algorithmic strategy exploits
it by superposing an exponentially large number of quantum components using only polynomial resources. For example, with \( n \) qubits and \( n \) rotations, one can create a uniform superposition of \( 2^n \) quantum components:

\[
|0\rangle^{\otimes n} \rightarrow \left( \frac{|0\rangle + |1\rangle}{\sqrt{2}} \right)^{\otimes n} = 2^{-n/2} \sum_{i=0}^{2^n-1} |i\rangle.
\]  

A quantum instruction applied to a superposed state processes all the superposed components together, in a manner analogous to the classical SIMD (single instruction multiple data) paradigm, but without the need for any extra parallel computation resources. Thus a single run of a quantum algorithm can take \( 2^n \) superposed inputs to \( 2^n \) superposed outputs. The caveat is that a projective measurement of the output can give only one of the output components while erasing all the rest, not unlike the situation that one can listen to only a single radio or television programme at a time from a superposition of a large number of available signals. The huge advantage inherent in superposition is therefore useful in those computational problems, where many different inputs need to be processed by the same instructions but only one specific property of the possible outputs is desired at the end. A clear criterion for identifying such problems has not been found, although pattern recognition problems are good candidates.

When the full exponential advantage provided by superposition can be used, the complexity classification of the quantum solution becomes exponentially better than the classical one. Indeed, a lot of research effort has been directed towards discovering problems whose classical solution is in class NP (non-deterministic polynomial), while the quantum solution would be in class P (polynomial). But even in cases where the advantage provided by superposition can only partially be used, the improvement in the scaling rules of the solutions can be substantial enough for real life applications.

Major boost to the subject of quantum computation was provided by the discovery of efficient quantum solutions to two problems of practical interest. One is Shor’s algorithm for factoring large integers [3], which is based on an exponentially faster quantum Fourier transform solution to the period finding problem compared to the classical fast Fourier transform one. The other is Grover’s algorithm for finding an object in an unsorted database [4], which provides a square root speed-up by cleverly using interference to enhance the amplitude at the desired location while suppressing the amplitudes at all other locations. Grover’s algorithm applies to unstructured problems, and assumes so little in terms of either the properties of the problem or the instructions to be executed, that it is generally believed that it will be a popular application on any quantum computer in one form or the other. The following sections provide an introduction to this wonderful algorithm and some of its variations.

## 2 The Database Search Problem

A database is a collection of items. These items possess certain properties, which can be used to distinguish them from each other. The problem of database search is to find an item with the desired properties from the collection. An efficient search process is the one which can locate the desired item in the database as quickly as possible. In practice, efficiency of the search process becomes more and more important as the database size grows.

To understand the optimisation of the search process, it is instructive to first look at a familiar game played by school children. In the game, two teams compete to find the names of famous persons. One team selects the name of a famous person and gives it to the referee. The other team has to discover this name by asking a set of questions to the first team. The game is made interesting by the condition that the first team only provides “yes or no” answers to the questions, i.e. the minimal amount of information—one bit—is released in response to every question. The two teams take turns choosing the names and asking the questions. After several rounds, the team which succeeds in discovering the names with a smaller number of questions is the winner.

The players quickly learn that specific questions such as “Is the person Richard Feynman?” are inefficient. They fail most of the time, and when they fail one does not learn much about who the person is. Efficient questions are of the type “Is the person a man or a woman?”, whence there is a substantial reduction in the number of possible names for the next step no matter what the answer to the question is. The best questions are the ones which reduce the number of possible names for the next step by a factor of two. This factor of two reduction is of course a consequence of the fact that the answers provided to the questions are binary.

A computer scientist would describe this game as “database search”. The list of possible names forms the database, the questions are referred to as queries, and the answers provided by the other team are called oracles. The winning strategy is the one that finds the hidden name with least number of oracle consultations. Binary search is the optimal classical algorithm, which finds the desired item in a database of size \( N \) using \( Q = \log_2 N \) binary queries. This algorithm can be used when the items in the database are sorted according to some order, so that at every step the items corresponding to “yes” answer can be easily separated from the items corresponding
to “no”. The ordering can be implicit (e.g. the team asking “man or woman” question already knows how to separate the two possibilities), or it can be explicit (e.g. the manner in which the words are arranged in a dictionary).

Sorting the items means arranging them in an ordered sequence according to their property values. Though property values along the real line are sufficient for establishing the sequence, the values are taken to be distinct, and without loss of generality they can be replaced by integer labels. The integer labels can be easily digitised, i.e. written as a string of letters belonging to a finite alphabet. When the alphabet has a letters, a string of n letters can label \( N = a^n \) items. (If the number of items in the database is not a power of \( a \), then the database can be padded up with extra labels to make \( N = a^n \). We also assume for simplicity that there are no duplicate entries.) In digital computers, this finite alphabet has the smallest size, i.e. \( a = 2 \), and the letters are called bits.

Sorting facilitates subsequent searching of a database, by factorisation of the search process. Though digitisation does not change the order of the items in the sequence, it simplifies the search process. To locate an item in the database with known properties, one does not look for the complete string of letters in one go, but sequentially inspects only one letter of the label at a time. With digitisation, the individual search steps have to distinguish amongst only a limited number of possibilities, and the maximum simplification of the search steps occurs when the alphabet has the smallest size, i.e. \( a = 2 \). Sorting requires significant effort—\( O(N \log_2 N) \) operations for a database of size \( N \) [5]. But once a database is sorted, all subsequent searches to locate any item in it require only \( O(\log_2 N) \) queries.

