Optimal parametrizations of adiabatic paths

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We show that, given a path of Hamiltonians and a fixed time to complete it, there are many parametrizations, i.e. time-tables for running along the path, such that the ground state of the initial Hamiltonian is mapped exactly on the final ground state. In contrast, we show that if dephasing is added to the dynamics there is a unique parametrization which maximizes the fidelity of the final state with the target ground state. The optimizing parametrization solves a variational problem of Lagrangian type and has constant tunneling rate along the path irrespective of the gap. Application to quantum search algorithms recovers the Grover result for appropriate scaling of the dephasing with the size of the data base. Lindbladians that describe wide open systems require special care since they may mask hidden resources that enable beating the Grover bound.

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In the theory of adiabatic quantum control and quantum computation, one is interested in reaching a target state from a (different) initial state with high fidelity, as quickly as possible, subject to given cap on the available energy. The initial state is assumed to be the ground state of a known Hamiltonian $H_0$ and the target state is the ground state of a known Hamiltonian $H_1$. The two are connected by a smooth interpolating path in the space of Hamiltonians. The interpolation is denoted by $H_q$ with $q \in [0, 1]$. An example is the linear interpolation

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

However, any smooth interpolation will do. We are interested in the optimal parametrization of the interpolating path. That is, a time-table for the path which optimizes the fidelity of the time-evolving state at the end time with the ground state of the target Hamiltonian. We will show that when the evolution is unitary, there is a unique optimizer—there are plenty of them. However, when dephasing is added to the dynamics there is a unique optimizer which we characterize and discuss.

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

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

$P_a(q)$ are the corresponding spectral projections.

A slow change of $q$ tends to maintain the system in its ground state up to an error due to tunneling. We are interested in getting as close as possible to the target state within the time $T$ allotted to traversing the path. The controls at our disposal are $a$. The total time $T$ and b. The parametrization of the path $q(s) = q_e(s), s \in [0, 1]$ for given $e$. Here $s = \varepsilon t$ is the slow time parametrization and $\varepsilon = 1/T$ the adiabaticity parameter.

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

$$T_{q,e}(s) = 1 - \text{tr}(P_0(q)\rho_{q,e}(s)). \tag{3}$$

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

A related but different optimization problem commonly considered in quantum information is to optimize upper bounds on the tunnelings. The difference is that the cost function is evaluated not for a fixed, given interpolation, but for the worst case for any (smooth) interpolation between any two Hamiltonians belonging to certain classes.

We consider two types of evolutions: (a) Unitary evolutions generated by $H_q$. (b) Non-unitary evolutions generated by appropriate Lindblad generators $L_{\rho}^{\Gamma}$. Since (a) is a special case of (b), both are of the form

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

where $\dot{} = d/ds$ and

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

with $\Gamma_j$, a-priori, arbitrary. Adiabatic evolutions are a singular limit of the evolution equations since $\varepsilon$ hits the leading derivative. Unitary evolutions are generated when $\Gamma_j = 0$.

In the case of unitary evolution the optimization problem has no unique solution, on the contrary, optimizers are ubiquitous. More precisely:

**Theorem 1** Let

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

be any smooth interpolation of a 2-level system where $\sigma$ is the vector of Pauli matrices and $\mathbf{g}(q)$ a smooth, vector valued function with a gap, $|\mathbf{g}(q)| \geq g_0 > 0$; let $\varepsilon/g_0$ be small. Then, in a neighborhood of order $\varepsilon$ of
any smooth parametrization, there are many non-smooth parametrizations with zero tunneling and therefore many smooth parametrizations with arbitrarily small tunneling.

We shall sketch the main idea behind the proof. 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 $\tau \leq 2\pi/|g(q^*)| \leq 2\pi/g_0$, will map the image on the Bloch sphere of the starting point $q_-$ to the image of the end point $q_+$. This says that there are many (non-smooth) paths, labelled by the continuous parameter $s_0$ in Fig. 1 that map the instantaneous state at the initial end point to the corresponding state at the final end point. These paths have zero tunneling. The existence of $q^*$ follows from the geometric construction in Fig. 1: $g(q^*)$ is a point of intersection of the path with the equatorial plane orthogonal to $g(q_+)-g(q_-)$. The resulting parametrization differs from the original one by at most $(\sup_{s} |q(s)|) \cdot 2\pi\varepsilon/g_0$, as seen from the mean-value theorem.

![Diagram](image)

**FIG. 1:** Left: $g_\pm$ 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 $g(q^*)$ (red) that maps the instantaneous state at the initial end point to the corresponding state at the final end point. Right: A non-smooth 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.

