Floquet-Fourier approach

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1 Floquet Theory

Consider a quantum system driven by a periodic external field with period T and fundamental frequency $\Omega = \frac{2\pi}{T}$. The Schrodinger equation for the time dependent Hamiltonian $\hat{\mathcal{H}}(r, t+T) = \hat{\mathcal{H}}(r, t)$ of the system is

$$\hat{\mathcal{H}}(r,t)\Psi(r,t) = 0 \tag{1}$$

where

$$\hat{\mathcal{H}}(r,t) = \hat{H}(r,t) - i\hbar\partial/\partial t \tag{2}$$

$\hat{H}(r,t)$ is the total Hamiltonian given by

$$\hat{H}(r,t) = \hat{H}_0(r) + V(r,t) \tag{3}$$

where $V(r,t)$ is the periodic perturbation due to the interaction between the system and the external field

$$V(r,t+T) = V(r,t) \tag{4}$$

and the unperturbed Hamiltonian $\hat{H}_0(r)$ is assumed to posses a complete orthonormal set of eigenfunctions $|\phi_\alpha\rangle$ with corresponding eigenvalues E_α.

$$\hat{H}_0(r)\,|\phi_\alpha(r)\rangle = E^0_\alpha\,|\phi_\alpha(r)\rangle \tag{5}$$

$$\langle\phi_\alpha(r)|\phi_\beta(r)\rangle = \int \phi^*_\alpha(r)\phi_\beta(r)dr = \delta_{\alpha\beta} \tag{6}$$

According to the Floquet Theorem !REF! there exist a complete set of Floquet solutions to the dynamics in Eq.(2.1) of the form

$$\Psi_\alpha(r,t) = exp(-i\varepsilon_\alpha t/\hbar)\Phi_\alpha(r,t) \tag{7}$$

where $\Phi_\alpha(r,t)$ is periodic in time $\Phi_\alpha(r,t) = \Phi_\alpha(r,t+T)$ and ε_α is a real energy parameter called the Floquet characteristic exponent or the quasienergy. It is the analogous of the quasimomentum k that characterize the Bloch eigenstates in a periodic solid. Substituting Eq.(7) in Eq.(1) we obtain the eigenvalue equation for the quasienergies ε_α

$$\begin{aligned}
\left[\hat{H}(r,t) - i\hbar\partial/\partial t\right] exp(-i\varepsilon_\alpha t/\hbar)\Phi_\alpha(r,t) &= 0\\
exp(-i\varepsilon_\alpha t/\hbar)\left[\hat{H}(r,t)\Phi_\alpha(r,t) - \varepsilon_\alpha\Phi_\alpha(r,t) - i\hbar\partial/\partial t\Phi_\alpha(r,t)\right] &= 0\\
\left[\hat{H}(r,t) - i\hbar\partial/\partial t\right]\Phi_\alpha(r,t) &= \varepsilon_\alpha\Phi_\alpha(r,t)
\end{aligned}$$

$$\hat{\mathcal{H}}(r,t)\Phi_\alpha(r,t) = \varepsilon_\alpha\Phi_\alpha(r,t) \tag{8}$$

Note that the following transformation

$$\varepsilon'_\alpha = \varepsilon_\alpha + n\hbar\Omega = \varepsilon_{\alpha n} \tag{9}$$

$$\Phi'_\alpha(r,t) = exp(in\Omega t)\Phi_\alpha(r,t) \tag{10}$$

with n being an integer number $n = 0, \pm 1, \pm 2, ...$ converts any eigenstate in Eq.(8) into another eigenstate but with shifted quasienergy. That means, the Floquet states are physically equivalent if their quasienergies differ by $n\hbar\Omega$. Thus, we can work in the first Brillouin zone $-\hbar\Omega/2 \leq \varepsilon_\alpha \leq \hbar\Omega/2$. The wavefunction $\Psi(r,t)$ in Eq.(1) on the other hand remains unchanged upon this transformation.

