Adiabatic evolution operator for periodic driven system and topological numbers

Ning Sun

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I. ADIABATIC EVOLUTION OPERATOR

For a quantum mechanics system, the evolution of any given initial state is totally determined by the evolution operatoe $U(t, t_0)$ which is defined as

$$U(t, t_0) = \mathcal{T} e^{-\mathrm{i}\int_{t_0}^{t} H(t')dt'}$$

where $\mathcal{T}$ is time-ordered operator, whose presice mathematical definition would be written down later. For a system governed by a static Hamiltonian $H(t) \equiv H_0$, it reduces to

$$U(t, t_0) = \exp[-\mathrm{i}H_0(t - t_0)]$$

Here the exponential for operator is in the familiar Taylor-expansion sence.

For a periodic driven system, i.e. $H(t) = H(t + T)$ for any time t, it's natural to consider evolution operator $U(t_0 + T, t_0)$. Due to the invariant property of eigenvalues of U under an unitary transformation we deal with $U(T, 0)$ in the following for convenient.

Definition 1. *Periodic evolution operator of a periodic driven system is defined as*

$$\begin{aligned} U(T) \equiv U(T,0) &= \mathcal{T} e^{-\mathrm{i}\int_0^T H(t')dt'} \\ &= \lim_{\substack{N\to\infty \\ \Delta t\to 0}} \exp\Big[-\mathrm{i}H(t_{N-1})\Delta t\Big] \exp\Big[-\mathrm{i}H(t_{N-2})\Delta t\Big] \cdots \exp\Big[-\mathrm{i}H(t_0)\Delta t\Big] \\ &= \lim_{\substack{N\to\infty \\ \Delta t\to 0}} \prod_{j=0}^{N-1} \exp\Big[-\mathrm{i}H(t_j)\Delta t\Big] \end{aligned}$$

Here $N\Delta t = T$, $t_j = j\Delta t$.

A. High frequency limit

In high frequency regime, we could expand the time evolution operator in terms of $1/\omega$, or T, and drop high order terms in $1/\omega$ to derive the effective Hamiltonian for one period evolution. Specifically,

$$\begin{aligned} U(T) &= \lim_{\substack{N\to\infty \\ \Delta t\to 0}} \prod_{j=0}^{N-1} \exp\Big[-\mathrm{i}H(t_j)\Delta t\Big] \\ &= \lim_{\substack{N\to\infty \\ \Delta t\to 0}} \prod_{j=0}^{N-1} \Big[1-\mathrm{i}H(t_j)\Delta t\Big] \\ &= \lim_{\substack{N\to\infty \\ \Delta t\to 0}} \left(1 - \sum_{j=0}^{N-1} H(t_j)\Delta t + \frac{1}{2}(-\mathrm{i}\Delta t)^2 \sum_{j,k} \Big[H(t_j)H(t_k)\Theta(t_j-t_k) + H(t_k)H(t_j)\Theta(t_k-t_j)\Big] + \cdots\right) \\ &= \lim_{\substack{N\to\infty \\ \Delta t\to 0}} \left(1 - \sum_{j=0}^{N-1} H(t_j)\Delta t + (-\mathrm{i}\Delta t)^2 \sum_{j>k} H(t_j)H(t_k) + \cdots\right) \\ &= 1 - \mathrm{i}\int_0^T H(t)dt + (-\mathrm{i})^2 \int_0^T dt_2 \int_0^{t_2} dt_1 H(t_2)H(t_1) + \cdots \end{aligned}$$

Definition 2. *Effective Hamiltonian for a periodic driven system is defined as*

$$U(T) = e^{-\mathrm{i}H_{\mathit{eff}}T}$$

We then obtain the effective Hamiltonian in high frequency regime to be

$$H_{\text{eff}} = H_0 + \frac{1}{\hbar\omega}\sum_{n>0}\frac{1}{n}[H_n, H_{-n}] + \mathcal{O}(\frac{1}{\omega^2})$$

where

$$H_n = \int_0^T H(t)e^{\mathrm{i}n\omega t}dt$$

B. Adiabatic limit

Adiabatic evolution assumes

- filled bands and empty bands are seperated by some energy gap.
- evolution period is so long compare to excitation process, or $\hbar\omega \ll E_{\text{gap}}$.

