Adiabatic evolution

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Definition. *Adiabatic evolution of a quantum system usually refers to its unitary evolution driven by external controls such that there is no probability change on its instantaneous eigenstates of the time-dependent system Hamiltonian.*

Keywords

Adiabatic theorem; geometric phase; shortcut to adiabaticity; holonomy; adiabatic quantum computing; circuit-to-Hamiltonian map; bang-bang; quantum control.

Abstract

We introduce the idea of adiabatic evolution (AE) in quantum mechanics and also in the context of quantum control. To begin with, we explain AE and the idea of shortcut to adiabaticity. For cyclic evolution, AE leads to geometric phase and the non-Abelian ones: holonomy, which is central for holonomic and anyonic quantum computing. We then focus on the adiabatic quantum computing, and explain the proof of universality based on circuit-to-Hamiltonian map. By viewing AE as a type of quantum control scheme, we explain various control schemes, and we also analyze the key differences between quantum control and quantum computing. Finally, we survey some frontiers and stories in the history of AE.

1 Minimal version of AE

1.1 Opening

The subject of this document is about *driven evolution*, which is the dynamics not induced by the system Hamiltonian itself, but instead by external means. Although sometime it might be hard to draw a boundary between external and internal means, usually this can be clearly made. Driven evolution is very common in our daily life, just like driving a car there are many ways to perform it. Imagine a car does not have a Hamiltonian, it can only be moved by a driver, can be slowly, abruptly, via zigzag path, circling, or any other forms.

Adiabatic evolution (AE) is an ideal but common type of driven evolution, originating from thermal physics. It refers to no exchange of heat of a system with an external bath. So there could be work and exchange of particles. This can be seen from the expression of energy $E = \mu N + \sum_i p_i E_i$: the change of energy δE can be from any of the variables in it. Heat refers to change of probability p_i, work refers to change of each energy level E_i, while particle exchange is due to δN. We could also apply this picture to quantum systems, except for new variables such as geometric phase.

AE has been very popular in quantum physics, from the early Landau-Zener study, to the seminal Berry phase, and the recent application in quantum computation via adiabatic passage, holonomy, or anyon braidings. In a more general picture, AE belongs to the field of *quantum control*, which aims to use external means to steer quantum systems to achieve some goals.

1.2 Primary

To introduce AE, we need a parameter-dependent Hamiltonian $H(\lambda)$, while λ depends on time t. For simplicity, we consider a model with $H(t)$. In general, the evolution $U := \mathcal{T} e^{i \int H(\tau) d\tau}$ is extremely hard to solve. Adiabaticity is one way to make this simple by just focusing on the Hamiltonian itself. Assume 1) $H(t)$ can be diagonalized for all t with bounded spectrum $\{E_n(t)\}$ and eigenstates $\{|n(t)\rangle\}$; we assume no degeneracy for now; 2) $H(t)$ is smooth for all t; 3) there is no level-crossing, i.e., eigenvalues can never be the same; 4) $\frac{d}{dt}|n(t)\rangle$ and $\frac{d^2}{dt^2}|n(t)\rangle$ are piecewise continuous. Write the model as

$$H(t) = \sum_n E_n(t)|n(t)\rangle\langle n(t)|. \tag{1}$$

Any state in the basis $\{|n(t)\rangle\}$ can be written as

$$|\psi(t)\rangle = \sum_n c_n(t) e^{-i\theta_n(t)} |n(t)\rangle. \tag{2}$$

Now comes the adiabatic part: the probability $p_n = |c_n(t)|^2$ on each state is required not to change. Hence we can assume $c_n \in \mathbb{R}^+$ and be fixed. AE will only change the phases $\theta_n(t)$ and the basis $\{|n(t)\rangle\}$, with the former containing a geometric part, and the latter refers to work. As p_n does not change, we can assume the initial state is a $|n(0)\rangle$, which evolves to $e^{-i\theta_n(t)}|n(t)\rangle$. Apply $H(t)$ on it and it is not hard to find