The advantage of sorting becomes obvious when one looks at the process of finding the desired item in an unsorted database, e.g. finding the name of the person with a given telephone number using a telephone directory. There is no classical quick search algorithm available—random pickings are as good as any other selection scheme. All one can do is to go through all the items one by one, asking the binary question “Is this the item that I want or not?”; no further reduction in search effort is possible. On the average, one requires \( \langle Q \rangle = N \) binary queries to locate the desired item in an unsorted database, since each query has a success probability of \( 1/N \). The number of queries can be reduced to \( \langle Q \rangle = (N + 1)/2 \), provided that the search process has a memory so that an item rejected once is not picked up again for inspection. Now we can understand that it is the large change in the number of queries, from \( O(N) \) to \( O(\log_2 N) \), that makes the laborious process of sorting worthwhile, to be carried out once and for all.

3 Grover’s Quantum Solution

Can one improve upon this classical analysis? The answer is yes, if we give up some implicit assumptions in the methodology. A crucial assumption in the classical analysis has been that one can inspect only one item of the database (or one letter of the label) at a time. This assumption can be bypassed in a quantum algorithm, where one can work with a superposition of states and “inspect” many—even all—items with a single query. Lov Grover exploited this superposition feature of quantum dynamics, and discovered the optimal quantum database search algorithm [4]. The quantum algorithm is far more interesting for an unsorted database than for a sorted one, and we look at that in detail first.

Quantum states are unit vectors in a Hilbert space (linear vector space with complex coefficients). They evolve in time by unitary transformations. These properties are totally different from classical states and their evolution, and they form the basis of the subject of quantum computation. Of course, to make contact with our problems defined in classical language, we require a mapping between classical and quantum states. That is achieved by identifying the orthogonal basis vectors of the Hilbert space with the set of distinct classical states. The complex components of a general vector in the Hilbert space can vary continuously, and they are called amplitudes of the quantum state. States with more than one non-zero amplitudes are superposed states. Quantum algorithms evolve the amplitudes from some initial values to some final values, by a sequence of unitary transformations. The measurement probability of obtaining a particular classical result from a quantum state is given by the absolute value squared of the corresponding amplitude.

The quantum database search algorithm works in an \( N \)-dimensional Hilbert space, whose basis vectors are identified with the individual items. It takes an initial state whose amplitudes are uniformly distributed over all the items, to a final state where all but one amplitudes vanish. Following Dirac’s notation, let \( \{ |i\rangle \} \) be the set of basis vectors, \( |s\rangle \) be the initial uniform superposition state, and \( |t\rangle \) be the final state corresponding to the desired item. Then

\[
|\langle i | s \rangle| = 1/\sqrt{N}, \quad \langle i | t \rangle = \delta_{it}.
\]

At any stage of the algorithm, the amplitude corresponding to a particular item can be obtained by projecting the quantum state along the corresponding basis vector, using the operator \( P_i = |i\rangle \langle i| \).

Since superposition of amplitudes is commutative, the quantum database can be taken to be unsorted without any loss of generality. The optimal solution to the quantum search problem is based on two properties: (i) the shortest path between two points on the unitary sphere is the geodesic great circle, and (ii) the largest step
one can take in a given direction, consistent with unitarity, is the reflection operation. The available reflection operators are:

\[ U_t = 1 - 2|t⟩⟨t|, \quad U_s = 1 - 2|s⟩⟨s|. \]  

(A projection operator satisfies \( P^2 = P \), which makes \( 1 - 2P \) a reflection operator, i.e. \( (1 - 2P)^2 = 1 \).) The operator \( U_t \) distinguishes between the desired state and the rest. It flips the sign of the amplitude in the desired state, and is the binary query or the quantum oracle. The operator \( -U_s \) treats all items on an equal footing; it flips the sign of the amplitudes relative to the initial uniform state. Note that applying \( P_s \) to any state \( |k⟩ \) averages all its component amplitudes, and so the operation \(-U_s\) is often called “reflection in the average”.

Grover’s algorithm is the discrete Trotter’s formula with these two operators, which locates the desired item in the database with \( Q \) queries,

\[ G^Q|s⟩ = (-U_sU_t)^Q|s⟩ = |t⟩. \]  

This iterative procedure is readily evaluated to yield the relation

\[ (2Q + 1)\sin^{-1}(1/\sqrt{N}) = \pi/2. \]

For a given \( N \), the solution for \( Q \) satisfying Eq.(5) may not be an integer. This means that the algorithm will have to stop without the final state being exactly \( |t⟩ \). There will remain a small admixture of other amplitudes in the output, implying an error in the search process. The size of the unwanted admixture is determined by how close one can get to \( \pi/2 \) on the r.h.s. of Eq.(5). That restricts the error rate to be smaller than \( 1/N \). Apart from this, the algorithm is completely deterministic.

### 3.1 Geometric Interpretation

The algorithm has a simple geometric structure. It follows from the definitions above that the evolving quantum state always remains in the 2-dimensional subspace spanned by the vectors \( |s⟩ \) and \( |t⟩ \). The state therefore proceeds from its initial value \( |s⟩ \) towards its target value \( |t⟩ \) along the geodesic connecting the two.

