Time Scale for Adiabaticity Breakdown in Driven Many-Body Systems and Orthogonality Catastrophe

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The adiabatic theorem is a fundamental result in quantum mechanics, which states that a system can be kept arbitrarily close to the instantaneous ground state of its Hamiltonian if the latter varies in time slowly enough. The theorem has an impressive record of applications ranging from foundations of quantum field theory to computational molecular dynamics. In light of this success it is remarkable that a practicable quantitative understanding of what "slowly enough" means is limited to a modest set of systems mostly having a small Hilbert space. Here we show how this gap can be bridged for a broad natural class of physical systems, namely, many-body systems where a small move in the parameter space induces an orthogonality catastrophe. In this class, the conditions for adiabaticity are derived from the scaling properties of the parameter-dependent ground state without a reference to the excitation spectrum. This finding constitutes a major simplification of a complex problem, which otherwise requires solving nonautonomous time evolution in a large Hilbert space.

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The adiabatic theorem (AT) is a profound statement that applies universally to all quantum systems having slowly varying parameters. It was originally conjectured by Born in 1926 [1], and its complete proof was given in a joint paper by Fock and Born two years later [2]. A number of refinements have been proposed over the years, see Ref. [3] and references therein. The theorem addresses the time evolution of a generic quantum system having a Hamiltonian $\hat{H}_\lambda$, which is a continuous function of a dimensionless time-dependent parameter $\lambda = \Gamma t$, where t is time and Γ is called the driving rate. For each λ one defines an instantaneous ground state, which is the lowest eigenvalue solution to Schrödinger's stationary equation

$$\hat{H}_\lambda \Phi_\lambda = E_\lambda \Phi_\lambda. \tag{1}$$

For simplicity, we assume that Φ_λ is unique for each λ. Imagine that at $t = 0$ the system is prepared in the Hamiltonian's instantaneous ground state Φ_0. Then, as the parameter λ changes with time, the wave function of the system, Ψ_λ, evolves according to Schrödinger's equation

$$i\Gamma \frac{\partial}{\partial \lambda} \Psi_\lambda = \hat{H}_\lambda \Psi_\lambda, \qquad \Psi_0 = \Phi_0. \tag{2}$$

It is natural to expect that as time goes by, the physical state Ψ_λ will depart from the instantaneous ground state Φ_λ; in other words, the quantum fidelity

$$\mathcal{F}(\lambda) = |\langle \Phi_\lambda | \Psi_\lambda \rangle|^2 \tag{3}$$

will decrease from its initial value of unity. The adiabatic theorem states that this departure can be made arbitrarily small provided that the driving is slow enough. In more rigorous terms, for any λ and for any small positive ϵ there exists small enough Γ such that $1 - \mathcal{F}(\lambda) < \epsilon$. A process in which the fidelity (3) remains within a prescribed vicinity of unity is called adiabatic.

The AT is a powerful tool in quantum physics, with applications ranging from the foundations of perturbative quantum field theory [4,5] to computational recipes in atomic and solid state physics [6]. The recent upsurge of interest in the AT has been driven by the ongoing developments in the theory of quantum topological order [7] and quantum information processing [8]. The universal applicability of the AT, however, comes at a cost. Making no use of any specific properties of the Hamiltonian, the AT's mathematical machinery does not provide a useful definition of what is meant by "slow enough." In particular, it leaves open the following two questions. (i) For a given displacement λ in the parameter space what is the maximum driving rate Γ allowing us to keep the evolution adiabatic? (ii) For a given driving rate Γ what is the system's adiabatic mean free path, that is the maximum distance, λ_*, in the parameter space that the system can travel while maintaining adiabaticity? With the advent of technologies that depend on coherent quantum state manipulation, these questions are becoming of ever increasing practical importance.

