Hall conductivity of Aubry-André system driven by rapidly oscillating magnetic field

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Abstract

Study of quantum hall effect in 2D square lattice driven by oscillatory magnetic field perpendicular to the plane. The time-dependent hamiltonian is solved in fourier space using Brillouin-Wigner perturbation theory, in the high frequency limit. Investigation of localization/delocalization transitions of time-averaged wavefunctions and calculation of hall conductivity of the system using TKNN invariant. Comparison of the results with the effective static hamiltonian picture carried out in the previous work.

Acknowledgements

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Declaration

I, Rajath Shashidhara, declare that this thesis titled, 'Hall conductivity of Aubry-André system driven by rapidly oscillating magnetic field' and the work presented in it is my original work. I affirm that all references are clearly attributed and any collaboration with others has been duly acknowledged.

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Certificate

This is to certify that the thesis titled, 'Hall conductivity of Aubry-André system driven by rapidly oscillating magnetic field' and submitted by Rajath Shashidhara 2012B5A7589P in partial fulfillment of the requirements of BITS F421T embodies the work done by him under my supervision.

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Chapter 2

Geometric Phase

Physical measurements or observations are extracted from quantum mechanical systems in the form of expectation values of hermitian operators $\langle\psi|\hat{A}|\psi\rangle$. Eigenvectors of the hamiltonian are only specified up to a phase factor. Expectation values and thereby, the physical observations are unaltered by a transformation of the form $\psi \rightarrow e^{i\phi}\psi$. Gauge-dependent quantities are considered unphysical and the phase of the eigenvectors is usually thrown away from analysis. Berry demonstrated the existence of a gauge-invariant phase called the geometric phase - a physically observable quantity.

2.1 Definition

Prof. M V Berry studied the adiabatic evolution of a quantum system described by the hamiltonian $\hat{H}(\mathbf{R})$, parameterized by external factors $\mathbf{R}$ – such as magnetic field, electric field, etc [1]. The hamiltonian is varied by slowly changing $\mathbf{R}$ from time $t = 0$ to $t = T$ such that $\mathbf{R}(0) = \mathbf{R}(T)$. This evolution is a closed loop in the parameter space. Apart from the adiabatic assumption, we also assume that the energy spectrum is discrete and there are no level crossings or degeneracies in the energy spectrum. Using the guage freedom, we enforce single-valuedness on the eigenvectors of the hamiltonian in the parameter space. Under the assumptions stated above, eigenvectors of the hamiltonian can be uniquely identified as $|n(\mathbf{R})\rangle$ at each point in parameter space without any ambiguity. The schrodinger equation is stated in this notation as

$$\hat{H}(\mathbf{R}(t))\,|n(\mathbf{R}(t))\rangle = E(\mathbf{R}(t))\,|n(\mathbf{R}(t))\rangle \tag{2.1}$$

$$i\hbar\frac{\partial}{\partial t}\,|\psi(t)\rangle = \hat{H}(t)\,|\psi(t)\rangle \tag{2.2}$$

In the case of static time-independent hamiltonian, any state expanded as a linear combination of stationary states is written as $|\psi(t)\rangle = \sum c_n e^{-\frac{iE_n(t)}{\hbar}}\,|n\rangle$. Taking cue from this, the expansion ansatz

$$|\psi(t)\rangle = \sum c_n(t) e^{-\frac{i}{\hbar}\int_0^t E_n(t)dt}\,|n(t)\rangle \tag{2.3}$$

is a valid generalization for a system with a time-dependent hamiltonian. When the ansatz is substituted into Eq. (2.2), we obtain

$$\dot{c}_m(t) = -c_m(t)\left\langle m(t)\left|\frac{\partial}{\partial t}m(t)\right.\right\rangle - \sum_n c_n(t)e^{i(\theta_n-\theta_m)}\frac{\langle m(t)|\dot{\hat{H}}|n(t)\rangle}{E_n - E_m} \tag{2.4}$$

where $\theta_n = \frac{-1}{\hbar}\int_0^t E_n(t')\,dt'$. In the adiabatic limit, the transition probability between states tends to zero. We ignore the second term in the general solution above to obtain the result

$$c_n(t) = e^{i\gamma_n(t)}\,c_n(0) \tag{2.5}$$

If we started in an eigenstate of the hamiltonian $|\psi(0)\rangle = |n(\mathbf{R}(0)\rangle$, then the state evolves as

$$|\psi(t)\rangle = e^{i\gamma_n(t)}e^{i\theta_n(\mathrm{R}(t))}\,|n(\mathbf{R}(t))\rangle \tag{2.6}$$

remaining in the nth eigenstate all along, only picking up phase factors. In the case of cyclic evolution, we write

$$|\psi(T)\rangle = e^{i\gamma_n(C)}e^{i\theta_n(T)}\,|\psi(0)\rangle \tag{2.7}$$

From Eq. (2.4), we note that

$$\gamma_n(C) = i\int_0^T \langle n(t)|\frac{\partial}{\partial t}n(t)\rangle\;dt = i\oint_c \langle n(\mathbf{R})|\boldsymbol{\nabla}_{\boldsymbol{R}}|n(\mathbf{R})\rangle\cdot\,d\mathbf{R} \tag{2.8}$$

$\gamma_n(C)$ is a real number and therefore $e^{i\gamma_n(C)}$ is a pure phase term. This simple fact can be demonstrated by taking the time-derivative of $\langle n(t)|n(t)\rangle = 1$.

$$\begin{gathered}\langle n(t)|n(t)\rangle = 1\\ \left[\frac{\partial}{\partial t}\langle n(t)|\right]|n(t)\rangle + \langle n(t)|\left[\frac{\partial}{\partial t}|n(t)\rangle\right] = 0\\ \langle n(t)|\left[\frac{\partial}{\partial t}|n(t)\rangle\right] = -\left(\langle n(t)|\left[\frac{\partial}{\partial t}|n(t)\rangle\right]\right)^*\end{gathered}$$

$\theta_n(T)$ is the familiar dynamical phase and $\gamma_n(C)$ is known as geometric phase or simply berry phase. While the dynamical phase is a time-dependent quantity, the geometric phase is a line integral, that only depends on path traversed in the parameter space. Another important observation is the fact that γ_n is a non-integrable quantity as it is not single valued - $\gamma_n(0) \neq \gamma_n(T)$ in the parameter space. Therefore, the geometric phase cannot be expressed as a field over the parameter space. By application of stokes theorem, the line integral can be convereted into a surface integral as shown below

$$\begin{aligned}\gamma_n(C) &= i\oint_C \langle n(\mathbf{R})|\boldsymbol{\nabla}_{\boldsymbol{R}}|n(\mathbf{R})\rangle\cdot\,d\mathbf{R}\\ &= i\int_S \boldsymbol{\nabla}_{\boldsymbol{R}}\wedge\langle n(\mathbf{R})|\boldsymbol{\nabla}_{\boldsymbol{R}}|n(\mathbf{R})\rangle\cdot\,d\mathbf{S} \qquad (2.9)\\ &= i\int_S (\boldsymbol{\nabla}_{\boldsymbol{R}}\langle n(\mathbf{R})|)\wedge\boldsymbol{\nabla}_{\boldsymbol{R}}|n(\mathbf{R})\rangle\cdot\,d\mathbf{S}\\ &= i\int_S \sum_{m\neq n}\frac{\langle n(\mathbf{R})|\boldsymbol{\nabla}_{\boldsymbol{R}}\hat{H}(\mathbf{R})|m(\mathbf{R})\rangle\wedge\langle m(\mathbf{R})|\boldsymbol{\nabla}_{\boldsymbol{R}}\hat{H}(\mathbf{R})|n(\mathbf{R})\rangle}{(E_n(\mathbf{R})-E_m(\mathbf{R}))^2}\cdot\,d\mathbf{S} \qquad (2.10)\end{aligned}$$

Eq. (2.10) has a remarkable property of being gauge independent. Any transformation of the form $|n(\mathbf{R})\rangle \to e^{i\delta(\mathrm{R})}|n(\mathbf{R})\rangle$, leaves Eq. (2.10) unchanged.

