Optimizing adiabaticity in quantum mechanics

R. MacKenzie, M. Pineault and L. Renaud-Desjardins

Physique des particules, Université de Montréal,
C.P. 6128, Succ. Centre-ville, Montréal, QC H3C 3J7

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A condition on the Hamiltonian of a time-dependent quantum mechanical system is derived which, if satisfied, implies optimal adiabaticity (defined below). The condition is expressed in terms of the Hamiltonian and in terms of the evolution operator related to it. Since the latter depends in a complicated way on the Hamiltonian, it is not yet clear how the condition can be used to extract useful information about the optimal Hamiltonian. The condition is tested on an exactly-soluble time-dependent problem (a spin in a magnetic field), where perfectly adiabatic evolution can be easily identified.

I. INTRODUCTION

The adiabatic theorem in quantum mechanics was developed when quantum mechanics was still in its infancy [1]. (See [2] for an early English-language reference, and [3] for a recent overview.) It is used in virtually every area of quantum physics. The essential idea underlying the theorem is very simple. Let the Hamiltonian be \( H(t) \) and define its instantaneous eigenstates \( |n(t)\rangle \) and eigenenergies \( E_n(t) \) as the solutions to the time-independent Schrödinger equation \( H(t)|\psi\rangle = E|\psi\rangle \) (where \( t \) is viewed as a parameter). The states \( |n(t)\rangle \) evolve in time, as does the solution \( |\psi(t)\rangle \) of the time-dependent Schrödinger equation

\[
i\frac{\partial}{\partial t}|\psi(t)\rangle = H(t)|\psi(t)\rangle.
\]

In general there is no obvious relation between these two evolutions. The adiabatic theorem states that the system follows the instantaneous eigenstates for infinitely slow evolution. More precisely, suppose the system starts in \( |n(0)\rangle \) at \( t = 0 \), and that \( |n(t)\rangle \) is gapped at all times (that is, \( |E_n(t) - E_m(t)| \geq E_0 > 0 \) for all \( t \) and for all \( m \neq n \)). Suppose that we can control the speed with which the Hamiltonian varies by making the replacement \( H(t) \rightarrow H_\lambda(t) \equiv H(\lambda t) \) with the time interval changed accordingly, \([0,T] \rightarrow [0,T/\lambda] \), so that the limit \( \lambda \rightarrow 0 \) corresponds to infinitely slow evolution. Then the adiabatic theorem states that the solution to the Schrödinger equation

\[
i\frac{d}{dt}|\psi_\lambda(t)\rangle = H_\lambda(t)|\psi_\lambda(t)\rangle, \quad |\psi_\lambda(0)\rangle = |n(0)\rangle
\]
satisfies

\[
\lim_{\lambda \rightarrow 0} |\psi_\lambda(T/\lambda)\rangle = (\text{phase}) |n(T)\rangle + O(\lambda).
\]

Thus, as \( \lambda \rightarrow 0 \), the probability for the system to make a transition to a different instantaneous eigenstate goes to zero. We then say that the evolution is adiabatic.

Infinitely slow evolution is time consuming, to say the least, so it is of interest to be able to make a statement about finitely slow evolution. Intuitively, if the evolution is sufficiently slow, the adiabatic approximation

\[
|\psi(t)\rangle \simeq (\text{phase}) |n(t)\rangle
\]

should be reasonable.

This begs the question: how slow must the evolution be for (1) to be a good approximation? In a situation where adiabatic evolution is desirable, it is obviously important to know just how slowly the system must evolve in order for this to be the case, in order to accomplish the task required as quickly as possible. (In the case of adiabatic quantum computing [4, 5], for instance, how the slowness required scales with the size of the system being studied enables comparison of this approach to conventional circuit-based quantum computing.)

There are two time scales at play: the time scale of the evolution of the Hamiltonian and a scale related to the difference in energies. The former is often estimated to be of order \( |\langle m(t)|\dot{n}(t)\rangle|^{-1} \); the latter can be written \( |E_m - E_n|^{-1} \). Usually, the evolution can be considered slow [6] if

\[
\frac{\langle m(t)|\dot{n}(t)\rangle}{E_m - E_n} \ll 1.
\]

But this condition does not guarantee that (1) is a good approximation. First, it does not necessarily imply slow evolution [6]. Secondly, even in circumstances where it does imply slow evolution, one cannot conclude that the adiabatic approximation is true indefinitely; rather, it implies that the system will “escape” from \( |n(t)\rangle \) more slowly than for a “generic” (non-slow) evolution. Much work has been done recently studying the adiabatic approximation and attempting to give one or more conditions guaranteeing its validity [7–28].

