
Chapter 2

Formalism: Floquet theory

Floquet theory is applied to study quantum systems with time-periodic Hamiltonian. The primary goal of this study is to derive an effective time independent Hamiltonian corresponding to the time-periodic Hamiltonian. This simply means that the dynamics of a quantum system described by the time-periodic Hamiltonian should also be equivalently described by its corresponding effective time independent Hamiltonian. In Floquet theory literature, this effective Hamiltonian is known as the Floquet Hamiltonian.

More than a half a century back, Shirley systematically investigated generic time-periodic Hamiltonian systems or the Floquet systems [21, 74]. This work mostly addressed how to calculate the transition probabilities among various states of the system under a time dependent perturbation theory. In order to include the assumption of the weak or strong field into the theory, this work suggested a generic form of any time dependent Hamiltonian, which should have two parts: one is a static part, and the another is the time dependent part. This work also demonstrated the advantages of the effective time independent description to formulate the periodically driven problem correctly. In order to derive this description, the Floquet theory was found appropriate. One important advantage of this formalism

is that it provides a possibility to include the effect of the time dependence for different frequency ranges. However, one has to pay the price for this by mapping the finite dimensional time-periodic problem into an infinite dimensional time independent problem [21, 74]. Later, Sambe studied this by extending the *standard* system Hilbert space into the so-called “Sambe space”, which also satisfies the properties of a Hilbert space. Therefore, the Sambe space is also known as the Floquet-Hilbert space. This extended space is defined as a tensor product of the system Hilbert space \mathbb{H} and a Hilbert space of time-periodic functions denoted by \mathbb{T} . This method is simpler than the other time dependent perturbation theory from both analytical and computational point of view.

A general prescription of the Floquet theory of studying a time-periodic quantum system is the following:

(1) the Floquet theory states that the time evolution operator corresponding to a quantum system described by a time-periodic Hamiltonian can always be expressed as a product of three unitary operators:

$$U(t_i \rightarrow t_f) = e^{-iG[t_f]} e^{-iH_{\text{eff}}(t_f - t_i)} e^{iG[t_i]}. \quad (2.1)$$

This expression was mentioned earlier in Eq. (1.1). Here, we are re-writing this for the sake of completeness. Here, t_i and t_f are the initial and the final time, respectively. The extreme right unitary operator $e^{iG[t_i]}$ and the left unitary operator $e^{-iG[t_f]}$ are determined by how one switches on and off the driving. The Hermitian operator $G[t]$ is also has the same time-periodicity as the driving period T , i.e., $G[t + T] = G[t]$. Our main interest is the central unitary operator, which describes the dynamics in terms of a time independent Hamiltonian or Floquet Hamiltonian H_{eff} [75], which is not dependent on the initial and the final time. If one probes the dynamics of the system stroboscopically, that is at time intervals $t_f = t_i + nT$,

where n are positive integers, then the two operators $G[t_f]$ and $G[t_i]$ become equal. Here, nT is defined as the stroboscopic time, measured in the units of the driving period T . For such cases, the full evolution operator is equivalent to the evolution of the system generated by the static Hamiltonian H_{eff} , i.e.,

$$U(t_i \rightarrow t_f = t_i + nT) = e^{-iG[t_i]} e^{-iH_{\text{eff}} nT} e^{iG[t_i]} \quad (2.2)$$

(2) This time evolution operator is exact. However, in most of the cases, it is not possible to derive H_{eff} exactly. One has to employ some perturbation techniques to evaluate H_{eff} . There are different perturbation theories at the high frequency limit proposed [26, 27, 41–48, 76, 77]. In this thesis, we shall study two perturbation schemes, one is based on the Van Vleck theory [27, 41], and the other one is based on the Brillouin-Wigner (BW) theory [76]. The later exploits Sambe’s idea and applies the BW theory, which was originally defined for the time independent Hamiltonian systems. Reference [43] has systematically established the connection between the different perturbation schemes.

