Driven Aubry-André-Harper systems

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Abstract

Investigation of variants of Aubry-André-Harper systems driven by electromagnetic fields in the high frequency limit. A time-independent effective Hamiltonian is obtained for the models using Floquet theory. The spectrum of the variant models is shown to retain the Hofstadter butterfly structure - a characteristic property of the pure Aubry-André-Harper model. The driven models are probed for topological phase transitions - indicators of drastic change in Hall conductivity. The localization-delocalization transition exhibted by Aubry-André-Harper like models is also obtained.

Acknowledgements

Hello, here is some text without a meaning. This text should show what a printed text will look like at this place. If you read this text, you will get no information. Really? Is there no information? Is there a difference between this text and some nonsense like "Huardest gefburn"? Kjift – not at all! A blind text like this gives you information about the selected font, how the letters are written and an impression of the look. This text should contain all letters of the alphabet and it should be written in of the original language. There is no need for special content, but the length of words should match the language.

Declaration

I, Rajath Shashidhara, declare that this thesis titled, 'Driven Aubry-André-Harper systems' and the work presented in it is my original work. I affirm that all references are clearly cited and any collaboration with others has been duly acknowledged.

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Certificate

This is to certify that the thesis titled, 'Driven Aubry-André-Harper systems' 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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Contents

Chapter 1

Introduction

Part I

Background

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

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

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

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

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

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

$\gamma_n(C)$ 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 $\langle n(t)|n(t)\rangle = 1$.

$$\langle n(t)|n(t)\rangle = 1$$

$$\left[\frac{\partial}{\partial t} \langle n(t)| \right] |n(t)\rangle + \langle n(t)| \left[\frac{\partial}{\partial t} |n(t)\rangle \right] = 0$$

$$\langle n(t)| \left[\frac{\partial}{\partial t} |n(t)\rangle \right] = -\left(\langle n(t)| \left[\frac{\partial}{\partial t} |n(t)\rangle \right] \right)^*$$

$\theta_n(T)$ 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

$$\gamma_n(C) = i \oint_C \langle n(\mathbf{R})|\boldsymbol{\nabla}_{\mathbf{R}}|n(\mathbf{R})\rangle \cdot d\mathbf{R}$$

$$= i \int_S \boldsymbol{\nabla}_{\mathbf{R}} \wedge \langle n(\mathbf{R})|\boldsymbol{\nabla}_{\mathbf{R}}|n(\mathbf{R})\rangle \cdot d\mathbf{S} \tag{2.9}$$

$$= i \int_S (\boldsymbol{\nabla}_{\mathbf{R}} \langle n(\mathbf{R})|) \wedge \boldsymbol{\nabla}_{\mathbf{R}} |n(\mathbf{R})\rangle \cdot d\mathbf{S}$$

$$= i \int_S \sum_{m \neq n} \frac{\langle n(\mathbf{R})|\boldsymbol{\nabla}_{\mathbf{R}}\hat{H}(\mathbf{R})|m(\mathbf{R})\rangle \wedge \langle m(\mathbf{R})|\boldsymbol{\nabla}_{\mathbf{R}}\hat{H}(\mathbf{R})|n(\mathbf{R})\rangle}{(E_n(\mathbf{R}) - E_m(\mathbf{R}))^2} \cdot d\mathbf{S} \tag{2.10}$$

Eq. (2.10) has a remarkable property of being gauge independent. Any transformation of the form $|n(\mathbf{R})\rangle \rightarrow e^{i\delta(\mathbf{R})} |n(\mathbf{R})\rangle$, 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 $|n(\mathbf{R})\rangle \rightarrow e^{i\delta(\mathbf{R})} |n(\mathbf{R})\rangle$, then the berry connection transforms as $\mathbf{A}_n(\mathbf{R}) \rightarrow \mathbf{A}_n(\mathbf{R}) - \boldsymbol{\nabla}_{\boldsymbol{R}}\delta(\mathbf{R})$, 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.

