

A simple proof of Floquet's theorem for the case of unitary evolution in quantum mechanics

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We present a constructive proof of Floquet's theorem for the special case of unitary time evolution in quantum mechanics. The proof is straightforward and suitable for study in courses on quantum mechanics.

Floquet's theorem [1, 2] tells us something useful about the solutions to the time-dependent Schrödinger equation (TDSE) for Hamiltonians that are periodic in time [3]. Specifically, given the TDSE:

$$i\hbar \frac{d\psi(t)}{dt} = H(t)\psi(t) \quad (1)$$

in a space of finite dimension n , with both $H(t) = H^\dagger(t)$ and $H(t+T) = H(t)$ for all t with period T , there are n orthonormal "Floquet" solutions of the form:

$$\psi_j(t) = \phi_j(t)e^{-i\epsilon_j t/\hbar} \quad (2)$$

where $\phi_j(t) = \phi_j(t+T)$ for all t , and the ϵ_j 's are real, so-called *quasi-energies*. For convenience here and in what follows, we consider $H(t)$, $U(t,0)$, etc... to be $n \times n$ matrix representations in an orthonormal basis; and likewise $\psi(t)$, $\phi_j(t)$, etc... to be $n \times 1$ column vectors.

The Floquet solutions may be used to construct a unitary time evolution operator:

$$U(t,0) = \sum_{j=1}^n \phi_j(t)e^{-i\epsilon_j t/\hbar} \phi_j^\dagger(0) \quad (3)$$

appropriate for any initial conditions at $t = 0$:

$$\psi(t) = U(t,0)\psi(0). \quad (4)$$

Equivalently, we may form the $n \times n$ matrix $\Phi(t) = [\phi_1(t) \ \phi_2(t) \ \dots \ \phi_n(t)]$, and condense Eq. 3 to

$$U(t,0) = \Phi(t)e^{-iEt/\hbar}\Phi^\dagger(0), \quad (5)$$

where E is a diagonal matrix containing the ϵ_j 's, and $\Phi(t)$ is periodic; i.e., $\Phi(t) = \Phi(t+T)$ for all t .

Despite the relative simplicity of this result, it is not standard quantum mechanics textbook fare (with at least one exception [4]). But due to the fundamental nature of this "time version" of Bloch's theorem and recent activity in time-periodic quantum-mechanical Floquet systems (see, for example, Ref. [5]), it may be desirable to study it in quantum mechanics courses.

The purpose of this short note is to present a simple, constructive proof of Floquet's theorem in the special case of quantum-mechanical unitary time evolution (Eq. 5), appropriate for physics undergraduate students. This proof arises naturally from consideration of how

one might numerically compute time-evolution in an efficient manner. The steps in the derivation are easily remembered, and involve only the standard results of basic quantum mechanics, as found in typical textbooks [6–8].

First note that for any positive integer N , the evolution from $t = NT$ to $t = (N+1)T$ as given by $U((N+1)T, NT)$ is the same as for from $t = 0$ to $t = T$ as given by $U(T, 0)$. This symmetry can be seen by replacing t by $t - T$ in the TDSE, since $H(t+T) = H(t)$ for all t . Since t in $U(t, 0)$ is potentially much greater than T , it makes sense to compute $U(T, 0)$, then raise it to the largest non-negative integer power N such that $NT \leq t$. Then finally, compute evolution over the "left-over" interval from NT to t (of duration less than T). In other words, we consider the factorization:

$$\begin{aligned} U(t,0) &= U(t,NT)U(NT,0) \\ &= U(t,NT)U(T,0)^N. \end{aligned} \quad (6)$$

Taking the matrix power will be more computationally efficient if we first diagonalize $U(T,0)$. Recall that any unitary operator has a complete orthonormal eigenbasis with complex eigenvalues of unit magnitude, a result that will be familiar to undergraduates (e.g., pg 39 of Ref. [6]). Thus we may write $U(T,0) = We^{iD}W^\dagger$, where D is a real, diagonal, $n \times n$ matrix, and W is unitary ($W^\dagger W = WW^\dagger = \mathbb{1}$). This diagonalized form of $U(T,0)$ is more efficient for computation because

$$\begin{aligned} U(T,0)^N &= (We^{iD}W^\dagger)^N \\ &= We^{iD}W^\dagger We^{iD}W^\dagger \dots We^{iD}W^\dagger \\ &= We^{iDN}W^\dagger. \end{aligned} \quad (7)$$

As it is unlikely that t is an exact integer multiple of T , we still need to compute time evolution over the remaining time interval from NT to t (the first "factor" on the RHS of Eq. 6). The time-periodic $H(t)$ allows us to write the remaining time evolution as:

$$U(t,NT) = U(t-NT,0). \quad (8)$$

It is convenient to introduce a notation for the "leftover" time (after Ref. [9]). Defining $[x]$ as the largest integer less than or equal to x , we have $N = [t/T]$. If we also define "mod", so that $x \bmod y := x - y[x/y]$, then $t - NT = t \bmod T$. Note that $t \bmod T$ is periodic in t , with period T .

Combining evolution from 0 to NT with evolution from NT to t gives:

$$U(t, 0) = U(t, NT) U(NT, 0) \quad (9)$$

$$= U(t \bmod T, 0) W e^{iDN} W^\dagger \quad (10)$$

and using $N = [t - (t \bmod T)]/T$ gives:

$$U(t, 0) = U(t \bmod T, 0) W e^{iD[t - (t \bmod T)]/T} W^\dagger. \quad (11)$$

Defining $\Phi(t) := U(t \bmod T, 0) W e^{-iD(t \bmod T)/T}$, we note that it is both periodic and unitary. Also defining $E := -D\hbar/T$, we note that it is real and diagonal. Using these

definitions we may rewrite Eq. 11 as

$$U(t, 0) = \Phi(t) e^{-iEt/\hbar} \Phi^\dagger(0), \quad (12)$$

the result that we were to show (Eq. 5) \square .

Given the periodicity of $\Phi(t)$, it is natural to consider its Fourier expansion. Shirley [3] followed this line of thought, showing that both the Fourier expansion of $\Phi(t)$ and the corresponding quasi-energies may be obtained by diagonalization of a *time-independent* Hamiltonian, constructed using the Fourier components of $H(t)$.

A preliminary version of this note appeared in the supplemental material for Ref. [10].

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