2.1 Floquet Analysis and Floquet Operator

The Hamiltonian $H(t)$ of a periodically driven systems satisfies the property

$$H(t + T) = H(t), \quad (2.3)$$

where $T = 2\pi/\omega$ is the time period of the periodic driving and ω is the corresponding frequency. The generic form of any time-periodic Hamiltonian is

$$H(t) = H_0 + V(t), \quad (2.4)$$

where H_0 is the Hamiltonian of the undriven or static part, and $V(t)$ is the time-periodic driving part, i.e., $V(t+T) = V(t)$. The time-periodic potential makes the total Hamiltonian time-periodic. The time dependent Schrödinger equation (TDSE) of this system

$$\left[H(t) - i\hbar \frac{d}{dt} \right] |\psi(t)\rangle = 0. \quad (2.5)$$

The solutions of the above equation $|\psi(t)\rangle$ can always be represented by a unitary time evolution operator $U(t_i \rightarrow t)$, i.e., $|\psi(t)\rangle = U(t_i \rightarrow t)|\psi(t_i)\rangle$, where $|\psi(t_i)\rangle$ is the initial state or the given state at the initial time t_i . One can now consider a unitary transformation

$$|\phi(t)\rangle = \mathcal{U}(t)|\psi(t)\rangle = e^{iG[t]}|\psi(t)\rangle, \quad (2.6)$$

where $G[t]$ is an explicitly time dependent Hermitian operator and satisfies the same time-periodic property as that of the system Hamiltonian, i.e., $G[t+T] = G[t]$. This is also known as the *kick* operator. The new state $|\phi(t)\rangle$ satisfies the Schrödinger equation

$$i\hbar \frac{d}{dt} |\phi(t)\rangle = H_{\text{eff}} |\phi(t)\rangle, \quad (2.7)$$

$$\text{where } H_{\text{eff}} = e^{iG[t]} H(t) e^{-iG[t]} - i\hbar e^{iG[t]} \left(\frac{d}{dt} e^{-iG[t]} \right). \quad (2.8)$$

Here, a time independent Hamiltonian H_{eff} is introduced. In literature, this Hamiltonian is known as the Floquet Hamiltonian. We shall refer this as the effective time independent Hamiltonian, because this generates the same time evolution as the time-periodic Hamiltonian. In recent times, from the so-called *Floquet engineering* point of view, it has become an important theoretical task to derive the effective Hamiltonian corresponding to a particular driving protocol, at least

within a suitable approximation. This helps experimentalists to design driving protocols depending on the initial static and the final desired Hamiltonians. Following Ref. [26], one can always construct a time independent H_{eff} , by transferring all time dependent terms into the operator $G[t]$. In terms of these operators, the time evolution operator is written for the situation when one switches on the driving at time t_i and switches off at time t_f as [21]:

$$U(t_i \rightarrow t_f) = e^{-iG[t_f]} e^{-iH_{\text{eff}}(t_f-t_i)} e^{iG[t_i]} = U_M(t_f) e^{-iH_{\text{eff}}(t_f-t_i)} U_M(t_i)^\dagger. \quad (2.9)$$

The above equation has already been given in Eq. (2.1), here we rewrite that to give it a proper context. This expression illustrates that the time evolution of periodically driven systems or the Floquet systems have two components: one is the so-called *micromotion* operator described by the evolution $U_M(t) = e^{-iG[t]}$, where the kick operator $G[t_i]$ describes how the driving is switching on, and $G[t_f]$ describes the process by which the driving is switching off. The other one is the time independent effective Hamiltonian H_{eff} , which describes the time evolution similar to any autonomous system.

Let us assume that the effective Hamiltonian satisfies the eigen relation

$$H_{\text{eff}}|\tilde{u}_\alpha\rangle = \epsilon_\alpha|\tilde{u}_\alpha\rangle, \quad (2.10)$$

where $\{\epsilon_\alpha\}$ s are called quasienergies. From this, one can construct the generalized stationary states or the Floquet states $|\psi_\alpha(t)\rangle$ of the TDSE. First, we define the Floquet modes:

$$|u_\alpha(t)\rangle = U_M(t)|\tilde{u}_\alpha\rangle = e^{-iG[t]}|\tilde{u}_\alpha\rangle, \quad \text{where } |u_\alpha(t+T)\rangle = |u_\alpha(t)\rangle. \quad (2.11)$$

The second relation is obtained trivially from the first relation by exploiting the time-periodic property of $G[t]$. The Floquet modes $|u_\alpha(t)\rangle$ describes the micromotion and the quasienergies ϵ_α describes the linear phase evolution. The Floquet states are then obtained as

$$|\psi_\alpha(t)\rangle = e^{-i\epsilon_\alpha t/\hbar}|u_\alpha(t)\rangle. \quad (2.12)$$

These states are the eigenstates of the time evolution operator over one period, i.e.,

$$|\psi_\alpha(t+T)\rangle = U(t \rightarrow t+T)|\psi_\alpha(t)\rangle = e^{-i\epsilon_\alpha T/\hbar}|\psi_\alpha(t)\rangle. \quad (2.13)$$

These states form a complete orthonormal basis at arbitrary any time t . Therefore, any initial state can be expanded on this basis, and then the time evolution will be determined by the quasienergies.