In other words, adiabatic evolution limits happens when there exists some energy gap between filled bands (for many-particle systems) and the empty bands, which would never close during evolution. And driven frequency are so low compare to the energy gap that excitation is very very small which we do not take into consideration. Then whole evolution is confined in the subspace of filled bands. We should deal with this subspace.

1. *single band*

First we consider the situation for a single band. Assume it is seperated by some never-close energy gap with high bands. Assume also driving frequency $\omega \ll E_{\text{gap}}$ and no excitation considered. For this single band n, periodic evolution operator becomes

$$\begin{aligned}
U_n(T) &= \mathcal{T} e^{-\mathrm{i}\int_0^T H(t')dt'} \\
&= \lim_{\substack{N\to\infty \\ \Delta t\to 0}} \exp\Big[-\mathrm{i}H(t_{N-1})\Delta t\Big] \exp\Big[-\mathrm{i}H(t_{N-2})\Delta t\Big]\cdots\exp\Big[-\mathrm{i}H(t_0)\Delta t\Big] \\
&= \lim_{\substack{N\to\infty \\ \Delta t\to 0}} \exp\Big[-\mathrm{i}H(t_{N-1})\Delta t\Big]|n(t_{N-1})\rangle\langle n(t_{N-1})| \exp\Big[-\mathrm{i}H(t_{N-2})\Delta t\Big]|n(t_{N-2})\rangle\langle n(t_{N-2})|\cdots \\
&\quad |n(t_{j+1})\rangle\underbrace{\langle n(t_{j+1})| \exp\Big[-\mathrm{i}H(t_j)\Delta t\Big]|n(t_j)\rangle}\langle n(t_j)|\cdots|n(t_1)\rangle\langle n(t_1)| \exp\Big[-\mathrm{i}H(t_0)\Delta t\Big]
\end{aligned}$$

by inserting a series of instantaneous projectors between exponentials. A typical element underlined above is

$$\begin{aligned}
\langle n(t_{j+1})| \exp\Big[-\mathrm{i}H(t_j)\Delta t\Big]|n(t_j)\rangle &= e^{-\mathrm{i}E_n(t_j)\Delta t}\langle n(t_{j+1})|n(t_j)\rangle \\
&= e^{-\mathrm{i}E_n(t_j)\Delta t}\left(\langle n(t_j)| + \Delta t\frac{\partial\langle n(t_j)|}{\partial t}\right)|n(t_j)\rangle \\
&= e^{-\mathrm{i}E_n(t_j)\Delta t}\Big(1+\Delta t\langle\partial_t n(t_j)|n(t_j)\rangle\Big) \\
&= e^{-\mathrm{i}E_n(t_j)\Delta t}\Big(1-\Delta t\langle n(t_j)|\partial_t n(t_j)\rangle\Big) \\
&\to e^{-\mathrm{i}E_n(t_j)\Delta t}\exp\Big(-\Delta t\langle n(t_j)|\partial_t n(t_j)\rangle\Big)
\end{aligned}$$

The last line is derived in the limit of $N\to\infty$, $\Delta t\to 0$. Then

$$\begin{aligned}
U_n(T) &= \lim_{\substack{N\to\infty \\ \Delta t\to 0}} |n(t_{N-1})\rangle e^{-\mathrm{i}E_n(t_{N-1})\Delta t} e^{-\langle n(t_{N-1})|\partial_t n(t_{N-1})\rangle\Delta t}\cdots e^{-\mathrm{i}E_n(t_0)\Delta t} e^{-\langle n(t_0)|\partial_t n(t_0)\rangle\Delta t}\langle n(t_0)| \\
&= \lim_{\substack{N\to\infty \\ \Delta t\to 0}} \prod_{j=0}^{N-1} \exp\Big[-\mathrm{i}E_n(t_j)\Delta t\Big]\exp\Big[-\langle n(t_j)|\partial_t n(t_j)\rangle\Delta t\Big]|n(t_{N-1})\rangle\langle n(t_0)| \\
&= \exp\left[-\int_0^T\langle n(t)|\partial_t n(t)\rangle dt\right]\exp\left[-\mathrm{i}\int_0^T E_n(t)dt\right]|n(T)\rangle\langle n(0)|
\end{aligned}$$