$$\theta_n(t) = \int_0^t E_n(\tau) d\tau - i \int_0^t \langle n(\tau)|\dot{n}(\tau)\rangle d\tau, \tag{3}$$

with the first term called "dynamical" phase and the second term called Berry's phase, i.e., the adiabatic geometric phase. As a global phase, the Berry's phase cannot be detected; however, superposition of different states can manifest the difference of it, which is indeed measurable. The condition of constant probability p_n can be expressed as $|\langle m(t)|\dot{n}(t)\rangle| = 0$ or $\ll 1$ $\forall m \neq n$, which is the condition for AE.

Actually, geometric phase goes beyond AE. The essence is that there should be a smooth sequence of states $|\psi(t)\rangle$ for $t \in [0, T]$ with $|\psi(0)\rangle = e^{-i\theta}|\psi(T)\rangle$. For a system, such states are called *cyclic solution*. We can define cyclic non-adiabatic geometric phase, which is known as Aharonov-Anandan (AA) phase. Given $H(t)$, if $|\psi(t)\rangle$ is a solution, then define the dynamical phase

$$\theta_{\mathrm{dy}}(t) := \int_0^t \langle \psi(\tau)|H(\tau)|\psi(\tau)\rangle d\tau, \tag{4}$$

and the geometric phase is the difference $\theta - \theta_{\mathrm{dy}}(t)$. However, the cyclic condition is no easier than the adiabatic condition. Note that the cyclic condition does not imply H itself is periodic.

Back to AE, the difficulty is that it cannot be realized exactly. Any slow change of external parameters will lead to a bit excitation, namely, the actual state will not be the form (2). It turns out the solution (2) becomes exact if a counterdiabatic (CD) term is added

$$H_{\mathrm{CD}}(t) = i \sum_{m \neq n} |m(t)\rangle\langle m(t)|\dot{n}(t)\rangle\langle n(t)|. \tag{5}$$

We can see the adiabatic condition from it easily. This CD term is found by defining

$$U(t) = \sum_n e^{-i\theta_n(t)} |n(t)\rangle\langle n(0)| \tag{6}$$

and $H(t) = i\dot{U}U^\dagger$. For non-AE, this term can be added, and in general $[H_{\rm CD}(t), H(t)] \neq 0$. We could use Trotter formula $\prod_k e^{it_k H_{\rm CD}(t_k)} e^{it_k H(t_k)}$ to approximate the total evolution, which can be much faster than the original AE. This is a central scheme for the shortcut to adiabaticity (STA). However, the CD term is usually too complicated to be applicable, or might be forbidden by some super-selection rules.

In the above, the exact scaling in the adiabatic condition is not specified. That is, we did not specify how AE is approached, e.g., how much time is needed, how difficult to realize a quasi-AE, or the degree of (non-)adiabaticity. A simple way to measure the degree is to use $\|H_{\rm CD}\|/\|H(t)\|$, or other operator norms. A better way is to use the uncertainty principle: the time-energy uncertainty specifies a tradeoff between time and energy. This has been widely used in many settings such as quantum speed limit, quantum estimation, and lower bound for quantum algorithm cost. One form of the time-energy uncertainty is

$$\tau \geq \frac{c}{\Delta H} \tag{7}$$

for some constant c and $\Delta H = \sqrt{\langle H^2\rangle - \langle H\rangle^2}$, which can be applied to a quasi-AE at any instance. The evolution time τ will be longer if the 'fluctuation' of the spectrum ΔH is tiny. A similar form using the gap value $\Delta(t)$ along the path is $\tau \sim O(\max_t \|\dot{H}(t)\|/\Delta(t)^2)$. From this formula, it is clear that gap-closing is forbidden for AE.