To each point in the parameter space, we associate a 1-dimensional complex vector space (spanned by all gauge choices of the eigenstate at that point). We call the parameter space a vector bundle for this reason. When we try to compare vectors from vector spaces associated with two different points in the parameter space, we need to use the Berry connection (akin to Levi-Cevita connection/ Christoffel symbols in General relativity). 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

$$e^{i\Delta\gamma} = \frac{\langle n(\mathbf{R})|n(\mathbf{R} + \delta\mathbf{R})\rangle}{|\langle n(\mathbf{R})|n(\mathbf{R} + \delta\mathbf{R})\rangle|} \tag{2.15}$$

$$\approx \frac{\langle n(\mathbf{R})| \ [|n(\mathbf{R})\rangle + \nabla_{\mathbf{R}}|n(\mathbf{R})\rangle \cdot \delta\mathbf{R} + \ldots]}{|\langle n(\mathbf{R})|n(\mathbf{R} + \delta\mathbf{R})\rangle|}$$

$$1 + i\Delta\gamma + \ldots \approx \frac{1 + \langle n(\mathbf{R})|\nabla_{\mathbf{R}}|n(\mathbf{R})\rangle \cdot \delta\mathbf{R} + \ldots}{|\langle n(\mathbf{R})|n(\mathbf{R} + \delta\mathbf{R})\rangle|}$$

$$\Delta\gamma \approx -i \langle n(\mathbf{R})|\nabla_{\mathbf{R}}|n(\mathbf{R})\rangle \cdot \delta\mathbf{R} \tag{2.16}$$

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

$$\gamma(C) = \oint_C \mathbf{A}_n(\mathbf{R}) \cdot \delta\mathbf{R} = -\oint_C \arg(\langle n(\mathbf{R})|n(\mathbf{R} + \delta\mathbf{R})\rangle)$$

$$= -\lim_{N\to\infty} \arg(\prod_{j=0}^{N-1} \langle n(\mathbf{R}(t + j\Delta t))|n(\mathbf{R}(t + (j + 1)\Delta t))\rangle) \tag{2.17}$$

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

$$\oint_Q \mathbf{A}_n(\boldsymbol{\lambda}) \cdot \delta\boldsymbol{\lambda} =$$

$$- \arg(\langle n(\boldsymbol{\lambda})|n(\boldsymbol{\lambda} + \delta\lambda_x\hat{\mathbf{x}})\rangle \langle n(\boldsymbol{\lambda} + \delta\lambda_x\hat{\mathbf{x}})|n(\boldsymbol{\lambda} + \delta\lambda_x\hat{\mathbf{x}} + \delta\lambda_y\hat{\mathbf{y}})\rangle$$

$$\langle n(\boldsymbol{\lambda} + \delta\lambda_x\hat{\mathbf{x}} + \delta\lambda_y\hat{\mathbf{y}})|n(\boldsymbol{\lambda} + \delta\lambda_y\hat{\mathbf{y}})\rangle \langle n(\boldsymbol{\lambda} + \delta\lambda_y\hat{\mathbf{y}})|n(\boldsymbol{\lambda})\rangle)$$

Using stokes theorem

$$\oint_Q \mathbf{A}_n(\boldsymbol{\lambda}) \cdot \delta\boldsymbol{\lambda} = \int_Q \mathbf{B}_n(\boldsymbol{\lambda}) \cdot d\mathbf{S}_{\boldsymbol{\lambda}}$$

$$= \mathbf{B}_n(\boldsymbol{\lambda})\delta\lambda_x\delta\lambda_y$$

Combining these two results, we infer that[8]

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

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

In the derivation of Berry's phase, we assumed that there is/are no degeneracy or level crossings in the spectrum. In this section, we shall lift this restriction and examine its consequences. If we assume that the ground state is N fold degenerate, and begin in one of the degenerate states, after varying the parameters in closed loop, we examine the effect of this evolution on the state in the adiabatic limit [5]. Unlike the previous discussion, the state can land up in a linear combination of the N-degenerate states.

The treatment of such systems require us to generalize the definition of a berry connection to

$$
(A_i)_{ab}(\mathbf{R}) = i \langle n_b | \frac{\partial}{\partial R_i} | n_a \rangle \quad (2.19)
$$

where $|n_a\rangle$ such that $a = 1 \ldots N$, are the degenerate eigenstates of the hamiltonian. Notice that $\mathbf{A}$ is a d-dimensional (parameter space dimensions) vector of which each individual component is a $N \times N$ matrix. Non-abelian Berry curvature is defined as

$$
F_{ij} = \frac{\partial A_i}{\partial R_j} - \frac{\partial A_j}{\partial R_i} - i[A_i, A_j] \quad (2.20)
$$

However, the Berry curvature is not a gauge invariant quantity. Instead, $tr(F_{ij})$ is gauge invariant.