For small or particularly simple systems questions, (i) and (ii) can be addressed microscopically, that is, through the explicit solution of Schrodinger's time-dependent equation [9]. The drawback of such a microscopic approach is that in larger systems it stumbles upon the issues of computational complexity, i.e., impossibility to solve the evolution in a huge Hilbert space, and redundancy, i.e., the disproportionate amount of irrelevant information encoded in the exact time-dependent wave function. As a way to bypass this problem, heuristic adiabaticity conditions [10] inspired by Landau and Zener's work on a two-level model [11,12] have been in use for several decades. The popularity of these conditions is due to their simplicity, intuitive appeal, and reliance on a small set of physical characteristics of a system. Unfortunately, these heuristic conditions were shown to fail even in elementary models [13,14]. Despite subsequent progress in mathematical theory of adiabatic processes [15–17] the relationship between the adiabaticity conditions and simple physical characteristics of a system remains largely unexplored. Here we show how this gap can be bridged for a broad natural class of physical systems, that is, many-body systems where a small move in the parameter space induces the orthogonality catastrophe. In this class, the adiabaticity loss rate has simple expression in terms of the scaling properties of the parameter-dependent ground state without a reference to the the excitation spectrum. This greatly simplifies theoretical investigation of the adiabaticity conditions by reducing a complex time-dependent problem in a large Hilbert space to the analysis of the ground state only.

We begin our analysis by noticing that new insight into the problem of adiabaticity can be obtained by enriching the general linear-algebraic construction of quantum mechanics with some additional structure. Such a structure appears naturally in many body systems, where the system size plays a role of an additional control parameter. Known examples of solvable driven many-body systems [18–21] point to the importance of this parameter for adiabaticity, although its general role is not yet understood and in some cases is a matter of debate [22–24]. To make further progress, we focus on a particular class of many-body systems where a small move in the parameter space induces a generalized orthogonality catastrophe. We define the latter as a phenomenon by which the overlap $\mathcal{C}(\lambda) \equiv |\langle \Phi_\lambda | \Phi_0 \rangle|^2$ has the following asymptotic behavior in the limit of a large particle number N

$$\ln \mathcal{C}(\lambda) = -C_N \lambda^2 + r(N, \lambda). \tag{4}$$

Here, $C_N \to \infty$ in the $N \to \infty$ limit, and r is the residual term satisfying $\lim_{N\to\infty} r(N, C_N^{-1/2}) = 0$.

We note that the class of many-body systems experiencing the orthogonality catastrophe in the form (4) is extremely wide. The theory of the orthogonality catastrophe is well developed, providing efficient tools for the calculation of C_N such as the linked cluster expansion, effective field theory methods, variational and Monte Carlo techniques [25,26]. These approaches have been underpinned by rigorous mathematical results for independent fermion systems [27,28]. It is worth noting that field-theoretical approaches to the calculation of C_N exploit the method of adiabatic evolution along the lines of the Gell-Mann and Low theorem. This requires extra care with taking the thermodynamic limit [29–32]. We emphasize that adiabatic evolution in such context is a formal device unrelated to any actual physical process. We further notice that in certain cases C_N can be linked to a direct experimental measurement, e.g., to the structure of the x-ray edge singularity [25]. Here we take Eq. (4) for granted and proceed to its implications for adiabaticity.

Our main result in its simplest and most useful form can be stated as follows. Consider a quantum system with a time-dependent Hamiltonian $\hat{H}_\lambda$, which possesses the following properties: (i) The system exhibits a generalized orthogonality catastrophe of the form (4) with $C_N \to \infty$ in the $N \to \infty$ limit. (ii) The uncertainty $\delta V_N \equiv \sqrt{\langle \hat{V}^2 \rangle_0 - \langle \hat{V} \rangle_0^2}$ of the driving potential

$$\hat{V} \equiv \left. \frac{\partial \hat{H}}{\partial \lambda} \right|_{\lambda=0}$$

in the initial state Φ_0 satisfies

$$\frac{\delta V_N}{C_N} \to 0, \qquad N \to \infty \tag{5}$$

(iii) The fidelity, Eq. (3), is a monotonically decreasing function of time [33]; therefore, one can define the adiabatic mean free path λ_* as the solution to $\mathcal{F}(\lambda_*) = 1/e$. Then we find that for a driving rate Γ independent of the system size the adiabatic mean free path tends to zero in the $N \to \infty$ limit with the leading asymptote given by

$$\lambda_* = C_N^{-1/2}. \tag{6}$$

It follows that for any fixed driving rate Γ and any fixed displacement λ adiabaticity fails if N is large enough to ensure $\lambda > \lambda_*$. To avoid the adiabaticity breakdown one has to allow the driving rate to scale down with increasing system size, $\Gamma = \Gamma_N$, where

$$\Gamma_N \leq \frac{\delta V_N}{2 C_N} \tag{7}$$

in the large N limit.