Actually, because of periodicity of the system, $|n(T)\rangle = |n(0)\rangle (= |n\rangle)$ (choosing some gauge). The first phase factor is just the Berry phase for a loop evolution, which is gauge-independent, while the second term is averaged

energy over one period of evolution. It could be written as

$$U_n(T) = e^{\mathrm{i}\gamma} e^{-\mathrm{i}\int_0^T E_n(t)dt} |n\rangle\langle n|$$
$$\gamma = \int_0^T \mathrm{i}\langle n(t)|\partial_t n(t)\rangle dt$$

2. *generalise to several bands*

What has been done could be easily generalised to manifolds consist of several bands (energy levels). In this case the adiabatic condition assume as well band gap seperate lower bands we are interested in and high bands. Mixing states within the subspaces we considered is allowed, while transition to high bands is forbidden. Driven frequency should meet these requirements.

Consider a subspace with m bands (energy levels), the evolution operator $U(T)$ within this manifold is an $m \times m$ unitary matrix. Could imagine that $(U)_{mn}$ element not always zero, there could be off-diagonal elements $[U(T)]_{mn} = e^{i\theta}|m\rangle\langle n|$.

The phase factor before consist of a part comes from non-Abelian berry phase, i.e.

$$\gamma_{mn} = \int_0^T \mathrm{i}\langle m(t)|\partial_t n(t)\rangle dt$$

Besides, there are some more complicated parts.

3. *additional parameters*

Suppose there are some good quantum numbers (systems possess some symmetries), for example, a lattice with discrete translational symmetry supports eigenmodes with good quantum number the quasi-momentum q. Do unitary transiformation with some good quantum number q could introduce some additional parameters to the evolution operator. Means we parametrizes the evolution operator $U(T)$ to become $U_q(T)$ with some good quantum number q. This describe physics in subspace q. Varying parameters q leads a way to looking into the topological property of $U(T)$, that is the system.

II. TOPOLOGICAL NUMBERS

A. Winding number

Consider a 1D lattice system. In the presence of translational symmetry, the invariant ν_1 is defined as[1]

$$\nu_1 = \frac{1}{2\pi}\int_{-\pi}^{\pi} dk Tr[U_k(T)^{-1}\mathrm{i}\partial_k U_k(T)]$$

whose value would not be changed under a k-dependent unitary transformation of U_k, that $\tilde{U}_k = V_k U_k V_k^{-1}$ gives the same value. This could be directly checked. Hence we understand the winding number in one dimension by a simple interpretation that ν_1 is adding over (trace out) the "winding" of all bands (energy levels), by which we mean the mapping from a circle ($-\pi < k \leq \pi$) to another circle ($-\pi < \varepsilon \leq \pi$) winds around how many times (number of loops).

This kind of characterization is connected to homotopy groups in math.

Similarly, we could define higher dimensional winding number[1, 2]. For example, in three dimension,

$$\nu_3 = \int \frac{d^3k}{24\pi}\varepsilon^{\alpha\beta\gamma}Tr[(U_k^{-1}\partial_{k_\alpha}U_k)(U_k^{-1}\partial_{k_\beta}U_k)(U_k^{-1}\partial_{k_\gamma}U_k)]$$

Winding numbers are only defined in odd dimensions ($\mathbb{Z}$), because in even dimension homotopy groups are trivial (identity).

B. Chern number

Chern numbers defined in even dimensions. Common examples are the first Chern number (defined in 2D) and the second Chern number (4D).

Linking Chern number to winding number as well as physical properties such as edge states, polarization and quantization of particle transport in different dimensions and different models are well illustrated in [1, 2].