As $\mathbf{A}$'s at different points in parameter space may not commute, we require the use of Path ordering operator (similar to Dyson series) to write the geometric phase as the integral of the berry connection

$$
U = \mathcal{P} \exp \left(\oint A_i dR_i \right) \quad (2.21)
$$

where

$$
|\psi_a\rangle (t) = U_{ab}(t) |n_b\rangle (t) \quad (2.22)
$$

We began with $|\psi_a(0)\rangle = |n_a(0)\rangle$.

2.4 Chern numbers

An important theorem of differential geometry, called the Gauss-Bonnet theorem states that the surface integral of Gaussian curvature over a closed surface is 2π times the

Euler characteristic of the surface [8, 9]. Euler characteristic of a polyhedra is defined as $\chi = V - E + F$, where V is the number of vertices, E is the number of edges and F is the number of faces. The Euler characteristic for a continuous surface can be obtained by triangulation of the surface. The Euler characteristic of a closed surface is equal to $2(1-g)$, g is the genus of the surface or intuitively the number of holes in the surface. Two surfaces that are continuously deformable into each other have the same genus. Therefore, χ for a closed surface is an integral topological invariant and from Gauss-Bonnet theorem, the integral of the curvature over a closed surface is an integral multiple of 2π.

$$\iint_S \mathbf{F}.d\mathbf{S} = 2\pi\chi(S) = 4\pi(1 - g(S)) = 2\pi C \tag{2.23}$$

The Berry curvature satisfies the Gauss-Bonnet theorem, thereby the surface integral over a closed parameter space is an integral multiple of 2π. The integers are called the Chern numbers of the first class[7]. We shall see that the geometric phase and the chern numbers are closely related to hall conductivity in Chapter 3.

Chapter 3

Quantum Hall Effect

It was observed in two-dimensional materials placed in strong magnetic fields, the hall conductivity is quantized[1] [12–14]. The striking feature is that the quantization is robust to disorder and independent of material or its geometry. Classical conduction theories such as the Drude's model failed to explain this strange phenomenon.

Eventually, the Landau problem that describes the cyclotron motion of electrons restricted to 2-dimensional plane in the presence of magnetic field was connected with the Quantum hall effect. The energy levels in the Landau problem are quantized, called the Landau levels, each level is degenerate by roughly the magnitude of magnetic flux (magnetic field times the area) passing through the sample. The quantization of hall conductance was linked to the filling fraction of the landau levels. Although this was successful in explaining the magnitude of hall conductance, it failed to explain the robustness of the phenomenon. The idea of edge states and the role of disorder was incorporated into heuristic explanations to explain the plateaus of hall conductance, based on localization of states in the presence of disorder. However, if only a fraction of all states are localized, and only the localized states contribute to conduction, the value of hall conduction as explained by the filling fraction of landau levels assuming each state contributed equally to conduction, is in direct contradiction to the idea of localized states. This puzzle was finally cracked by Laughlin using the idea of gauge invariance of electromagnetism and the concept of spectral flow [11, 12, 15–17].

The breakthrough result was established by Thouless et al., as they demonstrated that hall conductivity is indeed a topological invariant which is an integral quantity[2] [7, 18, 19]. The topology of the hilbert space parameterized by the crystal momentum of the lattice, manifests as the hall conductance of the material. This explanation supplanted all the previous theories, unveiled the deeper topological links to conduction and launched a whole branch of physics called topological insulators. We shall study techniques in this thesis to calculate the topological invariant and identify topological phase transitions in quantum systems.