Next we sketch our derivation of the asymptotic formula for the mean free path, Eq. (6), and the necessary condition for a given process to be adiabatic in a large many-body system, Eq. (7). They both follow from a rigorous inequality

$$|\mathcal{F}(\lambda) - \mathcal{C}(\lambda)| \leq \mathcal{R}(\lambda) \quad \text{with}$$
$$\mathcal{R}(\lambda') \equiv \int_0^{\lambda'} \frac{d\lambda}{|\dot{\lambda}|} \sqrt{\langle \Psi_0 | \hat{H}_\lambda^2 | \Psi_0 \rangle - \langle \Psi_0 | \hat{H}_\lambda | \Psi_0 \rangle^2}. \tag{8}$$

Here, λ can be an arbitrary smooth function of time and $\dot{\lambda}$ is its derivative. In the large N limit and for $\dot{\lambda} = \Gamma$ the leading asymptote for $\mathcal{R}(\lambda)$ is $\lambda^2\delta V_N/(2\Gamma)$. Thus, the inequality (8) implies that the fidelity $\mathcal{F}$ and the orthogonality overlap function $\mathcal{C}$ stay close to each other for a certain path length determined by the ground state uncertainty of the driving potential δV_N and the driving rate Γ. When the system has traveled the distance λ_* given in Eq. (6), then $\mathcal{C}$ departs significantly from its inital value $\mathcal{C} = 1$, according to Eq. (4). If at the same time the right-hand side (r.h.s) of Eq. (8) is still small, which is ensured by Eq. (5) in the case of a fixed Γ, the fidelity $\mathcal{F}$ will follow $\mathcal{C}$ and the adiabaticity will be lost. This adiabaticity breakdown can be avoided if one allows the driving rate to scale with the system size. In this case one imposes the condition (7) to ensure that the r.h.s. of Eq. (8) is greater than one and thus $\mathcal{F}$ and $\mathcal{C}$ are unrelated.

The proof of the inequality (8) is given in the Supplemental Material [34]. Here we outline the main idea behind this proof. First, we recall that the space of quantum states can be endowed by a natural sense of distance, the Bures angle distance [35]

$$D(\Phi, \Psi) = \frac{2}{\pi} \arccos |\langle \Phi | \Psi \rangle|, \tag{9}$$

where Φ and Ψ are any two states represented by normalized wave functions in the system's Hilbert space. As the parameter λ changes the physical state Ψ_λ and the instantaneous ground state Φ_λ each describe a continuous trajectory in this metric space as illustrated in Fig. 1. At any given λ the states Φ_0, Ψ_λ, and Φ_λ form a triangle with sides a, b, and c. The sides a and c characterize the fidelity and the orthogonality overlap, respectively. In order to estimate the side b we employ the quantum speed limit [36,37], which provides an upper bound on the length of b in terms of the quantum uncertainty of the driving potential. The inequality (8) then follows from the triangle inequality $|a - c| \le b$.

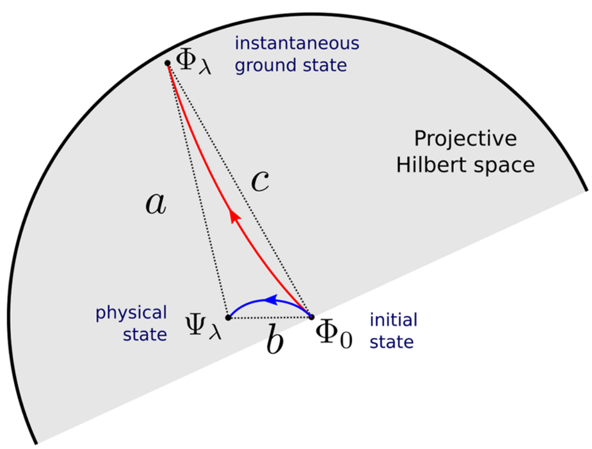

FIG. 1. Triangle inequality resulting in the estimate Eq. (8). States are shown as points in the projective Hilbert space. The red trajectory shows the evolution of the instantaneous ground state, Eq. (1), while the blue trajectory corresponds to the physical evolution given in Eq. (2). The length of side b is bounded by the quantum speed limit, while the length of side c approaches the maximally possible distance of 1 in the large N limit.