Before we proceed, it is useful to define two important quantities called the berry connection and the berry curvature. *Berry connection* is defined as

$$\mathbf{A}_n(\mathbf{R}) = i\,\langle n(\mathbf{R})|\boldsymbol{\nabla}_{\boldsymbol{R}}|n(\mathbf{R})\rangle \tag{2.11}$$

and the *Berry curvature* is given by

$$\mathbf{B}_n(\mathbf{R}) = i\,\boldsymbol{\nabla}_{\boldsymbol{R}} \wedge \langle n(\mathbf{R})|\boldsymbol{\nabla}_{\boldsymbol{R}}|n(\mathbf{R})\rangle = \boldsymbol{\nabla}_{\boldsymbol{R}} \wedge \mathbf{A}_n(\mathbf{R}) \tag{2.12}$$

Berry phase is conveniently expressed in terms of these quantities as

$$\gamma_n(C) = \oint_C \mathbf{A}_n(\mathbf{R}) \cdot\, d\mathbf{R} = \int_S \mathbf{B}_n(\mathbf{R}) \cdot\, d\mathbf{S} \tag{2.13}$$

If we transform the states as $|n(\mathbf{R})\rangle \to e^{i\delta(\mathrm{R})}|n(\mathbf{R})\rangle$, then the berry connection transforms as $\mathbf{A}_n(\mathbf{R}) \to \mathbf{A}_n(\mathbf{R}) - \boldsymbol{\nabla}_{\boldsymbol{R}}\delta(\mathbf{R})$, but the berry curvature remains unchanged. This shows an uncanny resemblance between magnetic vector potential and the berry connection and consequently the magnetic field strength and the berry curvature. However, it must be kept in mind that the berry connection and the berry curvature are defined over the parameter space (could be more than 4-dimensional) and not the real space.

Geometric phase was overlooked as physically irrelevant as the expectation values are independent of the phase of eigenfunctions. As opposed to the then prevalent notion, Prof. Berry, in his seminal paper, demonstrated that the geometric phase is in fact, physically observable [1, 2]. Several assumptions imposed by Prof. Berry in defining the geometric phase can be relaxed and definition of geometric phase has been generalized to nonadiabatic, noncyclic, nonunitary and nonabelian situations [3–6].

2.2 Bargmann invariants

A remarkable feature of the berry phase is that it is a geometric quantity, i.e., it is a property arising by virtue of the geometry of the underlying hilbert space. In [6], it is demonstrated that the berry phase is both gauge and reparameterization invariant (thereby a geometric property) using purely kinematic arguments. Geometric phase is akin to parallel transport of vectors on a non-trivial manifold. Just as the co-variant derivative of a vector on a manifold has contributions purely arising from the underlying geometry, the geometric phase is acquired by a state evolving in the hilbert space by virtue of its geometry [7]. Precisely, berry phase is the holonomy in a hermitian line bundle in the language of differential geometry.

In this section, our intention is to express the berry phase in terms of gauge invariant quantities called Bargmann invariants. Bargmann invariant of order j of a series of j normalized states $|\psi_j\rangle$ such that $\langle\psi_j|\psi_{j+1}\rangle \neq 0$ is defined as

$$\Delta^{(j)}(\psi_1, \ldots, \psi_j) = \langle\psi_1|\psi_2\rangle\,\langle\psi_2|\psi_3\rangle \ldots \langle\psi_{j-1}|\psi_j\rangle\,\langle\psi_j|\psi_1\rangle \tag{2.14}$$

It is apparent from the definition that $\Delta^{(j)}$ is invariant under a $U(1) \times U(1) \ldots j$ *times* transformation. Consider the space of eigenfunctions parameterized (under the assumptions as described in the previous section) by $\mathbf{R}$, the inner product

$$\begin{aligned} e^{i\Delta\gamma} &= \frac{\langle n(\mathbf{R})|n(\mathbf{R}+\delta\mathbf{R})\rangle}{|\langle n(\mathbf{R})|n(\mathbf{R}+\delta\mathbf{R})\rangle|} \qquad (2.15) \\ &\approx \frac{\langle n(\mathbf{R})|\ [|n(\mathbf{R})\rangle + \boldsymbol{\nabla}_{\boldsymbol{R}}|n(\mathbf{R})\rangle \cdot \delta\mathbf{R} + \ldots]}{|\langle n(\mathbf{R})|n(\mathbf{R}+\delta\mathbf{R})\rangle|} \\ 1 + i\Delta\gamma + \ldots &\approx \frac{1 + \langle n(\mathbf{R})|\boldsymbol{\nabla}_{\boldsymbol{R}}|n(\mathbf{R})\rangle \cdot \delta\mathbf{R} + \ldots}{|\langle n(\mathbf{R})|n(\mathbf{R}+\delta\mathbf{R})\rangle|} \\ \Delta\gamma &\approx -i\langle n(\mathbf{R})|\boldsymbol{\nabla}_{\boldsymbol{R}}|n(\mathbf{R})\rangle \cdot \delta\mathbf{R} \qquad (2.16) \end{aligned}$$

We have established that

$$\arg(\langle n(\mathbf{R})|n(\mathbf{R}+\delta\mathbf{R})\rangle) \approx -\mathbf{A}_n(\mathbf{R}) \cdot \delta\mathbf{R}$$

which means that

$$\begin{aligned} \gamma(C) = \oint_C \mathbf{A}_n(\mathbf{R}) \cdot \delta\mathbf{R} &= -\oint_C \arg(\langle n(\mathbf{R})|n(\mathbf{R}+\delta\mathbf{R})\rangle) \\ &= -\lim_{N\to\infty} \arg\Big(\prod_{j=0}^{N-1} \langle n(\mathbf{R}(t+j\Delta t))|n(\mathbf{R}(t+(j+1)\Delta t))\rangle\Big) \qquad (2.17) \end{aligned}$$

where $\Delta t = \frac{T}{N} \ni \mathbf{R}(0) = \mathbf{R}(T)$. Immediately we recognize that the RHS of Eq. (2.17) is the argument of Bargmann invariant of states lying on the path C.

