

Computational leakage: Grover's algorithm with imperfections

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Abstract. We study the effects of dissipation or leakage on the time evolution of Grover's algorithm for a quantum computer. We introduce an effective two-level model with dissipation and randomness (imperfections), which is based upon the idea that ideal Grover's algorithm operates in a 2-dimensional Hilbert space. The simulation results of this model and Grover's algorithm with imperfections are compared, and it is found that they are in good agreement for appropriately tuned parameters. It turns out that the main features of Grover's algorithm with imperfections can be understood in terms of two basic mechanisms, namely, a diffusion of probability density into the full Hilbert space and a stochastic rotation within the original 2-dimensional Hilbert space.

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Recently, quantum computing has emerged as one of the most challenging fields of physics both for theoreticians and experimentalists (see Ref. [1] for a review). At the core of the theoretical side, a few quantum algorithms are now available, which can solve a certain class of problems faster than any available classical counterparts: for example, Shor's algorithm [2] factorizes a given large number N at $\sim (\log N)^2$ time steps with an exponential speed-up. Using Grover's algorithm (GA [3]), one can find a specific item on a long list of size N at $\sim \sqrt{N}$ time steps, which is a considerable gain in speed as compared with $\sim N$ in classical algorithms.

These quantum algorithms operate perfectly only on ideal quantum computers. On the other hand, a certain amount of dissipation or uncontrolled coupling to the environment is clearly inevitable on real quantum computers. For example, any deviation from ideal operation in quantum gates, which may result from various origins, including fluctuation in the excitation energies of two-level systems (qubits), can be considered as "imperfections". The imperfections will affect the efficiency of a quantum computer, and the operability of a given quantum algorithm may break down to the point of losing its advantage over a classical counterpart. Therefore, it is of vital importance to have a sound picture of how an error due to the presence of imperfections evolves in quantum algorithms. Obviously, a reasonable picture of the basic mechanisms given by the imperfections will be very crucial

in constructing an appropriate quantum error correction method [4–7].

In general, the quantum state in a quantum computer is essentially a many-body (or network) state, the time evolution of which is delicately controlled by a given quantum algorithm. From such a point of view, the study of imperfection effects on quantum algorithms would belong to a more general research field which investigates disorder effects on the dynamics of a many-body state. Their exact treatment is actually a complicated subject, and only a few results have been obtained giving either general frameworks for understanding the effects or general methodologies for calculation.

There exist several theoretical, mainly numerical, investigations in this direction. The main stress has been given, from a practical point of view, on the stability of quantum algorithms with respect to the presence of imperfections. Cirac and Zoller [8] reported that the operability of quantum computing is rather safe against disorders available in the quantum Fourier transform process. In references [9,10], the disorder effect in Shor's algorithm applied to the factorization of the number 15 was studied and by using the fidelity being defined as the square of the overlap of the actual quantum state with the ideal one, it was found that the operability of the Shor's algorithm can be destroyed due to a very small strength of the disorder in the modular exponentiation part [10]. More systematic results have recently been obtained in reference [11] from the study of quantum computing of quantum chaos and imperfection effects: by considering the presence of imperfections in the quantum Fourier transform, it was

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obtained that the imperfection strength scales polynomially with the number of qubits for the inverse participation ratio (IPR), which measures the strength of localization of quantum state and plays a role of the fidelity in reference [10]. Nevertheless, it still remains at a primitive stage regarding an understanding of basic mechanisms carried by the imperfections in quantum algorithms. So far, the main policy has been simply to watch a deviation of the quantum state from the ideal one and to analyze its parameter dependence.

In this paper, we investigate the time evolution of a state governed by Grover's algorithm with imperfections, with a main emphasis on an understanding of interplay of the imperfections with the algorithm operator. Based on the idea that the ideal GA operates in an effective 2-dimensional Hilbert space, a stochastic two-level model with dissipation will be introduced, and then its simulation results will be compared to those of the GA with imperfections, which operates in a larger relevant Hilbert space resulting from the presence of the imperfections. They are in a good agreement *via* an appropriate fit of parameters. An analytic solution of the two-level model is given with some modification and provides a comprehensive picture of imperfection effects on the GA.