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[1]Knowledge of Classical Hall effect is assumed in this discussion. [10–12] contain excellent review of the subject

[2]This work was awarded the Nobel prize in 2016 - incidentally the period during which this document was compiled

3.1 Brillouin zone as the parameter space

Consider a particle moving on a rectangular lattice. By application of bloch theorem, the wavefunction can be factorized as

$$|\psi_{\mathbf{k}}(\mathbf{x})\rangle = e^{i\mathbf{x}\cdot\mathbf{x}}|u_{\mathbf{k}}(\mathbf{x})\rangle$$

such that $|u_{\mathbf{k}}(\mathbf{x})\rangle = |u_{\mathbf{k}}(\mathbf{x}+\mathbf{R})\rangle$ where $\mathbf{R}$ is a lattice translation vector. The crystal momentum $\mathbf{k}$ is bounded in the first Brillouin zone[3]

$$\frac{-\pi}{a} < k_x \leq \frac{\pi}{a} \text{ and } \frac{-\pi}{b} < k_y \leq \frac{\pi}{b}$$

The Hamiltonian $\hat{H}(\mathbf{k})$ is also parametrized by the crystal momentum. The Brillouin zone is a torus $\mathbf{T}^2$ and by changing the parameters k_x and k_y, we can apply the idea of Berry described in the previous chapter.

3.2 Kubo formula for conductivity

We shall use the Brillouin zone as the arena and calculate the transverse electrical conductivity on a 2D rectangular lattice. Bands are labelled by α and the crystal momentum by $\mathbf{k}$. The linear response of current in the transverse direction to the applied electric field was derived by Kubo [11, 18–21]. Kubo's result is a relationship like Ohm's law, the electric field (stimulus) and the current density (response) are correlated linearly as[4]

$$J_x = \sigma_{xy} E_y \tag{3.1}$$

$$\sigma_{xy} = i\hbar \sum_{\alpha,\beta|E_\alpha < E_F < E_\beta} \int_{\mathbf{T}^2} \frac{d^2k}{(2\pi)^2} \frac{\langle u_k^\alpha|J_y|u_k^\beta\rangle \langle u_k^\beta|J_x|u_k^\alpha\rangle - \langle u_k^\alpha|J_x|u_k^\beta\rangle \langle u_k^\beta|J_y|u_k^\alpha\rangle}{(E_\beta(\mathbf{k}) - E_\alpha(\mathbf{k}))^2} \tag{3.2}$$

E_F is the Fermi energy.

3.3 TKNN Invariant

Thouless et al. in their seminal paper, using the Kubo formula for electric conductivity, showed that the hall conductivity of landau level problem on a lattice is a topological property and it is quantized.

The kubo formula can be recast into this form [11, 19]

$$\sigma_{xy} = \frac{ie^2}{\hbar} \sum_{\alpha|E_\alpha < E_F} \int_{\mathbf{T}^2} \frac{d^2k}{(2\pi)^2} \langle \partial_y u_{\mathbf{k}}^\alpha|\partial_x u_{\mathbf{k}}^\alpha\rangle - \langle \partial_x u_{\mathbf{k}}^\alpha|\partial_y u_{\mathbf{k}}^\alpha\rangle \tag{3.3}$$

The integral in the above equation is the integral of Berry curvature, already familiar to us from our discussion on geometric phase, as the chern number (See Chapter 2).

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[3]In the presence of magnetic field, we shall use the magnetic Brillouin zone. See Chapter 6.

[4]At absolute zero $T = 0$.

Therefore, we can express the hall conductivity as the sum of chern numbers of filled bands

$$\sigma_{xy} = -\frac{e^2}{2\pi\hbar} \sum_{\alpha|E_\alpha < E_F} C_\alpha \tag{3.4}$$

Now it is clear why the integer hall effect is robust - chern numbers are discrete integers and any deformation of the system that does not change the underlying topology of the hilbert space does not affect the hall conductivity.

3.4   Topological phase transitions

As shown above, topology is deeply connected with conduction properties of the material. Changes to topological invariants when a physical parameter of the system is varied indicates sharp changes in conduction properties. This kind of tuning of electronic properties has immense applications in the domain of high-performance electronics and quantum computing. In this thesis, we introduce some driving or perturbations in the Aubry-Andre-Harper model to discover topological phase transitions.