The Berry curvature surface integral can also be expressed in terms of the Bargmann invariant. We derive the relationship below for a 2-dimensional parameter space labeled by $\boldsymbol{\lambda} = (\lambda_x, \lambda_y)$. This result can be easily generalized to arbitrary dimensions. Consider an infinitesimal square Q in the parameter space consisting of points $(\lambda_x, \lambda_y), (\lambda_x + \delta\lambda_x, \lambda_y), (\lambda_x + \delta\lambda_x, \lambda_y + \delta\lambda_y), (\lambda_x, \lambda_y + \delta\lambda_y)$ in anti-clockwise order. The integral of berry connection around this closed loop is

$$\begin{aligned} \oint_Q \mathbf{A}_n(\boldsymbol{\lambda}) \cdot \delta\boldsymbol{\lambda} = \\ &- \arg(\langle n(\boldsymbol{\lambda})|n(\boldsymbol{\lambda} + \delta\lambda_x\hat{\mathbf{x}})\rangle \langle n(\boldsymbol{\lambda} + \delta\lambda_x\hat{\mathbf{x}})|n(\boldsymbol{\lambda} + \delta\lambda_x\hat{\mathbf{x}} + \delta\lambda_y\hat{\mathbf{y}})\rangle \\ &\qquad \langle n(\boldsymbol{\lambda} + \delta\lambda_x\hat{\mathbf{x}} + \delta\lambda_y\hat{\mathbf{y}})|n(\boldsymbol{\lambda} + \delta\lambda_y\hat{\mathbf{y}})\rangle \langle n(\boldsymbol{\lambda} + \delta\lambda_y\hat{\mathbf{y}})|n(\boldsymbol{\lambda})\rangle) \end{aligned}$$

Using stokes theorem

$$\begin{aligned} \oint_Q \mathbf{A}_n(\boldsymbol{\lambda}) \cdot \delta\boldsymbol{\lambda} &= \int_Q \mathbf{B}_n(\boldsymbol{\lambda}) \cdot d\mathbf{S}_{\boldsymbol{\lambda}} \\ &= \mathbf{B}_n(\boldsymbol{\lambda})\delta\lambda_x\delta\lambda_y \end{aligned}$$

Combining these two results, we infer that

$$\begin{aligned} \mathbf{B}_n(\boldsymbol{\lambda})\delta\lambda_x\delta\lambda_y = \\ &- \arg(\langle n(\boldsymbol{\lambda})|n(\boldsymbol{\lambda} + \delta\lambda_x\hat{\mathbf{x}})\rangle \langle n(\boldsymbol{\lambda} + \delta\lambda_x\hat{\mathbf{x}})|n(\boldsymbol{\lambda} + \delta\lambda_x\hat{\mathbf{x}} + \delta\lambda_y\hat{\mathbf{y}})\rangle \\ &\qquad \langle n(\boldsymbol{\lambda} + \delta\lambda_x\hat{\mathbf{x}} + \delta\lambda_y\hat{\mathbf{y}})|n(\boldsymbol{\lambda} + \delta\lambda_y\hat{\mathbf{y}})\rangle \langle n(\boldsymbol{\lambda} + \delta\lambda_y\hat{\mathbf{y}})|n(\boldsymbol{\lambda})\rangle) \qquad (2.18) \end{aligned}$$

This result is particularly useful when numerically evaluating the surface integral of a berry phase in discretized parameter space.

2.3 Non-abelian Berry connection

Chapter 3

Quantum Hall Effect

3.1 Phenomenon

3.2 Landau levels

3.3 Corbino geometry and Lauglin's argument

3.4 Kubo formula and the TKNN invariant

Chapter 4

Brillouin-Wigner Perturbation Theory

When encountered with an analytically intractable quantum mechanical problem, perturbation techniques may be used to obtain approximate solutions. Formally, the problem can be stated as follows : Given a hamiltonian $\hat{H} = \hat{H}_0 + \hat{V}$ where $\hat{H}_0$ is exactly solvable and $\hat{V}$ is the perturbation term, and the eigendecomposition of $\hat{H}_0$ —

$$\begin{aligned} \hat{H}_0 |n\rangle &= \epsilon_n |n\rangle \\ \langle m|n\rangle &= \delta_{mn} \\ \sum_m |m\rangle \langle m| &= 1 \end{aligned}$$

using Brillouin-Wigner (BW) perturbation theory, we express $\{|\psi_n\rangle, \dots\}$ and $\{E_n, \dots\}$, such that $\hat{H}|\psi_n\rangle = E_n|\psi_n\rangle$, in terms of $\hat{V}$ and $\{|n\rangle, \dots\}$.

4.1 Introduction

To obtain the BW perturbative expansion, we begin with the eigenvalue equation.

$$\hat{H}|\psi_n\rangle = (\hat{H}_0 + \hat{V})|\psi_n\rangle = E_n|\psi_n\rangle$$

The wavefunctions $|\psi_n\rangle$ are normalized as $\langle n|\psi_n\rangle = 1$, as discussed in [8]. On contracting with $\langle n|$,

$$\begin{aligned} \langle n|(\hat{H}_0 + \hat{V})|\psi_n\rangle &= E_n \langle n|\psi_n\rangle \\ \epsilon_n \langle n|\psi_n\rangle + \langle n|\hat{V}|\psi_n\rangle &= E_n \langle n|\psi_n\rangle \\ E_n &= \epsilon_n + \langle n|\hat{V}|\psi_n\rangle \end{aligned} \tag{4.1}$$

Rewriting the eigenvalue equation as

$$\begin{aligned}(E_n - \hat{H}_0)\,|\psi_n\rangle &= \hat{V}\,|\psi_n\rangle \\ &= 1\,\hat{V}\,|\psi_n\rangle \\ &= \sum_m |m\rangle\,\langle m|\,\hat{V}\,|\psi_n\rangle \\ &= |n\rangle\,\langle n|\hat{V}|\psi_n\rangle + (1 - |n\rangle\,\langle n|)\hat{V}\,|\psi_n\rangle \end{aligned}$$

Using Eq. 4.1,

$$\begin{aligned} &= (E_n - \hat{H}_0)\,|n\rangle + (1 - |n\rangle\,\langle n|)\hat{V}\,|\psi_n\rangle \\ (E_n - \hat{H}_0)(|\psi_n\rangle - |n\rangle) &= (1 - |n\rangle\,\langle n|)\hat{V}\,|\psi_n\rangle \\ |\psi_n\rangle &= |n\rangle + (E_n - \hat{H}_0)^{-1}(1 - |n\rangle\,\langle n|)\hat{V}\,|\psi_n\rangle \end{aligned}$$

Define resolvent operator as $\hat{R}_n = (E_n - \hat{H}_0)^{-1} = \sum_n |n\rangle\,(E_n - \epsilon_n)^{-1}\,\langle n|$,

$$|\psi_n\rangle = |n\rangle + \hat{R}_n(1 - |n\rangle\,\langle n|)\hat{V}\,|\psi_n\rangle \tag{4.2}$$

The above equation is the main result of BW perturbation theory. Peculiarity of the above equation is that it depends on the undertermined parameter E_n, and this is unlike the Rayleigh-Schrodinger perturbation theory. Solving Eq. (4.2) self-consistently with Eq. (4.1), solutions to the eigenvalue equation are obtained. Using the equation, we obtain an iterative solution to the schordinger equation. In each iteration, we obtain a new estimate of $|\psi_n\rangle$ by substituting the old estimate of $|\psi_n\rangle$ on the righthand side of Eq. (4.2)

$$\begin{aligned} |\psi_n^{(j)}\rangle &= |n\rangle + \hat{R}(E_n)\,(\hat{\mathbb{I}} - |n\rangle\,\langle n|)\hat{V}\,|\psi_n^{(j-1)}\rangle \\ |\psi_n^{(0)}\rangle &= |n\rangle \\ \lim_{j\to\infty} |\psi_n^{(j)}\rangle &= |\psi_n\rangle \end{aligned} \tag{4.3}$$

No approximation has been used until this point, and exact solution can be obtained if iterated infinitely. In practice, approximate solution is obtained by truncating the iteration.

