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Optimal time schedule for adiabatic evolution

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We show that, provided dephasing is taken into account, there is a unique timetable which maximizes the fidelity with a target state in adiabatic evolutions. The optimum has constant tunneling rate along the path. Application to quantum search algorithms recovers the Grover result for appropriate scaling of the dephasing with the size of the database. Moreover, the Grover bound imposes constraints on the dephasing rates of systems coupled to a universal Markovian bath.

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Quantum computation holds a promise of solving some of the most challenging problems in computational science, e.g., integer factorization [1]. The adiabatic model of quantum computation introduced by Farhi *et al.* [2] is equivalent [3] to the standard circuit model of a quantum computer [1] while having a built-in protection from decoherence associated with the exchange of energy with the environment. This protection comes from the (assumed) energy gap of the quantum system. The simplicity and physical character of the model led to a resurgence of interest in adiabatic control of both isolated [4] and open quantum systems [5] and gave rise to new and interesting optimization problems in the context of adiabatic evolutions [6]: One is interested in minimizing the requisite time to reach a target state with given fidelity and given cap on the available energy. Equivalently, one is interested in minimizing the tunneling out of the ground state given a cap on the energy and the time duration $\mathcal{T}$. For unitary evolution, path optimization problems have been studied by several authors analyzing various *upper bounds* on the tunneling; see [4] and references therein. A variational ansatz for the optimal path has been proposed by Rezakhani *et al.* [6].

Dephasing is a special case of decoherence which leads to a loss of information that does not depend on exchange of energy. The role of dephasing in adiabatic quantum computation is, at present, less well understood than that of decoherence in general [7]. Our aim is to describe a simple model where the role of dephasing in adiabatic quantum computation can be studied in detail. Surprisingly, it turns out to be an elixir for the path optimization problem: It allows one to solve the optimal time-scheduling problem.

The time-scheduling problem is to determine the optimal time parametrization of a *given* path of Hamiltonians. In the absence of dephasing, there is no unique optimizer—there are plenty of them. Dephasing singles out a unique optimizer. The optimizer turns out to have a "local" characterization: It has a *fixed tunneling rate* along the path. This means that monitoring the tunneling rate (or, equivalently, the purity of the state) allows one to adhere to an optimal time schedule. No *a priori* knowledge about the governing dynamics is required.

As an application we derive relations between Lindblad operators [8] and the Grover bound [9] on the time for searching an unstructured data base. Lindblad operators describe the quantum evolution of a system coupled to a memoryless (Markovian) bath. The formal theory of Lindblad operators allows one to choose the Hamiltonian and the terms responsible for decoherence independently. In particular, "wide open" systems with large dephasing rates are as legitimate as weakly coupled ones. We show that Markovian baths which are universal, i.e., do not anticipate any properties of the system, must have dephasing rates that are bounded by the spectral gaps in the Hamiltonian for consistency with the Grover bound and cannot be wide open.

Let us now describe the setting and results in more detail. Let H_q, $q \in [0,1]$, be a path in the space of Hamiltonians, e.g., a linear interpolation,

$$H_q = (1-q)H_0 + qH_1 \quad (0 \leqslant q \leqslant 1). \tag{1}$$

We are interested in the optimal parametrization of the interpolating path. That is, a timetable $q(s)$, which optimizes the fidelity of the state, initially in the ground state of H_0, with the ground state of the target Hamiltonian at the end time $\mathcal{T}$. Here $s = \varepsilon t \in [0,1]$ is the *slow time* parametrization and $\varepsilon = 1/\mathcal{T}$ the adiabaticity parameter.

For the sake of simplicity we assume that the Hilbert space has a dimension N (finite) and that H_q is a self-adjoint matrix-valued function of q with ordered simple eigenvalues $e_a(q)$, so that

$$H_q = \sum_{a=0}^{N-1} e_a(q) P_a(q). \tag{2}$$

$P_a(q) = |\psi_a(q)\rangle\langle\psi_a(q)|$ are the corresponding spectral projections.

The cost function is the tunneling $T_{q,\varepsilon}(1)$ at the end point defined by

$$T_{q,\varepsilon}(s) = 1 - \mathrm{tr}[P_0(q)\rho_{q,\varepsilon}(s)]. \tag{3}$$

$\rho_{q,\varepsilon}(s)$ is the quantum state at slow time s which has evolved from the initial condition $\rho_{q,\varepsilon}(0) = P_0(0)$.

We consider the quantum evolution generated by a Lindbladian

$$\varepsilon\dot{\rho} = L_q(\rho), \tag{4}$$

where the overdot indicates d/ds and [8]

$$L(\rho) = -i[H,\rho] + \sum_{j=1}^{M}(2\Gamma_j\rho\Gamma_j^* - \Gamma_j^*\Gamma_j\rho - \rho\Gamma_j^*\Gamma_j) \tag{5}$$

with Γ_j, *a priori*, arbitrary. Unitary evolutions are generated when $\Gamma_j = 0$.