In this paper, our goal will be to devise a criterion which implies that a Hamiltonian is optimal in the sense that the evolution is optimally adiabatic. If \( |\psi(0)\rangle =
|n(0)) then we define the adiabaticity as

\[ A(t) = |\langle n(t) | \psi(t) \rangle|^2 . \]  

(2)

A cannot exceed unity, and \( A = 1 \) corresponds to perfectly adiabatic evolution (that is, evolution where the adiabatic approximation is exactly satisfied).

The specific question we will address is as follows. Suppose we are given a physical system described by a time-dependent Hamiltonian, and that the duration of evolution (call it \( T \)) and the initial and final Hamiltonians \( (H(0) \) and \( H(T)) \) are given. Suppose furthermore that, as above, the system is initially in the state \( |n(0)\rangle \). The question is: Can we determine an interpolating Hamiltonian \( H(t) \) which maximizes the (final) adiabaticity,

\[ A[H(t)] = |\langle n(T) | \psi(T) \rangle|^2 \]  

(3)

In what follows, we will devise such a criterion, and will test it on an exactly-solvable system. Unfortunately, as will be seen below, the criterion is expressed in terms of the evolution operator. Thus, it is not clear how it can be used on a system for which this operator cannot be determined. In the next section we begin by observing that there is a trivial, but impractical, way of obtaining perfectly adiabatic evolution. We then restrict and formalize the question addressed above. In the following section we explain the optimization procedure which results in our main result, \( (\ref{eq:optimization}) \). Following this, we test the result on what is probably the simplest case of a time-dependent Hamiltonian, one which can be solved exactly: a spin in a rotation magnetic field. We end with a summary and concluding remarks.

II. STATEMENT OF THE PROBLEM

Before we begin, note that there is actually a trivial (although impractical) way of attaining perfectly adiabatic evolution \[ (\ref{eq:adiabaticity}). \] Suppose \( H_s \) (where \( s : 0 \to 1 \)) is a sufficiently smooth family of Hamiltonians which interpolates between \( H(0) \) and \( H(T) \) (so that \( H_0 = H(0) \) and \( H_T = H(T) \)) and for which the instantaneous eigenstate \( |n_s\rangle \) is always gapped. Then the following time-dependent Hamiltonian will give perfectly adiabatic evolution in the limit \( \Lambda \to \infty \):

\[
H_\Lambda(t) = \begin{cases} 
(1 + \frac{3\Lambda}{T}(\Lambda - 1)) \ H_0 & t : 0 \to \frac{T}{4}, \\
(2 - \frac{3\Lambda}{T}) \ \Lambda H_0 + (-1 + \frac{3\Lambda}{T}) \ \Lambda H_1 & t : \frac{T}{4} \to \frac{3T}{4}, \\
(3\Lambda - 2 + \frac{3\Lambda}{T}(1 - \Lambda)) \ H_1 & t : \frac{3T}{4} \to T
\end{cases}
\]

The evolution is divided into three steps. During the first step, the Hamiltonian is simply multiplied by a linear function of time, going from \( H_0 \) to \( \Lambda H_0 \); \( |n(t)\rangle \) remains an eigenstate of the Hamiltonian so the state of the system only changes by a phase. During the second step, the Hamiltonian evolves (again linearly) from \( \Lambda H_0 \) to \( \Lambda H_1 \); as \( \Lambda \) goes towards infinity, the probability of making a transition from \( |n(t)\rangle \) to a different state drops to zero, so in this limit the state of the system at the end of this stage is a phase times \( |n(T)\rangle \). During the third step, the Hamiltonian is again multiplied by a linear function of time, going from \( \Lambda H_1 \) to \( H_1 \), and as in the first stage the state of the system only changes by a phase.

We then begin by observing that there is a trivial, but impractical, way of attaining perfectly adiabatic evolution \( (\text{adiabatic approximation is exactly satisfied}). \)

The specific question we will address is as follows. Suppose we restrict ourselves to situations where the energy eigenvalues are constant, \( E_n(t) = E_n; \) this eliminates the trivial way just described, and simplifies the analysis to follow. The Hamiltonian then evolves via a unitary transformation

\[ H(t) = V(t) H(0) V(t)^\dagger, \]

where \( V^\dagger V = 1 \). We can assume \( V(0) = 1 \), and the final value \( V(T) \) is fixed since the final Hamiltonian is presumed to have been specified in advance; the instantaneous eigenstates are \( |n(t)\rangle = V(t) |n(0)\rangle \). We write \( A[H(t)] \to A[V(t)] \).

