TCM315 Fall 2022: Introduction to Open Quantum Systems

Lecture 10: Qualitative analysis of unitary time evolution

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CONTENTS

1. INTRODUCTION

We review some general mathematical results which allows us to circumscribe dynamics compatible with unitary evolution. In particular, we identify a theoretical scenario to account for the exponential decay of the survival probability often observed in experiments.

An insightful qualitative analysis of the dynamics generated by unitary evolution is Complement $\mathrm{A}_{\mathrm{III}}$ of [3]. A pedagogic review including extensive reference to the literature, is also offered in [1].

2. SPECTRAL THEOREM AND UNITARY EVOLUTION

Let us consider a quantum system governed by an infinite dimensional self-adjoint Hamiltonian. We suppose that the spectrum is bounded from below say by the zero energy level $E = 0$. We also suppose that the spectrum contains a countable discrete component $\{\epsilon_i\}_{i\geq 0}$ with $\epsilon_0 = 0$ and corresponding eigenvectors $\{\phi_i\}_{i\geq 0}$. In addition we surmise that the spectrum has a continuous component taking values for $[\lambda, 0)$ for some $\lambda > 0$ with corresponding generalized eigenvectors φ_y of energy $y \in [\lambda, 0)$.

Based on these hypotheses the unitary evolution operator acts on a test function (i.e. sufficiently integrable so that all the ensuing steps are well defined) f as

$$\mathbb{U}_t f = \sum_{i\geq 0} e^{-\imath\,\epsilon_i\,t}\phi_i \,\langle\,\phi_i\,,f\,\rangle + \int_{\lambda}^{\infty} \mathrm{d}y\,n(y)\,e^{-\imath\,y\,t}\,\varphi_y\,\langle\,\varphi_y\,,f\,\rangle \tag{1}$$

In general the integral over the continuous is modulated by a positive definite function

$$n\colon \mathbb{R}_+ \mapsto \mathbb{R}_+$$

characterizing the **density of energy eigenstates** at y (see e.g. § 3 of chapter 4 [5]). We wish to inquire the time asymptotic behavior of this expression.

2.1. Discrete spectrum: almost periodic functions

We first restrict the attention to a pure point spectrum. The survival amplitude of a state $\boldsymbol{\psi}$ at time t is

$$\langle \boldsymbol{\psi} , \mathbb{U}_t \boldsymbol{\psi} \rangle = \sum_{i \geq 0} e^{-\imath \epsilon_i t} | \langle \boldsymbol{\phi}_i , \boldsymbol{\psi} \rangle |^2$$

In order to analyze the qualitative behavior of the survival amplitude we need the notion of **almost periodic function**.

Definition. *(**Harald Bohr**) A continuous function $f : \mathbb{R} \mapsto \mathbb{R}$ is called an **almost periodic** function if, for every $\varepsilon > 0$, there exists a T_ε such that **for every** t the interval $[t , t + T_\varepsilon)$ **contains at least one** τ such that*

$$|f(t) - f(t + \tau)| < \varepsilon$$

In other words, an almost periodic function after a sufficiently long time will return arbitrarily closely to any value it has taken.

Let us consider the function

$$f(t) = \sum_{k=0}^{N} r_n \, e^{\imath E_n t} \qquad r_n \geq 0 \ \forall n \tag{2}$$

Then the chain of equalities

$$|f(t+T) - f(t)| = \left| \sum_{k=0}^{N} r_n \left(e^{\imath E_n (t+T)} - e^{\imath E_n t} \right) \right| \leq \sum_{k=0}^{N} r_n \left| e^{\imath E_n T} - 1 \right| = 2 \sum_{k=0}^{N} r_n \left| \sin\left(\frac{E_n T}{2} \right) \right|$$

holds true. It is readily seen that the absolute value of the difference does not depend upon t. A standard result of the theory of the almost-periodic functions states then that for all ε for any f of the form (2) **it is always possible to find a** T_ε such that

$$|f(t + T_\varepsilon) - f(t)| < \varepsilon \qquad \text{for all } t$$

The conclusion is that the survival amplitude in finite dimensional Hilbert spaces specifies an almost periodic function. The result can be extended also to countable point spectra. In particular [2, 9] proved that