The time-periodic micromotion operator $U_M(t)$ is not unique for a given time evolution operator and consequently does not give a unique H_{eff} . One can construct a new micromotion operator $U'_M(t)$ starting from $U_M(t)$ by applying certain unitary operations. Since the Floquet states are the eigenstates of the time evolution operator, they will remain the same if one uses a different form of the micromotion operator. The simplest possibility which one can think of constructing a new micromotion operator of the form $U'_M(t) = U_M(t)U_0$ where U_0 is a time independent unitary operator. Then the effective Hamiltonian will become $H'_{\text{eff}} = U_0^\dagger H_{\text{eff}} U_0$. One can assume $U_0 = U_M^\dagger(t_i) \equiv U_M(t, t_i)$, where $U_M(t_i)$ is defined at a fixed time t_i which is here just the initial time and therefore it is a time independent operator. The new micromotion operator satisfies the condition $U'_M(t_i) = U_M(t_i, t_i) = \mathbb{1}$.

This allows one to write the time evolution operator

$$U(t_i \rightarrow t_f) = U_M(t_f, t_i) \exp\left(-\frac{i}{\hbar} H_{\text{eff}}^{[t_i]}\right), \quad (2.14)$$

with the effective Hamiltonian

$$H_{\text{eff}}^{[t_i]} = U_M(t_i) H_{\text{eff}} U_M^\dagger(t_i) \quad (2.15)$$

and the two point (or at two different time) micromotion operator

$$U_M(t_f, t_i) = U_M(t_f) U_M^\dagger(t_i). \quad (2.16)$$

Particularly for the situation when one probes the system stroboscopically at time intervals $t_f = t_i + nT$, where n are positive integers, then Eq. (2.14) becomes much simpler:

$$U(t_i \rightarrow t_f) \equiv U(nT) = \exp\left(-\frac{i}{\hbar} nT H_{\text{eff}}^{[t_i]}\right) = U(T)^n, \quad (2.17)$$

where $U(T)$ is the time evolution operator defined over one time period T . Here, the Hamiltonian $H_{\text{eff}}^{[t_i]}$ depends parametrically on the initial time t_i ; but according to Eq. (2.15), it is related to H_{eff} by a unitary transformation. Therefore, the spectrum of effective or Floquet Hamiltonian is independent of t_i .

Another way to construct a new micromotion operator is

$$U'_M(t) = U_M(t) e^{im\omega t |\tilde{u}_\alpha\rangle\langle\tilde{u}_\alpha|}, \quad (2.18)$$

where m is integer. This choice of the micromotion operator will modify the effective Hamiltonian as

$$H'_{\text{eff}} = H_{\text{eff}} + m\hbar\omega |\tilde{u}_\alpha\rangle\langle\tilde{u}_\alpha|. \quad (2.19)$$

The above operation changes the quasienergies as well as the Floquet modes as

$$\epsilon_{m\alpha} = \epsilon_\alpha + m\hbar\omega, \quad |u_{\alpha m}(t)\rangle = e^{im\omega t}|u_\alpha(t)\rangle. \quad (2.20)$$

One can easily show that the above new solutions labeled by m ensure that the Floquet states will remain the same, i.e.,

$$|\psi_\alpha(t)\rangle = e^{-i\epsilon_\alpha t/\hbar}|u_\alpha(t)\rangle = e^{-i\epsilon_{m\alpha} t/\hbar}|u_{\alpha m}(t)\rangle. \quad (2.21)$$

Equation (2.20) is showing that the quasienergies are not unique and defined up to an integer multiples of $\hbar\omega$. This is in agreement that the effective or Floquet Hamiltonian is not unique for a given time-periodic Hamiltonian. This is an important result. Because this gives the freedom to choose m independently for each Floquet state $|\psi_\alpha\rangle$ so that all quasienergies can lie within the same interval of width $\hbar\omega$, this interval is called *Floquet-Brillouin zone* (FBZ). The concept of Brillouin zone is well known in solid state physics where, instead of time, the system has periodicity in space.