Dephasing Lindblad operators belong to a special class of Lindblad operators that share with unitary evolutions the existence of $N$ stationary states. (In contrast with generic Lindblad operators that have a unique equilibrium state.) More precisely, $\mathcal{L}$ is a dephasing Lindblad operator, if all the spectral projections $P_a$ of $H$ are stationary states, namely $P_a \in \ker \mathcal{L}$. This is the case when $[\Gamma, H] = 0$, and the condition is also necessary when $H$ has simple eigenvalues, as can be seen by expanding $\text{tr}(P_a \mathcal{L}(P_a)) = 0$. We can then write

$$\Gamma_j = \sum_{a=0}^{N-1} \sqrt{\gamma_{ja}} P_a,$$

where $\mathcal{L}$ is a rectangular, $M \times N$, matrix (without loss, $M = N^2 - 1$). It follows that dephasing Lindbladians have the form:

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

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

The motion of $\ker \mathcal{L}_q$ with $q$ can be interpreted geometrically as follows: The space of (unnormalized) states is a fixed $N^2$ dimensional convex cone. The normalized instantaneous stationary states are a simplex whose vertices are the instantaneous spectral projections $P_a(q)$. This simplex rotates with $q$ like a rigid body, since the vertices remain orthonormal, $\text{tr}(P_a P_b) = \delta_{ab}$ and the motion is purely orthogonal to the kernel, $\text{tr}(P_a^2 P_b) = 0$ where $P_a^\prime = dP_a/dq$. This follows from the fact that for orthogonal projections $P_a^\prime$ is off-diagonal

$$P_a^\prime(q) = \sum_{\delta \neq c} P_b(q) P_a^\prime(q) P_c(q). \quad (8)$$

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

$$\rho_{q,\varepsilon}^{(a)}(s) = P_a(s) + O(\varepsilon), \quad (s > 0). \quad (9)$$

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

$$\mathcal{L}_q(\rho) = -i[H_q, \rho] - \gamma(q) \sum_{j \neq k} P_j(q) \rho P_k(q). \quad (10)$$

Our main results follow from:

**Theorem 2** Let $\mathcal{L}_q$ be the dephasing Lindblad of Eq. (10), and $\rho_{q,\varepsilon}$ a solution of (3) 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. (4), is given by

$$T_{q,\varepsilon}(1) = 2\varepsilon \int_0^1 M(q) \; dq^2 \; ds + O(\varepsilon^2), \quad (11)$$

where the $q$ dependent mass term

$$M(q) = \sum_{a \neq 0} \frac{\gamma(q) \text{tr}(P_a P_a^2)}{(e_a(q) - e_{a}(q))^2 + \gamma^2(q)} \geq 0 \quad (12)$$

is independent of the parametrization. $P_0^\prime(q)$ denotes a derivative with respect to $q$ and $q(s)$ with respect to $s$. 
In the special case of a 2-level system, Eq. (11), where \( \mathbf{g}(q) \) is a 3-vector valued function parametrized by its length \( dg(q) \cdot dg(q) = (dq)^2 \) the “mass” term of Eq. (12) takes the simple form

\[
M(q) = \frac{\gamma(q)}{4} \frac{|\dot{g}'(q)|^2 + |g''(q)|^2}{g''(q)}
\]

(13)

\(|\dot{g}'|\) is the velocity w.r.t. \( q \) on the Bloch sphere ball and \( g(q) = |\mathbf{g}(q)| \) is the gap.

Remark: For a 2-level system undergoing unitary evolution a similar variational principle to Eq. (11), but with a different \( M(q) \), was proposed, as an ansatz, in \(^2\) the purpose of determining an optimal path, rather than an optimal parametrization of a given path.

Before proving the theorem let us discuss some of its consequences: Note first, that the tunneling rate, \( 2\varepsilon M(q)\dot{q}^2 \geq 0 \), is local and uni-directional. It follows that whatever has tunnelled cannot be recovered, in contrast with unitary evolutions. Eq. (11) has the standard form of variational Euler-Lagrange problems with a Lagrangian that is proportional to the adiabaticity \( \varepsilon \) and with the interpretation of kinetic energy 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 by Theorem \(^1\) has no unique minimizer.

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. The optimal speed along the path is then

\[
\dot{q} = \sqrt{\frac{\tau}{M(q)}},
\]

(14)

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. The optimal tunneling, \( T_{\text{min}} \), is then

\[
T_{\text{min}} = 2\varepsilon \tau + O(\varepsilon^2), \quad \sqrt{\tau} = \int_0^1 dq \sqrt{M(q)}.
\]

(15)

This formulas will play a role in our analysis of Grover search algorithm.

We now turn to proving Theorem \(^2\). Evidently

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

(16)

Using Eq. (4), the defining property of dephasing Lindbladians, \( \mathcal{L}_q(P_0(q)) = 0 \), and by Eq. (17), the concomitant \( \mathcal{L}_q'(P_0(q)) = 0 \), one finds

\[
\frac{d}{ds} \text{tr}(P_0(q) \rho_{q,\varepsilon}(s)) = \text{tr}\left( P_0'(q) \rho_{q,\varepsilon}(s) \right) \dot{q}(s).
\]

(17)

Now, the identity,

\[
\mathcal{L}^\ast(P_a A P_b) = (i(e_a - e_b) - \gamma) P_a A P_b, \quad (a \neq b)
\]