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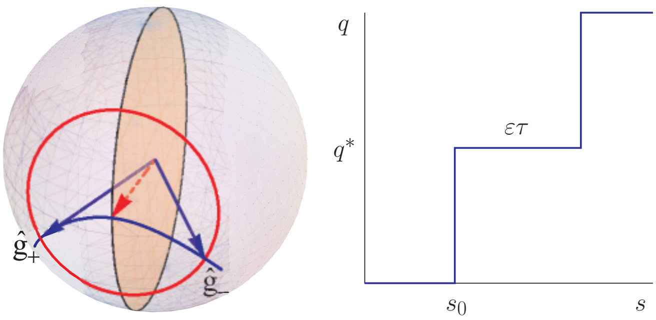

FIG. 1. (Color online) Left: $\hat{\mathbf{g}}_\pm$ are the images on the Bloch sphere of the end points of an interval of size $O(\varepsilon)$ of a given parametrization (blue). The intersection of the associated interpolating path with the equatorial plane (shaded) determines the point q^* and thereby the axis of precession $\hat{\mathbf{g}}(q^*)$ (dashed red) that maps the instantaneous state at the initial end point to the corresponding state at the final end point. Right: A nonsmooth interpolating path that takes the instantaneous eigenstate at the beginning of the interval to the instantaneous eigenstate at the end of the interval with no tunneling.

In the case of unitary evolution the time-schedule optimization problem has no unique solution; on the contrary, optimizers are ubiquitous. To see this consider the two-level system

$$2H_q = \mathbf{g}(q)\cdot\sigma, \tag{6}$$

where σ is the vector of Pauli matrices and $\mathbf{g}(q)$ a smooth, vector-valued function with a gap, $|\mathbf{g}(q)| \geqslant g_0 > 0$; let ε/g_0 be small. Then, in a neighborhood of order ε of any smooth parametrization, there are many nonsmooth parametrizations with zero tunneling and therefore many smooth parametrizations with arbitrarily small tunneling.

To see why this must be so, consider a discretization of any given parametrization to (slow) time intervals of size $2\pi\varepsilon/g_0$. In each interval one can find a point q^*, such that the time-independent Hamiltonian H_{q^*} acting for appropriate time $\tau \leqslant 2\pi/|\mathbf{g}(q^*)| \leqslant 2\pi/g_0$ will map the image on the Bloch sphere of the starting point q_- to the image of the end point q_+ (Fig. 1). The existence of q^* follows from the geometric construction in Fig. 1: $\mathbf{g}(q^*)$ is a point of intersection of the path with the equatorial plane orthogonal to $\hat{\mathbf{g}}(q_+) - \hat{\mathbf{g}}(q_-)$. The resulting parametrization differs from the original one by at most $[\sup_s |\dot{q}(s)|]2\pi\varepsilon/g_0$, as seen from the mean-value theorem. This says that there are many (nonsmooth) paths having zero tunneling.

Dephasing Lindblad operators belong to a special class of Lindblad operators which share with unitary (time-independent) evolutions the existence of N stationary states and conservation of energy $\mathcal{L}^*(H) = 0$. [General Lindblad operators allow for energy exchange $\mathcal{L}^*(H) \neq 0$ and generically have a *unique* equilibrium state.[1]] They can be interpreted as representing a monitoring of the energy of the system. Explicitly, dephasing Lindbladians have the form [10]

$$\mathcal{L}(\rho) = -i[H,\rho] + \sum_{a,b} 2\gamma_{ba}\, P_a \rho P_b - \sum_a \gamma_{aa}\{P_a,\rho\}, \tag{7}$$

where $0 \leqslant \gamma$ is a positive matrix. Time-dependent dephasing Lindblad operators [11] are then defined by setting $H \to H_q$ and $P_a \to P_a(q)$ and $\gamma \to \gamma(q)$.

An adiabatic theorem for dephasing Lindblad operators can be inferred from [12]. It says that the solution $\rho^{(a)}_{q,\varepsilon}$ of the adiabatic evolution, Eq. (4), for the parametrization $q(s)$ and initial condition $\rho^{(a)}_{q,\varepsilon}(0) = P_a(0)$, adheres to the instantaneous spectral projection[2]

$$\rho^{(a)}_{q,\varepsilon}(s) = P_a(s) + O(\varepsilon) \quad (s > 0). \tag{8}$$

For the sake of writing simple formulas we shall, from now on, restrict ourselves to the special case where the positive matrix $\gamma(q) > 0$ of Eq. (7) is a multiple of the identity

$$\mathcal{L}_q(\rho) = -i[H_q,\rho] - \gamma(q)\sum_{j\neq k} P_j(q)\rho P_k(q). \tag{9}$$