Proposition. *for any $\varepsilon > 0$ there **exists at least one** T_ε such the unitary evolution in the Schrödinger picture according generated by a time-autonomous self-adjoint Hamiltonian with pure point spectrum satisfies*

$$\|\boldsymbol{\psi} - \mathbb{U}_{T_\varepsilon} \boldsymbol{\psi}\| < \varepsilon$$

for any state vector $\boldsymbol{\psi}$

Proof.
The norm squared is by definition

$$\|\boldsymbol{\psi} - \mathbb{U}_T \boldsymbol{\psi}\|^2 = \langle \boldsymbol{\psi} - \mathbb{U}_T \boldsymbol{\psi} , \boldsymbol{\psi} - \mathbb{U}_T \boldsymbol{\psi} \rangle = 2 - 2 \operatorname{Re} \langle \boldsymbol{\psi} , \mathbb{U}_T \boldsymbol{\psi} \rangle$$

We get into

$$\|\boldsymbol{\psi} - \mathbb{U}_T \boldsymbol{\psi}\|^2 \leq 2 \sum_{n \geq 0} | \langle \boldsymbol{\phi}_n , \boldsymbol{\psi} \rangle |^2 \big(1 - \cos(E_n T) \big)$$

The convergence of the series imposes that for any T there is an N_T such that

$$\sum_{n \geq N_T} | \langle \boldsymbol{\phi}_i , \boldsymbol{\psi} \rangle |^2 \big(1 - \cos(E_n T) \big) < \frac{\varepsilon}{2}$$

The theory of almost periodic functions grants us the existence of a T_ε such that

$$\sum_{n \leq N-1} | \langle \boldsymbol{\phi}_i , \boldsymbol{\psi} \rangle |^2 \big(1 - \cos(E_n T_\varepsilon) \big) < \frac{\varepsilon}{2}$$

Combining the two observations yields the claim □

The conclusion is that we cannot expect any irreversible decay from Hamiltonians with pure point spectrum.

Remark. *Existence of recurrence cycles proves that in a finite system information can never disappear [10]. It must be also emphasized that for macroscopic environments the recurrence time T_ε may actually prove longer than the lifetime of the Universe.*

*A plausible scenario is that in a system with $N \gg 1$ degrees of freedom the state autocorrelation function (or similar indicators) "decreases to zero on what one may call a correlation decay time scale" [10]. This regime decay of correlations is followed by a presumably much longer period during which the indicator fluctuate around zero having apparently lost coherence. Only on extermely long time scales almost periodicity become manifest giving rise to **quantum revival phenomena**.*

2.2. Continuous spectrum: decay

Unitary evolution is compatible with asymptotic decay of the survival amplitude if the spectrum is continuous. This is a consequence of the Riemann–Lebesgue lemma. Namely

Proposition. ***(Riemann–Lebesgue)***

$$\lim_{t \nearrow \infty} \int_{\mathbb{R}} \mathrm{d}\epsilon\, e^{-\imath\,\epsilon\,t}\, g(\epsilon) = 0$$

if $g(\epsilon)$ is integrable in $\mathbb{R}$ i.e. $g \in L^1(\mathbb{R})$

$$\int_{\mathbb{R}} \mathrm{d}\epsilon\, |g(\epsilon)| < \infty$$

a. Idea of the Proof:

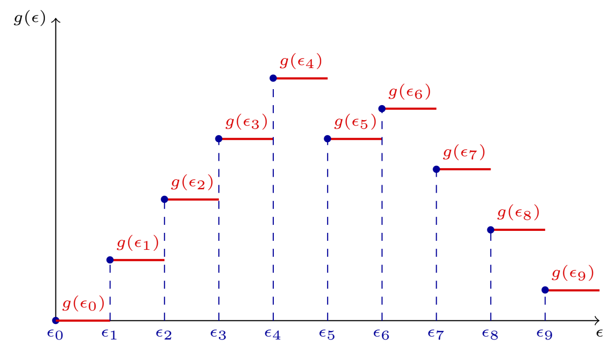
Any function in $L^1(\mathbb{R})$ can be approximated with arbitrary accuracy with a sequence of step functions.

$$g(\epsilon) = \lim_{N \nearrow \infty} \sum_k g_k^{(N)} \chi_{\mathbb{I}_k^{(N)}}(\epsilon)$$

where for all finite N, $\chi_{\mathbb{I}_k^{(N)}}(\epsilon)$ is the indicator function of the set $\mathbb{I}_k^{(N)}$ and

$$\sum_k \mathbb{I}_k^{(N)} = \mathbb{R}$$

In other words the disjoint union of the $\mathbb{I}_k$'s forms a partition of the real axis.