Let the initial angle between \( |s⟩ \) and \( |t_⊥⟩ \) be \( \theta \). Fig.1 depicts how a state \( |k⟩ \) in the \( |t⟩ - |s⟩ \) subspace transforms under the action of the two operators, \( U_t \) and \( -U_s \). When the angle between \( |k⟩ \) and \( |t_⊥⟩ \) is \( \phi \), one application of \( U_t \) changes it to \( -\phi \), and one application of \( (-U_sU_t) \) changes that to \( \phi + 2\theta \). Thus the quantum state rotates at a uniform rate of \( 2\theta \) per query in the direction \( |t_⊥⟩ \rightarrow |t⟩ \). It is easy to figure out that the eigenvalues of the rotation operator \( G \) are \( e^{\pm 2i\theta} \), and the corresponding eigenvectors are \((1, \pm i)/\sqrt{2}\) in the \((|t⟩, |t_⊥⟩)\) basis.

![Figure 1: The steps of the quantum database search algorithm as rotations in the plane formed by the states |s⟩ and |t⟩. The angle θ is defined by the relation ⟨t|s⟩ = sin θ.](image)

Clearly, successive applications of \( G \) to \( |s⟩ \) change the angle from \( \theta \) to \( 3\theta, 5\theta, 7\theta, 9\theta, \ldots \). We obtain the result in Eq.(5), noting that the initial angle is determined by

\[ \sin \theta = ⟨t|s⟩ = 1/\sqrt{N}, \]

and the total desired rotation after \( Q \) queries is \( \pi/2 - \theta \). In general, \( \pi/2 \) is not an odd-integral multiple of \( \theta \). Then the best approximation to the desired state is obtained by running the algorithm till the quantum state gets within angle \( \theta \) of \( |t⟩ \). Note that to obtain the optimal solution, one has to know precisely when to stop the algorithm, i.e. the value of \( Q \) (or equivalently \( N \)) should be known apriori. In case \( N \) is known only in order of magnitude and not precisely, one can stop the algorithm randomly after \( O(\sqrt{N}) \) queries. Since the iterative algorithm rotates the state at a uniform rate in the \( |t⟩ - |s⟩ \) subspace, the success probability over a number of random attempts is \( (\sin^2 \phi) = 1/2 \). That is still much larger than the initial value \( 1/N \) and only a factor of two worse than the best result.
This picture makes it clear that the algorithm is optimal, i.e. it proceeds along the shortest geodesic path and takes the largest possible steps (operators other than reflection operators would produce rotation angle less than $2\theta$). No other algorithm, classical or quantum, can locate the desired object in an unsorted database with a fewer number of queries [6, 7].

### 3.2 The Smallest Solution

It is also interesting to visualise the evolution of amplitudes in case of the smallest solution to Eq.(5). This solution is exact and corresponds to locating the desired item in a database of four items with a single query. It is quite a contrast to the classical case, where a single binary query can distinguish only two items. Fig.2 illustrates how the evolution operators change various amplitudes in the 4-dimensional Hilbert space. The algorithm amplifies the desired amplitude and eliminates the unwanted amplitudes, by a clever interference amongst them. Note that this is possible only when the amplitudes have both positive and negative values—a characteristic wave feature that is absent in Boolean logic operations. Thus the algorithm illustrates a quantum amplification process, where the desired amplitude grows at the expense of the rest. This internal rearrangement of amplitudes is unusual, in stark contrast to conventional amplifiers that require the help of an external energy source.

![Figure 2: The steps of the quantum database search algorithm for the simplest case of 4 items, when the first item is desired by the oracle. The left column depicts the amplitudes along the 4 basis vectors, with the dashed lines showing their average values. The middle column describes the algorithmic steps, and the right column mentions their physical implementation in the wave language.](image)

### 3.3 Salient Features

There are several noteworthy features of this algorithm:

- The iterative steps of the algorithm can be viewed as the discretised evolution of the quantum state in the Hilbert space, governed by a Hamiltonian containing two terms, $|t\rangle\langle t|$ and $|s\rangle\langle s|$. The former represents a potential energy attracting the state towards $|t\rangle$, while the latter represents a kinetic energy isotropically diffusing the state throughout the Hilbert space [8]. The alternate application of $U_t$ and $U_s$ in the discretised evolution steps is then reminiscent of Trotter’s formula, generated by exponentiating the terms in the Hamiltonian when constructing the the transfer matrix from a discretised path integral.

- Asymptotically, $Q = \pi\sqrt{N}/4$. The best that the classical algorithms can do is to random walk through all the possibilities, and that produces $Q = O(N)$ as mentioned above. With the use of superposition of all possibilities at the start, the quantum algorithm performs a directed walk along the geodesic to the final result and achieves a square-root speed-up. Rather rarely one comes across such truly optimal algorithms.

- It is easy to see that the result in Eq.(5) depends only on $|t\langle s|$ and not on $\langle t|s$. The phases of various components of $|s\rangle$ can therefore be arbitrary (e.g. they can have the symmetry of bosons, fermions or even anyons). The starting point of the algorithm can therefore be generalised from the state with all amplitudes equal to the state with all probabilities equal.
• It is straightforward to convert the algorithm to the situation where there are \( M \) marked items in the database instead of just one. Then \( |t\rangle \) is replaced by \( \sum_{k=1}^{M} |t_k\rangle/\sqrt{M} \), and the algorithm yields one of the marked items after \( O(\sqrt{N/M}) \) queries.

• In case the quantum database permits factorised queries, i.e. inspection of one letter of the item label at a time, the algorithm can be speeded up just as in the classical situation. Mere digitisation of item labels is sufficient for efficient search, however, sorting becomes redundant with the quantum superposition of states. Since a single quantum query can distinguish one of four items, the factorised quantum search algorithm can locate the desired item with \( \log_4 N \) queries. This is a factor of two improvement on the best classical algorithm applied to a sorted database [9].

