Floquet theory

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Floquet theory in the temporal dimension *Apply the Floquet theory of differential equation to how a wave function evolves according to a periodic Hamiltonian. What are counterparts of* $\mathbf{k}$ *and* $\mathbf{G}$ *vectors in band theory?*

we know it is possible to expand an arbitrary state that evolves according to a Hamiltonian H with period T into a linear combination (the coefficients are constants) of $\{ |\psi_n(t)\rangle \}$ where

$$|\psi_n(t)\rangle = \mathrm{e}^{-\mathrm{i}\varepsilon_n t/\hbar} |\Phi_n(t)\rangle \,, \quad |\Phi_n(t+T)\rangle = |\Phi_n(t)\rangle \,. \tag{1}$$

By discrete periodicity of $|\Phi_n(t)\rangle$ we make Fourier expansion

$$|\Phi_n(t)\rangle = \sum_m \mathrm{e}^{-\mathrm{i}m\omega t} |\phi_n^{(m)}\rangle \,, \tag{2}$$

where m goes over all integers. The quasienergies ε_n are comparable to the crystal momentum, and $m\omega$ are comparable to $\mathbf{G}$ vectors. Note that here $|\phi_n^{(m)}\rangle$ are *Fourier coefficients* and are not eigenstates of anything; there is no normalization or orthogonality condition for them.

Floquet effective Hamiltonian *Rewrite the Schrodinger equation*

$$\mathrm{i}\hbar \frac{\mathrm{d}}{\mathrm{d}t} |\psi_n(t)\rangle = H |\psi_n(t)\rangle \tag{3}$$

in a form that doesn't explicitly contain time. The resulting matrix is known as the Floquet effective Hamiltonian.

The Schrodinger equation now reads

$$\mathrm{i}\hbar \sum_m (-\mathrm{i}\varepsilon_n/\hbar - \mathrm{i}m\omega) \mathrm{e}^{-\mathrm{i}(\varepsilon_n/\hbar + m\omega)t} |\phi_n^{(m)}\rangle = \sum_{m'} \mathrm{e}^{-\mathrm{i}\varepsilon_n/\hbar - \mathrm{i}m'\omega t} H |\phi_n^{(m')}\rangle \,,$$

and by cancelling the $\mathrm{e}^{-\mathrm{i}\varepsilon_n t/\hbar}$ factor and doing inverse Fourier transform, we get

$$(\varepsilon_n + m\hbar\omega) |\phi_n^{(m)}\rangle = \sum_{m'} H^{(m-m')} |\phi_n^{(m')}\rangle \,, \tag{4}$$

where

$$H(t) = \sum_m \mathrm{e}^{-\mathrm{i}m\omega t} H^{(m)}, \quad H^{(m)} = \frac{1}{NT} \int_0^{NT} \mathrm{d}t \, \mathrm{e}^{\mathrm{i}m\omega t} H(t), \tag{5}$$

N is a large positive integer. Thus we find

$$\varepsilon_n |\phi_n^{(m)}\rangle = \sum_{m'} (H^{(m-m')} - m\hbar\omega \delta_{mm'}) |\phi_n^{(m')}\rangle \,. \tag{6}$$

ε_n and the structure of $|\psi_n\rangle$ can then be solved by diagonalizing (6).

The non-equilibrium nature of Floquet effective Hamiltonian *Compare the Floquet effective Hamiltonian with an ordinary effective Hamiltonian, say a two band model or a two-level atom model. Is there any substantial difference?*

Although we may want to interpret (6) as an effective Hamiltonian where photon degrees of freedom have been integrated out, unlike conventional effective Hamiltonians whose eigenstates can in principle be obtained by applying a projection operator on a subset of eigenstates of the full Hamiltonian, eigenstates of (6) *do not* correspond to any eigenstate of the full, time-independent Hamiltonian that contains both light and matter degrees of freedom. If we consider the state of the full Hamiltonian corresponding to an eigenstate of (6), we find that the light part of the former is in a coherent state, which is far from any eigenstate of the linear electromagnetic Hamiltonian $\hbar\omega(n + \frac{1}{2})$. Instead, Floquet formalisms is to be understood in a more generic framework of non-equilibrium physics: Floquet Green function can be calculated within the Keldysh formalism, and (6) can be understood as the non-equilibrium self-energy [1, 2] and therefore is not necessarily an equilibrium effective Hamiltonian.