Our main results follow from the following theorem. *Theorem 1.* Let $\mathcal{L}_q$ be the dephasing Lindbladian of Eq. (9), and $\rho_{q,\varepsilon}$ a solution of (4) with initial condition $\rho(0) = P_0(0)$ for the parametrization $q(s)$. Assume a gap condition $e_a(q) \neq e_b(q)$, $(a \neq b)$. Then the tunneling defined by Eq. (3) is given by

$$T_{q,\varepsilon}(1) = 2\varepsilon \int_0^1 M(q)\,\dot{q}^2\, ds + O(\varepsilon^2), \tag{10}$$

where the q-dependent *mass* term

$$M(q) = \sum_{a\neq 0} \frac{\gamma(q)\,\mathrm{tr}\big(P_a P_0'^2\big)}{[e_0(q) - e_a(q)]^2 + \gamma^2(q)} \geqslant 0 \tag{11}$$

is independent of the parametrization. $P_0'(q)$ denotes a derivative with respect to q and $\dot{q}(s)$ with respect to s.

In the special case of a two-level system, Eq. (6), where $\mathbf{g}(q)$ is a three-vector-valued function parametrized by its length $d\mathbf{g}(q)\cdot d\mathbf{g}(q) = (dq)^2$, the "mass" term of Eq. (11) takes the simple form

$$M(q) = \frac{\gamma(q)}{4}\,\frac{|\hat{\mathbf{g}}'|^2(q)}{g^2(q) + \gamma^2(q)}. \tag{12}$$

$|\hat{\mathbf{g}}'|$ is the velocity with respect to q on the Bloch sphere ball and $g(q) = |\mathbf{g}(q)|$ is the gap.

Before proving the theorem let us discuss some of its consequences.

1. The tunneling rate $2\varepsilon M(q)\dot{q}^2 \geqslant 0$ is local and unidirectional: Whatever has tunneled cannot be recovered, in contrast with unitary evolutions.

2. Equation (10) has the standard form of variational Euler-Lagrange problems with a Lagrangian that is proportional to the adiabaticity ε and with the interpretation of kinetic energy

[1] $\mathcal{L}$ always has a nonempty kernel since $\mathcal{L}^*(1) = 0$. Since $\mathcal{L}$ can be represented as a matrix, its kernel is generically one dimensional by a simple argument of perturbation theory.

[2] Since there are several energy scales in the problem: ε, γ, and the minimal g_0, the remainder term is guaranteed to be small provided $\varepsilon \ll \gamma, g_0$ is the smallest energy scale.

with position-dependent mass. This variational problem has a unique minimizer $q_0(s)$ in the adiabatic limit, in contrast with the case for unitary evolutions, which as we have seen, has no unique minimizer.

3. Since the Lagrangian is s independent, $q_0(s)$ conserves "energy" and the tunneling rate is constant along the minimizing orbit. This gives a local algorithm for optimizing the parametrization: Adjust the speed $\dot{q}(s)$ to keep the tunneling rate constant.

4. The optimal speed along the path is then

$$\dot{q} = \sqrt{\frac{\tau}{M(q)}}, \tag{13}$$

where $\tau > 0$ is a normalization constant. This formula quantifies the intuition that the optimal velocity is large when the gap is large and the projection on the instantaneous ground state changes slowly.

5. The optimal tunneling $T_{\min}$ is then

$$T_{\min} = 2\varepsilon\tau + O(\varepsilon^2), \quad \sqrt{\tau} = \int_0^1 dq\, \sqrt{M(q)}. \tag{14}$$

We now turn to proving Theorem 1. Evidently

$$1 - \mathrm{tr}(P_0\rho_{q,\varepsilon})(1) = -\int_0^1 \frac{d}{ds}\mathrm{tr}[P_0(q)\rho_{q,\varepsilon}(s)]\, ds. \tag{15}$$

Using Eq. (4), the defining property of dephasing Lindbladians, $\mathcal{L}_q\big(P_0(q)\big) = 0$, and by Eq. (7), the concomitant $\mathcal{L}_q^*\big(P_0(q)\big) = 0$, one finds

$$\frac{d}{ds}\mathrm{tr}[P_0(q)\rho_{q,\varepsilon}(s)] = \mathrm{tr}[P_0'(q)\,\rho_{q,\varepsilon}(s)]\,\dot{q}(s). \tag{16}$$

Now, the identity

$$\mathcal{L}^*(P_a A P_b) = [i(e_a - e_b) - \gamma]P_a A P_b \quad (a \neq b) \tag{17}$$

together with $P_a P_0' P_a = 0$ shows that

$$X = \sum_{a\neq b} \frac{P_a P_0' P_b}{i(e_a - e_b) - \gamma} \tag{18}$$

solves the equation

$$P_0'(q) = \mathcal{L}_q^*\big(X(q)\big). \tag{19}$$

Substituting this in Eq. (16) gives the identity

$$\frac{d}{ds}\mathrm{tr}[P_0(q)\rho_{q,\varepsilon}(s)] = \varepsilon\, \mathrm{tr}[X(q)\,\dot{\rho}_{q,\varepsilon}(s)]\,\dot{q}(s). \tag{20}$$

Integrating by parts the last identity gives an expression involving ρ but no $\dot{\rho}$. This allows us to use the adiabatic theorem and replace ρ by $P + O(\varepsilon)$. We then undo the integration by parts to get Theorem 1.