For the Hermitian operator $\hat{\mathcal{H}}$ we have an eigenvalue problem in the direct-product Floquet space $\mathscr{R} \otimes \mathscr{T}$. $\mathscr{R}$ being the usual Hilbert space spanned by the orthonormal basis set of square-integrable functions in the configuration space

$$\langle \phi_\alpha | \phi_\beta \rangle = \delta_{\alpha\beta} \tag{11}$$

and $\mathscr{T}$ being the space spanned by the complete orthonormal basis set of periodic temporal functions $\xi_n(t) = exp(in\Omega t)$ where $n = 0, \pm 1, \pm 2, ...$ is the Fourier index and

$$\frac{1}{T}\int_0^T \xi_n^*(t)\xi_m(t)dt = \delta_{nm} \tag{12}$$

The eigenvectors of $\hat{\mathcal{H}}$ satisfy the orthonormality condition

$$\langle \Phi_{\alpha n}(r,t) | \Phi_{\beta m}(r,t) \rangle = \frac{1}{T}\int_0^T dt \int_{-\infty}^{\infty} dr \Phi_{\alpha n}^*(r,t)\Phi_{\beta m}(r,t) = \delta_{\alpha\beta}\delta_{nm} \tag{13}$$

and form a complete set in the composite Hilbert space $\mathscr{R} \otimes \mathscr{T}$

$$\sum_\alpha \sum_n \Phi_{\alpha n}^*(r,t)\Phi_{\alpha n}(r',t') = \delta(r-r')\delta(t-t') \tag{14}$$

1.1 Time-independent Floquet Hamiltonian Method

The state $\Psi_\alpha(r,t)$ in Eq.(7) can be expanded in a Fourier series using the Fourier mode expansion of $\Phi_\alpha(r,t)$

$$\Psi_\alpha(r,t) = exp(-i\varepsilon_\alpha t) \sum_{n=-\infty}^{n=\infty} |C_\alpha^{(n)}(r)\rangle \, \xi_n(t) \tag{15}$$

The functions $|C_\alpha^{(n)}(r)\rangle$ of Eq.(15) can be further expanded in terms of the orthonormal set of unpertrbed eigenfunctions of $\hat{H}_0(r)$, namely $|\phi_\beta(r)\rangle$

$$|C_\alpha^{(n)}(r)\rangle = \sum_\beta \Lambda_{\alpha\beta}^{(n)} \, |\phi_\beta\rangle \tag{16}$$

Substituting Eq.(15) and Eq.(16) into Eq.(1) we have

$$\begin{aligned} \left[\hat{H}(r,t) - i\hbar\partial/\partial t\right] exp(-i\varepsilon_\alpha t) \sum_n \sum_\beta \Lambda_{\alpha\beta}^{(n)} \, |\phi_\beta\rangle \, \xi_n(t) &= 0 \\ \hat{H}(r,t) \sum_n \sum_\beta \Lambda_{\alpha\beta}^{(n)} \, |\phi_\beta\rangle \, \xi_n(t) - \sum_n \sum_\beta \Lambda_{\alpha\beta}^{(n)} \, |\phi_\beta\rangle \, \xi_n(t) \, (\varepsilon_\alpha - n\hbar\Omega) &= 0 \end{aligned}$$

Multiplication from the left by $\langle \phi_\alpha | \, \xi_m^*(t)$ and average over one temporal period leads to

$$\sum_n \sum_\beta \left[\langle \alpha | \hat{H}^{(m-n)}(r) | \beta \rangle - (\varepsilon_\alpha - n\hbar\Omega) \, \delta_{\alpha\beta}\delta_{nm}\right] \Lambda_{\alpha\beta}^{(n)} = 0 \tag{17}$$

where we have used the simplifying notation $|\alpha\rangle \equiv |\phi_\alpha\rangle$ and

$$\hat{H}^{(n)}(r) = \frac{1}{T}\int_0^T \hat{H}(r,t) exp(i\Omega t n) dt \tag{18}$$

