Generalized quantum search Hamiltonian

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There are Hamiltonians that solve the search problem of finding one of N items in $O(\sqrt{N})$ steps. These are Hamiltonians describing an oscillation between two states. In this paper we propose a generalized search Hamiltonian H_g. Then the known search Hamiltonians become special cases of H_g. For the generalized search Hamiltonian, we present the remarkable result that searching with 100% success is subject only to the phase factor in H_g and independent of the number of states or initialization.

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Grover proposed the quantum search algorithm that finds one of N unsorted items in $O(\sqrt{N})$ steps [1]. Since it is known that classical search algorithms take $O(N)$ steps to solve a search problem, the quadratic speedup in the Grover algorithm is remarkable. The reason for the speedup is the result of quantum mechanics. To apply quantum mechanics to a search problem, each item needs to be mapped to a state in N-dimensional Hilbert space. Then the search problem can be transformed to finding one of N states. We can use quantum mechanical characteristics, for instance, superposition and parallelism. The Grover algorithm in fact finds the state that corresponds to a target item. An iteration of the Grover algorithm is composed of two operations: the first is to flip the target state about 0 and the next to invert all states about the average state [2]. An oracle, the heart of the quadratic speedup, is applied in the first operation. Grover iterations amplify the amplitude of the target state to be nearly one in $O(\sqrt{N})$ times, when the initial state is a uniform superposition of N states. Zalka showed that the Grover algorithm is optimal when unstructured items are considered [3].

On the other hand, there are search algorithms based on Hamiltonian evolution via the Schrödinger equation. While the Grover algorithm operates on a state in discrete time, a search Hamiltonian operates on a state in continuous time. These are Hamiltonians describing an oscillation between two states. Farhi and Gutmann suggested a harmonic-oscillation Hamiltonian, exactly $H_{fa}=E(|w\rangle\langle w|+|s\rangle\langle s|)$, where $|w\rangle$ is a target state and $|s\rangle$ is an initial state [4]. Fenner provided another Hamiltonian, $H_{fe}=2iEx(|w\rangle\langle\psi|-|\psi\rangle\langle w|)$, where x is the overlap between an initial state and a target state, i.e., $\langle w|s\rangle=x(>0)$ [5]. A state under these Hamiltonians evolves from an initial state to a target state in the half period of oscillation $O(\sqrt{N})$. This oscillation is a process to amplify the amplitude of a target state. It is noted that the initial state should be prepared as a superposition of all states, since one of the initially superposed states becomes the target state via the Hamiltonian evolution.

We expect that there exists a more general search Hamiltonian including the known Hamiltonians. We then write down a possible combination of a target state and an initial state as follows:

$$H=E(a|w\rangle\langle w|+b|w\rangle\langle s|+c|s\rangle\langle w|+d|s\rangle\langle s|).$$

The initial state can be written as $|s\rangle=x|w\rangle+\sqrt{1-x^2}|r\rangle$, where $|r\rangle$ is the state orthogonal to the target state (so $\langle w|r\rangle=0$) and x is the overlap between the initial state and the target state, i.e., $x=\langle w|s\rangle$. The Hamiltonian and the initial state can be written in matrix representation:

$$\mathbf{H}=\mathbf{E}\begin{pmatrix} a+(b+c)x+dx^2 & (b+dx)\sqrt{1-x^2} \\ (c+dx)\sqrt{1-x^2} & d(1-x^2) \end{pmatrix},$$

$$|\mathbf{s}\rangle=\begin{pmatrix} x \\ \sqrt{1-x^2} \end{pmatrix}.$$

The state $|\psi(t)\rangle$ is governed by the time-dependent Schrödinger equation

$$i\frac{d}{dt}|\psi(t)\rangle=H|\psi(t)\rangle,$$

where the initial condition is $|\psi(t=0)\rangle=|s\rangle$ (we let $\hbar=1$ for convenience). At time t, the probability of finding the target state is

$$P=|\langle w|e^{-iHt}|s\rangle|^2=x^2\cos^2 EDt+CC^*\sin^2 EDt, \quad (1)$$

where

$$q=\tfrac{1}{2}[(a+d)+(b+c)x],$$

$$D=\sqrt{q^2-(ad-bc)(1-x^2)},$$

and

$$C=\left[\frac{(d(1-x^2)-q)^2+x(c+dx)(d(1-x^2)-q)-D^2}{(c+dx)D}\right].$$

The postulate of quantum mechanics that any observable should be Hermitian requires that $H=H^\dagger$. Then we obtain the results that (1) a and d are real; and (2) $b=c^*=re^{i\phi}$, where r and ϕ are real.