2.2 Perturbation theory to generate the effective Hamiltonian: High frequency case

A major requirement of the Floquet engineering is to compute the effective Hamiltonian. However, in general, it is not possible to compute exactly by any analytical means. Therefore, one has to develop perturbation schemes at some suitable approximation. One such approximation is the high frequency driving limit. Here, the high frequency suggests that the corresponding energy $\hbar\omega$ is larger than all the energy scales of the undriven system. Mathematically, this means $\hbar\omega$ is much

larger compared to all the matrix elements of the undriven Hamiltonian. The low frequency limit can be another extreme approximation, but this thesis is only considering the high frequency case. We now discuss two perturbation techniques: based on the Van Vleck expansion [24, 26, 27] and on the Brillouin-Wigner (BW) perturbative expansion [76].

2.2.1 Van Vleck expansion

Since we assume that the frequency $\omega = 2\pi/T$ is large, the effective Hamiltonian H_{eff} and the kick operator $G[t]$ can be expanded in perturbation series of $(1/\omega)$ up to a desired accuracy $\mathcal{O}(\omega^{-n})$ as [26]

$$\begin{aligned} H_{\text{eff}} &= \sum_{0 \leq n < \infty} \frac{1}{\omega^n} H^{(n)} \\ G[t] &= \sum_{1 \leq n < \infty} \frac{1}{\omega^n} G^{(n)}[t]. \end{aligned} \quad (2.22)$$

One has to use the following identities

$$e^{iG} H e^{-iG} = H + i[G, H] - \frac{1}{2}[G, [G, H]] - \frac{i}{6}[G, [G, [G, H]]] + \dots, \quad (2.23)$$

$$\left(\frac{\partial}{\partial t} e^{iG} \right) e^{-iG} = i \left[\frac{\partial G}{\partial t} \right] - \frac{1}{2} \left[G, \frac{\partial G}{\partial t} \right] - \frac{i}{6} \left[G, \left[G, \frac{\partial G}{\partial t} \right] \right], \quad (2.24)$$

where $G = G[t]$, and the Fourier series expansion of the time-periodic Hamiltonian

$$H(t) = H_0 + V(t) = H_0 + V_0 + \sum_{n=1}^{\infty} (V_n e^{in\omega t} + V_{-n} e^{-in\omega t}) \quad (2.25)$$

to derive the operators H_{eff} and $G[t]$. Following the above expansions, one can obtain the general expressions up to $\mathcal{O}(\omega^{-2})$ for the effective Hamiltonian

$$\begin{aligned} H_{\text{eff}} = & H_0 + V_0 + \frac{1}{\omega} \sum_{n=1}^{\infty} \frac{1}{n} [V_n, V_{-n}] + \frac{1}{2\omega^2} \sum_{n=1}^{\infty} \left(\left[[V_n, H_0], V_{-n} \right] + \text{h.c.} \right) \\ & + \frac{1}{3\omega^2} \sum_{n,m=1}^{\infty} \frac{1}{nm} \left(\left[V_n, [V_m, V_{-(n+m)}] \right] - 2 \left[V_n, [V_{-n}, V_{(n-m)}] \right] + \text{h.c.} \right) \dots \end{aligned} \quad (2.26)$$

and for the kick operator at time t as

$$\begin{aligned} G[t] = & \frac{1}{i\omega} \sum_{n=1}^{\infty} \frac{1}{n} \left(V_n e^{in\omega t} - V_{-n} e^{-in\omega t} \right) + \frac{1}{i\omega^2} \sum_{n=1}^{\infty} \frac{1}{n^2} \left([V_n, H_0 + V_0] e^{in\omega t} - \text{h.c.} \right) \\ & + \frac{1}{2i\omega^2} \sum_{n,m=1}^{\infty} \frac{1}{n(n+m)} \left([V_n, V_m] e^{i(n+m)\omega t} - \text{h.c.} \right) \\ & + \frac{1}{2i\omega^2} \sum_{n \neq m=1}^{\infty} \frac{1}{n(n-m)} \left([V_n, V_{-m}] e^{i(n-m)\omega t} - \text{h.c.} \right) \dots \end{aligned} \quad (2.27)$$

A more detailed derivation of the above equations is given in Appendix A.1.