Discretization of an integrable function on the positive real axis

It follows that for any finite N

$$\int_{\mathbb{R}} \mathrm{d}\epsilon\, e^{-\imath\,\epsilon\,t} \sum_k g_k^{(N)} \chi_{\mathbb{I}_k^{(N)}}(\epsilon) = \sum_k g_k^{(N)} \int_{\mathbb{I}_k^{(N)}} \mathrm{d}\epsilon\, e^{-\imath\,\epsilon\,t} = \sum_k g_k^{(N)} \frac{e^{-\imath\,E_k\,t} - e^{-\imath\,E_{K+1}\,t}}{\imath\,t} \overset{t \nearrow \infty}{\to} 0$$

□

3. KHALFIN'S RESULT: LARGE TIME ASYMPTOTICS OF THE CONTINUOUS SPECTRUM

The conclusion we can draw from Riemann–Lebesgue's lemma is that **irreversibility is in principle compatible with unitary evolution** in the following sense. An unit wave vector f with non-vanishing projection on all components of the spectrum of a self-adjoint time autonomous Hamiltonian $\mathbb{H}$ will asymptotically have non vanishing projection only on the eigenfunctions of the discrete spectrum. The question which is left open pertains the speed with which this decay can occur.

Khalfin's [4] provided a rigorous argument ruling out exponential decay from unitary evolution. Khalfin's argument relies on a theorem by Paley–Wiener which can be stated as follows:

Theorem. *(**Paley–Wiener**[7]) If $a(t)$ and $\check{a}(E)$ are Fourier transform of each other such that*

$$\check{a}(E) = \begin{cases} 0 & \forall\, E \,\leq\, \lambda \\ g(E) \,\neq\, 0 & \forall\, E \,>\, \lambda \end{cases}$$

and $a(t)\, in\, \mathbb{L}^2(\mathbb{R})$ i.e.

$$\int_{\mathbb{R}} \mathrm{d}t\, |a(t)|^2 \,<\, \infty$$

then

$$\int_{R} \mathrm{d}t\, \frac{\ln |a(t)|}{1+t^2} \,<\, \infty$$

In [4] Khalfin argued that Paley–Wiener's result strongly constrains the long time behavior of a quantum state survival probability. The argument is based on the following observations (which we report following supplement II of [8]).

i Any interacting quantum-mechanical system must have a ground state. More explicitly, there must be a state vector ψ_0 satisfying

$$\mathbb{H}\, \psi_0 \,=\, \epsilon_0\, \psi_0$$

where ϵ_0 is the smallest eigenvalue of $\mathbb{H}$. If this was not the case, it would be possible to extract arbitrarily large amounts of energy from the system by interactions that send it to eigenstates of increasingly lower energy. The existence of the ground state obviously implies that the spectral density of a physically acceptable model must vanish below a value of the energy bounded from below by the ground state:

$$g(\epsilon) = n(\epsilon)\, |\, \langle\, \varphi_\epsilon \,,\, f\, \rangle\, |^2\, \chi_{[\lambda,\infty)}(\epsilon) \tag{3}$$

for $\epsilon_0 \,\leq\, \lambda$.

ii If the spectrum is continuous, Riemann-Lebesgue theorem predicts for the amplitude a $O(1/t)$ upper bound on the time asymptotic behavior so that

$$\int_{\mathbb{R}} \mathrm{d}t\, |a(t)|^2 \,<\, \infty$$

and, consequently, the Fourier transform pair $a(t)$ and $\check{a}(E)$ satisfies the conditions for the Paley–Wiener theorem.

Thus, for large times, is required to increase slower than linearly

$$\ln |a(t)| \overset{t \nearrow \infty}{\lessapprox} t^b \qquad \text{for some}\, b \,<\, 1$$

which precludes an exact asymptotic exponential behavior for $|a(t)|$

$$|a(t)| \,<\, K\, e^{-r\, t^b}$$

for some positive K and r.

4. SHORT TIME ASYMPTOTICS: ZENO EFFECT

It is straightfoward to see that short time unitary evolution it is not compatible with exponential decay, neither.

Proposition. *For any state vector in $\mathbb{H}$*

$$\left.\frac{\mathrm{d}}{\mathrm{d}t}\right|_{t=0} \left|\, \langle\, \boldsymbol{\psi} \,,\, e^{-\imath\, \mathbb{H}\, t} \boldsymbol{\psi}\, \rangle\, \right|^2 = 0$$

Proof.
We use the definition of norm in an Hilbert space to write

$$\left|\left\langle \boldsymbol{\psi}\,, e^{-\imath\,\mathbb{H}\,t}\boldsymbol{\psi}\right\rangle\right|^2 = \left\langle \boldsymbol{\psi}\,, e^{-\imath\,\mathbb{H}\,t}\boldsymbol{\psi}\right\rangle^* \left\langle \boldsymbol{\psi}\,, e^{-\imath\,\mathbb{H}\,t}\boldsymbol{\psi}\right\rangle = \left\langle e^{-\imath\,\mathbb{H}\,t}\boldsymbol{\psi}\,, \boldsymbol{\psi}\right\rangle \left\langle \boldsymbol{\psi}\,, e^{-\imath\,\mathbb{H}\,t}\boldsymbol{\psi}\right\rangle$$