As an example consider the interaction of a quantum system with a linearly polarized monochromatic field. In this case $V(r,t) \sim cos(\Omega t)$ and only the matrix elements $\langle\alpha|\hat{H}^{(n)}(r)|\beta\rangle$ with $n = 0, \pm 1$ are non-vanishing. Now we introduce the Floquet-state nomenclature $|\alpha n\rangle = |\alpha\rangle \otimes |n\rangle$ where α represents an atomic state and n represents a Fourier component. The system of Eq.(17) can be recast into the form of a matrix eigenvalue equation

$$\sum_{\gamma k} \langle\alpha n|\hat{H}_F|\gamma k\rangle\, \Lambda^{(k)}_{\gamma\beta} = \varepsilon_\beta \Lambda^{(n)}_{\alpha\beta} \tag{19}$$

where $\hat{H}_F$ is the *time-independent Floquet Hamiltonian* whose matrix elements are defined by

$$\begin{aligned} \langle\alpha n|\hat{H}_F|\beta m\rangle &= \hat{H}^{n-m}_{\alpha\beta} + n\hbar\Omega\delta_{\alpha\beta}\delta_{nm} & (20)\\ &= \hat{H}_0\delta_{\alpha\beta}\delta_{nm} + n\hbar\Omega\delta_{\alpha\beta}\delta_{nm} + \frac{1}{T}\int_0^T V_{\alpha\beta}(r,t)exp(i\Omega t(n-m))dt & (21) \end{aligned}$$

The operator $\hat{H}_F$ is therefore an infinite Hermitian matrix that possesses a block tridiagonal form as shown in the matrix representation below. Then, the quasienergies ε are the eigenvalues of the secular equation

$$det\left|\hat{H}_F - \varepsilon I\right| = 0 \tag{22}$$

$\cdots$	m=-2	m=-1	m=0	m=1	m=2	$\cdots$	
·	·	·	·	·	·	·	$\vdots$
·	$\hat{H}_0 - 2\hbar\Omega$	$\tilde{V}$	0	0	0	·	n=-2
·	$\tilde{V}^\dagger$	$\hat{H}_0 - \hbar\Omega$	$\tilde{V}$	0	0	·	n=-1
·	0	$\tilde{V}^\dagger$	$\hat{H}_0$	$\tilde{V}$	0	·	n=0
·	0	0	$\tilde{V}^\dagger$	$\hat{H}_0 + \hbar\Omega$	$\tilde{V}$	·	n=1
·	0	0	0	$\tilde{V}^\dagger$	$\hat{H}_0 + 2\hbar\Omega$	·	n=2
·	·	·	·	·	·	·	$\vdots$

Floquet Hamiltonian on matrix representation

Consider now the transition from an initial quantum state $|\alpha\rangle$ to a final quantum state $|\beta\rangle$. The time-evolution operator $\hat{U}(t,t_0)$, in matrix form, can be expressed as

$$\begin{aligned} \hat{U}_{\beta\alpha}(t,t_0) &= \langle\beta|\hat{U}(t,t_0)|\alpha\rangle \\ &= \sum_n \langle\beta n|exp\left[-i\hat{H}_F(t-t_0)\right]|\alpha 0\rangle\, exp(in\Omega t) \end{aligned} \tag{23}$$

Eq.(23) shows that $\hat{U}_{\beta\alpha}(t,t_0)$ can be seen as the amplitude that a system initially in the Floquet state $|\alpha 0\rangle$ at time t_0 evolve to the Floquet final state $|\beta n\rangle$ by time t according to the time-independent Floquet Hamiltonian $\hat{H}_F$, summing over n with weighting factors $exp(in\Omega t)$. Based on this interpretation, we can use methods applicable to time-independent Hamiltonians in order to solve problems involving Hamiltonians periodic in time.