Next, we discuss, without going too deeply into the mathematical detail, the scaling properties of C_N and δV_N and explain why applicability conditions (i) and (ii) hold in a broad class of many-body systems. For simplicity, we limit ourselves to the case of a standard thermodynamic limit taken at a fixed particle density. We recall that typical physical observables in a many-body system are generated by quasilocal operators having a finite-range support in the configuration space. We denote one such operator $\hat{v}(x)$, where x is a point in a D-dimensional space and take

$$\hat{V} = \int_{\text{vol}} d^D x f(x) \hat{v}(x), \tag{10}$$

where the integral is taken over the volume of the system and $f(x)$ is a support function, which satisfies

$$\int_{\text{vol}} d^D x f(x) \sim N^{d/D}, \qquad N \to \infty. \tag{11}$$

For example, if $f(x)$ constraints driving to the boundary of the sample we have $d = D - 1$, for driving localized near a given point of space we have $d = 0$, while for driving homogeneously distributed in the bulk we have $d = D$. It is straightforward to see that in *all* systems with rapidly decaying local correlation functions, for example, in systems with a spectral gap, $\delta V_N \sim N^{d/(2D)}$ while $C_N \sim N^{d/D}$, which immediately ensures conditions (i) and (ii) for $d > 0$. For localized driving, $d = 0$, conditions (i) and (ii) are violated unless the spectrum of the system is gapless. For example, in a metal $C_N \sim \log N$ [27,38] (other scaling laws may apply in dirty metals [39,40] or near quantum critical points [41]) and $V_N \sim 1$.

To illustrate our general findings, we consider the Rice-Mele model, describing a system of fermions on a half-filled one-dimensional bipartite lattice with the Hamiltonian

$$H_{\text{RM}} = \sum_{j=1}^{N} [-(J + U) a_j^\dagger b_j - (J - U) a_j^\dagger b_{j+1} + \text{H.c.}] + \sum_{j=1}^{N} \Delta (a_j^\dagger a_j - b_j^\dagger b_j). \tag{12}$$

Here, a_j and b_j are the fermion annihilation operators on the a and b sublattices, and j labels the lattice cites. The Rice-Mele Hamiltonioan is an archetypal model of the adiabatic Thouless pump, that is, a system where exactly one particle is transferred from one end to another if a topologically nontrivial cycle is performed in the Hamiltonian's parameter space [42]. In the present case such a cycle would be any loop in the (U, Δ) plane enclosing the origin. The reasoning of Ref. [42] guarantees quantization of the pumped charge provided the evolution is adiabatic; however, the adiabatic conditions are not elaborated upon in Ref. [42].

The Thouless pump protocol in a Rice-Mele system was recently implemented in a parabolically confined ultracold atomic system [43] (see also Ref. [44] for pumping in a Bose-Mott insulator). The particle transport was measured by the direct observation of the center-of-mass displacement of the atomic cloud using *in situ* absorption imaging. The authors of Ref. [43] emphasize the importance of adiabaticity for the observation of the Thouless quantization. In order to ensure slow enough driving, they use a heuristic condition $\Gamma < \Gamma_{\mathrm{LZ}}$. Here, Γ_{LZ} is obtained in the Landau-Zener spirit from the condition $2\pi(D_{\min}/2)^2/(\dot{D}_{\max}) = 1$, where $D_{\min}$ is the smallest value of the time-dependent band gap $D(t)$, and $\dot{D}_{\max}$ is the maximal derivative of $D(t)$ during the cycle. We note that this condition is insensitive to the system size, in particular it does not predict any problems with adiabaticity in the thermodynamic limit. In contrast, our exact result (6), together with the scaling laws $C_N \sim N$ and $\delta V_N \sim \sqrt{N}$ (see Ref. [34]) imply that for any given $\Gamma < \Gamma_{\mathrm{LZ}}$ adiabaticity fails to survive even a single cycle of pumping when the number of particles is too large [45]. To illustrate the effect of the system size on adiabaticity we numerically simulate the evolution of the fidelity $\mathcal{F}$ in the Rice-Mele model (12) for various system sizes, with parameters J, U, Δ taken from the experiment [43]. While for $N = 10$, which is close to the experimental value, the bound (8) is too weak to relate the fidelity to the orthogonality catastrophe [34], for $N = 1000$ the bound is strong enough to ensure an e-fold decay of the fidelity over a mean-free path, which turns out to be only a small fraction of the complete cycle; see Fig. 2(a).