At the high frequency limit, the convergence is expected to be fast; then the above series expansion may be treated as a regular perturbation series with finite order of corrections. In this thesis, we particularly consider periodic δ -kick driving

$$V(t) = V \sum_n \delta(t - nT). \quad (2.28)$$

From Eq. (2.26), we obtain the effective time independent Hamiltonian as:

$$H_{\text{eff}} = H_0 + \frac{V}{T} + \frac{1}{24} [[V, H_0], V] + \mathcal{O}\left(\frac{1}{\omega^3}\right). \quad (2.29)$$

A complete derivation is provided in appendix A.1.1.

2.2.2 Brillouin-Wigner (BW) perturbation theory

Van Vleck perturbation theory provides a systematic and consistent high frequency expansion that correctly reproduces the expansion for effective Hamiltonian H_{eff} . However, sometimes it is cumbersome to compute higher-order terms in $(1/\omega)$ with this method. An alternative approach based on the Brillouin-Wigner perturbation theory is proposed [76, 78]. This perturbation theory is developed on the idea of expanded Hilbert space or Sambe space [22], and thus this space can be called Floquet-Hilbert (FH) space.

A Sambe space or a FH space \mathbb{H}_{FH} is a tensor product of the ‘standrad’ system Hilbert space \mathbb{H} and the Hilbert space of time-periodic functions \mathbb{T} defined by the period T , i.e., $\mathbb{H}_{FH} = \mathbb{H} \otimes \mathbb{T}$. The Hilbert space of time-periodic functions \mathbb{T} is a direct sum space of the subspaces \mathbb{T}_m , i.e., $\mathbb{T} = \bigoplus_m \mathbb{T}_m$, and the subspaces spanned by $\mathbb{T}_m = \{e^{-im\omega t}\}$, (where $m \in \mathbb{Z}$). In the FH space, the TDSE can be transformed in to the following eigenvalue problem

$$\sum_{n \in \mathbb{Z}} (H_{mn} - m\omega \delta_{mn}) |u_{\alpha m}\rangle = \epsilon_{\alpha} |u_{\alpha m}\rangle, \quad (2.30)$$

where the general solution of the original TDSE will be

$$|\phi_{\alpha}(t)\rangle = \sum_{m \in \mathbb{Z}} c_m e^{-i(\epsilon_{\alpha} + m\omega)t} |u_{\alpha m}\rangle, \quad (2.31)$$

and

$$H_{m,n} = \frac{1}{T} \int_0^T H(t) e^{i(m-n)\omega t} dt. \quad (2.32)$$

The above time independent eigen representation of the TDSE in the FH space can be written in a matrix form as

$$(\mathcal{H} - \mathcal{M}) |\mathbf{u}_{\alpha}\rangle = \epsilon_{\alpha} |\mathbf{u}_{\alpha}\rangle, \quad (2.33)$$

where $[\mathcal{M}]_{mn} = m\delta_{mn}$ is a diagonal matrix. Here, $(\mathcal{H} - \mathcal{M})$ plays the role of a time independent Hamiltonian defined in the FH space.

In the BW theory, a key concept is the *model* space, which is a smaller Hilbert space and can be chosen arbitrarily. In general, the model space \mathbb{M} is constructed by spanning some eigenstates, but not all, of the Hamiltonian, i.e., $\mathbb{M} = \{|\mathbf{u}_\alpha\rangle\}$. Let us denote \mathbb{Q} as the space formed by the orthogonal components of \mathbb{M} . If \mathcal{P} is a projection operator to the model space, then the orthogonal projection operator $\mathcal{Q} \in \mathbb{Q}$ will satisfy $\mathcal{Q} = \mathbb{1} - \mathcal{P}$. If $\mathcal{P}|\mathbf{u}_\alpha\rangle$ is the projection of the eigenstate $|\mathbf{u}_\alpha\rangle$ to the model space, then there exists another projection operator Ω which projection back the eigenstate from the model space to the full Hilbert space, which is here the FH space. The operator Ω is called the wave operator. Therefore,

$$|\mathbf{u}_\alpha\rangle = \Omega\mathcal{P}|\mathbf{u}_\alpha\rangle. \quad (2.34)$$