Let us begin with a brief sketch of the GA. The final goal is to identify $|j\rangle$ (target state) among $N = 2^{n_q}$ quantum states, where n_q is the number of qubits. Initially, the state of quantum register is prepared as a superposition of all states with the same amplitude. The GA may be broken up into two steps:

- (i) rotation of phase of $|j\rangle$ by π
- (ii) and application of a diffusion operator D which is defined, in matrix form, as $D_{kl} = -\delta_{kl} + 2/N$ with $k, l = 0, 1, \dots, N-1$, and δ_{kl} denoting the Kronecker delta.

The step (ii) is achieved by applying the Hadamard operation to each single qubit and then performing a conditional phase shift on the computer with every computational basis state except $|k=0\rangle$ receiving a phase shift of -1 followed by the second Hadamard operation to each single qubit. Then, the quantum state during time evolution can be expressed as [12]

$$|\Psi(\vartheta)\rangle = \sin \vartheta |j\rangle + \frac{\cos \vartheta}{\sqrt{N-1}} \sum_{k \neq j} |k\rangle. \quad (1)$$

The initial state is characterized by $\vartheta = \vartheta_0$ with $\sin \vartheta_0 = 1/\sqrt{N}$. Each iteration transforms $|\Psi(\vartheta)\rangle$ into $|\Psi(\vartheta + \omega)\rangle$, where $\sin \omega = 2\sqrt{N-1}/N$. Then, after $m \approx (\pi/4)\sqrt{N}$ iterations, ϑ becomes very close to $\pi/2$, and a measurement of the state yields $|j\rangle$ with an error $O(1/N)$. We note that the evolution of $|\Psi(\vartheta)\rangle$ according to the GA is restricted to a 2-dimensional Hilbert space which is spanned by $|x\rangle = (1/\sqrt{N-1}) \sum_{k \neq j} |k\rangle$ and $|y\rangle = |j\rangle$. Each iteration represents a rotation of the quantum state by the angle ω in the x - y -plane and the Grover's operator for a

single iteration can be written in a familiar form

$$\hat{R}(\omega) = \begin{pmatrix} \cos \omega & -\sin \omega \\ \sin \omega & \cos \omega \end{pmatrix} \quad (2)$$

on the basis $\{|x\rangle, |y\rangle\}$.

Imperfections are introduced in the GA as follows: the ideal Hadamard operator in the step (ii) is given by $\mathbf{n} \cdot \hat{\boldsymbol{\sigma}}$, where $\mathbf{n} = (1/\sqrt{2}, 0, 1/\sqrt{2})$, and $\hat{\sigma}_{x(y,z)}$ denotes the Pauli spin matrix. We now replace \mathbf{n} by

$$\mathbf{m}_q = \frac{1}{\sqrt{2}} (\cos \varphi_q \sin \delta_q + \cos \delta_q, \sqrt{2} \sin \varphi_q \sin \delta_q, -\cos \varphi_q \sin \delta_q + \cos \delta_q), \quad (3)$$

where $q = 1, 2, \dots, n_q$ represent each single qubit. Here, δ_q and φ_q with $|\delta_q| < \epsilon/2$ and $0 \leq \varphi_q < 2\pi$ are randomly chosen in an iteration of the GA and also vary randomly from iteration to iteration. Then, it turns out that \mathbf{m}_q is a unit vector tilted from \mathbf{n} by $\sim \epsilon$. It should be noted that, in spite of the imperfections, since the quantum state evolves without coupling to the additional environment, the qubit rotations remain unitary, keeping the normalization condition $\langle \Psi | \Psi \rangle = 1$ for any iteration number t . The presence of the imperfections will provide an additional coupling between the 2-dimensional Hilbert space spanned by $\{|x\rangle, |y\rangle\}$ ("computational space") and the rest part of the total Hilbert space with 2^{n_q} dimensions, leading to the *quantum leakage* [13] from the computational space as an intrinsic source of error in ideal gate operations.