In the theory of Lindblad operators H and Γ_j of Eq. (5) can be chosen independently. However, as we shall now show, if one makes some natural assumptions about the bath, the dephasing rate γ of Eq. (9) is constrained by the gaps of H.

To see this we turn to quantum search with dephasing [11,13]. Grover has shown [9] that $O(\sqrt{N})$ queries of an oracle suffice to search an unstructured database of size $N \gg 1$. The adiabatic formulation of the problem leads to the study of a two-level system with a small gap given by [4,14]

$$g^2(q) = 4\frac{(1-q)q}{N} + (1-2q)^2 \tag{21}$$

and large velocity on the Bloch sphere

$$|\hat{\mathbf{g}}'(q)| = \sqrt{\frac{1}{N} - \frac{1}{N^2}}\,\frac{2}{g^2(q)}. \tag{22}$$

The time scale τ, which determines the optimal tunneling, can be estimated by evaluating the integrand in Eq. (14) at its maximum, $q = 1/2$, and taking the width to be $1/\sqrt{N}$. This gives

$$\tau = O\left(\frac{M(1/2)}{N}\right) \tag{23}$$

to leading order in the adiabatic approximation.

The adiabatic formulation of Grover search [2] fixes the scaling of the minimal gap $g_0 \sim \frac{1}{\sqrt{N}}$ but does not fix the scaling of the dephasing rate γ with N. We shall now address the issue of what physical principles determine the scaling of the dephasing with N. To this end we consider various cases.

The regime $\gamma \ll \varepsilon$ is outside the framework of the adiabatic theory described here. [For the adiabatic expansion and Eq. (23) to hold ε must be the smallest energy scale in the problem.] This is essentially the unitary scenario [2,4].

The regime $\varepsilon \ll \gamma \ll g_0$ is trivially consistent with the Grover bound since $\mathcal{T} \gg \gamma^{-1} \gg O(\sqrt{N})$.

Optimal scheduling recovers the Grover bound when dephasing is comparable to the gap, $\gamma \sim g_0$. One finds $M(1/2) \sim 1/g_0^3$, and from Eqs. (23) and (21) the search time

$$\mathcal{T} = O\left(\frac{1}{g_0^3 N}\right) = O(\sqrt{N}). \tag{24}$$

The most interesting regime is the dominant dephasing case: $\gamma \gg g_0$. Here $M \sim \gamma^{-1}/g_0^2$, and from Eqs. (23) and (21) one finds

$$\mathcal{T} = O(\gamma^{-1}). \tag{25}$$

If γ scaled as $\gamma \sim N^{-\alpha/2}$, then $\mathcal{T} = O(N^{\alpha/2})$, which seems to beat Grover time whenever $\alpha < 1$.

The accelerated search enabled by strong dephasing is in apparent conflict with the optimality of the Grover bound [17,18]: Consider the joint Hamiltonian dynamics of the system and the bath, which underlies the Lindblad evolution. By an argument of [14] for a universal bath, the Grover search time is optimal. How can one reconcile Eq. (25) with this result? Before doing so, however, we want to point out that Eq. (25) is not an artifact of perturbation theory: While $T_{\min} = 2\varepsilon\tau$ is valid in first order in ε, an estimate $T_{\min} \lesssim \varepsilon\tau$, with τ as in Eq. (14), remains true for all ε provided $\gamma \gtrsim g_0$.

The resolution is that a Markovian bath with $\gamma \gg g_0$ cannot be universal and must be system specific: The bath has a premonition of what the solution to the problem is. (Formally, this "knowledge" is reflected in the dephasing in the instantaneous eigenstates of H_q.) Lindbladians with dephasing rates that dominate the gaps mask resources hidden in the bath. This can also be seen by the following argument: Dephasing can be interpreted as the monitoring of the observable H_q. The *time-energy* uncertainty principle [15] says that if H_q is unknown, then the rate of monitoring is bounded by the gap. The accelerated search occurs when the monitoring rate exceeds this bound, which is only possible if the bath already "knows" what H_q is. When H_q is known, the bath can freeze the system in the instantaneous ground state arbitrarily fast. Consequently, the Zeno effect [16] then allows for the speedup of the evolution without paying a large price in tunneling.

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