1.3 More: holonomy

Recall that above we assumed no degeneracy. Instead, the degenerate case is more interesting, which leads to 'non-Abelian geometric phases', also called holonomy. For a set of orthonormal states $|\psi_m\rangle$ with parameter r and fixed energy, the matrix-element of the holonomy is

$$\gamma_{mn} = -i \int dr \langle\psi_m|\partial_r|\psi_n\rangle. \tag{8}$$

The degeneracy condition is necessary to avoid dynamical effects. This plays important roles for holonomic quantum computing (HQC) and anyonic (topological) quantum computing (TQC).

The HQC is usually realized in small systems, and gates via holonomy are realized by tuning parameters in Hamiltonian. The degeneracy of states has to be fine-tuned. A seminal system is the atom-laser coupled system, with laser variables such as frequency, strength, and phase as external parameters, there could be degenerate 'dark states'. A holonomy, which is a unitary operator, can be applied on the subspace of dark states via a path of external parameters. Such holonomy is geometrical but not topological.

In TQC, the holonomy from anyon braidings is topological. In this case, the external parameter is the location of anyons in a topological system. The degeneracy of states arises from the fusion space of anyons. The nature of topology is similar with the Aharonov-Bohm (AB) phase, which is also topological. In the AB effect, the trapped flux serves as a nontrivial defect in the configuration space of an electron, whose trajectory cannot be shrunk to a point. This relates to the nontrivial homotopy of a circle, which counts the number of windings. The topology is physically due to the gauge invariance of electromagnetic fields, or in general, gauge fields. As we know, gauge theory can be used to describe topological systems.

A final question is: is this topological holonomy adiabatic? Namely, does the motion of an electron or anyon have to be adiabatic? For the AB phase, it is not easy to tell. The spectrum of electron is gapless. AE would imply a constant energy, but a circling electron might emit radiations. Using the AA phase, it seems there is no need to be adiabatic. The trajectory of an electron is just a cyclic solution for the AA phase. Similarly, anyon braidings do not have to be adiabatic. However, non-AE of anyons, realized by some external 'dragger', might cause thermal excitation of other anyons, which could interfer with the desired braidings. There is a time window for anyon braiding: it shall be faster than the possible dynamical effects due to non-degeneracy of the fusion space, but slower that the creation of thermal excitation. So, roughly speaking, anyons have to be moved quasi-adiabatically.

2 Advanced topics: adiabatic quantum computing

The adiabatic quantum computing (AQC) is a direct application of AE which does not reply on geometric phases. In AQC, the solution to a problem is encoded in a complicated quantum state $|\psi_f\rangle$, which can be evolved adiabatically from an easily prepared state $|\psi_0\rangle$. Here, we analyze the most central issue: how can AQC be universal? The *universality* means that it is able to realize any unitary operator $U \in SU(2^n)$ acting on n qubits.

Usually, U is decomposed as a product of primary one and two-qubit gates. If we simulate each primary gate by an adiabatic process, the whole sequence of them may not be adiabatic anymore. Instead, the common simulation method is to prepare arbitrary state $|\psi_f\rangle$ generated by a random U. The required time-dependent Hamiltonian is of the form

$$H(s) = (1-s)H_i + sH_f \tag{9}$$

for $s \in [0,1]$ as the effective time, and the model remains gapped for all s. The solution is highly non-unique: given some states, there could be vast kinds of Hamiltonians taking them as eigenstates. But the difficult part is to prove the model is *gapped*.

Here we review the method based on Feynman-Kitaev space-time circuit-to-Hamiltonian map. Instead of requiring $|\psi_f\rangle$ as the unique ground state of H_f, it uses the history state

$$|\Phi\rangle = \frac{1}{\sqrt{L+1}} \sum_{\ell=0}^{L} |\psi_\ell\rangle|\ell\rangle \tag{10}$$

with $|\psi_\ell\rangle = \prod_{a=0}^{\ell} U_a|\psi_0\rangle$ as the computation state at step ℓ, with $U = U_L \cdots U_2 U_1$, $U_0 = \mathbb{1}$. The states $|\ell\rangle$ are 'clocks' that times the computation. The history state can be formally written as a column-vector $(\psi_0, \psi_1, \ldots, \psi_L)^t$. Now if we define terms