III. THOULESS CHARGE PUMPING

Consider the following time-dependent tight-binding model[4]

$$H(t) = \sum_j -(J+\delta\sin(\omega t))a_j^\dagger b_j - (J-\delta\sin(\omega t))a_{j+1}^\dagger b_j + h.c. + \Delta\cos(\omega t)(a_j^\dagger a_j - b_j^\dagger b_j)$$

$\mathcal{F}.\mathcal{T}.$ of the Hamiltonian:

$$\mathcal{H}(q,t) = -2J\cos(\frac{qa}{2})\sigma_x - 2\delta\sin(\omega t)\sin(\frac{qa}{2})\sigma_y + \Delta\cos(\omega t)\sigma_z$$

In the adiabatic limit, we calculate the evolution operator for each of the two bands.

$$\begin{aligned} U_n(q,T) &= e^{\mathrm{i}\gamma(q)}e^{-\mathrm{i}\int_0^T E_n(q,t)dt}|n\rangle\langle n| \\ \gamma(q) &= \int_0^T \mathrm{i}\langle n(q,t)|\partial_t n(q,t)\rangle dt \end{aligned} \tag{1}$$

Evaluate the winding number for each band, we find that the winding comes from two parts, the Berry phase $\gamma(q)$ and averaged band energy $\int_0^T E_n(q,t)dt$ over one period. Explicitly,

$$U(q,T)^{-1}\mathrm{i}\partial_q U(q,T) = -\partial_q\gamma(q) + \int_0^T \partial_q E_n(q,t)dt$$

then

$$\begin{aligned} \nu_1^{(n)} &= \frac{1}{2\pi}\int_{-\pi}^{\pi} dq U_n(q,T)^{-1}\mathrm{i}\partial_q U_n(q,T) \\ &= -\frac{1}{2\pi}\gamma(q)\Big|_{-\pi}^{\pi} \\ &= \frac{1}{2\pi}\int_{-\pi}^{\pi} dq\int_0^T dt\,\mathrm{i}\Big[\langle\partial_q n(q,t)|\partial_t n(q,t)\rangle - \langle\partial_t n(q,t)|\partial_q n(q,t)\rangle\Big] \end{aligned}$$

which is the same as the result of the quantized Thouless charge pumping[3–5]. Note that the average energy part cancelled during the calculation.

This integer gives ± 1 by a simple argument that the evolution enclose the degeneracy point once during one period. We could also numerically verified it.

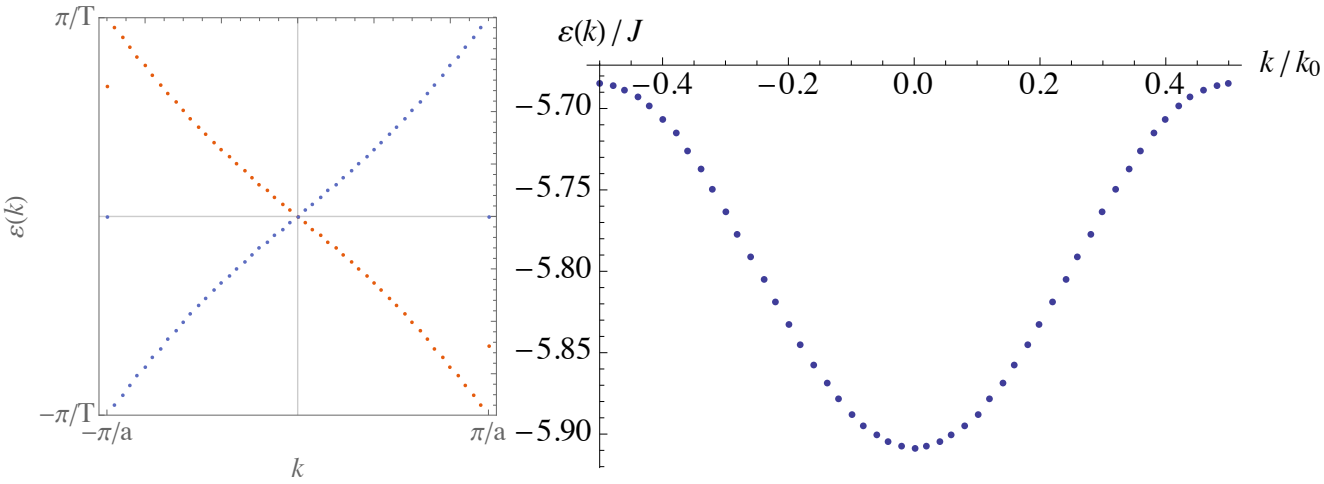
1. *Floquet spectrum*

Actually, above gives a method to extract the Floquet quasi-energy spectrum in adiabatic limit. We see clearly from Eq. (1) that there are two parts contribution, one of which comes from the Berry phase$\gamma(q)$ and another from averaged energy.