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 $\hat{H}_0$ ——

$$\hat{H}_0 \ket{n} = \epsilon_n \ket{n}$$
$$\braket{m|n} = \delta_{mn}$$
$$\sum_m \ket{m}\bra{m} = 1$$

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

4.1 Introduction

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

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

The wavefunctions $\ket{\psi_n}$ are normalized as $\braket{n|\psi_n} = 1$, as discussed in [22]. On contracting with $\bra{n}$,

$$\bra{n}(\hat{H}_0 + \hat{V})\ket{\psi_n} = E_n\braket{n|\psi_n}$$
$$\epsilon_n\braket{n|\psi_n} + \bra{n}\hat{V}\ket{\psi_n} = E_n\braket{n|\psi_n}$$
$$E_n = \epsilon_n + \bra{n}\hat{V}\ket{\psi_n} \tag{4.1}$$

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)

$$
|\psi_n^{(j)}\rangle = |n\rangle + \hat{R}(E_n)\,(\hat{\mathbb{I}} - |n\rangle\,\langle n|)\hat{V}\,|\psi_n^{(j-1)}\rangle \tag{4.3}
$$

$$
|\psi_n^{(0)}\rangle = |n\rangle
$$

$$
\lim_{j\to\infty} |\psi_n^{(j)}\rangle = |\psi_n\rangle
$$

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

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

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 [23].

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 [23]. In fact, RS theory can be obtained as an approximation to BW theory by power series expansion of the resolvent operator [24]. 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 R $\equiv \{|\phi_n\rangle \dots\}$ is the set of reference states, $|\phi_0\rangle \in$ 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 [24] for multi-reference partitioning.

$$\hat{H}_{eff} \ket{\phi} = P\hat{H}\Omega P \ket{\phi}$$
$$= P\hat{H}\Omega PP \ket{\psi}$$
$$= P\hat{H} \ket{\psi}$$
$$= E\,P \ket{\psi}$$
$$= E \ket{\phi}$$

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 $\ket{\psi} = \Omega \ket{\phi}$.

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

$$Q\hat{H} \ket{\psi} = E\,Q \ket{\psi}$$
$$Q \ket{\psi} = \frac{Q\hat{H}}{E} \ket{\psi}$$

Therefore,

$$\ket{\psi} = (P + Q) \ket{\psi}$$
$$= P \ket{\psi} + Q \ket{\psi}$$
$$= P \ket{\psi} + \frac{Q\hat{H}}{E} \ket{\psi} \tag{4.6}$$
$$P \ket{\psi} = \left(1 - \frac{Q\hat{H}}{E} \right) \ket{\psi}$$
$$\ket{\psi} = \left(1 - \frac{Q\hat{H}}{E} \right)^{-1} P^2 \ket{\psi} \tag{4.7}$$

Eq. (4.6) has the familiar iterative form as Eq. (4.2) with the choice of $P = \ket{n}\bra{n}$. From Eq. (4.7),

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

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 $E_i(i = 1 \dots \dim(H))$, 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 [24].

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 [25]. 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

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

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

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

$|\phi_\alpha(t)\rangle$ 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

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

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 [26–30]. 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 [27, 28, 31].

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 [28, 31]. $\hat{H}_F$ 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

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

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 $\frac{1}{\omega^n}$ [27].

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

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

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

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

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

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

where ϵ 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,

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

$$= \sum_n \tilde{\Phi}_{n,\alpha\beta}e^{in\omega t}e^{-i\epsilon_\beta t} \tag{5.32}$$

Inserting these expansions into the Schrodinger equation

$$
i\frac{\partial}{\partial t}\Psi_{\alpha\beta}(t) = i\frac{\partial}{\partial t}\left(\sum_n \tilde{\Phi}_{n,\alpha\beta}e^{in\omega t}e^{-i\epsilon_\beta t}\right)
$$

$$
= i\sum_n \tilde{\Phi}_{n,\alpha\beta}e^{in\omega t}e^{-i\epsilon_\beta t}(in\omega - i\epsilon_\beta)
$$

$$
= \sum_n \tilde{\Phi}_{n,\alpha\beta}e^{in\omega t}e^{-i\epsilon_\beta t}(\epsilon_\beta - n\omega)
$$

$$
(H\Phi)_{\alpha\beta}(t) = \sum_\gamma \left(\sum_r \tilde{H}_{r,\alpha\gamma}e^{ir\omega t}\sum_s \tilde{\Phi}_{s,\gamma\beta}e^{is\omega t}e^{-i\epsilon_\beta t}\right)
$$