Let the time evolution operator associated with \( H(t) \) be \( U(t) \), so the state is given by \( |\psi(t)\rangle = U(t) |n(0)\rangle \). Then \( (\ref{eq:adiabaticity}) \) becomes

\[ A[V(t)] = |\langle n(0) | V(T) U(T) | n(0) \rangle|^2, \]  

(4)

and we wish to find a condition on \( V(t) \) for which the adiabaticity is maximal.

III. OPTIMIZATION

We will adopt a variational approach to find a condition on \( V(t) \). Suppose that the adiabaticity is optimized for a certain matrix \( V_0(t) \) (to be determined). Then for any variation of \( V(t) \) about \( V_0(t) \) which is zero initially and finally \( (\text{so that the initial and final Hamiltonians are unaffected}) \), \( A \) is stationary to first order:

\[
\left. \frac{\delta A}{\delta V(t)} \right|_{V(t)=V_0(t)} = 0.
\]

(Of course, solutions to this equation will be local extrema, not necessarily global minima, of the adiabaticity.)

We write \( H_0(t) = V_0(t) H(0) V_0^\dagger(t) \), with \( U_0(t) \) the corresponding evolution operator and \( A_0 \) the optimal \( (\text{assumed maximal}) \) adiabaticity.

Now consider a small variation of \( V(t) \):

\[ V(t) = (1 + i h(t)) V_0(t), \]

where \( h(t) = h^\dagger(t) \) (in order for \( V(t) \) to be unitary), \( h(t) \ll 1 \) \( (\text{meaning the matrix elements are much less than 1}) \) and \( h(0) = h(T) = 0 \). Then

\[
\left. \frac{\delta A}{\delta V(t)} \right|_{V(t)=V_0(t)} \to \left. \frac{\delta A}{\delta h(t)} \right|_{h(t)=0} .
\]

In \( (\ref{eq:adiabaticity}) \), \( V(T) = V_0(T) \) is independent of \( h(t) \) \( (\text{so in what follows we will write} \langle n(0) | V(T) = \langle n(T) \rangle) \); but \( U(T) \) depends non-trivially on \( h(t) \).
The change \( V_0(t) \rightarrow V(t) \) will induce a small change in the evolution, so we can write

\[
U(t) = (1 + ik(t))U_0(t),
\]

where \( k(t) = k^\dagger(t), k(0) = 0 \) and \( k \ll 1 \). Then

\[
A = \left| \langle n(T)| (1 + ik(T))U_0(T)|n(0) \rangle \right|^2
= A_0 + 2\text{Im} \left\{ \langle n(T)| k(T)U_0(T)|n(0) \rangle \times \langle n(0)| U_0^\dagger(T)|n(T) \rangle \right\} + O(k^2).
\]

That \( A \) is stationary implies

\[
\text{Im} \left\{ \langle n(T)| k(T)U_0(T)|n(0) \rangle \langle n(0)| U_0^\dagger(T)|n(T) \rangle \right\} = 0
\]

for any \( h(t) \).

We must now express \( k(T) \) in terms of \( h(t) \). We note that for the unperturbed problem

\[
i \frac{d}{dt} U_0(t) = H_0(t)U_0(t), \quad U_0(0) = 1,
\]

while for the perturbed problem

\[
i \frac{d}{dt} U(t) = H(t)U(t), \quad U(0) = 1,
\]

with the Hamiltonians and evolution operators related by

\[
H(t) = (1 + ih(t))H_0(t)(1 - ih(t)),
\]

\[
U(t) = (1 + ik(t))U_0(t).
\]

Direct substitution and taking linear terms in both \( h \) and \( k \) yields

\[
i \frac{d}{dt} k(t) = [H_0, k] - [H_0, h], \quad k(0) = 0.
\]

Standard techniques yield the following solution, as can be verified directly:

\[
k(T) = U_0(T)i \int_0^T dt U_0^\dagger (t)[H_0(t), h(t)]U_0(t)U_0^\dagger (T)
\]

Substituting in \((5)\), we see that

\[
\text{Re} \int_0^T dt \left\{ \langle n(T)| U_0(T)U_0^\dagger (t)[H_0(t), h(t)]U_0(t)|n(0) \rangle \times \langle n(0)| U_0^\dagger (T)|n(T) \rangle \right\} = 0
\]

for any Hermitian \( h(t) \). Each of the factors in the braces can be analyzed semi-intuitively. The second, which can be loosely described as the “square root” of \( A_0 \), is simply the amplitude for the optimal evolution to be adiabatic. The first factor, read right to left, is: starting in the initial state, evolving optimally for a time \( t \), an effect of the perturbation acting on the state at time \( t \), evolving for the remaining time \( T - t \), and projecting onto the final instantaneous eigenstate. Thus, roughly speaking, the sum of all possible first-order changes to \( A \) must be zero.