4.2 BW theory as an Operator series

Further, Eq. (4.2) can be simplified by expanding the recurrence relation

$$|\psi_n\rangle = |n\rangle + \hat{R}_n\hat{Q}_n\hat{V}\,|\psi_n\rangle$$

where $\hat{Q}_n = 1 - |n\rangle\,\langle n|$,

$$\begin{aligned} &= |n\rangle + \hat{R}_n\hat{Q}_n\hat{V}\,|n\rangle + \hat{R}_n\hat{Q}_n\hat{V}\hat{R}_n\hat{Q}_n\hat{V}\,|n\rangle + \dots \\ &= \sum_{k=0}^{\infty} \{\hat{R}_n\hat{Q}_n\hat{V}\}^k\,|n\rangle \\ &= (1 - \{\hat{R}_n\hat{Q}_n\hat{V}\})^{-1}\,|n\rangle \end{aligned} \tag{4.4}$$

When higher order term contributions are diminishingly small, truncating the series produces approximate solutions to the problem. However, in certain specialized problem settings, operator inverse in the above equation can be analytically obtained [9].

4.3 Comparison with Rayleigh-Schrodinger theory

Rayleigh-Schrodinger (RS) perturbation theory is a more popular perturbation theory and is used widely in practice. But, RS theory is not without its shortcomings. Unlike the RS theory, BW theory does not require separate treatment in the case degenerate spectrum. A thorough comparative study of RS and BW theory can be found in [9]. In fact, RS theory can be obtained as an approximation to BW theory by power series expansion of the resolvent operator [10]. A major problem with the BW theory is that Eq. (4.2) is an implicit equation in E_n and it must be solved in conjunction with Eq. (4.1). Solving this system of equations is usually tricky as compared to the simple perturbation terms obtained from RS theory.

4.4 Effective Hamiltonian

Recent efforts to extend the theory to many-body systems has led to systematization of BW theory in terms of model space and effective hamiltonian formalism. This new representation requires the introduction of a model space with respect to a set of reference states. Any complete set of orthonormal states of the hilbert space is chosen as a set of reference states. Usually, the set of eigenstates of the unperturbed hamiltonian $\hat{H}_0$ is chosen as a set of reference states. The hilbert space is partitioned into model space and orthogonal space, by choosing one state from the set of reference states as the model state [1].

Let $\mathrm{R} \equiv \{|\phi_n\rangle \dots\}$ is the set of reference states, $|\phi_0\rangle \in \mathrm{R}$ is the model state, then $P = |\phi_0\rangle \langle\phi_0|$ is the corresponding projection operator of the model space and $Q = 1 - P$ is the projection operator corresponding to orthogonal space. A state $|\psi\rangle$ in the hilbert space can be projected onto the model space using operator P, $|\phi\rangle = P|\psi\rangle$ and a wavefunction $|\phi\rangle$ in model space can be reconstructed in hilbert space using the wave operator Ω as $|\psi\rangle = \Omega|\phi\rangle$.

Some useful relationships between operators P, Q and Ω are

1. $P + Q = 1$ (by definition)
2. $P^2 = P$ and $Q^2 = Q$ (property of projection operators)
3. $PQ = QP = 0$ (using Property 1)
4. $\Omega^2|\phi\rangle = \Omega|\phi\rangle$ (by definition)
5. $\Omega P|\phi\rangle = \Omega|\phi\rangle$ and $P\Omega|\psi\rangle = P|\psi\rangle$ (by definition)

Provided the eigenvalue equation $\hat{H}|\psi\rangle = E|\psi\rangle$, then $|\phi\rangle = P|\psi\rangle$ satisfies the equation $\hat{H}_{eff}|\phi\rangle = E|\phi\rangle$, where

$$\hat{H}_{eff} = P\hat{H}\Omega P \tag{4.5}$$

[1] In this treatment, a single reference state is chosen as the model function. See [10] for multi-reference partitioning.

$$\begin{aligned}\hat{H}_{eff}\,|\phi\rangle &= P\hat{H}\Omega P\,|\phi\rangle \\ &= P\hat{H}\Omega PP\,|\psi\rangle \\ &= P\hat{H}\,|\psi\rangle \\ &= E\,P\,|\psi\rangle \\ &= E\,|\phi\rangle\end{aligned}$$

Therefore, the eigenvalues of the effective hamiltonian are equal to the eigenvalues of the original hamiltonian and the eigenfunctions of the original hamiltonian can be obtained by application of the wave operator Ω on the eigenfunctions of the effective hamiltonian $|\psi\rangle = \Omega\,|\phi\rangle$.

How do we obtain the wave operator Ω ? Operating Q on the eigenvalue equation,

$$\begin{aligned}Q\hat{H}\,|\psi\rangle &= E\,Q\,|\psi\rangle \\ Q\,|\psi\rangle &= \frac{Q\hat{H}}{E}\,|\psi\rangle\end{aligned}$$

Therefore,

$$\begin{aligned}|\psi\rangle &= (P+Q)\,|\psi\rangle \\ &= P\,|\psi\rangle + Q\,|\psi\rangle \\ &= P\,|\psi\rangle + \frac{Q\hat{H}}{E}\,|\psi\rangle \qquad (4.6) \\ P\,|\psi\rangle &= \left(1 - \frac{Q\hat{H}}{E}\right)|\psi\rangle \\ |\psi\rangle &= \left(1 - \frac{Q\hat{H}}{E}\right)^{-1} P^2\,|\psi\rangle \qquad (4.7)\end{aligned}$$

Eq. (4.6) has the familiar iterative form as Eq. (4.2) with the choice of $P = |n\rangle\,\langle n|$. From Eq. (4.7),

$$\Omega = \left(1 - \frac{Q\hat{H}}{E}\right)^{-1} P \qquad (4.8)$$

The inverse operation in the wave operator can be expanded to obtain the perturbative expansion.

Usually, the effective hamiltonian is parameterized by energy. To obtain the solutions, we must diagonalize the effective hamiltonian by treating E as a free parameter to obtain the eigenvalue expressions $E_i (i = 1 \ldots \dim(H))$, and solve the equations $E = E_i$ to obtain the numerical values of energy eigenvalues.

Above discussion is an abridged version of the theory of BW perturbation presented in [10].

Chapter 5

Floquet theory

Although Rayleigh-Schrodinger perturbation theory can be extended to time-dependent situations, it is not well suited for periodic systems as it relies on power-series expansions. Approximate solutions obtained from RS theory may not retain the periodic character - necessitated by physical conditions - at all perturbation orders [11]. A relatively new class of techniques based on the application of floquet theory have been developed to alleviate this problem. This approach effectively converts a time-dependent problem into a time-independent problem, which is much easier to tackle both analytically and numerically.

5.1 Statement

The time-dependent Schrodinger equation is

$$i\hbar\frac{\partial}{\partial t}\left|\psi(t)\right\rangle = \hat{H}\left|\psi(t)\right\rangle \tag{5.1}$$

We are interested in periodically driven systems, i.e., the hamiltonian satisfies

$$\hat{H}(t+T) = \hat{H}(t) \quad \forall t \tag{5.2}$$

where $T = \frac{2\pi}{\omega}$ is the time period of the driving. Floquet theory establishes the general form of the solution to such periodic linear differential equations.