It is instructive to investigate what happens to the Thouless pumping in the regime where the particle number is large enough to ensure the collapse of adiabaticity within one cycle, but the driving is slow compared to the band gap. First, we consider this question qualitatively assuming, for simplicity, a two-terminal geometry where the ends of the Rice-Mele lattice are attached to two infinite particle reservoirs. In such a geometry the charge is pumped between the two reservoirs. We recall that the adiabatic mean free path $\lambda_* \sim 1/\sqrt{N}$ is the typical distance the Thouless pump travels in the parameter space before an elementary excitation is created in the bulk. For λ_* much shorter than the length of the loop that the system describes in the parameter space, a large number of elementary excitations is born in one cycle. These excitations form a dilute gas of mobile quasiparticles, which travel in both directions, left and right. If the pump is initiated in the equilibrium state and performs one cycle, then during the period T of the cycle the number of such excitations reaching the left or right end of the system will be $\delta N = \rho v T$, where $\rho \sim 1/(\lambda_* N)$ is the number of elementary excitations created during the cycle per lattice site and v is the typical group velocity. Clearly, $\delta N \ll 1$ in the large N limit; therefore, the charge pumped in one cycle will be close to the quantized value despite the violation of adiabaticity conditions. A completely different picture will, however, be seen if the pump operates continuously performing one cycle after another. The number of quasiparticles in the bulk will then

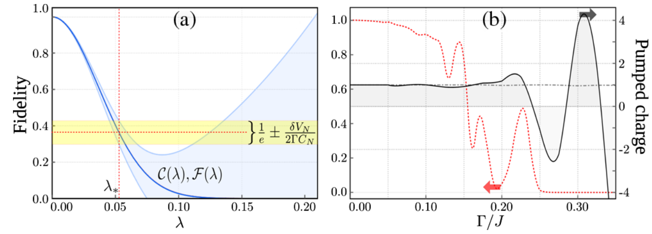

FIG. 2. Adiabaticity, orthogonality catastrophe, and transport in a Thouless pump described by the Hamiltonian (12) with $N = 1000$ particles. (a) Illustration of the inequality (8). Solid blue—the orthogonality overlap $\mathcal{C}(\lambda)$. The shaded region is the one which has to contain the $\mathcal{F}(\lambda)$ curve due to the inequality (8). This bound is tight enough to guarantee the adiabaticity breakdown for the chosen set of parameters, $J = 0.4E_R$, $U = 0.4E_R$, $\Delta = \lambda E_R$ with $\lambda = \Gamma t$ and $\Gamma = 0.7E_R$. For $E_R = 6.4\ \mathrm{ms}^{-1}$ these parameters coincide with those of the effective Hamiltonian describing the optical lattice in the experiment Ref. [43] at the $\Delta = 0$ point of the pumping cycle. Remarkably, true adiabatic fidelity $\mathcal{F}(\lambda)$ calculated numerically follows $\mathcal{C}(\lambda)$ even closer than what can be expected from the bound (8), so that the two curves look indistinguishable in the figure. The latter fact indicates that sides b and c of the triangle depicted in Fig. 1 are in fact nearly orthogonal in the present case. (b) Operation of the Thouless pump in the first cycle as compared to a steady-state regime, for different values of the driving rate, Γ. The cycle is given by $\Delta = (J/2)\sin\lambda$, $U = (J/2)\cos\lambda$ with $\lambda = \Gamma t$. Initially the system is in equilibrium. Dash-dotted gray—charge transferred in the first cycle. Dashed red—the adiabatic fidelity $\mathcal{F}$ at the end of the first cycle. Solid black—charge transferred per cycle in a continuous regime after the stationary state is reached. One can see that the charge transferred in the first cycle is quantized even when the many-body adiabaticity has gone completely ($\mathcal{F} \simeq 0$), while the quantization of the charge in the continuous regime disappears as soon as the many-body adiabaticity is broken.

keep increasing until the amount of elementary excitation particles leaving the system through the boundary per unit time gets equal to the production rate $N\rho/T$. Since $N\rho \gg 1$, the Thouless quantization should be completely destroyed in such a steady state. To summarize, in the considered regime of slow but nonadiabatic driving the quantization of the transferred charge is a transient phenomenon which fades away with time if the pump is operated continuously. This conclusion is supported by a microscopic calculation as illustrated in Fig. 2(b).

To conclude, we have established a simple quantitative relationship between the orthogonality catastrophe and the adiabaticity breakdown in a driven many-body system. We have illustrated the utility of this finding by determining conditions for quantization of transport in a Thouless pump.

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[45] This scaling exemplifies a remarkable fact: In a many-body system a finite energy gap is not sufficient to protect adiabaticity in the thermodynamic limit. This fact can be easily inferred from our general scaling analysis for $d \geq 1$.