• Applicability of the algorithm has been extended to the much wider context of amplitude amplification [10]. In this case, the state \( |s\rangle \) is replaced by \( V|s\rangle \), where \( V \) is any unitary operator. The overlap \( \langle t|s\rangle \) then gets replaced by \( \langle t|V|s\rangle \), and the operator \( U_s \) gets replaced by \( VU_sV^{-1} \). This generalised algorithm amplifies the initial probability \( |V_{ts}|^2 \) towards unity, and can be used to improve the situation where \( V \) is another algorithm with a small success probability.

• The algorithm does not require the full power of quantum dynamics. It only needs superposition of states and interference of amplitudes. So it can very well be implemented using any system—not necessarily quantum—that obeys the superposition principle. For example, explicit examples using classical waves in the form of coupled oscillators have been constructed [11, 12]. In such mechanical systems, the role of the uniform superposition state \( |s\rangle \) is played by the centre-of-mass mode. Fig.2 also describes the individual steps of the algorithm in the wave language. The number of queries required in the wave scenario and in the quantum case is the same. The difference is that to represent \( N \) items of the database one requires \( N \) wave modes but only \( \log_2 N \) qubits.

• The quantum algorithm for searching an unsorted database does not assume any specific structure or pattern as far as the input data are concerned. This makes it highly versatile with broad utility. The algorithm has been incorporated, either in full or in part, in the quantum solutions of a variety of problems. Some of such applications are: square-root speed-up of solutions to NP-complete problems, finding mean and median of statistical distributions, locating minimum of a function, quantum counting, deciphering cryptographic codes, and so on. Details can be found in the literature [13, 14].

• The solutions of Eq.(5) for \( Q = 1, 2, 3, \) viz. \( N = 4, 10, 5, 20, 2 \) respectively, are of special significance for the number of building blocks involved in genetic information processing [15, 16]. Living organisms generally do not have access to desired biomolecules in a ready-made form. They first break down the ingested food into small building blocks, and then assemble the pieces in a precise manner to synthesise the desired biomolecules. The desired pieces are selected by pattern recognition binary oracles (i.e. whether correct molecular bonds will be formed or not) provided by the master template available in DNA. Such assembly processes follow the unsorted database search algorithm with factorised queries.

The DNA alphabet has four letters identified by a single base-pairing, and the amino acid alphabet has twenty letters identified by three consecutive base-pairings. Both these languages are universal, i.e. the same all the way from viruses and bacteria to human beings. The numbers involved fit Grover’s algorithm, and not the powers of two associated with the classical binary search. The binary alphabet is certainly simpler, and hence likely to appear earlier during evolution. So did the living organisms evolve more complicated genetic languages because of the advantage offered by Grover’s optimal algorithm? That is a tantalising possibility which can explain the unanswered mystery at the origin of life—why do genetic languages have the structure that they do?—not as an accident of history but as the optimal solution to the implemented task.

4 The Spatial Search Problem

It can happen that the items belonging to a physical database are spread over distinct locations instead of being in one place, and one still needs to find the desired item among them. When there is a restriction that one can proceed from any location to only its neighbours, while inspecting the unsorted items, we have the spatial search problem. This problem is conveniently represented using a graph, with the vertices denoting the locations of items and the edges labeling the connectivity of neighbours. Boolean algorithms for this problem are \( O(N) \), since they can do no better than inspect one location after another until reaching the desired item. Grover’s algorithm illustrates that one can do better in search problems by working with a superposition of states, but it uses the global operator \( U_s \), with the property \( \langle j|U_s|i\rangle = -2/N \) for any \( i \neq j \). That is tantamount to moving between any two locations, not just neighbours, with equal ease. To solve spatial search problems, therefore, we need to investigate algorithms where the operator \( U_s \) is replaced by a local operator that connects only neighbouring
locations. The scaling behaviour of such algorithms is expected to depend on the database size $N$ as well as the connectivity of the graph.

Working with a regular graph (i.e., the same number of neighbours for every vertex) keeps the problem tractable. In fact, most investigations of spatial search problems have been carried out on hypercubic lattices, where the dimensionality $d$ specifies the connectivity of the graph. In this geometry, $N = L^d$ and each vertex has $2d$ neighbours. Grover’s algorithm can then be looked up on as the $d \to \infty$ limit, i.e., the mean-field-theory limit of statistical mechanics where any vertex is a neighbour of any other one. Furthermore, by varying both $N$ and $d$ independently, we can develop a broad picture of how the dimension of the database influences the scaling behaviour of the spatial search problem, and how various limits are approached.

Complexity of quantum spatial search on a hypercubic lattice obeys two simple lower bounds. One arises from the fact that while the marked vertex could be anywhere on the lattice, a local step can move from any vertex to only its neighbours. Since the marked vertex cannot be located without reaching it, the worst case scenario requires $\Omega(dL)$ steps. This bound weakens with increasing $d$, and is the strongest in one dimension where a quantum algorithm cannot improve on the $O(N)$ classical algorithm. The other bound follows from the fact that spatial search cannot outperform Grover’s optimal algorithm, which has no restriction on movement. Quantum spatial search therefore must require $\Omega(\sqrt{N})$ oracle queries. This bound is independent of $d$, and stronger than the first bound for $d > 2$. Combined together, the two bounds make the complexity of quantum spatial search $\Omega(dN^{1/d} \sqrt{N})$. Note that the two bounds are of the same magnitude, $\Omega(\sqrt{N})$, for the critical case of $d = 2$.