Theorem 5.1.1 (Floquet Theorem)**.** A periodic linear differential equation

$$\frac{\partial \vec{x}}{\partial t} = \mathbf{A}(t)\vec{x} \qquad \forall t\ \mathbf{A}(t+T) = \mathbf{A}(t)$$

has solutions of the form

$$\vec{x} = e^{-i\mu t}\vec{p}(t) \quad \ni \quad \vec{p}(t+T) = \vec{p}(t)$$

Using floquet theory, solutions to Eq. (5.1) have the form

$$\left|\psi_\alpha(t)\right\rangle = e^{-i\epsilon_\alpha t}\left|\phi_\alpha(t)\right\rangle \tag{5.3}$$

$|\phi_\alpha(t)\rangle$ are periodic in time and they are called the *floquet modes*. ϵ_α are real parameters known as *quasienergies*, and they are analogous to quasimomentum k in bloch theory.

$$\begin{aligned}|\psi_\alpha(t+T)\rangle &= e^{-i\epsilon_\alpha(t+T)}\,|\phi_\alpha(t+T)\rangle \\ &= e^{-i\epsilon_\alpha T}e^{-i\epsilon_\alpha t}\,|\phi_\alpha(t)\rangle \\ &= e^{-i\epsilon_\alpha T}\,|\psi_\alpha(t)\rangle\end{aligned}$$

Three interesting properties can be inferred from the above snippet

1. ϵ_n is real. This is due to the fact that $|\psi_\alpha(t)\rangle$ is normalized to 1 at all times.
2. If $\hat{U}(t_2, t_1)$ is the time evolution operator, then

$$\hat{U}(t+T, t)\,|\psi_\alpha(t)\rangle = e^{-i\epsilon_\alpha T}\,|\psi_\alpha(t)\rangle \tag{5.4}$$

   Therefore, $|\psi_\alpha(t)\rangle$, also known as the *floquet states*, are the eigenvectors of the time evolution operator over one period. This also means that at any fixed time t, the floquet states form a complete orthonormal basis.

3. ϵ_α may be replaced by $\epsilon_\alpha + n\omega$ without affecting the above equations. We define $\epsilon_{\alpha n} = \epsilon_\alpha + n\omega$ and restrict $\epsilon_\alpha \in \left[\frac{-\omega}{2}, \frac{\omega}{2}\right)$, called the *Brillouin zone*.

The time evolution operator can be further simplified using the complete and orthonormal set of floquet states

$$\begin{aligned}\hat{U}(t_2, t_1) &= \sum_{\alpha_2} |\psi_{\alpha_2}(t_2)\rangle \langle\psi_{\alpha_2}(t_2)|\hat{U}(t_2, t_1) \sum_{\alpha_1} |\psi_{\alpha_1}(t_1)\rangle \langle\psi_{\alpha_1}(t_1)| \\ &= \sum_{\alpha_1,\alpha_2} |\psi_{\alpha_2}(t_2)\rangle \langle\psi_{\alpha_2}(t_2)|\psi_{\alpha_1}(t_2)\rangle \langle\psi_{\alpha_1}(t_1)| \\ &= \sum_{\alpha} e^{-i\epsilon_\alpha(t_2-t_1)}\,|\phi_\alpha(t_2)\rangle \langle\phi_\alpha(t_1)|\end{aligned} \tag{5.5}$$

This is a remarkable result as we can express any state $|\psi(t)\rangle$ as

$$|\psi(t)\rangle = \sum_{\alpha} \langle\phi_\alpha(t_0)|\psi(t_0)\rangle\, e^{-i\epsilon_\alpha(t-t_0)}\,|\phi_\alpha(t)\rangle \tag{5.6}$$

i.e., the contribution of each floquet state remains constant through as the state evolves in time.

5.2 Floquet Hamiltonian

The time evolution over one period is given by the *stroboscopic operator* $\hat{U}(t_0 + T, t_0)$. We know from elementary linear algebra that any unitary operator can be expressed in terms of exponential of a hermitian operator. The generator of stroboscopic evolution, identified by the relation

$$\exp\left(-iT\hat{H}^F_{t_0}\right) = \hat{U}(t_0 + T, t_0) \tag{5.7}$$

is known as the *Floquet Hamiltonian*. The floquet hamiltonian is time-independent, but parameterized by the initial time t_0. It is then obvious from Eq. (5.4) that,

$$\hat{H}^F_{t_0} = \sum_\alpha \epsilon_\alpha \left|\phi_\alpha(t_0)\right\rangle \left\langle\phi_\alpha(t_0)\right|$$

and subsequently

$$\hat{H}^F_{t_0} \left|\phi_\alpha(t_0)\right\rangle = \epsilon_\alpha \left|\phi_\alpha(t_0)\right\rangle \tag{5.8}$$

This eigenvalue equation proves the corollary of floquet theory stating that there exists a one-to-one mapping between the quasienergies and the floquet modes. This fact has been inherently assumed in our analysis up to this point, as the quasienergies and floquet modes were indexed by the same variable.

We can obtain an alternate definition of floquet hamiltonian also known as the *Quasienergy operator* by substitution of Eq. (5.3) in Eq. (5.1),

$$\left[\hat{H} - i\frac{\partial}{\partial t}\right] \left|\phi_\alpha\right\rangle = \epsilon_\alpha \left|\phi_\alpha\right\rangle \tag{5.9}$$

Therefore, we identify $\hat{H}^F_t$ as

$$\hat{H}^F_t = \left[\hat{H}(t) - i\frac{\partial}{\partial t}\right] \tag{5.10}$$

We also introduce the *micromotion operator*

$$\left|\phi_\alpha(t_2)\right\rangle = \hat{U}_F(t_2, t_1) \left|\phi_\alpha(t_1)\right\rangle \tag{5.11}$$

$$\hat{U}_F(t_2, t_1) = \sum_\alpha \left|\phi_\alpha(t_2)\right\rangle \left\langle\phi_\alpha(t_1)\right| \tag{5.12}$$

which describes the time evolution of periodic floquet modes.

Further, the time evolution operator from Eq. (5.5) can be written in terms of the floquet hamiltonian and the micromotion operator.

$$\hat{U}(t_2, t_1) = e^{-i(t_2-t_1)\hat{H}^F_{t_2}} \hat{U}_F(t_2, t_1) = \hat{U}_F(t_2, t_1) e^{-i(t_2-t_1)\hat{H}^F_{t_1}} = e^{i\hat{K}(t_2,t_1)} e^{-i(t_1-t_2)\hat{H}^F_{t_1}} \tag{5.13}$$

In the final expression, the micromotion operator (unitary operator) is expressed in terms of an exponential.

By diagonalizing the floquet hamiltonian, both quasienergies and the floquet modes can be determined. Floquet hamiltonian is amenable to analysis as it is time independent as opposed to the original time dependent hamiltonian. Unfortunately, our discussion to this point, does not provide a procedure to calculate the floquet hamiltonian without knowing the quasienergies and the floquet modes! A myriad of approximation schemes have been devised to obtain the floquet hamiltonian for high-frequency driving [12–16]. We shall only briefly discuss two such methods in the forthcoming sections.

5.3 Effective Hamiltonian

We have already noted that the floquet hamiltonian is parameterized by initial time. However, this idea of initial time is absurd in many situations. Instead, a static hamiltonian without reference to any initial time parameter may be defined without losing the physical interpretation of macromotion associated with the floquet hamiltonian [13, 14, 17].