By identifying $e^{-i\varepsilon(q)T}$ with the eigenvalues of $U(q,T)$, we derived

$$\varepsilon_1(q) = -\gamma(q)/T = -\frac{1}{T}\int_0^T i\langle n(q,t)|\partial_t n(q,t)\rangle$$
$$\varepsilon_2(q) = \frac{1}{T}\int_0^T E_n(q,t)dt$$

We conclude that:



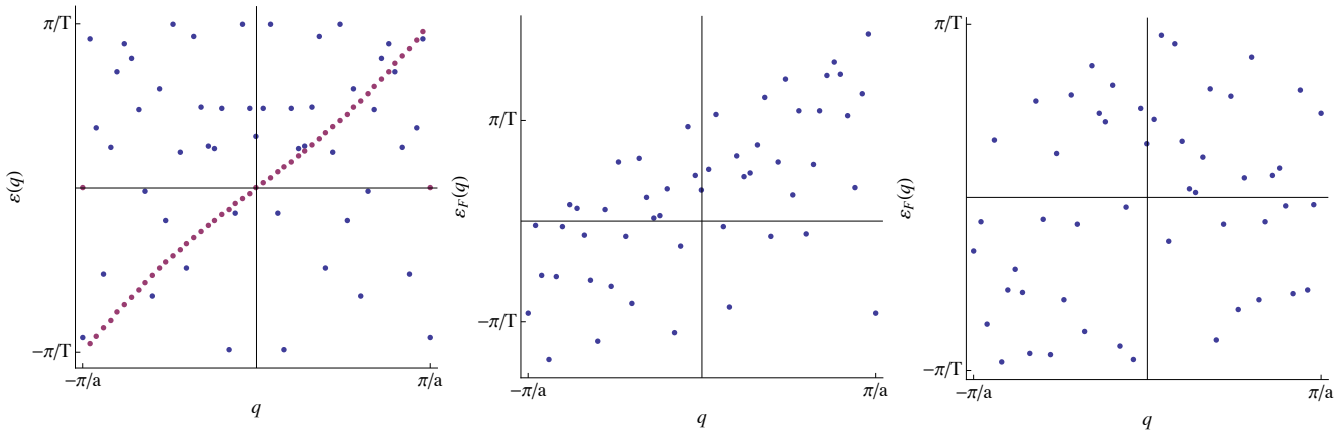
(a)$\varepsilon_1(q)$ blue(orange) for lower(higher) band.

(b)$\varepsilon_2(q)$ for lower band.

FIG. 1: Time-dependent RM with $\delta/J = -0.85$, $\Delta/J = 8.5$, see Ref.[4]

- The Berry phase part always "winds" around one loop, no matter how large or small is ω and doesn't depend on any other energy scales of the system J, δ, Δ. Means that it always comparable with ω.
- The averaged energy part, on contrast, depends only on J, δ, Δ, but not ω.

This could explain why Floquet spectrum so mess in the adiabatic limit. If we take the adiabatic limit[6], we should fold $\varepsilon_2(q)$ part into the first quasi-energy Brillioun Zone and add up ε_1 part to get ε_F. (see Fig. 2)