(18)

together with Eq. (8) shows that

\[
X = \sum_{a \neq b} P_a P_b^\ast P_b \frac{i(e_a - e_b) - \gamma}{i(e_a - e_b) - \gamma}.
\]

(19)

solves the equation

\[
P_0'(q) = \mathcal{L}^\ast_q(X(q))
\]

(20)

Substituting this in Eq. (17) gives the identity

\[
\frac{d}{ds} \text{tr}(P_0(q) \rho_{q,\varepsilon}(s)) = \varepsilon \text{tr}\left( X(q) \rho_{q,\varepsilon}(s) \right) \dot{q}(s).
\]

(21)

Integrating by parts the last identity gives an expression involving \( \rho \) but no \( \dot{\rho} \). This allows us to use the adiabatic theory and replace \( \rho \) by \( P + O(\varepsilon) \). We then undo the integration by parts to get Theorem \(^2\).

In the theory of Lindblad operators \( H \) and \( \Gamma_j \) 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 \( \gamma \) of Eq. (10) is constrained by the gaps of \( H \).

To see this we turn to quantum search with dephasing. \(^7,10\) Grover has shown \(^11\) that \( O(\sqrt{N}) \) queries of an oracle suffice to search an unstructured data base of size \( N \gg 1 \). The adiabatic formulation of the problem leads to the study of a 2-level system with a small gap given by \(^4,12\)

\[
g^2(q) = 4\frac{(1 - q)q}{N} + (1 - 2q)^2
\]

(22)

and large velocity on the Bloch sphere

\[
|\dot{\hat{g}}(q)| = \sqrt{\frac{1}{N} - \frac{1}{N^2} \frac{2}{g^3(q)}}.
\]

(23)

The time scale \( \tau \), which determines the optimal tunneling, can be estimated by evaluating the integrand in Eq. (15) at its maximum, \( q = 1/2 \), and taking the width to be \( 1/\sqrt{N} \). This gives

\[
\tau = O\left( \frac{M(1/2)}{N} \right)
\]

(24)

to leading order in the adiabatic approximation.

The adiabatic formulation \(^2\) fixes the scaling of the minimal gap \( g_0 \sim \frac{1}{\sqrt{N}} \) but does not fix the scaling of the dephasing rate \( \gamma \) with \( N \). We shall now address the issue of what physical principles determines 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, but is close to the unitary scenario. \(^3,4\) For the adiabatic expansion and Eq. (21) to hold \( \varepsilon \ll \gamma \). This means that in case of small dephasing,
\( \gamma < g_0 \), the allotted time, \( T \gg \gamma^{-1} \gg O(\sqrt{N}) \), is longer than Grover search time. For such times the theory developed here can be used to estimate the tunneling, but it is not appropriate for optimizing the search time. To optimize the search time one needs to study bounds on the tunneling rather than a first order term in \( \varepsilon \).

When dephasing is comparable to the gap, \( \gamma \sim g_0 \), one finds \( M(1/2) \sim 1/g_0^2 \) and from Eqs. [24] [22] one recovers Grover’s result for the search time

\[
T = O\left(\frac{1}{g_0^2 N}\right) = O(\sqrt{N}).
\]

Finally, consider the dominant dephasing case: \( \gamma \gg g_0 \). Here \( M \sim \gamma^{-1}/g_0^2 \) and from Eqs. [24] [22] one finds

\[
T = O\left(\gamma^{-1}\right).
\]

If \( \gamma \) scaled like \( \gamma \sim N^{-\alpha/2} \), \( 1 > \alpha \), then \( T = O\left(N^{\alpha/2}\right) \) which seems to beat Grover time.

The accelerated search enabled by strong dephasing in apparent conflict with the optimality of Grover bound[15,16]: Consider the Hamiltonian dynamics of the joint system and 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. [26] with this result? Before doing so, however, we want to point out that Eq. [20] is not an artefact of perturbation theory: While \( T_{\text{min}} = 2\varepsilon T \) is valid in first order in \( \varepsilon \), an estimate \( T_{\text{min}} \lesssim \varepsilon T \), with \( T \) as in Eq. [19], remains true for all \( \varepsilon \) provided \( \gamma \gtrsim g_0 \).

The resolution is that a Markovian bath with \( \gamma \gg g_0 \) can not 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[17] says that if \( H_q \) is unknown, then the rate of monitoring is bounded by the gap. The accelerated search occurs when 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[14] then allows for the speedup of the evolution without paying a large price in tunneling.

The formal theory of Lindblad operators allows one to choose the operators, \( H \) and \( \Gamma \), in Eq. [4], independently. From the discussion in the last paragraph one learns that one must exercise care in using Lindbladians for systems that are wide open. Markovian baths which are universal, i.e. oblivious of the state of the system, give rise to dephasing Lindbladians, with dephasing rates that are bounded by the spectral gaps of the system.

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17. Since there are several energy scales in the problem: \( \varepsilon, \gamma \) and the minimal \( g_0 \), the remainder term is guaranteed to be small provided \( \varepsilon \ll \gamma, g_0 \) is the smallest energy scale.