Typical results of the GA with imperfections are shown in Figure 1: $\langle p_j \rangle$ and F denote an ensemble-averaged probability of the target state $|j\rangle$ and an ensemble-averaged fidelity over 100 random runs, respectively, each of which is here given for $n_q = 13$ and for imperfection strengths $\epsilon = 0, 0.005, 0.01$ and 0.02 , respectively, as a function of iteration number t . Clearly, they are given by

$$\begin{aligned} \langle p_j \rangle_\epsilon(t) &= \langle |\langle j | \Psi(\epsilon, t) \rangle|^2 \rangle, \\ F_\epsilon(t) &= \langle |\langle \Psi(\epsilon = 0, t) | \Psi(\epsilon, t) \rangle|^2 \rangle, \end{aligned} \quad (4)$$

respectively, where the outer bracket represents the ensemble average. In the case of $\epsilon = 0$, $\langle p_j \rangle_0(t)$ oscillates between 0 and 1 and reaches 1 at $t \approx (m + 1/2)(\pi/2)\sqrt{N} \approx 71, 213, 355, \dots$ with $m = 0, 1, 2, \dots$. When ϵ is non-zero, one still finds oscillating features with the same period as in the ideal case, however, with an envelope decaying nearly exponentially with time t . As t increases, the system approaches a saturated regime, where the noise completely dominates the ideal system dynamics, and accordingly $\langle p_j \rangle_\epsilon(t)$ fluctuates around $1/N$. A novel feature is that the decay affects not only the shape of the upper envelope but also that of the lower envelope such that the lower envelope is not simply given by $\langle p_j \rangle_\epsilon(t) = 0$. This means that the probability for the system to remain at the target state is still available even at the time it originally vanishes in the ideal unperturbed system. Furthermore, $F_\epsilon(t)$ is found to approximately equal the upper envelope of $\langle p_j \rangle_\epsilon(t)$.

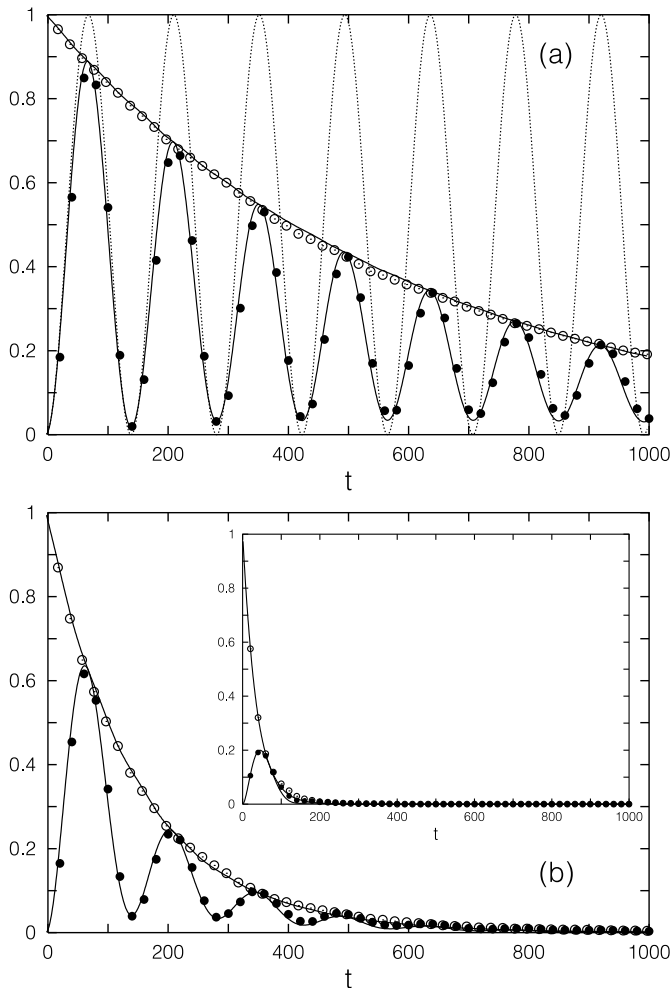


Fig. 1. Behaviors of $\langle p_j \rangle$ (\bullet) and F (\circ) in the Grover's algorithm for the qubit number $n_q = 13$ with the imperfection strength (a) $\epsilon = 0.005$, (b) $\epsilon = 0.01$ and $\epsilon = 0.02$ (inset). Each data point is given, for every 20 iterations, by an ensemble-average over 100 realizations. The dotted line of (a) represents $\langle p_j \rangle$ for $n_q = 13$ in the ideal case ($\epsilon = 0$). The solid lines result from the stochastic two-level model described in the text with parameters (a) $\gamma = 7.6 \times 10^{-4}$, (b) 3.0×10^{-3} and 1.3×10^{-2} (inset), and (a) $W_\phi = 0.089$, (b) 0.19 and 0.25 (inset), respectively.