The sesquilinearity of the inner product then implies

$$\begin{aligned}&\left.\frac{\mathrm{d}}{\mathrm{d}t}\right|_{t=0} \left|\left\langle \boldsymbol{\psi}\,, e^{-\imath\,\mathbb{H}\,t}\boldsymbol{\psi}\right\rangle\right|^2 = \\ &\left\langle -\imath\,\mathbb{H}\,\boldsymbol{\psi}\,, \boldsymbol{\psi}\right\rangle\left\langle \boldsymbol{\psi}\,, \boldsymbol{\psi}\right\rangle + \left\langle \boldsymbol{\psi}\,, \boldsymbol{\psi}\right\rangle\left\langle \boldsymbol{\psi}\,, -\imath\,\mathbb{H}\,\boldsymbol{\psi}\right\rangle = \imath\left\langle \boldsymbol{\psi}\,, \mathbb{H}\,\boldsymbol{\psi}\right\rangle - \imath\left\langle \boldsymbol{\psi}\,, \mathbb{H}\,\boldsymbol{\psi}\right\rangle = 0\end{aligned}$$

□

In fact, the Taylor expansion for short time of a state vector survival amplitude

$$a(t) = \left\langle \boldsymbol{\psi}\,, e^{-\imath\,\mathbb{H}\,t}\boldsymbol{\psi}\right\rangle = 1 + \imath\,t\,\left\langle \boldsymbol{\psi}\,, \mathbb{H}\boldsymbol{\psi}\right\rangle - \frac{t^2}{2}\left\langle \boldsymbol{\psi}\,, \mathbb{H}^2\boldsymbol{\psi}\right\rangle + \dots$$

yields for the "survival probability" of the state ψ the short time expression

$$|a(t)|^2 = 1 - t^2\left(\left\langle \boldsymbol{\psi}\,, \mathbb{H}^2\boldsymbol{\psi}\right\rangle - |\left\langle \boldsymbol{\psi}\,, \mathbb{H}\boldsymbol{\psi}\right\rangle|^2\right) + O(t^3) \tag{4}$$

We relate the characteristic time-scale of the short time expansion to the **variance of the energy** in the probability ensambles associated to the initial state vector

$$\frac{1}{\tau} = \left\langle \boldsymbol{\psi}\,, \mathbb{H}^2\boldsymbol{\psi}\right\rangle - |\left\langle \boldsymbol{\psi}\,, \mathbb{H}\boldsymbol{\psi}\right\rangle|^2$$

This result has some important physical consequences: **the quantum Zeno effect**. We follow here the presentation of [6]. Suppose we perform N measurements at equal time intervals t, in order to ascertain whether the system is still in its initial state. After each measurement, the system is "projected" onto the quantum mechanical state representing the result of the measurement, and the evolution starts anew. The total duration of the experiment is $T = Nt$. Based on (4) we can compute the probability of observing the initial state at time T, after having performed the N above-mentioned measurements, as

$$|a_N(T)|^2 = \left|a\left(\frac{T}{N}\right)\right|^{2N} \simeq \left(1 - \frac{T^2}{N^2\,\tau}\right)^N \overset{N \gg 1}{\approxeq} e^{-\frac{T^2}{\tau\,N}}$$

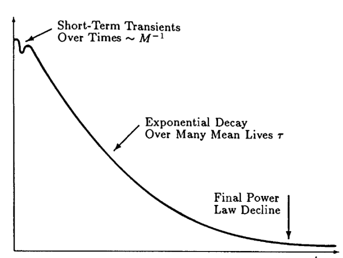
with both T and N finite. This is the **quantum Zeno effect**: Repeated observations "slow down" the evolution and increase the probability that the system is still in the initial state at time T . In the limit of continuous observation ($N \uparrow \infty$) one obtains the quantum **Zeno paradox**

$$\lim_{N \nearrow \infty} |a_N(T)|^2 = 1$$

It must be emphasized that the limit $N \uparrow \infty$ is a mathematical abstraction. It presupposes instantaneous duration of measurements and, a more severe obstruction towards physical attainability, it can be argued to clash with uncertainty relations. We refer to [6] for a detailed discussion of the Zeno effect.

5. EXPONENTIAL DECAY: INTERMEDIATE ASYMPTOTICS

The previous results rule out exponential decay of an indicator undergoing unitary evolution for very short and very large time. The conclusion, summarized in the picture below, is that the experimentally observed exponential decay is compatible with an **intermediate asymptotics** of unitary evolution.



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