The way these lower bounds arise in spatial search illustrates an interplay of two distinct physical principles, special relativity (or no faster than light signalling) and unitarity. The locality constraint on movement is the result of the finite propagation speed in relativity. On the other hand, the optimality of Grover’s algorithm is a consequence of unitarity [6, 7]. It is known that the two principles are compatible, although just barely, and so the best spatial search algorithms should arise in a framework that respects both the principles, i.e. relativistic quantum mechanics.

The concepts of critical phenomena in statistical mechanics turn out to be useful in understanding the scaling behaviour of spatial search algorithms in different dimensions: (i) Universality of scaling suggests that the scaling exponents depend on the dimensionality of the database but not on further details of graph connectivity. (ii) Increasing the number of neighbours for a vertex makes the local movement restriction less relevant and takes the system toward its mean-field-theory limit. (Note that the maximum value of $d$ is $\log_2 N$ for finite $N$.) (iii) Interplay of different dynamical features produces logarithmic correction factors in critical dimensions due to infrared divergences. Indeed, spatial search algorithms in $d = 2$ are slowed down by extra logarithmic factors, whose suppression by clever algorithm design (including use of additional parameters) is an interesting exercise.

We point out that preparation of the unbiased initial state for the quantum spatial search problem, i.e., preparation of the translationally invariant uniform superposition state $|s\rangle = \sum_x |\vec{x}\rangle/\sqrt{N}$, does not add to the complexity of the problem. $|s\rangle$ can easily be prepared using local directed steps. For instance, one can start at the origin, then step by step transfer the amplitude to the next vertex along an axis, and achieve an amplitude $L^{-1/2}$ at all the vertices on the axis after $L$ steps. Thereafter, repeating the procedure for each remaining coordinate direction produces the state $|s\rangle$ after $dL$ steps in total. This cost is smaller than the lower bounds on quantum spatial search mentioned above.

5 Quantum Random Walk Based Solution

We follow Grover’s quantum algorithmic strategy for spatial search as well, i.e., construct a Hamiltonian evolution where the kinetic part of the Hamiltonian diffuses the amplitude distribution all over the lattice and the potential part of the Hamiltonian attracts the amplitude distribution toward the marked vertex [8]. The change is that we have to replace the global evolution operator $U_s$ (corresponding to the kinetic part of the Hamiltonian) by a local movement operator $W$, and then optimise $W$ to achieve the fastest diffusion [17]. The typical discrete method for exploring an unstructured space, with the constraint of local movements, is random walk. In the “particle” form, that is a diffusion process which spreads according to $\text{distance} \propto \sqrt{\text{time}}$. On the other hand, a coherent “wave” form can spread faster according to $\text{distance} \propto \text{time}$, and we certainly want to use that in a quantum algorithm.

Classical random walks evolve the given probability distribution in a non-deterministic manner at every time step. They have been used to tackle a wide variety of graph theory problems, usually with a local and translationally symmetric evolution rule. We use a quantum version of this process, i.e. quantum random walks [18]. It provides a unitary evolution of the quantum amplitude distribution, such that the amplitude at each vertex gets redistributed over itself and its neighbours at every time step. Quantum random walks are deterministic, unlike classical random walks, with quantum superposition allowing simultaneous exploration of multiple possibilities. Several quantum algorithms have used them as important ingredients, and an introductory overview can be found in Ref.[19].
The spatial propagation modes of a quantum random walk are characterized by their wave vectors $\vec{k}$. Quantum diffusion depends on the energy of these modes according to

$$U(\vec{k}, t) = \exp(-iE(\vec{k})t) .$$

The lowest energy mode, $\vec{k} = 0$, corresponding to a uniform distribution, is an eigenstate of the diffusion operator and does not propagate. The slowest propagating modes are the ones with the smallest nonzero $|\vec{k}|$. The commonly used diffusion operator is the Laplacian, e.g. it appears in the non-relativistic Schrödinger equation. That gives $E(\vec{k}) \propto |\vec{k}|^2$ corresponding to the distance $\propto \sqrt{\text{time}}$ spread. On the other hand, the relativistic massless Dirac operator has the dispersion relation $E(\vec{k}) \propto |\vec{k}|$ corresponding to the distance $\propto \text{time}$ spread. Its quadratically faster diffusion of the slowest modes makes it better suited to quantum spatial search algorithms [20, 21].

### 5.1 Spatial Search with the Dirac Operator

An automatic consequence of the Dirac operator is the appearance of an internal degree of freedom corresponding to spin, whereby the quantum state becomes a multi-component spinor. These spinor components can guide the wavefunction to spin, whereby the quantum state becomes a multi-component spinor. These spinor components can guide the search. Just as in Grover’s algorithm, the largest potential evolution step corresponds to making the evolution phase change of $(\pi/2)$. The search algorithm is completed by alternating the kinetic evolution step with the potential evolution step.