$$
= \sum_\gamma \sum_r \sum_s \tilde{H}_{r,\alpha\gamma}\tilde{\Phi}_{s,\gamma\beta}e^{i(r+s)\omega t}e^{-i\epsilon_\beta t}
$$

making change of variable $n = r + s$

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

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

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* [28, 32, 33], 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 [28, 33]. 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 [28] 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 [29]. 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, $\mathcal{Q}_{mn} = 1 - \mathcal{P}_{mn} = \delta_{mn}(1 - \delta_{m0})$, $(\mathcal{P}\mathcal{M})_{mn} = k\delta_{mk}\delta_{m0}\delta_{kn} = 0$ and $(\mathcal{Q}\mathcal{M})_{mn} = k\delta_{mk}(1 - \delta_{m0})\delta_{kn} = m\delta_{mk}\delta_{kn}(1 - \delta_{k0}) = (\mathcal{M}\mathcal{Q})_{mn}$. 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

$$\mathcal{Q}(\mathcal{H} - \mathcal{M}\omega) |\phi_\alpha\rangle = \epsilon_\alpha \mathcal{Q} |\phi_\alpha\rangle$$
$$\mathcal{Q}\mathcal{H} |\phi_\alpha\rangle = \mathcal{Q}\mathcal{M}\omega |\phi_\alpha\rangle + \epsilon_\alpha \mathcal{Q} |\phi_\alpha\rangle$$
$$\mathcal{Q}\mathcal{H} |\phi_\alpha\rangle = \mathcal{M}\omega\mathcal{Q} |\phi_\alpha\rangle + \epsilon_\alpha \mathcal{Q} |\phi_\alpha\rangle$$
$$(\epsilon_\alpha + \mathcal{M}\omega)\mathcal{Q} |\phi_\alpha\rangle = \mathcal{Q}\mathcal{H} |\phi_\alpha\rangle$$
$$\mathcal{Q} |\phi_\alpha\rangle = \frac{\mathcal{Q}}{\epsilon_\alpha + \mathcal{M}\omega}\mathcal{H} |\phi_\alpha\rangle \tag{5.40}$$
$$\tag{5.41}$$

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

---

[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 [29].

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

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

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

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

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

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

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

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

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

$$(1 - \mathcal{P})\Omega(\epsilon)\epsilon + \mathcal{M}\omega\Omega(\epsilon) - \mathcal{Q}\mathcal{H}\Omega(\epsilon) = \mathcal{M}\omega\mathcal{P}$$

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

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

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

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 $\mathcal{P}|\phi_\alpha\rangle$.

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 [29].

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 wave-functions 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 [29].

Chapter 6

Aubry-Andre-Harper Model

The study of motion of electrons (spinless, non-relativistic) in a periodic 2-dimensional lattice subject to a constant magnetic field perpendicular to the plane of the lattice, or simply the Landau level problem on a lattice, has generated a lot of interest due to the fractal nature of the spectrum, presence of a sharp metal-insulator phase transition and its connection to quantum hall effect. We shall systematically explore this problem and its close connection to the research work carried out in this thesis.

Several interesting properties of this system are attributed to the competing driving forces in the problem - the cyclotron motion due to the magnetic field and the wave properties of periodic potential. In the limiting cases, the system maps to Landau problem and free electron motion in a lattice system respectively.

The coordinate axes are oriented such that the periodic lattice lies in the x-y plane and the perpendicular magnetic field is $\mathbf{B} = B\hat{\mathbf{z}}$. Further, the $\hat{\mathbf{x}}$ and $\hat{\mathbf{y}}$ lie along the perpendicular edges of the square lattice unit cell. The magnetic vector potential in Landau gauge is written as $\mathbf{A} = Bx\hat{\mathbf{y}}$. This choice of gauge is for convenience and does not alter the results derived in this section. The square lattice is defined by the set of lattice translation vectors $\mathbf{R} = md\hat{\mathbf{x}} + nd\hat{\mathbf{y}}$ such that $m, n \in \mathbb{Z}$.