Suppose the initial state is a uniform superposition of all states and we read out the final state at time T. In Eq. (1), the contribution of $x^2\cos^2 EDT$ to the probability is so small that it can be neglected. Moreover, $x^2\cos^2 EDT$ becomes zero at

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time T, since the readout time T comes from $EDT=\pi/2$. We find that $T=O(\sqrt{N})$, where the quadratic speedup is shown. Thus it is essential to make the value of C^*C as large as possible, to find the target state with high probability at time T:

$$P=CC^*=\frac{u_0+u_1x+u_2x^2+u_3x^3+u_4x^4+u_5x^5+u_6x^6}{l_0+l_1x+l_2x^2+l_3x^3+l_4x^4}, \tag{2}$$

$$\begin{aligned}
u_0&=r^4,\\
u_1&=(a+3d)r^3\cos\phi,\\
u_2&=\frac{1}{4}r^2[a^2+6ad+9d^2-4r^2+4(ad+d^2+r^2)\cos 2\phi],\\
u_3&=\frac{1}{2}dr\cos\phi(a^2+4ad+3d^2-4r^2+4r^2\cos 2\phi),\\
u_4&=\frac{1}{4}[a^2d^2+2ad^3+d^4-4d^2r^2+2r^4+(4d^2r^2\\
&\quad-2r^4)\cos 2\phi],\\
u_5&=2dr^3\cos\phi\, sin^2\phi,\\
u_6&=d^2r^2\sin^2\phi,\\
l_0&=\frac{1}{4}(a^2r^2-2adr^2+d^2r^2+4r^4),\\
l_1&=\frac{1}{2}r(a^2d-2ad^2+d^3+2ar^2+6dr^2)\cos\phi,\\
l_2&=\frac{1}{4}[a^2d^2+d^4+8d^2r^2-2r^4-2a(d^3-4dr^2)+2r^2(2ad\\
&\quad+2d^2+r^2)\cos 2\phi],\\
l_3&=dr\,cos\,\phi(3ad+d^2-r^2+r^2cos\,2\phi),\\
l_4&=\frac{1}{2}d^2(2ad-r^2+r^2cos\,2\phi).
\end{aligned} \tag{3}$$

In Eq. (2), to consider the zeroth order terms of x, u_0, and l_0, is crucial. Thus we obtain the condition $a=d$ by setting $u_0=l_0$, which automatically gives $u_1=l_1$. Under the condition $a=d$, the probability becomes

$$P_g=1-O(x^2). \tag{4}$$

The corresponding Hamiltonian is

$$H_g=E_1(|w\rangle\langle w|+|s\rangle\langle s|)+E_2(e^{i\phi}|w\rangle\langle s|+e^{-i\phi}|s\rangle\langle w|), \tag{5}$$

where $E_1=Ea$ and $E_2=Er$. The probability of getting the target state under this Hamiltonian is not exactly but is nearly 1. Therefore it is allowed to use the Hamiltonian H_g when 100% success of searching is not required.

We here pursue the condition for higher probability, which is $l_2=u_2$. It makes us choose a specific phase, $\phi=n\pi$. This automatically gives the useful relations $l_3=u_3, l_4=u_4$, and $u_5=u_6=0$. Then the probability under these relations is

$$P_p=\frac{u_0+u_1x+u_2x^2+u_3x^3+u_4x^4}{u_0+u_1x+u_2x^2+u_3x^3+u_4x^4}=1.$$

The Hamiltonian is

$$H_p=E_1(|w\rangle\langle w|+|s\rangle\langle s|)\pm E_2(|w\rangle\langle s|+|s\rangle\langle w|). \tag{6}$$

That is, the Hamiltonian H_p can search for a target state with probability 1.

We now have the generalized search Hamiltonian H_g, and the perfect search Hamiltonian H_p. H_p is in particular produced from H_g by fixing the phase $\phi=n\pi$. Here, we can show that known search Hamiltonians are special forms of H_g. For $E_2=0$, it becomes Farhi and Gutmann Hamiltonian, and Fenner's Hamiltonian for $E_1=0$, $\phi=\pi/2$, and $r=2x$. Moreover, we provide the additional quantum search Hamiltonian

$$H_{add}=E_2(e^{i\phi}|w\rangle\langle\psi|+e^{-i\phi}|\psi\rangle\langle w|). \tag{7}$$

When the Grover algorithm is applied to a search problem, the probability 1 appears if and only if two assumptions are satisfied: (1) the target items are $N/4$ among N items, and (2) the initial state is a uniform superposition of all states in the system. Here we present the remarkable result that the Hamiltonian H_p does not depend on the number of states and the initialization. There is no condition on H_p about the number of states or the initialization. This implies that H_p finds target states with probability 1 regardless of the number of target states, although the initial state is prepared as an arbitrary superposition of all states. When a generalized search Hamiltonian is used in a search problem, the probability 1 in readout procedure depends only on the phase condition.

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