The Dirac Hamiltonian in the continuum theory is well-known, and we need to construct a discrete time evolution operator corresponding to its kinetic part. Note that even when the Hamiltonian $H$ is local, the associated unitary evolution operator $U = \exp(-iH\tau)$ may connect arbitrarily far apart vertices. To make $U$ also local, we split $H$ in to block-diagonal Hermitian parts and then exponentiate each part separately [23]. For a bipartite lattice, partitioning of $H$ in to two parts (which we label “odd” and “even”) is sufficient for this purpose:

$$H = H_o + H_e .$$

Each part then contains all the vertices, but only half of the links attached to each vertex. Each link is associated with a term in $H$ providing propagation along it, and appears in only one of the two parts. On a hypercubic lattice, $H$ gets divided in to a set of non-overlapping blocks of size $2^d \times 2^d$ (each block corresponds to an elementary hypercube) that can be exactly exponentiated. After this bipartite decomposition, we let the quantum random walk evolve according to

$$\psi(\vec{x}; t) = W^t\psi(\vec{x}; 0) , \quad W = U_e U_o = e^{-iH_o\tau} e^{-iH_e\tau} .$$

Each block of the unitary matrices $U_{o(e)}$ mixes amplitudes of vertices belonging to a single elementary hypercube, and the amplitude distribution spreads in time because the two alternating matrices do not commute. Note that $W$ does not perform evolution according to $H$ exactly. Instead, $W = \exp(-iH\tau) + O(\tau^2)$. Still, the truncation is such that $W$ is exactly unitary, i.e. $W = \exp(-iH\tau)$ for some $H$.

The search algorithm is completed by alternating the kinetic evolution step with the potential evolution step. Just as in Grover’s algorithm, the largest potential evolution step corresponds to making the evolution phase change maximally different from 1. That is the binary oracle reflection operator,

$$R = I - 2|0\rangle\langle 0| ,$$

when the marked vertex is chosen to be the origin. Thus the spatial search algorithm evolves the amplitude distribution according to

$$\psi(\vec{x}; t_1, t_2) = [W^{t_1}R]^{t_2}\psi(\vec{x}; 0, 0) .$$

Here $t_2$ is the number of oracle queries, and $t_1$ is the number of quantum random walk steps between queries. Both should be minimised to find the quickest solution to the spatial search problem.

Grover’s algorithm is designed to evolve the quantum state in the two-dimensional subspace spanned by the initial and the desired states. It strides along the geodesic arc from $|s\rangle$ to $|0\rangle$ perfectly, and reaches the marked vertex with the maximum probability $P_{\text{max}} = 1$. That does not hold for spatial search. The amplitude distribution evolving with a local operator $W$ (instead of the global operator $U_o$) does not remain fully confined to the two-dimensional subspace. The maximum probability to reach the marked vertex is therefore reduced, $P_{\text{max}} < 1$. The remedy is to augment the algorithm by the amplitude amplification procedure [10], and reach the marked vertex with $\Theta(1)$ probability. The complexity of the algorithm then increases to the effective number of oracle queries, $t_2/\sqrt{P_{\text{max}}}$.
To obtain the best results, one can tune parameters such that \( W^{t_1} \) approximates \(-U_s\) as closely as possible, i.e. maximise the overlap \( Tr(-W^{t_1}U_s)\). This condition can be recast as the minimisation of \( \langle \vec{0}|W^{t_1}|\vec{0}\rangle \), which is the quantum random walk amplitude to return to the starting point. In practice, this has to be performed numerically, depending on the parameters appearing in \( W^{t_1} \).

5.2 Numerical Results

We have performed numerical simulations of the quantum spatial search algorithm in various dimensions \([25, 26, 27]\), as per the theoretical considerations described above, and observed the following:

- For large values of \( t_1 \), the amplitude distribution diffuses too much out of the two-dimensional subspace, and the algorithm fails to reach the marked vertex with any meaningful probability. The best results for complexity as well as total computational cost are obtained with \( t_1 = 2 \) or 3.

- The eigenvalues of \( U_s \) are \( \pm 1 \), while those of \( W \) are spread around the unit circle. We find that, with optimal tuning of the parameters, \( W^{t_1} \) approximates \(-U_s\) in the average sense, i.e. \( W^{t_1} \) is a reflection operator for the average eigenvalue of the associated \( \tilde{H}^2 \). Appearance of the average eigenvalue in this result indicates that all spatial modes contribute to the search process with roughly equal strength.

- For \( d > 2 \), the optimised quantum spatial search algorithm has the same scaling behaviour as Grover’s algorithm. As \( N \to \infty \), \( P_{\text{max}} \) approaches a constant and \( t_2 \) is proportional to \( \sqrt{N} \). The locality restriction on movement does not matter much, and the slow down with respect to Grover’s optimal algorithm is only in the scaling prefactor. Looking at it differently, the square-root speed-up provided by relativity (through change in dispersion relation) is perfectly compatible with that provided by unitarity.

- With increasing \( d \), the prefactor in complexity scaling approaches its optimal value \( \pi/4 \). Moreover, we can get pretty close to the optimal value for all \( d > 2 \). In particular, the scaling prefactor for \( d = 3 \) exceeds \( \pi/4 \) by about 25\%, and that for \( d = 7 \) by about 10\%. The approach to the asymptotic scaling behaviour as a function of \( d \) is illustrated in Fig.3, where \( N \) is changed by keeping \( L \) fixed and changing \( d \). It can also be seen that for fixed \( N \), it is best to implement the algorithm using the smallest \( L \) and hence the largest \( d \).