Hamiltonian in the presence of magnetic field is obtained by replacing $\hat{\mathbf{p}}$ by $\hat{\mathbf{p}} - e\mathbf{A}$.

$$\hat{H}(x, y) = \frac{1}{2m}(\hat{\mathbf{p}} - e\mathbf{A})^2 + \hat{V}(x, y) \tag{6.1}$$

6.1 Magnetic Translation Operators

In absence of magnetic field, the set of lattice translation operators form an abelian group and they commute with the translationally invariant hamiltonian. This implies that the translation operators and the hamiltonian can be simultaneously diagonalized.

$$\hat{H}(\mathbf{r}) = \hat{H}(\mathbf{r} + \mathbf{R})$$

$$\hat{T}_{\mathbf{R}} |\psi(\mathbf{r})\rangle = |\psi(\mathbf{r} + \mathbf{R})\rangle \tag{6.2}$$

$$\hat{T}_{\mathbf{R}} = e^{-\frac{i}{\hbar}\mathbf{R}\cdot\hat{\mathbf{p}}} \tag{6.3}$$

$$\hat{T}_{\mathbf{R}_1}\hat{T}_{\mathbf{R}_2} = \hat{T}_{\mathbf{R}_2}\hat{T}_{\mathbf{R}_1} = \hat{T}_{\mathbf{R}_1+\mathbf{R}_2} \tag{6.4}$$

$$\hat{T}_{\mathbf{R}}\hat{H}(\mathbf{r})\,|\psi(\mathbf{r})\rangle = \hat{H}(\mathbf{r}+\mathbf{R})\,|\psi(\mathbf{r}+\mathbf{R})\rangle$$
$$= \hat{H}(\mathbf{r})\,|\psi(\mathbf{r}+\mathbf{R})\rangle$$
$$= \hat{H}(\mathbf{r})\hat{T}_{\mathbf{R}}\,|\psi(\mathbf{r})\rangle$$
$$\hat{T}_{\mathbf{R}}\hat{H}(\mathbf{r}) = \hat{H}(\mathbf{r})\hat{T}_{\mathbf{R}} \tag{6.5}$$

The above properties imply that [12, 34, 35]

$$\hat{H}(\mathbf{r})\,|\psi_{\mathbf{k}}(\mathbf{r})\rangle = E_{\mathbf{k}}\,|\psi_{\mathbf{k}}(\mathbf{r})\rangle \tag{6.6}$$

$$\hat{T}_{\mathbf{R}}\,|\psi_{\mathbf{k}}(\mathbf{r})\rangle = e^{i\mathbf{k}\cdot\mathbf{R}}\,|\psi_{\mathbf{k}}(\mathbf{r})\rangle \tag{6.7}$$

$$|\psi_{\mathbf{k}}(\mathbf{r})\rangle = e^{i\mathbf{k}\cdot\mathbf{r}}\,|u_{\mathbf{k}}(\mathbf{r})\rangle \text{ such that } |u_{\mathbf{k}}(\mathbf{r})\rangle = |u_{\mathbf{k}}(\mathbf{r}+\mathbf{R})\rangle \tag{6.8}$$

This is the essence of *Bloch theorem*. $\mathbf{k}$ is the crystal momentum and it is confined to the limits $k_x, k_y \in [0, 2\pi/d)$.

However, in the presence of uniform magnetic field, the hamiltonian is no longer translationally invariant, because $\mathbf{A}(\mathbf{r}) \neq \mathbf{A}(\mathbf{r}+\mathbf{R})$. Therefore, a new set of translation operators called the *Magnetic translation operators* must be defined [12, 19, 36–40], that commutes with the new hamiltonian.