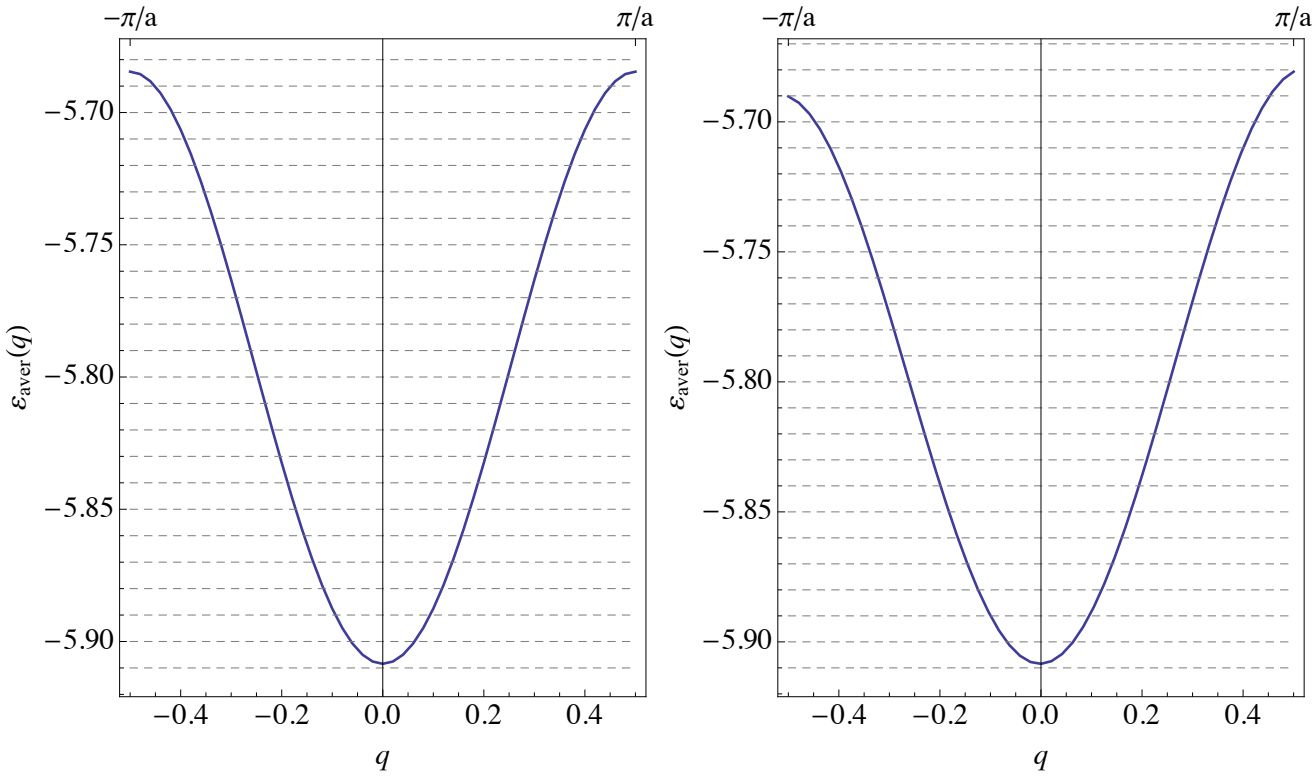
(a)ε_1(red) and ε_2(blue) in first quasi-energy band

(b)adding $\varepsilon_1(q)$ and $\varepsilon_2(q)$

(c)$\varepsilon_F(q)$ foldding into first QBZ

FIG. 2: $\delta/J = -0.85$, $\Delta/J = 8.5$, $\omega/J = 0.01$

This could also explain why a so mess Floquet spectrum couldn't vary the quantization of particle transport process because the net "winding" of the averaged energy part ε_2 is always zero. (see Fig. 3) This part contributes nothing to the periodic particle transport.



(a)averaged energy part (ε_2)

(b)adding the Berry phase (ε_1) to averaged energy (ε_2)

FIG. 3: averaged energy of the lower band winding around quasi-energy BZ

[1] Takuya Kitagawa, Erez Berg, Mark Rudner, and Eugene Demler, *Topological characterization of periodically driven quantum systems*, Phys. Rev. B **82**, 235114 (2010).

[2] Mark S. Rudner, Netanel H. Lindner, Erez Berg, and Michael Levin, *Anomalous Edge States and the Bulk-Edge Correspondence for Periodically Driven Two-Dimensional Systems*, Phys. Rev. X **3**, 031005 (2013).

[3] D. J. Thouless, *Quantization of particle transport*, Phys. Rev. B **27**, 6083 (1983).

[4] Yoshiro Takahashi's group, *Topological Thouless pumping of ultracold fermions*, Nat. Phys. **12** 296300 (2016).

[5] Di Xiao, Ming-Che Chang, and Qian Niu, *Berry phase effects on electronic properties*, Rev. Mod. Phys. **82**, 1959 (2010).

[6] In Ref.[4] their parameters for experiments is of order $\omega/V_{\text{depth}} \sim 1/1000$. In the tight-binding model analysis, it's of order $1/50$.