As noted earlier, in the absence of imperfections, the wave-function of quantum register evolves within a very small part (of dimension 2) of the total Hilbert space (of dimension 2^{n_q}). Furthermore, since the amplitudes of $|x\rangle$ and $|y\rangle$ remain real or at least keep the same phase over the time evolution, the actual relevant space is even smaller than the 2-dimensional entire Hilbert space. Let us denote the 2-dimensional Hilbert space spanned by $|x\rangle$ and $|y\rangle$ and the total Hilbert space by \mathcal{H}_2 and \mathcal{H}_t , respectively. The above results suggest that in general, the disordered GA operator yields states which are not restricted in \mathcal{H}_2 but spread over a larger space \mathcal{H}_t (“computational leakage”). In other words, the presence of imperfections induces a probability density flow from \mathcal{H}_2 to \mathcal{H}_t with

diffusion-like nature. Then, let us define $|w_2(t)|^2$ as the probability that the state remains in \mathcal{H}_2 at time t with an exponentially decaying function of t ,

$$w_2(t) = e^{-\gamma t}, \quad (5)$$

where γ represents the strength of the diffusion which depends on system parameters such as the strength of imperfections and the qubit numbers. Also, the imperfections affect the dynamics of the state within \mathcal{H}_2 : in general, the phases of the two amplitudes of $|x\rangle$ and $|y\rangle$ are not equal to each other, and it is reasonable to assume that random phases are introduced during each iteration. Therefore, we would now like to adopt an effective two-level model which can encapsulate the effects of imperfections in the GA living in \mathcal{H}_t . Here, the time evolution of a quantum state $|\psi(t)\rangle = c_m(t)|m\rangle + c_n(t)|n\rangle$ on the basis $\{|m\rangle, |n\rangle\}$ is described by

$$\begin{pmatrix} c_m(t+1) \\ c_n(t+1) \end{pmatrix} = e^{-\gamma} \hat{R}(\omega) \hat{U}(\phi_m, \phi_n) \begin{pmatrix} c_m(t) \\ c_n(t) \end{pmatrix}, \quad (6)$$

where $\hat{U}(\phi_m, \phi_n)$ is a diagonal matrix with $U_{mm} = e^{i\phi_m}$ and $U_{nn} = e^{i\phi_n}$, and $\phi_m(t)$ and $\phi_n(t)$ are assumed to be two independent random variables without any time correlation. Let each of these phase variables be chosen from a box distribution $[-W_\phi/2, W_\phi/2]$ for a given W_ϕ . The frequency $\omega = \sin^{-1}(2\sqrt{N-1}/N)$ is the same as in the GA, and the initial conditions are given by $c_m(0) = \cos\vartheta_0$ and $c_n(0) = \sin\vartheta_0$ with $\vartheta_0 = \sin^{-1}(1/\sqrt{N})$. This is a stochastic two-level model with dissipation and we refer to it as STLM hereafter. Here, we obtain, after a minor calculation, an ensemble-averaged probability of the target state $|j\rangle$ and an ensemble-averaged fidelity, respectively:

$$\begin{aligned} \langle p_j \rangle_{W_\phi}^{(\gamma)}(t) &= \langle |c_n(t)|^2 \rangle, \\ F_{W_\phi}^{(\gamma)}(t) &= \langle |c_m(t) \cos(\omega t + \vartheta_0) \\ &\quad + c_n(t) \sin(\omega t + \vartheta_0)|^2 \rangle. \end{aligned} \quad (7)$$

It is noteworthy to consider the difference between the STLM and the original GA with imperfections. First, the finite fraction 2^{-n_q+1} occupied by \mathcal{H}_2 in \mathcal{H}_t is neglected in the STLM so that $w_2(t)$ decays to zero instead of $\sim \sqrt{2^{-n_q+1}}$. Since we are interested mainly in the regime before saturation, this is clearly not a significant difference. Secondly, the stochastic features of γ are not considered. But, this is not critical, either, since those features will contribute a negligible correction to γ after an ensemble-average in equation (7).