$$H_\ell = \begin{pmatrix} \mathbb{1} & -U_\ell^\dagger \\ -U_\ell & \mathbb{1} \end{pmatrix} \tag{11}$$

in the subspace $\{|\ell-1\rangle, |\ell\rangle\}$, we find it satisfies $H_\ell^2 = 2H_\ell$, so $\frac{1}{2}H_\ell$ is a projector, and $H_\ell|\Phi\rangle = 0$. This leads to the model $H = \sum_\ell H_\ell$ which takes $|\Phi\rangle$ as a ground state.

Now we apply this method to AQC. First, we need to design the clock. It turns out there are many ways, and a geometric way is to let $|\ell\rangle = |0^\ell 1^{L-\ell}\rangle$ using L qubits, and there are $(L+1)$ clock states which are product states. It is simple to see the state $|\Phi\rangle$ is prepared by the circuit

$$\wedge U = \prod_{\ell=1}^{L} (P_\ell^1 \otimes U_\ell) F |0^L\rangle |\psi_0\rangle, \tag{12}$$

for the initial computation state $|\psi_0\rangle$ usually set as $|0^n\rangle$, P_ℓ^1 as the projector $|1\rangle\langle 1|$ on the ℓth clock qubit. The gate F generates the clock state $\frac{1}{\sqrt{L+1}} \sum_\ell |\ell\rangle$. The initial state is the ground state of

$$H_i = H_{\rm in} + H_c + H_{\rm co}, \tag{13}$$

where $H_{\rm in} = \sum_{r=1}^n P_r^1 \otimes P_1^0$ projects out $|0^L 0^n\rangle$, $H_c = \sum_{\ell=1}^L P_\ell^0 \otimes P_{\ell+1}^1$ projects out the clock subspace $\{|\ell\rangle\}$, $H_{\rm co} = P_1^1$ projects out the clock state $|0^L\rangle$. The final model H_f is

$$H_f = \frac{1}{2} H_{\rm cir} + H_{\rm in} + H_c, \tag{14}$$

with $H_{\rm cir} = \sum_\ell H_\ell$. Here H_1 and H_L in it are edge terms with $H_1 = h_1 \otimes P_2^0$, $H_L = P_{L-1}^1 \otimes h_L$; all other $H_\ell = P_{l-1}^1 \otimes h_l \otimes P_{\ell+1}^0$, and h_ℓ are of the form (11). It is not hard to see $H_f |\Phi\rangle = 0$.

Now we have a model for AQC, the next task is to prove it is gapped. The model H contains a set of projectors, the dynamic ground subspace of H is spanned by $\{|\psi_\ell\rangle|\ell\rangle\}$, which is of dimension $2^n(L+1)$. The idea to prove the gap is first to prove the gap of the effective model of H on the ground subspace, which is a simple quantum walk. We would not study the details here. This subspace gap then will imply the gap of the model as

$$\Delta(H) \geq \Omega(1/L^3), \tag{15}$$

so the AE time scales as $O(L^3)$, independent of n, which means the simulation of a circuit U is efficient. The cost due to n shows up in the number of terms of H. Note that during the AE the exact form of the instantaneous ground state of $H(s)$ is unknown and not required. That is, the AE does not simulate U step by step, instead it only simulates the input-output map $|\psi_0\rangle \mapsto |\psi_f\rangle$.

This is not the end of the story. Given $|\Phi\rangle$, we still need to extract $|\psi_f\rangle$ from it. Apparently, we have to measure the clock state and we only obtain

$|\psi_f\rangle$ with probability $1/(L+1)$, which is tiny! This appears as a flaw of the method, but there is a naive way out: we could boost the success probability by repeat it many times, namely, we attach a long string of identity gates to the circuit U. Of course, there are also other clever ways, including other designs of the clock. Besides, the above construction has been improved in many ways, e.g., reducing the locality of terms, enforcing translation-invariance etc.