To achieve this, we have to conceive of a unitary transformation $\hat{U}_F(t)$, such that

$$\hat{H}_F = \hat{U}_F(t)\hat{H}_t^F\hat{U}_F^\dagger(t) = \hat{U}_F(t)\hat{H}(t)\hat{U}_F^\dagger(t) - i\hat{U}_F(t)\frac{\partial}{\partial t}\hat{U}_F^\dagger(t) \tag{5.14}$$

is time independent [14, 17]. $\hat{H}_F$ is known as the effective hamiltonian. Under this unitary transformation, quite obviously the floquet modes would transform to

$$|\phi_\alpha^F\rangle = \hat{U}_F(t)\,|\phi_\alpha(t)\rangle \tag{5.15}$$

$|\phi_\alpha^F\rangle$s are time independent as they are the eigenfunctions of static $\hat{H}_F$. The micromotion operator written in terms of the unitary transformation is

$$\begin{aligned}\hat{U}_F(t_2,t_1) &= \sum_\alpha |\phi_\alpha(t_2)\rangle\langle\phi_\alpha(t_1)| \\ &= \sum_\alpha \hat{U}_F^\dagger(t_2)\,|\phi_\alpha^F\rangle\langle\phi_\alpha^F|\,\hat{U}_F(t_1) \\ &= \hat{U}_F^\dagger(t_2)\left(\sum_\alpha |\phi_\alpha^F\rangle\langle\phi_\alpha^F|\right)\hat{U}_F(t_1) \\ &= \hat{U}_F^\dagger(t_2)\hat{U}_F(t_1)\end{aligned} \tag{5.16}$$

In the time-independent gauge, time evolution is simply $e^{-i\hat{H}_F(t_2-t_1)}$. To propagate any state in the time-independent gauge, it has to be transformed to time-independent gauge first. The propagated state must then be transformed back to the time-dependent gauge. This means that the time-evolution operator is

$$\hat{U}(t_2,t_1) = \hat{U}_F^\dagger(t_2)e^{-i\hat{H}_F(t_2-t_1)}\hat{U}_F(t_1) \tag{5.17}$$

Further, we enforce a periodicity constraint $\hat{U}_F(t) = \hat{U}_F(t+T)$. It is conventional to represent the operator $\hat{U}_F(t)$ as $e^{i\hat{K}(t)}$ and call $\hat{K}(t)$ as the kick operator. To obtain the expressions for $\hat{H}_F$ and $\hat{H}_F$, we expand them perturbatively under the high-frequency limit.

$$\hat{H}(t) = \hat{H}_{(0)} + \sum_{j=1}^{\infty}\hat{H}_{(j)}e^{ij\omega t} + \hat{H}_{(-j)}e^{-ij\omega t} \tag{5.18}$$

$$\hat{H}_F(t) = \sum_{j=0}^{\infty}\frac{1}{\omega^j}\hat{H}_F^{(j)} \tag{5.19}$$

$$\hat{K}(t) = \sum_{j=0}^{\infty}\frac{1}{\omega^j}\hat{K}^{(j)} \tag{5.20}$$

With this ansatz, on equating terms of the same order on both sides of Eq. (5.14), the effective hamiltonian is determined up to a suitable order of $\frac{1}{\omega^n}$ [13].

5.4 Brillouin-Wigner perturbative expansion of Floquet Hamiltonian

We shall exploit the periodicity of the problem and conveniently write the Schrodinger equation in terms of fourier components. Let $\{|\alpha\rangle, \dots\}$ be a complete orthonormal set of basis states. The components of the hamiltonian are written in this basis as $H_{\alpha\beta} = \langle\alpha|\hat{H}|\beta\rangle$. From results discussed in previous sections, we know that the time-dependent Schrodinger equation has $n = rank(\hat{H})$ linearly independent solutions - one corresponding to each of the quasienergies in the Brillouin zone. We define the fundamental matrix of Schrodinger equation as a matrix constructed by concatenating n eigenvectors as the columns of a $n \times n$ matrix.

$$\mathbf{\Psi}(t) = \left[\left[|\psi_1\rangle\right]\left[|\psi_2\rangle\right]\dots\left[|\psi_n\rangle\right]\right]$$

The result of Floquet theory can be expressed in this notation as

$$\mathbf{\Psi}(t) = \mathbf{\Phi}(t)e^{-i\boldsymbol{\epsilon}t} \tag{5.21}$$

$$i\frac{\partial}{\partial t}\mathbf{\Psi}(t) = \mathbf{H}(t)\mathbf{\Psi}(t) \tag{5.22}$$

$$\Psi_{\alpha\beta}(t) = \langle\alpha|\psi_\beta(t)\rangle \tag{5.23}$$

$$\epsilon_{\alpha\beta} = \epsilon_\alpha\delta_{\alpha\beta} \tag{5.24}$$

$$\Phi_{\alpha\beta}(t) = \langle\alpha|\phi_\beta(t)\rangle \tag{5.25}$$

where $\boldsymbol{\epsilon}$ is a constant real diagonal matrix and $\mathbf{\Phi}(t+T) = \mathbf{\Phi}(t)$.

Expanding $\mathbf{H}(t)$ and $\mathbf{\Phi}(t)$ in fourier series

$$\mathbf{H}(t) = \sum_n \tilde{\mathbf{H}}_n e^{in\omega t} \tag{5.26}$$

$$\tilde{\mathbf{H}}_n = \frac{1}{T}\int_0^T \mathbf{H}(t)e^{-in\omega t}dt \tag{5.27}$$

$$H_{\alpha\beta}(t) = \sum_n \tilde{H}_{n,\alpha\beta}e^{in\omega t} \tag{5.28}$$

$$\mathbf{\Phi}(t) = \sum_n \tilde{\mathbf{\Phi}}_n e^{in\omega t} \tag{5.29}$$

$$\tilde{\mathbf{\Phi}}_n = \frac{1}{T}\int_0^T \mathbf{\Phi}(t)e^{-in\omega t}dt \tag{5.30}$$

$$\Phi_{\alpha\beta}(t) = \sum_n \tilde{\Phi}_{n,\alpha\beta}e^{in\omega t} \tag{5.31}$$

Subsequently,

$$\begin{aligned}\Psi_{\alpha\beta}(t) &= \sum_\gamma \left(\sum_n \tilde{\Phi}_{n,\alpha\gamma}e^{in\omega t}\right)\delta_{\gamma\beta}e^{-i\epsilon_\beta t} \\ &= \sum_n \tilde{\Phi}_{n,\alpha\beta}e^{in\omega t}e^{-i\epsilon_\beta t}\end{aligned} \tag{5.32}$$

