Quasienergies and Quantum Chaos

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(Dated: December 2022)

I. INTRODUCTION

These are notes to obtain the propagator in the case of a periodic time-dependent Hamiltonian and then use the propagator to obtain the quasienergies. With the quasienergies, we can check if the system is chaotic or not.

II. PROPAGATOR FOR A TIME-DEPENDENT HAMILTONIAN

If the Hamiltonian is dependent, $H(t)$, we need to take into account that it may not commute with itself at different instants of times, that is

$$[H(t_2), H(t_1)] \neq 0.$$

This is at the heart of the time-ordering operator, $\mathcal{T}$, when we write the propagator,

$$U(T,0) = \mathcal{T} \exp\left(-i \int_0^T H(u) du\right).$$

The equation above can also be written in terms of tiny increments of time, dt as

$$U(T,0) = U\left(n\Delta t, (n-1)\Delta t\right) \dots U(3\Delta t, 2\Delta t)\, U(2\Delta t, \Delta t)\, U(\Delta t, 0) \tag{1}$$

where

$$\Delta t = \frac{T}{n} \tag{2}$$

ATTENTION! Do not choose a tiny value of Δt, choose instead a large integer n, as written in the equation above. This will guarantee that you do reach T exactly and not approximately.

A. Example

Let us consider the time-dependent Hamiltonian given in the QuTiP link
https://qutip.org/docs/latest/guide/dynamics/dynamics-floquet.html

The Hamiltonian is

$$H(t) = [A + B\sin(\omega t)]\, \sigma_z + C\sigma_x \tag{3}$$

$$A = -\pi \qquad B = 2.5\pi \qquad C = -0.2\pi \qquad \omega = 2\pi$$

We can separate the Hamiltonian in its time-independent and time-dependent part to use Trotter-Suzuki decomposition, that is

$$H(t) = H_1 + H_2(t)$$

$$H_1 = A\sigma_z + C\sigma_x \qquad H_2(t) = B\sin(\omega t)\sigma_z$$

The propagator is then given by

$$\begin{aligned} U(T,0) &= \exp\left(-iH_1\frac{\Delta t}{2}\right)\exp\left(-iB\left[\int_{(n-1)\Delta t}^{n\Delta t}\sin(\omega u)du\right]\sigma_z\right)\exp\left(-iH_1\frac{\Delta t}{2}\right) \\ &\quad \dots \\ &\quad \exp\left(-iH_1\frac{\Delta t}{2}\right)\exp\left(-iB\left[\int_{\Delta t}^{2\Delta t}\sin(\omega u)du\right]\sigma_z\right)\exp\left(-iH_1\frac{\Delta t}{2}\right) \\ &\quad \exp\left(-iH_1\frac{\Delta t}{2}\right)\exp\left(-iB\left[\int_{0}^{\Delta t}\sin(\omega u)du\right]\sigma_z\right)\exp\left(-iH_1\frac{\Delta t}{2}\right). \end{aligned} \tag{4}$$

We have used the symmetrized form of the Trotter-Suzuki expansion, that is valid to cubic order of Δt [1]. ATTENTION! The time interval for the integrals change! To expedite the code, a good idea is to solve the integral beforehand, instead of and having it in the loop to obtain the propagator, that is

$$\int_a^b \sin(\omega u)du = \frac{1}{\omega}[-\cos(\omega b) + \cos(\omega a)]$$

$$\begin{aligned} U(T,0) &= \exp\left(-iH_1\frac{\Delta t}{2}\right)\exp\left(i\frac{B}{\omega}\left[\cos(n\omega\Delta t) - \cos((n-1)\omega\Delta t)\right]\sigma_z\right)\exp\left(-iH_1\frac{\Delta t}{2}\right) \\ &\quad \dots \\ &\quad \exp\left(-iH_1\frac{\Delta t}{2}\right)\exp\left(i\frac{B}{\omega}\left[\cos(2\omega\Delta t) - \cos(\omega\Delta t)\right]\sigma_z\right)\exp\left(-iH_1\frac{\Delta t}{2}\right) \\ &\quad \exp\left(-iH_1\frac{\Delta t}{2}\right)\exp\left(i\frac{B}{\omega}\left[\cos(\omega\Delta t) - \cos(0)\right]\sigma_z\right)\exp\left(-iH_1\frac{\Delta t}{2}\right). \end{aligned} \tag{5}$$

III. QUASIENERGIES

https://qutip.org/docs/latest/guide/dynamics/dynamics-floquet.html

The analysis of quantum chaos is based on the quasienergies, as we now explain. According to the Floquet theorem, for a periodic drive, where

$$H(t) = H(t+T),$$

the solutions for the Schrödinger equation are the Floquet states,

$$\psi_\alpha(t) = e^{-i\epsilon_\alpha t}\phi_\alpha(t),$$

where

$$\phi_\alpha(t) = \phi_\alpha(t+T)$$

are the Floquet modes and ϵ_α are the quasienergies. Notice that the quasienergies are constants in time and unique values only in the interval

$$\epsilon_\alpha \in [0, 2\pi/T] \quad \text{or equivalently} \quad \epsilon_\alpha \in [-\pi/T, \pi/T]$$