3 Most relevant theory: quantum control

We could put AE in a broader perspective, which is quantum control. Quantum control is an important subject in quantum engineering and quantum physics, which aims to use external (sometimes internal) controllers to steer a quantum system for some goals. Here 'external' usually means the control parameters are classical variables, while 'internal' could mean the controllers are also quantum or controllers can significantly modify the coherence of the controlled system. In this way, AE is a simple quantum control that uses adiabatic changes of classical variables to convert between states or generate geometric phases.

Quantum control problem could be formalized as an optimization

$$\max_c \ f(c) \tag{16}$$

for c as the controller and $f(c)$ as the objective function. This appears simple but it isn't. There are nontrivial issues for all of its components:

1. The choices of c; e.g., it can be external fields, interaction strength, etc, can be external or internal.

2. The choices of f. It depends on the goal of the control; e.g., the set of desirable unitary operations. A key concept is *controllability*, which asks if a target can be realized given a control scheme.

3. The choices of $f(c)$. There are many functions that can be used, sometimes multiple ones are used to confine a range of optimal controls.

4. The set of $f(c)$; e.g., if they are linear, convex or other special forms.

5. The algorithms to realize 'max'. As usually is the case, optimization problems are very complicated and there are tons of algorithms.

Besides, some control problems do not focus on optimization at all.

In quantum physics, a seminal control problem is to use lasers to manipulate the dynamics of an atom. This can be used to realize geometric phase, quantum gates, a small heat engine, or for cooling, making BEC etc. We have discussed quantum computing a lot above, so an immediate question is: what is the difference between quantum control and quantum computing? This is a difficult question since they overlap a lot. Below we list some of their key concepts:

- QComp: information processing; logic; computational complexity; computing models; universality; set of problems an algorithm can solve; focus on states instead of Hamiltonian.
- QCont: system manipulation; mechanism of control schemes; controllability; robustness; usually assume Hamiltonian; optimal control.

Probably the primary difference is this: QComp relies on *information*, while QCont relies on *system*, with the former connects with information theory, the latter with system theory. A system is a collection of physical objects with features, which can be states, observable, statistical properties etc. Information is carried by physical objects but an *encoding* is needed to specify the (logical) information, which is usually encoded in quantum states (rather than Hamiltonian or observable). Because of this, QComp and information theory need to study error correction to protect information, while Qcont and system theory usually focus on robustness against perturbations or avoid errors instead of correcting them. The notion of universality is stronger than controllability, since the latter does not have to realize a whole unitary group $SU(d)$; on the other hand, the latter usually assumes a stringent set of controls while the former does not.
From Fig. 1, you could see the connections among different fields. Try to figure out what they are, or if there are more connections.

4 Frontiers

It seems there is no fundamental open problems relating to AE. The subject of AE and quantum control nowadays is mostly concerned for quantum technology. Here we mention several frontiers.

More advanced control schemes are developed for quantum technology. For instance, as the opposite of AE, a system can be acted upon 'brutally':

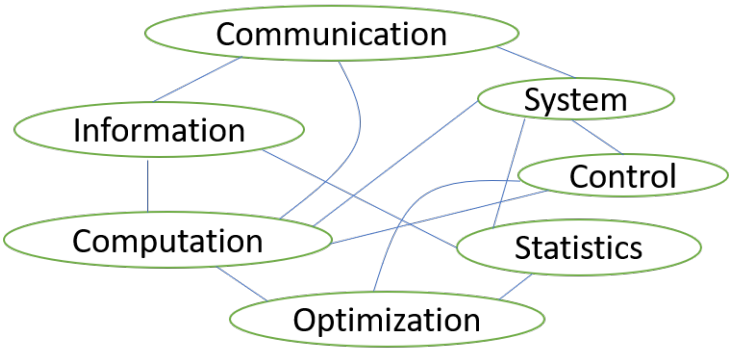

Figure 1: Kaleidoscope of research fields.