Now, we perform a numerical simulation to obtain $\langle p_j \rangle_{W_\phi}^{(\gamma)}(t)$ and $F_{W_\phi}^{(\gamma)}(t)$, which will be compared with $\langle p_j \rangle_\epsilon(t)$ and $F_\epsilon(t)$ of the GA with imperfections, respectively. In Figure 1, the results from the STLM are shown as solid lines: they are given by ensemble-averages over 1000 realizations, respectively. We find that these results from the STLM provide an impressive agreement with the results of the GA after a proper adjustment of γ and W_ϕ .

This suggests that the main physical ingredients of the disordered GA are correctly incorporated in the STLTM. Nevertheless, the origin of the novel feature in the lower envelopes is still unclear.

Without loss of generality, $(c_m(t), c_n(t))$ in the STLTM during the time evolution can be written by $(e^{-\gamma t} \cos \vartheta(t), e^{-\gamma t+i\phi(t)} \sin \vartheta(t))$ with $\phi(t) := \phi_n - \phi_m$ up to an overall phase. In case of $\phi(t) \equiv 0$ for arbitrary t , the angle $\vartheta(t)$ increases by ω after each iteration and is then given just by $\omega t + \vartheta_0$. However, if $\phi(t)$ does not vanish, then from its stochastic nature, it follows that $\vartheta(t) - \vartheta(t-1)$ is not constant but would fluctuate around ω [14]. Now, under the assumption that $\vartheta(t)$ and $\phi(t)$ are not correlated with each other, but simply two random variables, we can find analytic expressions of $\langle p_j \rangle_{W_\phi}^{(\gamma)}(t)$ and $F_{W_\phi}^{(\gamma)}(t)$, respectively; let $\vartheta(t)$ increase by $\omega + \eta_{t-1}$ between $t-1$ and t such that

$$\vartheta(t) = \vartheta_0 + \omega t + \sum_{k=0}^{t-1} \eta_k, \quad (8)$$

where η_k forms a Gaussian distribution with mean 0 and width Δ_ϑ , and then $\sum_{k=0}^{t-1} \eta_k$ also satisfies a Gaussian distribution with mean 0 and width $\Delta_\vartheta \sqrt{t}$. From this and equation (7), we get:

$$\begin{aligned} \langle p_j \rangle^{(\gamma)}(t) &= |w_2(t)|^2 \langle \sin^2 \vartheta(t) \rangle \\ &= \frac{|w_2(t)|^2}{\Delta_\vartheta \sqrt{\pi t}} \int_{-\infty}^{\infty} \sin^2(\omega t + \vartheta_0 + x) e^{-x^2/(\Delta_\vartheta^2 t)} dx \\ &= \frac{e^{-2\gamma t}}{2} \left[1 - \cos(2\omega t + 2\vartheta_0) e^{-\Delta_\vartheta^2 t} \right] \end{aligned} \quad (9)$$

(note that no subindex W_ϕ appears in $\langle p_j \rangle^{(\gamma)}(t)$). If we further assume that $\phi(t)$ also is of a Gaussian distribution with mean 0 and width Δ_ϕ , we then arrive at

$$\begin{aligned} F^{(\gamma)}(t) &= \frac{e^{-2\gamma t}}{2} \left[1 + e^{-\Delta_\phi^2 t} \right. \\ &\quad \left. \times \left\{ 1 - \sin^2(2\omega t + 2\vartheta_0) \left(1 - e^{-\Delta_\phi^2/4} \right) \right\} \right]. \end{aligned} \quad (10)$$

Figure 2 shows a comparison between the results of the GA with imperfections and those of equations (9, 10). The good agreement in $\langle p_j \rangle(t)$ would provide an explanation of why its lower envelope is not simply given by $\langle p_j \rangle = 0$ in the GA with imperfections; the uncertainty in the rotation angle during a single iteration accumulates as the iteration proceeds. Then, $\vartheta(t)$ does not represent a definite direction on a 2-dimensional plane but spreads over an interval range $(-\Delta_\vartheta \sqrt{t}, \Delta_\vartheta \sqrt{t})$. This offers an additional decay channel into the target state $|j\rangle$ after ensemble-averaging (see the term $e^{-\Delta_\vartheta^2 t}$ in Eq. (9)). Also, in equation (10) with $\Delta_\phi = 0$ we have $F^{(\gamma)}(t) = (e^{-2\gamma t}/2) (1 + e^{-\Delta_\phi^2 t})$, which is given by the solid lines in Figure 2 as the best fit of $F_\epsilon(t)$ of the GA with imperfections. From equation (10), it immediately follows that $F(\Delta_\phi \neq 0)$ is always less than $F(\Delta_\phi = 0)$.