With the Floquet states, we have any arbitrary evolved state

$$\Psi(t) = \sum_\alpha C_\alpha \psi_\alpha(t).$$

In terms of the propagator, we can show that

$$U(T+t,t)\Psi(t) = \Psi(T+t)$$

$$U(T+t,t)e^{-i\epsilon_\alpha t/\hbar}\phi_\alpha(t) = e^{-i\epsilon_\alpha(T+t)}\phi_\alpha(T+t).$$

Since $\phi_\alpha(T+t)=\phi_\alpha(t)$, we see that the Floquet modes are the eigenstates of the propagator after one period, which we can write as

$$
\begin{aligned}
U(T)|\phi_\alpha\rangle &= e^{-i\epsilon_\alpha T}|\phi_\alpha\rangle \\
U(T)|\phi_\alpha\rangle &= e^{-i\theta_\alpha}|\phi_\alpha\rangle \\
U(T)|\phi_\alpha\rangle &= \eta_\alpha|\phi_\alpha\rangle
\end{aligned}
\tag{6}
$$

A. Recipe to Extract the Quasienergies

The procedure to get the quasienergies, taking into account that they are defined only in $[0, 2\pi/T]$ (or equivalently in $[-\pi/T, \pi/T]$), goes as follows.

1. Diagonalize the propagator $U(T)$ at the completion of a period T and get its eigenvalues η_α,
$$U(T)|\phi_\alpha\rangle = \eta_\alpha|\phi_\alpha\rangle$$
2. Get the phases
$$\theta_\alpha = \frac{\ln(\eta_\alpha)}{-i}.$$
3. Compute
$$\text{mod }[\theta_\alpha, 2\pi] \quad \text{or equivalently} \quad \text{mod }[\theta_\alpha, 2\pi, -\pi].$$
ATTENTION!!
$$\text{mod }[\theta_\alpha, 2\pi, -\pi] \quad \neq \quad \text{mod }[\theta_\alpha, 2\pi] - \pi.$$
What mod $[\theta_\alpha, 2\pi, -\pi]$ does it to take any θ_α in the bottom half of the unit circle, that is, $\pi < \theta_\alpha < 2\pi$, and subtract it by 2π. For example, if $\theta_\alpha = 3\pi/2$, we will get $\theta_\alpha = 3\pi/2 - 2\pi = -\pi/2$, which is indeed in the interval $[-\pi, \pi]$.
4. We now have the quasienergies,
$$\epsilon_\alpha = \frac{\text{mod }[\theta_\alpha, 2\pi]}{T} = \frac{\text{mod }\left[\frac{\ln(\eta_\alpha)}{-i}, 2\pi\right]}{T}, \tag{7}$$
or equivalently
$$\epsilon_\alpha = \frac{\text{mod }[\theta_\alpha, 2\pi, -\pi]}{T} = \frac{\text{mod }\left[\frac{\ln(\eta_\alpha)}{-i}, 2\pi, -\pi\right]}{T}, \tag{8}$$
which should be sorted in increasing order.

B. Example

Let us use the Hamiltonian in Eq. (3) as an example. The results for the quasienergies given in the QuTiP site are

$$\epsilon_1 = -2.83131212 \qquad \epsilon_2 = 2.83131212,$$

which means that they chose to stay in the interval $[-\pi, \pi]$. Use the propagator as written in Eq. (5). The convergence is faster if one use Trotter-Suzuki as in this equation. And the code runs faster if we solve the integral before entering the loop. The Table below gives the approach to the values ± 2.83131212 as we increase n in Eq. (2)

n	$\epsilon_{1,2}$
100	$\pm$ 2.8313599409933654
500	$\pm$ 2.831314005888662
800	$\pm$ 2.8313128395371345
1000	$\pm$ 2.8313125703788744
2000	$\pm$ 2.83131221150107
5000	$\pm$ 2.831312111015257

IV. QUANTUM CHAOS

To determine whether the quasienergies are or not correlated, we need to focus on one symmetry sector. After sorting the quasienergies from lowest to largest values, the quantity that we use to determine the onset of chaos is

$$r_\alpha = \frac{\min(\delta_\alpha, \delta_{\alpha+1})}{\max(\delta_\alpha, \delta_{\alpha+1})}, \tag{9}$$

where

$$\delta_\alpha = \epsilon_{\alpha+1} - \epsilon_\alpha$$

is the spacing between neighboring quasienergy levels.

When the average value

$$\langle r \rangle = \frac{1}{D-2} \sum_{\alpha=1}^{D-2} r_\alpha \tag{10}$$

is close to 0.53, we have chaos, and when it is close to 0.39, that indicates a Poisson distribution. In the equation above, D could be the dimension of the Hilbert space.

[1] N. Hatano and M. Suzuki, Finding exponential product formulas of higher orders, in *Quantum Annealing and Other Optimization Methods*, edited by A. Das and B. K. Chakrabarti (Springer Berlin Heidelberg, Berlin, Heidelberg, 2005) pp. 37–68.