Inserting these expansions into the Schrodinger equation

$$\begin{aligned} i\frac{\partial}{\partial t}\Psi_{\alpha\beta}(t) &= i\frac{\partial}{\partial t}\left(\sum_n \tilde{\Phi}_{n,\alpha\beta}e^{in\omega t}e^{-i\epsilon_\beta t}\right) \\ &= i\sum_n \tilde{\Phi}_{n,\alpha\beta}e^{in\omega t}e^{-i\epsilon_\beta t}(in\omega - i\epsilon_\beta) \\ &= \sum_n \tilde{\Phi}_{n,\alpha\beta}e^{in\omega t}e^{-i\epsilon_\beta t}(\epsilon_\beta - n\omega) \\ (H\Phi)_{\alpha\beta}(t) &= \sum_\gamma \left(\sum_r \tilde{H}_{r,\alpha\gamma}e^{ir\omega t}\sum_s \tilde{\Phi}_{s,\gamma\beta}e^{is\omega t}e^{-i\epsilon_\beta t}\right) \\ &= \sum_\gamma\sum_r\sum_s \tilde{H}_{r,\alpha\gamma}\tilde{\Phi}_{s,\gamma\beta}e^{i(r+s)\omega t}e^{-i\epsilon_\beta t} \end{aligned}$$

making change of variable $n = r + s$

$$\begin{aligned} &= \sum_\gamma\sum_n\sum_s \tilde{H}_{n-s,\alpha\gamma}\tilde{\Phi}_{s,\gamma\beta}e^{in\omega t}e^{-i\epsilon_\beta t} \\ &= \sum_n \left(\sum_\gamma\sum_s \tilde{H}_{n-s,\alpha\gamma}\tilde{\Phi}_{s,\gamma\beta}\right)e^{in\omega t}e^{-i\epsilon_\beta t} \end{aligned}$$

Rearranging terms

$$\sum_n\sum_\gamma\sum_s [\tilde{H}_{n-s,\alpha\gamma} + n\omega\delta_{\alpha\gamma}\delta_{ns}]\tilde{\Phi}_{s,\gamma\beta}e^{in\omega t}e^{-i\epsilon_\beta t} = \sum_n \epsilon_\beta\tilde{\Phi}_{n,\alpha\beta}e^{-i\epsilon_\beta t}$$

Matching coefficients of the $e^{in\omega t}$, we obtain

$$\sum_{\gamma,s} [\tilde{H}_{n-s,\alpha\gamma} + n\omega\delta_{\alpha\gamma}\delta_{ns}]\tilde{\Phi}_{s,\gamma\beta} = \epsilon_\beta\tilde{\Phi}_{n,\alpha\beta} \tag{5.33}$$

The above equation is an eigenvalue written the *Sambe space* [14, 18, 19], in a basis constituting states from the direct product of hilbert space $\mathcal{H}$ and the $\mathcal{L}_T$ space of square integrable periodic functions with time period T. The fourier basis forms a complete and orthonormal set of basis states for $\mathcal{L}_T$. We identify the basis states as $|\alpha n(t)\rangle = |\alpha\rangle\, e^{in\omega t}$. Two indices or a 2-tuple (α, n) are/is required to identify the basis states uniquely. In this notation, we represent

$$\tilde{H}^F_{(\alpha,n),(\gamma,s)} = \tilde{H}_{n-s,\alpha\gamma} + n\omega\delta_{\alpha\gamma}\delta_{ns} \tag{5.34}$$

Then, the eigenvalue equation for above is written as

$$\sum_{(\gamma,s)} \tilde{H}^F_{(\alpha,n),(\gamma,s)}\tilde{\Phi}_{(\gamma,s),\beta} = \epsilon_\beta\tilde{\Phi}_{(\alpha,n),\beta} \tag{5.35}$$

Note that, $\tilde{\Phi}_\beta$ is an eigenvector associated with eigenvalue ϵ_β. It is not too surprising to see that $\tilde{H}^F$ is actually the floquet hamiltonian written in terms of fourier components. One major difference is that, it is now infinite dimensional, and it allows for all quasienergies extending beyond the brillouin zone [14, 19]. Another straight forward observation is, if $\tilde{\Phi}_{(\alpha,n),\beta}$ are the components of the eigenvector corresponding to ϵ_β, then the components

of the eigenvector corresponding to $\epsilon_\beta + m\omega$ are $\tilde{\Phi}_{(\alpha,n+m),\beta}$. This is established by the following steps

$$\hat{H}_F |\phi\rangle = \epsilon |\phi\rangle$$
$$\hat{H}_F e^{im\omega t} |\phi\rangle = (\epsilon + m\omega) e^{im\omega t} |\phi\rangle$$

Refer to [14] for techniques on how to diagonalize or block-diagonalize the floquet hamiltonian. Block diagonalizing the floquet hamiltonian is equivalent to calculating the effective hamiltonian, as $\tilde{\mathbf{H}}_{n-s} = \frac{1}{T}\int_0^T \hat{H}(t) e^{-i(n-s)\omega t}$ is non-zero only when $n = s$, because, $\hat{H}$ under the unitary transformation, is static in time.

Next step in our discourse is to apply Brillouin-Wigner perturation theory (See Chapter 4) to diagonalize the floquet hamiltonian. This is a very recent technique developed by Mikami et al. in [15]. We begin with the floquet eigenvalue equation, written in matrix form [1]

$$(\mathcal{H} - \mathcal{M}\omega) |\phi_\alpha\rangle = \epsilon_\alpha |\phi_\alpha\rangle \tag{5.36}$$
$$\mathcal{H}_{mn} = \frac{1}{T}\int_0^T \hat{H}(t) e^{i(m-n)\omega t} dt \tag{5.37}$$
$$\mathcal{M}_{mn} = m\delta_{mn} \tag{5.38}$$

Partitioning is done with the choice of $\mathcal{P}_{mn} = \delta_{mn}\delta_{m0}$, which essentially maps the eigenfunctions into a space devoid of the micromotion information. As a result, $\mathcal{Q}_{mn} = 1 - \mathcal{P}_{mn} = \delta_{mn}(1-\delta_{m0})$, $(\mathcal{PM})_{mn} = k\delta_{mk}\delta_{m0}\delta_{kn} = 0$ and $(\mathcal{QM})_{mn} = k\delta_{mk}(1-\delta_{m0})\delta_{kn} = m\delta_{mk}\delta_{kn}(1-\delta_{k0}) = (\mathcal{MQ})_{mn}$. The Brillouin-wigner effective hamiltonian is defined as

$$H_{eff} = \mathcal{P}(\mathcal{H} - \mathcal{M}\omega)\Omega\mathcal{P} \tag{5.39}$$

We determine the Ω wave operator as follows

$$\begin{aligned}
\mathcal{Q}(\mathcal{H} - \mathcal{M}\omega) |\phi_\alpha\rangle &= \epsilon_\alpha \mathcal{Q} |\phi_\alpha\rangle \\
\mathcal{QH} |\phi_\alpha\rangle &= \mathcal{QM}\omega |\phi_\alpha\rangle + \epsilon_\alpha \mathcal{Q} |\phi_\alpha\rangle \\
\mathcal{QH} |\phi_\alpha\rangle &= \mathcal{M}\omega\mathcal{Q} |\phi_\alpha\rangle + \epsilon_\alpha \mathcal{Q} |\phi_\alpha\rangle \\
(\epsilon_\alpha + \mathcal{M}\omega)\mathcal{Q} |\phi_\alpha\rangle &= \mathcal{QH} |\phi_\alpha\rangle \\
\mathcal{Q} |\phi_\alpha\rangle &= \frac{\mathcal{Q}}{\epsilon_\alpha + \mathcal{M}\omega}\mathcal{H} |\phi_\alpha\rangle
\end{aligned} \tag{5.40}$$

$$\tag{5.41}$$

$$\begin{aligned}
|\phi_\alpha\rangle &= \mathcal{P} |\phi_\alpha\rangle + \mathcal{Q} |\phi_\alpha\rangle \\
&= \mathcal{P} |\phi_\alpha\rangle + \frac{\mathcal{Q}}{\epsilon_\alpha + \mathcal{M}\omega}\mathcal{H} |\phi_\alpha\rangle \\
\mathcal{P} |\phi_\alpha\rangle &= |\phi_\alpha\rangle - \frac{\mathcal{Q}}{\epsilon_\alpha + \mathcal{M}\omega}\mathcal{H} |\phi_\alpha\rangle \\
|\phi_\alpha\rangle &= \left(1 - \frac{\mathcal{Q}}{\epsilon_\alpha + \mathcal{M}\omega}\mathcal{H}\right)^{-1} \mathcal{P} |\phi_\alpha\rangle
\end{aligned} \tag{5.42}$$

[1] In this analysis, the definition of $|m(t)\rangle$ is inverted to $e^{-im\omega t}$ to match the notation used by the original authors [15].