this includes the sudden quench, bang-bang control, Zeno effect etc. Various schemes of STA to avoid AE are also frontiers. Our way of running is an example of bang-bang control: you cannot run with one leg, instead, we use the two legs alternatively and each with full strength, then we can run forward. To realize the dynamics of a Hamiltonian $H = \sum_n H_n$, with $[H_n, H_m] \neq 0$, we can use short Trotter pulses $e^{i\tau_n H_n}$ sequentially. The Zeno effect uses a sequence of projective measurements which strongly disturb the coherence of a system. The sudden quench is mostly implemented on cold atoms in optical lattices, which is used to study non-equilibrium dynamics by suddenly changing some external parameters such as potential depth etc. To realize a goal, sometimes these schemes can be combined together to form highly nonlinear control paths: it may starts and ends suddenly but evolve adiabatically in between, or be the opposite. It is worthy to also mention another emerging technique known as Floquet engineering, which drives a bare system periodically.

In AQC, there are focuses to look for more adiabatic algorithms. This includes the study of other types of circuit-to-Hamiltonian maps, other forms of universal AQC schemes beyond the Feynman-Kitaev method, the design of more adiabatic algorithms; e.g., the AQC based on stoquastic Hamiltonian and speedup proofs. The famous D-Wave machines realize AQC as a quantum annealer, which can tune two-body interaction forms between qubits and evolve a large system of qubits from simple states to more complicated ones. Using quantum tunneling or excited states may provide speedups, but these are more difficult to control than the ground state.

Geometric phases are important part of AE, even some geometric phases

do not have to be adiabatic. The holonomy proves to be powerful than the Abelian case. The holonomy for small systems is geometrical, so sensitive to the control path. The holonomy for many-body systems (via anyon braidings) is topological, but it is extremely hard to find non-Abelian anyons! So there is the problem to look for other systems supporting holonomy which can be robust stronger than geometrical ones but may be weaker than topological ones. This robustness might be protected by a certain symmetry, redundancy, or freedom to make changes. For instance, the symmetry-protected topological order (e.g., valence-bond solids and topological insulators) is a novel type of systems beyond anyonic topological systems and trivial symmetry-breaking systems. The study of holonomy in this setting is a frontier.

5 History, people, and story

Although the idea of AE is apparent, in practice people need some criterion to tell if a process is AE. About fifteen years ago, there was some arguments about the necessary and sufficient condition for AE. The confusion comes from the ignorance of the assumptions/requirements to define AE, which we explained explicitly. With the requirements, the condition for AE is merely $\|H_{\rm CD}\|$ is much smaller than $\|H(t)\|$. In practice, it is better to specify the time needed to realize an AE, which needs the gap value instead of the whole Hamiltonian.

For quantum open systems, AE and geometric phases both have been studied. This appears as a paradox since AE requires no exchange of heat with the environment. Open-system dynamics such as Lindblad master equation $\dot{\rho} = \mathcal{L}\rho$ is due to exchange of energy, so AE implies that this dissipative process must be very slow or weak, $\dot{\mathcal{L}} \approx 0$. This could be formally done but has limited implications. Open-system geometric phases were also defined but have less apparent physical meanings. Sometimes it is hard to draw a boundary between math and physics: the math could be sound but the physical meaning is confusing, but lots of progress of physics are driven by beautiful mathematics.

The first quantum computing company is the famous *D-Wave* Systems, founded twenty years ago in Vancouver, Canada. It uses thousands of superconducting qubits to build a quantum annealer realizing AQC. Ironically, it is not recognized as a universal quantum computer for many reasons. The qubits are very noisy, there is no error correction, and the annealer seems

do not show quantum speedup. These arguments continue till today and they are updating their systems constantly. Nowadays there are more quantum computing companies, but they normally employ the standard circuit model, instead of AQC. What will be the future? We cannot tell. The situation may change slowly or adiabatically, or even abruptly, depending on what the driving forces are.

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Concept map