![Figure 3: Effective number of oracle queries as a function of the database size for \( d = 3 \) to 9 and different lattice sizes. The points are the data for \( t_1 = 3 \), and the curves are the fits \( t_2/\sqrt{NP} = a + b/d \). Also shown is the limiting value corresponding to Grover’s optimal algorithm.](image)

- For \( d \leq 2 \), the evolution operator arising from the massless Dirac operator is infrared divergent (as \( \int d^dk/k^2 \) in the continuum formulation). That slows down spatial search algorithms, altering the behaviour of both \( P_{\text{max}} \) and \( t_2 \) compared to their optimal scaling forms, by logarithmic factors in the critical dimension \( d = 2 \) and by power law factors in \( d < 2 \). In particular, the infrared divergence causes the amplitude distribution to evolve too much out of the two-dimensional subspace, and the maximum probability to reach the marked vertex plummets to zero as the database size increases. One way to regulate the infrared divergence is to introduce a non-zero mass term in the Dirac operator. That regulates the infrared divergence through \( k^2 \to k^2 + m^2 \), but also slows down the diffusion process. For small enough \( m \), the diffusion speed (and
hence $t_2$ may not change much, but substantial change in the contribution of the $|\vec{k}| \leq m$ modes can modify the scaling of $P_{\text{max}}$. Then an optimal value of $m$ can be obtained by trading off the increase in $t_2$ against the increase in $P_{\text{max}}$. For a finite lattice, the lattice size acts as the infrared cutoff, and so we expect the optimal value of $m$ to be a function of the database size $N$.

- Tulsi constructed an infrared regulated spatial search algorithm possessing the above described properties [24]. In his algorithm the $R$ and $W$ operations are controlled by an ancilla qubit such that the quantum walk pauses (i.e. misses some $W$ steps) when it passes through the marked vertex. This concentration of the quantum walk at the marked vertex can also be looked up on as the appearance (only at the marked vertex) of an effective mass in the propagator or a self-loop in the evolution graph. The effect is controlled by a mixing parameter $\cos \delta$ ($\cos \delta = 1$ means no pausing). Tulsi showed that for $\cos \delta = \Theta(1/\sqrt{\ln N})$, the amplitude concentration at the marked vertex cuts down the amplitude diffusion out of the two-dimensional subspace, and increases $P_{\text{max}}$ to $\Theta(1)$ without affecting the scaling of $t_2$.

- The scaling behaviour of the infrared regulated quantum spatial search algorithm in $d = 2$ is illustrated in Fig.4. Our best result for the complexity is $t_2/\sqrt{P} \approx 0.45 \sqrt{N \log_2 N}$.

![Figure 4: Effective number of oracle queries as a function of the database size for $d = 2$. The points are the data for $t_1 = 3$ and different values of the ancilla control parameter $\cos \delta$. The curves are the fits $t_2/\sqrt{PN \log_2 N} = a + b/L$.](image)

- Scaling behaviour of spatial search algorithms in non-integer dimensions can be studied using fractal lattices. That is useful for understanding the complexity scaling bounds, particularly for $1 < d < 2$, and testing the analogy with critical phenomena in statistical mechanics. Fractal lattices do not have translational invariance or a definition of the Dirac operator. Nevertheless, relativistic diffusion can be produced on regular lattices using the flip-flop operator [20]. Our numerical results for the infrared regulated algorithm on Sierpinski gaskets show that the complexity does scale as $N^{1/d}$, where $d$ is the spectral dimension (i.e. the dimension of the reciprocal lattice modes $\vec{k}$) and not the fractal (i.e. Hausdorff) dimension.

- The spatial search algorithm with a trap at the marked vertex has a potential application in understanding dynamics of photosynthesis. Light harvesting complexes of photosynthetic organisms have energy transport efficiency exceeding 95%, and the exciton motion is experimentally found to be quantum coherent for more than 400 fs [28, 29]. The complex consists of a reaction centre surrounded by light absorbing pigment molecules in an antenna structure. The energy of the absorbed photon is transported to the reaction centre in a wave motion, and has to remain there long enough till it is used in chemical reactions. The details of how this occurs without dissipation are still to be understood. But a coupled system of wave modes, in a specific geometry and with a trap at a particular location, can be a good model for understanding the phenomenon as an optimised solution.

6 Outlook

All known quantum algorithms are constructed in the SIMD paradigm, with the quantum parallelism superposing $N$ amplitudes using only $\log_2 N$ qubits. At its best, that can reduce the complexity of quantum algorithms...
compared to classical ones by a factor of $N/\log_2 N$. Efficient quantum algorithms also need factorisation of the unitary operations in the $N$-dimensional Hilbert space in to smaller blocks. That can also provide a speed-up of $O(N/\log_2 N)$ under the best circumstances. (With full factorisation, $N$ terms can be produced by multiplying $\log_2 N$ two-term factors.) Factorisation is however a classical computational procedure, and the advantage provided by it may or may not overlap with that provided by quantum parallelism. Efficiency of a quantum algorithm therefore depends on how these two features interplay.

In case of Shor’s solution to the period finding problem [3], complete classical factorisation converts the Fourier transform operation to FFT, yielding a speed-up of $O(N/\log_2 N)$. When FFT is converted to QFT, the quantum parallelism provides another non-overlapping gain of $O(N/\log_2 N)$. The result is a large separation between the classical and the quantum complexity of the problem. In the database search problem, gains of factorisation (i.e. sorting) and quantum parallelism overlap. So one cannot obtain two speed-up factors of $O(N/\log_2 N)$—the quantum factorised algorithm provides only a factor of two speed-up over the classical factorised algorithm. In case of Grover’s algorithm, the oracle is not factorised. That limits the gain that can be extracted from quantum parallelism, and only a square-root speed-up can be achieved. We do not know any systematic procedure to identify the problems amenable to both quantum parallelism and classical factorisation, and generic problems would have neither. Still, problems that possess both these features form an interesting hunting territory for efficient quantum algorithms, and we must explore that to come up with new quantum algorithms.