The structure of the eigensystem of the Floquet effective Hamiltonian *It can be seen that even when the dimension of the Hilbert space of matter is finite, the dimension of the Floquet effective Hamiltonian, if written as a matrix, is still infinite, as we have the the index of "photon number". Analyze the structure of the eigensystem of the Floquet effective Hamiltonian; compare it with the eigensystem in a spatially periodic system.*

If ε_n is a solution of (1), then so is $\varepsilon_n + m\hbar\omega$. As for the relation between quasi-stationary eigenstates corresponding to ε_n and $\varepsilon_n + m\hbar\omega$, we note that

$$|\psi_n(t)\rangle = \mathrm{e}^{-\mathrm{i}\varepsilon_n t/\hbar} \sum_m \mathrm{e}^{-\mathrm{i}m\omega t} |\phi_n^{(m)}\rangle = \mathrm{e}^{-\mathrm{i}(\varepsilon+\hbar m'\omega)t/\hbar} \sum_m \mathrm{e}^{-\mathrm{i}m\omega t} |\phi_n^{(m+m')}\rangle . \tag{7}$$

Therefore, if $(\varepsilon, \{ |\phi^{(m)}\rangle\}_m)$ is a solution of (6), then so is $(\varepsilon + \hbar m'\omega, \{ |\phi^{(m+m')}\rangle\}_m)$. This can also be directly shown from the form of (6).

Although $(\varepsilon, \{ |\phi^{(m)}\rangle\}_m)$ and $(\varepsilon + \hbar m'\omega, \{ |\phi^{(m+m')}\rangle\}_m)$ seem to be independent solutions of (6), they correspond to the the *same* $|\psi_n(t)\rangle$. Therefore the fact that a Floquet quasienergy plus an integer times ω is also a Floquet quasienergy is not a symmetry of the system, but merely a redundancy. Suppose we keep M_m choices of m when diagonalizing (6); (6) then has $N_m \times N$ solutions, where N is the dimension of the Hilbert space of the matter degrees of freedom. Since one solution of (6) has $N_m - 1$ physically equivalent counterparts, (6) eventually has

$$N \times N_m / N_m = N$$

physically independent solutions. There however is no redundant information in $\{ |\phi_n^{(m)}\rangle\}$, because every $|\phi_n^{(m)}\rangle$ is needed to determine $|\Phi_n(t)\rangle$ and thus $|\psi_n(t)\rangle$.

In conclusion, for each $|\psi_n(t)\rangle$ we have countable infinite quasi-energies, the difference between the nearest two being $\hbar\omega$; thus all distinct Floquet quasi-eigenstates can be indexed by quasi-energies that are within one "Floquet-Brillouin zone". Unlike the case in solid state physics, the state with quasienergy ε_n is equivalent to the state with quasienergy $\varepsilon_n + m\hbar\omega$, while in solid state physics of course $\mathrm{e}^{\mathrm{i}\mathbf{k}\cdot\mathbf{r}}$ is *not* equivalent to $\mathrm{e}^{\mathrm{i}(\mathbf{k}+\mathbf{G})\cdot\mathbf{r}}$; the number of physically non-equivalent $|\psi_n(t)\rangle$ is the same as the dimension of the Hilbert space. (And therefore, in the ARPES spectrum of a Floquet system, the signature at $\varepsilon_{n\mathbf{k}} + \hbar m\omega$ *does not* correspond to a new band other than the nth band: it's just a satellite in the signature of the Floquet-renormalized nth band that comes from the $\phi_{n\mathbf{k}}^{(m)}$ Floquet component of $|\psi_{n\mathbf{k}}\rangle (t)$).

Orthogonal relations *Under which condition are the Floquet quasi-stationary states orthogonal to each other?*

Although there is no generic orthogonal relation pertaining to $\{ |\psi_n(t)\rangle\}$, after time averaging an orthogonal relation can be obtained. From the fact that (6) is Hermitian, we have

$$\sum_m \langle\phi_n^{(m)}|\psi_{n'}^{(m)}\rangle = \delta_{nn'}, \tag{8}$$

and therefore the time average of $\langle\psi_n(t)|\psi_{n'}(t)\rangle$ is

$$\begin{aligned} \overline{\langle\psi_n(t)|\psi_{n'}(t)\rangle} &= \lim_{T\to\infty} \frac{1}{T} \int_0^T \mathrm{d}t\, \mathrm{e}^{\mathrm{i}(\varepsilon_n - \varepsilon_{n'})t} \sum_{m,m'} \mathrm{e}^{\mathrm{i}(m-m')t} \langle\phi_n^{(m)}|\phi_{n'}^{(m')}\rangle \\ &= \sum_{m,m'} \delta_{\varepsilon_n,\varepsilon_{n'}} \delta_{mm'} \langle\phi_n^{(m)}|\phi_{n'}^{(m')}\rangle \\ &= \delta_{\varepsilon_n,\varepsilon_{n'}} \sum_m \langle\phi_n^{(m)}|\psi_{n'}^{(m)}\rangle = \delta_{nn'}. \end{aligned} \tag{9}$$

Therefore, after time averaging, the Floquet quasi-stationary states are orthogonal to each other.

References

[1] Andreas Lubatsch and Regine Frank. "Evolution of Floquet topological quantum states in driven semiconductors". In: *The European Physical Journal B* 92 (2019), pp. 1–9.

[2] Hideo Aoki et al. "Nonequilibrium dynamical mean-field theory and its applications". In: *Reviews of Modern Physics* 86.2 (2014), p. 779.