We recognize the wave operator from the above expression as

$$\Omega(\epsilon) = \left(1 - \frac{\mathcal{Q}}{\epsilon + \mathcal{M}\omega}\mathcal{H}\right)^{-1} \tag{5.43}$$

and consequently the effective hamiltonian as

$$\begin{aligned} H_{eff}(\epsilon) &= \mathcal{P}(\mathcal{H} - \mathcal{M}\omega)\left(1 - \frac{\mathcal{Q}}{\epsilon + \mathcal{M}\omega}\mathcal{H}\right)^{-1}\mathcal{P} \\ &= \mathcal{P}\mathcal{H}\left(1 - \frac{\mathcal{Q}}{\epsilon + \mathcal{M}\omega}\mathcal{H}\right)^{-1}\mathcal{P} - \omega\mathcal{P}\mathcal{M}\left(1 - \frac{\mathcal{Q}}{\epsilon + \mathcal{M}\omega}\mathcal{H}\right)^{-1}\mathcal{P} \\ &= \mathcal{P}\mathcal{H}\left(1 - \frac{\mathcal{Q}}{\epsilon + \mathcal{M}\omega}\mathcal{H}\right)^{-1}\mathcal{P} \end{aligned} \tag{5.44}$$

We look to extend this theory by defining an ϵ-independent effective hamiltonian.

$$\begin{aligned} \Omega(\epsilon) = \Omega(\epsilon)\mathcal{P} &= \left(1 - \frac{\mathcal{Q}}{\epsilon + \mathcal{M}\omega}\mathcal{H}\right)^{-1}\mathcal{P} \\ \left(1 - \frac{\mathcal{Q}}{\epsilon + \mathcal{M}\omega}\mathcal{H}\right)\Omega(\epsilon) &= \mathcal{P} \\ \Omega(\epsilon) - \frac{\mathcal{Q}}{\epsilon + \mathcal{M}\omega}\mathcal{H}\Omega(\epsilon) &= \mathcal{P} \\ (\epsilon + \mathcal{M}\omega)\Omega(\epsilon) - \mathcal{Q}\mathcal{H}\Omega(\epsilon) &= \epsilon\mathcal{P} + \mathcal{M}\omega\mathcal{P} \\ \Omega(\epsilon)\epsilon - \mathcal{P}\epsilon + \mathcal{M}\omega\Omega(\epsilon) - \mathcal{Q}\mathcal{H}\Omega(\epsilon) &= \mathcal{M}\omega\mathcal{P} \\ \Omega(\epsilon)\epsilon - \mathcal{P}\Omega(\epsilon)\epsilon + \mathcal{M}\omega\Omega(\epsilon) - \mathcal{Q}\mathcal{H}\Omega(\epsilon) &= \mathcal{M}\omega\mathcal{P} \\ (1 - \mathcal{P})\Omega(\epsilon)\epsilon + \mathcal{M}\omega\Omega(\epsilon) - \mathcal{Q}\mathcal{H}\Omega(\epsilon) &= \mathcal{M}\omega\mathcal{P} \\ \mathcal{Q}\Omega(\epsilon)\epsilon + \mathcal{M}\omega\Omega(\epsilon) - \mathcal{Q}\mathcal{H}\Omega(\epsilon) &= \mathcal{M}\omega\mathcal{P} \\ \mathcal{M}\omega\mathcal{P} + \mathcal{Q}\mathcal{H}\Omega(\epsilon) - \mathcal{Q}\Omega(\epsilon)\epsilon &= \mathcal{M}\omega\Omega(\epsilon) \end{aligned}$$

$$\Omega(\epsilon) = \mathcal{P} + \frac{\mathcal{Q}}{\mathcal{M}\omega}\mathcal{H}\Omega(\epsilon) - \frac{\mathcal{Q}}{\mathcal{M}\omega}\Omega(\epsilon)\epsilon \tag{5.45}$$

We can replace the ϵ in the above equation with H_{eff}.

$$\Omega(\epsilon) = \mathcal{P} + \frac{\mathcal{Q}}{\mathcal{M}\omega}\mathcal{H}\Omega(\epsilon) - \frac{\mathcal{Q}}{\mathcal{M}\omega}\Omega(\epsilon)\mathcal{P}\mathcal{H}\Omega(\epsilon)\mathcal{P}$$

We omit the $\mathcal{P}$ in the last term, as it Ω is anyway acted on $\mathcal{P}\left|\phi_\alpha\right\rangle$.

ϵ independent wave operator is defined by the recursive relation

$$\Omega(\epsilon) = \mathcal{P} + \frac{\mathcal{Q}}{\mathcal{M}\omega}\mathcal{H}\Omega(\epsilon) - \frac{\mathcal{Q}}{\mathcal{M}\omega}\Omega(\epsilon)\mathcal{P}\mathcal{H}\Omega(\epsilon) \tag{5.46}$$

and the ϵ independent effective hamiltonian is obtained from the solution Ω_{BW}, of the preceding equation.

$$H_{BW} = \mathcal{P}\mathcal{H}\Omega_{BW}\mathcal{P} \tag{5.47}$$

Ω_{BW} is obtained by substitution of the $1/\omega$ series,

$$\Omega_{BW} = \sum_{N=0}^{\infty} \Omega_{BW}^{(N)}$$

where $\Omega_{BW}^{(N)}$ corresponds to order $1/\omega^N$ coefficient in the iterative solution to Ω_{BW}. Similarly, the effective hamiltonian is also expanded in a series

$$H_{BW} = \sum_{N=0}^{\infty} H_{BW}^{(N)}$$

and $H_{BW}^{(N)} = \mathcal{P}\mathcal{H}\Omega_{BW}^{(N)}\mathcal{P}$. Expansion up to 4th order can be found in [15].

Under the limit $\omega \to \infty$, the operators tend to their $0th$ order terms, $\Omega_{BW} \to \mathcal{P}$ and $H_{BW} \to H_{0,0}$. This guarantees that the eigenvalues of H_{BW} are in the first brillouin zone, as the contributions from higher order terms in the series is very small to transport the eigenvalues to the next brillouin zone.

The wave operator obtained from the above discussion was written in terms of the fourier components. Using fourier series, we can go back to time domain and express our wavefunctions as a function of time. This operator is defined as

$$\Xi(t) = \sum_{n\in\mathbb{Z}} e^{-in\omega t}[\Omega_{BW}]_{n,0} \tag{5.48}$$

and

$$|\psi_\alpha(t)\rangle = e^{-i\epsilon_\alpha t}\Xi(t)\,|\phi_\alpha^0\rangle \tag{5.49}$$

A nuanced discussion of this theory and its connections to other approximation techniques based on the floquet theory can be found in [15].

Appendices

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