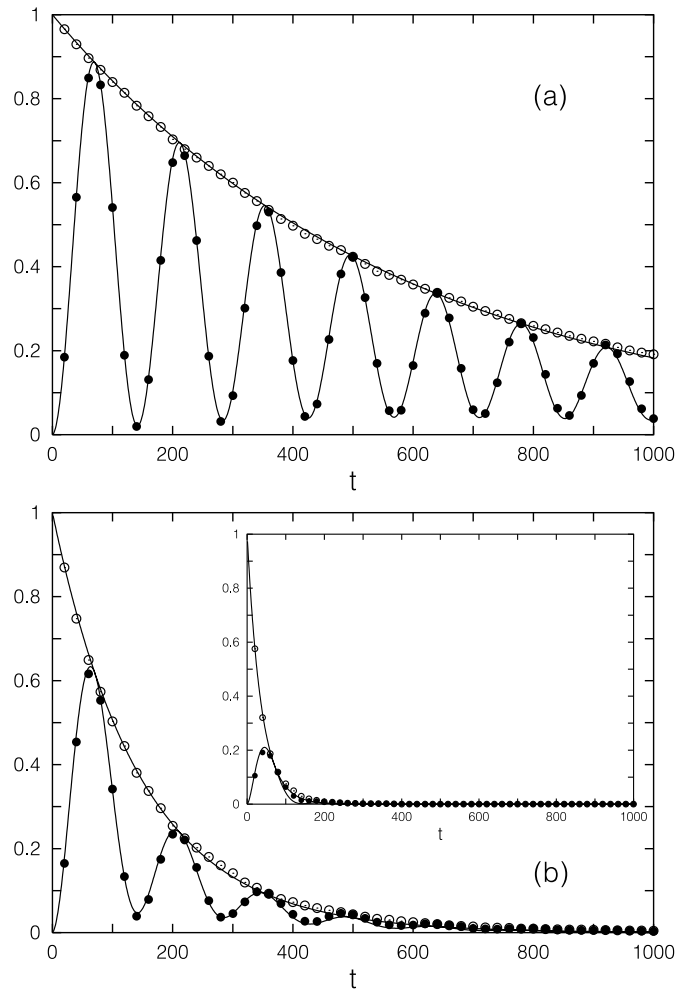


Fig. 2. Comparison between the results of the Grover's algorithm with imperfections and the theoretical predictions given by equations (9, 10). The symbols indicate the same data as in Figure 1. The parameters γ 's are the same as in Figure 1 with (a) $\Delta_\vartheta = 2.0 \times 10^{-2}$, (b) 4.2×10^{-2} and 3.5×10^{-2} (inset), respectively, and $\Delta_\phi = 0$ for all three.

In summary, we have investigated imperfection effects on the time evolution of the Grover's algorithm both numerically and analytically. An effective two-level model with dissipation and randomness has been introduced and the results show a good agreement with the simulation results of the disordered Grover's algorithm. It turns out that the main features in the results of the disordered Grover's algorithm can be understood through the diffusion-like behavior of quantum states from the original partial Hilbert space into the full Hilbert space. The two main decaying mechanisms found in this work are its direct manifestations. Our finding will provide a useful basis for study of more general imperfection effects in quantum algorithms.

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14. After some calculations from equation (6), we actually obtain $\vartheta(t+1) = \frac{1}{2} \cos^{-1}[\cos(2\omega + 2\vartheta(t)) - \sin(2\omega) \sin(2\vartheta(t))(\cos \phi(t) - 1)]$, which is, for general cases, clearly different from $\vartheta(t+1) = \vartheta(t) + \omega$