References

[1] J. von Neumann, *The Computer and the Brain*, (Yale University Press, 1958).

[2] R.P. Feynman, *There’s Plenty of Room at the Bottom*, Talk at the 1959 Annual Meeting of the American Physical Society, Published in Caltech’s Engineering and Science (1960).

[3] P. Shor, *Polynomial-time Algorithms for Prime Factorisation and Discrete Logarithms on a Quantum Computer*, SIAM J. Comp. 26 (1997) 1484, arXiv:quant-ph/9508027.

[4] L.K. Grover, *A Fast Quantum Mechanical Algorithm for Database Search*, Proceedings of the 28th Annual ACM Symposium on Theory of Computing, Philadelphia (1996), p.212, arXiv:quant-ph/9605043.

[5] D.E. Knuth, *The Art of Computer Programming, Vol.3: Sorting and Searching*, Second Edition, (Addison-Wesley, 1998).

[6] C. Bennett, E. Bernstein, G. Brassard and U. Vazirani, *Strengths and Weaknesses of Quantum Computing*, SIAM J. Comput. 26 (1997) 1510, arXiv:quant-ph/9701001.

[7] C. Zalka, *Grover’s Quantum Searching Algorithm is Optimal*, Phys. Rev. A60 (1999) 2746, arXiv:quant-ph/9711070.

[8] L. Grover, *From Schrödinger’s Equation to the Quantum Search Algorithm*, Pramana 56 (2001) 333, arXiv:quant-ph/0109116.

[9] A. Patel, *Quantum Database Search can do without Sorting*, Phys. Rev. A64 (2001) 034303, arXiv:quant-ph/0012149.

[10] G. Brassard, P. Hoyer, M. Mosca and A. Tapp, *Quantum Amplitude Amplification and Estimation*, AMS Contemporary Mathematics Series Vol. 305, Eds. S.J. Lomonaco and H.E. Brandt, (AMS, 2002), p.53, arXiv:quant-ph/0005055.

[11] L.K. Grover and A. Sengupta, *From Coupled Pendulums to Quantum Search*, in *Mathematics of quantum computation*, Eds. R.K. Brylinski and G. Chen, (CRC press, 2002), arXiv:quant-ph/0109123.

[12] A. Patel, *Optimal Database Search: Waves and Catalysis*, Int. J. Quant. Inform. 4 (2006) 815; Erratum ibid. 5 (2007) 437, arXiv:quant-ph/0401154.

[13] See for example: M.A. Nielsen and I.L. Chuang, *Quantum Computation and Quantum Information*, (Cambridge University Press, 2000).

[14] Most of the articles on the subject of quantum computation are available at the e-print web archive, http://arXiv.org/, under the category quant-ph.

[15] A. Patel, *Quantum Algorithms and the Genetic Code*, Pramana 56 (2001) 367, arXiv:quant-ph/0002037.
[16] A. Patel, Towards Understanding the Origin of Genetic Languages, Chapter 10 in Quantum Aspects of Life, Eds. D. Abbott, P.C.W. Davies and A.K. Pati, (Imperial College Press, 2008), p.187, arXiv:0705.3895.

[17] N. Shenvi, J. Kempe and K. Birgitta Whaley, A Quantum Random Walk Search Algorithm, Phys. Rev. A67 (2003) 052307, arXiv:quant-ph/0210064.

[18] Y. Aharonov, L. Davidovich and N. Zagury, Quantum Random Walks, Phys. Rev. A48 (1993) 1687.

[19] J. Kempe, Quantum Random Walks: An Introductory Overview, Contemporary Physics 44 (2003) 307, arXiv:quant-ph/0303081.

[20] A. Ambainis, J. Kempe and A. Rivosh, Coins Make Quantum Walks Faster, Proceedings of ACM-SIAM SODA’05, (ACM Press, 2005), p.1099, arXiv:quant-ph/0402107.

[21] A.M. Childs and J. Goldstone, Spatial Search and the Dirac Equation, Phys. Rev. A70 (2004) 042312, arXiv:quant-ph/0405120.

[22] L. Susskind, Lattice Fermions, Phys. Rev. D16 (1977) 3031.

[23] A. Patel, K.S. Raghunathan and P. Rungta, Quantum Random Walks do not need a Coin Toss, Phys. Rev. A71 (2005) 032347, arXiv:quant-ph/0405128.

[24] A. Tulsi, Faster Quantum-walk Algorithm for the Two-dimensional Spatial Search, Phys. Rev. A78 (2008) 012310, arXiv:0801.0497.

[25] A. Patel and Md.A. Rahaman, Search on a Hypercubic Lattice using a Quantum Random Walk: I. d > 2, Phys. Rev. A82 (2010) 032330, arXiv:1003.0065.

[26] A. Patel, K.S. Raghunathan and Md.A. Rahaman, Search on a Hypercubic Lattice using a Quantum Random Walk: II. d = 2, Phys. Rev. A82 (2010) 032331, arXiv:1003.5564.

[27] A. Patel and K.S. Raghunathan, Search on a Fractal Lattice using a Quantum Random Walk, (in preparation).

[28] G.S. Engel et al., Evidence for Wavelike Energy Transfer through Quantum Coherence in Photosynthetic Systems, Nature 446 (2007) 782.

[29] E. Collini et al., Coherently Wired Light-harvesting in Photosynthetic Marine Algae at Ambient Temperature, Nature 463 (2010) 644.