We can progress further by analyzing what we mean by the statement “for any Hermitian \( h(t) \).” We can write \( h(t) = \lambda_i f_i(t) \) (sum on \( i \) implicit), where \( \{\lambda_i\} \) is a basis of Hermitian matrices of the appropriate dimension and \( f_i(t) \) are arbitrary functions (except that they are zero initially and finally). We can vary these functions independently, and indeed if one of them is nonzero at one instant and the rest are zero for all times, the above condition becomes

\[
\text{Re} \int_0^T dt \left\{ \langle n(T)| U_0(T)U_0^\dagger (t)[H_0(t), \lambda_i]U_0(t)|n(0) \rangle \times \langle n(0)| U_0^\dagger (T)|n(T) \rangle \right\} = 0,
\]

an equation which must be true for all intermediate times \( t \) and for all \( i \). This is in principle an equation to be solved for \( H_0 \). However, as mentioned above, \( U_0 \) depends in a highly non-trivial way on \( H_0 \). Thus it is far from obvious how to use it to learn something about a system for which the time evolution operator is unknown (and if it is known, then the adiabatic approximation is of limited use).

**IV. TEST OF THE CONDITION**

We can at least test the condition on an exactly soluble model: the much-studied case of a spin-1/2 particle in a constantly rotating magnetic field. The geometry is illustrated in Figure 1.

![Rotating Magnetic Field](image)

**FIG. 1.** Rotating magnetic field with angular frequency \( \omega \) and angle with respect to axis of rotation \( \theta \).

The Hamiltonian is

\[
H(t) = -\frac{\omega_0}{2} \hat{n}(t) \cdot \mathbf{\sigma}
= -\frac{\omega_0}{2} e^{-i\frac{\omega_0}{2} \sigma_3} e^{-i\frac{\omega_0}{2} \sigma_2} e^{-i\frac{\omega_0}{2} \sigma_1}
\]

(7)

where \( \hat{n} \) is a unit vector in the direction of the magnetic field and \( \omega_0 \) is the Larmor frequency. The time evolution operator is

\[
U(t) = e^{-i\frac{\omega_0}{2} \sigma_3} e^{i\frac{\omega_0}{2} (c_2 \sigma_2 + c_3 \sigma_3)}
\]

(8)
where $\beta$, $\bar{\omega}$ are defined in Figure 2.

Since the model can be solved exactly, the adiabaticity can be calculated analytically as a function of $t$; the result (supposing we have started in an eigenstate of the initial Hamiltonian, e.g. $\exp(-i\theta\sigma_2/2)|+\rangle$) is

$$A(t) = 1 - \left(\frac{\omega s_0}{\bar{\omega}}\right)^2 s_{2t/2}^2$$

$A$ is obviously maximized when $\bar{\omega} t = 2\pi m$, where $m \in \mathbb{Z}$.

Thus, we can imagine being asked to find a Hamiltonian which optimizes the adiabaticity for the following parameters of the problem:

- system: spin 1/2
- $H(0) = -\frac{\omega}{2} e^{-i\frac{3}{2}\sigma_2} e^{i\frac{3}{2}\sigma_2}$
- $H(T) = -\frac{\omega}{2} e^{-i\frac{3}{2}\sigma_3} e^{-i\frac{3}{2}\sigma_2} e^{i\frac{3}{2}\sigma_2} e^{i\frac{3}{2}\sigma_3}$
- $T = 2m\pi/\bar{\omega}$ with $\bar{\omega}$ as defined in Figure 2

In principle, we would like to use (6) to determine an optimal Hamiltonian $H_0(t)$. We have not found a way to do so directly, but we can at least check that (7) is indeed optimal. This is simply a matter of substituting (7) and (8) into (6). This is somewhat tedious but absolutely straightforward, and we see that indeed for $T = 2m\pi/\bar{\omega}$, (7) does indeed result in a solution of (6), as expected.

V. CONCLUSIONS

A condition was derived which implies that the adiabaticity (defined in (2)) is maximal. This condition in principle determines which Hamiltonian or Hamiltonians give rise to perfectly adiabatic evolution. However the condition is expressed in terms of the evolution operator, which depends on a complicated way on the Hamiltonian, so it is not yet clear how to extract useful information about a system for which the evolution operator cannot be determined. We verified that the optimization condition is indeed satisfied when the evolution is optimal, in the case of an exactly-solvable system: a spin in a uniformly rotating magnetic field.

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![FIG. 2. Illustration of $\beta$, $\bar{\omega}$.

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