Since the rank $\Omega < \dim \mathcal{P}$, the above relation is not valid for all α . After defining the model space and all the projection operators, the BW theory gives the corresponding effective Hamiltonian as

$$H_{\text{eff}} = \mathcal{P}(\mathcal{H} - \mathcal{M})\Omega\mathcal{P}. \quad (2.35)$$

The eigenstates and the eigenenergies of this Hamiltonian are $\mathcal{P}|\mathbf{u}_\alpha\rangle$ and ϵ_α , respectively. In the context of Floquet formalism, when one is interested to compute a time independent effective Hamiltonian, a natural choice for the model space will be the so called *zero photon* subspace \mathbb{T}_0 , and therefore the projection operator becomes $[\mathcal{P}]_{mn} = \delta_{mn}\delta_{m0}$. The orthogonal projection operator then becomes $[\mathcal{Q}]_{mn} = \delta_{mn}(1 - \delta_{m0})$. This choice of \mathcal{P} averages out the micromotion or the periodic oscillations of the quasienergy eigenstates.

Since the operator \mathcal{Q} commutes with \mathcal{M} , then from Eq. (2.33), we get

$$\mathcal{Q}|\mathbf{u}_\alpha\rangle = \frac{\mathcal{Q}}{\epsilon_\alpha + \mathcal{M}\omega} \mathcal{H}|\mathbf{u}_\alpha\rangle, \quad (2.36)$$

and this implies

$$\begin{aligned} |\mathbf{u}_\alpha\rangle &= \mathcal{P}|\mathbf{u}_\alpha\rangle + \frac{\mathcal{Q}}{\epsilon_\alpha + \mathcal{M}\omega} \mathcal{H}|\mathbf{u}_\alpha\rangle \\ &= \left(\mathbb{1} - \frac{\mathcal{Q}}{\epsilon_\alpha + \mathcal{M}\omega} \mathcal{H} \right)^{-1} \mathcal{P}|\mathbf{u}_\alpha\rangle. \end{aligned} \quad (2.37)$$

Comparing the above relation with the relation given in Eq. (2.34), we get

$$\Omega(\epsilon) = \left(\mathbb{1} - \frac{\mathcal{Q}}{\epsilon + \mathcal{M}\omega} \mathcal{H} \right)^{-1}. \quad (2.38)$$

From Eq. (2.35) and noting that $\mathcal{P}\mathcal{M} = 0$, we get the expression of the effective Hamiltonian as

$$H_{\text{eff}}(\epsilon) = \mathcal{P}\mathcal{H} \left(\mathbb{1} - \frac{\mathcal{Q}}{\epsilon_\alpha + \mathcal{M}\omega} \mathcal{H} \right)^{-1} \mathcal{P}. \quad (2.39)$$

Since in the above expression, the quasienergy ϵ is at the both sides, one has to solve it self-consistently and thus one get the effective Hamiltonian as a perturbative expansion as:

$$H_{BW} = \sum_{n=0}^{\infty} H_{BW}^{(n)} \quad (2.40)$$

where

$$\begin{aligned} H_{BW}^{(0)} &= H_{0,0} \\ H_{BW}^{(1)} &= \sum_{n_i \neq 0} \frac{H_{0,n_1} H_{n_1,0}}{n_1 \omega} \\ H_{BW}^{(2)} &= \sum_{n_i \neq 0} \left(\frac{H_{0,n_1} H_{n_1,n_2} H_{n_2,0}}{n_1 n_2 \omega^2} - \frac{H_{0,n_1} H_{n_1,0} H_{0,0}}{n_1^2 \omega^2} \right) \end{aligned} \quad (2.41)$$

and H_{mn} are the Fourier components of the time-periodic Hamiltonian as defined in Eq. (2.32). For further details, see A.2.

In case of the single δ -kicked driving, we get the effective Hamiltonian from the BW perturbation theory up to order of ω^{-2} as

$$H_{BW} = H_0 + \frac{V}{T} + \frac{1}{12}VH_0V, \quad (2.42)$$

where H_0 is the static part of the Hamiltonian and V is the δ -kicked driven potential part.