As demonstrated in [12, 19], the consequence of uniform magnetic field is that the vector potential can be expressed as

$$\mathbf{A}(\mathbf{r}+\mathbf{R}) = \mathbf{A}(\mathbf{r}) + \nabla\mathcal{G}(\mathbf{r},\mathbf{R})$$

Therefore, the operation of translation operator on the hamiltonian is equivalent to a gauge transformation

$$\hat{T}_{\mathbf{R}}\left(\frac{1}{2m}(\hat{\mathbf{p}}-e\mathbf{A}(\mathbf{r}))^2\right) = \left(\frac{1}{2m}(\hat{\mathbf{p}}-e\mathbf{A}(\mathbf{r})-e\nabla\mathcal{G}(\mathbf{r},\mathbf{R}))^2\right)\hat{T}_{\mathbf{R}} \tag{6.9}$$

$$\left(\frac{1}{2m}(\hat{\mathbf{p}}-e\mathbf{A}(\mathbf{r})-e\nabla\mathcal{G}(\mathbf{r},\mathbf{R}))^2\right) = e^{\frac{ie}{\hbar}\mathcal{G}(\mathbf{r},\mathbf{R})}\left(\frac{1}{2m}(\hat{\mathbf{p}}-e\mathbf{A}(\mathbf{r}))^2\right)e^{\frac{-ie}{\hbar}\mathcal{G}(\mathbf{r},\mathbf{R})} \tag{6.10}$$

Now we know that

$$\hat{\mathcal{T}}_{\mathbf{R}} = e^{\frac{-ie}{\hbar}\mathcal{G}(\mathbf{r},\mathbf{R})}\hat{T}_{\mathbf{R}} \tag{6.11}$$

commutes with $\hat{H}$, and we call them magnetic translation operators. In Landau gauge, $\nabla\mathcal{G}(\mathbf{r},\mathbf{R}) = BR_x\hat{\mathbf{y}}$, which means that $\mathcal{G}(\mathbf{r},\mathbf{R}) = BR_x y$ and $\hat{\mathcal{T}}_{\mathbf{R}} = e^{\frac{-ie}{\hbar}BR_x y}\hat{T}_{\mathbf{R}}$. But, the magnetic translation operators do not form a group. On explicit calculation, one can show that

$$\hat{\mathcal{T}}_{\mathbf{R}}\hat{\mathcal{T}}_{\mathbf{R}'} = e^{\frac{-ie}{\hbar}BR_x' R_y}\hat{\mathcal{T}}_{\mathbf{R}+\mathbf{R}'}$$

If $\hat{\mathcal{T}}_x$ and $\hat{\mathcal{T}}_y$ translate by unit length along $\hat{\mathbf{x}}$ and $\hat{\mathbf{y}}$ respectively, then

$$\hat{\mathcal{T}}_x\hat{\mathcal{T}}_y = e^{i2\pi\frac{e}{h}Bd^2}\hat{\mathcal{T}}_y\hat{\mathcal{T}}_x$$

If we assume that the magnetic flux through a unit cell is rational

$$\alpha = \frac{e}{h}Bd^2 = \frac{p}{q} \text{ such that } p, q \in \mathcal{Z}^+ \text{ and } gcd(p,q) = 1 \tag{6.12}$$

and define magnetic translation vectors

$$\mathcal{R} = qmd\hat{\mathbf{x}} + nd\hat{\mathbf{y}} \text{ such that } m, n \in \mathcal{Z} \tag{6.13}$$

then, a subset of magnetic translation operators, that translate by units of magnetic unit cell form a group

$$\hat{\mathcal{T}}_{\mathcal{R}}\hat{\mathcal{T}}_{\mathcal{R}'} = e^{-i2\pi\frac{e}{h}Bm_1n_2qd^2}\hat{\mathcal{T}}_{\mathcal{R}+\mathcal{R}'} = e^{-i2\pi pm_1n_2}\hat{\mathcal{T}}_{\mathcal{R}+\mathcal{R}'} = \hat{\mathcal{T}}_{\mathcal{R}+\mathcal{R}'} \tag{6.14}$$

When the magnetic flux is irrational it is incommensurate with the periodicity of the lattice. The magnetic translation group can no longer be defined. The case of irrational magnetic flux is studied in [41]. Operators in the magnetic translation group commute with each other. Also, translation by magnetic unit cell $x = qd$ and $y = d$ gives

$$\hat{\mathcal{T}}_{qx}\hat{\mathcal{T}}_y = e^{i2\pi\alpha q}\hat{\mathcal{T}}_y\hat{\mathcal{T}}_{qx} = e^{i2\pi p}\hat{\mathcal{T}}_y\hat{\mathcal{T}}_{qx} = \hat{\mathcal{T}}_y\hat{\mathcal{T}}_{qx} \tag{6.15}$$

Now we have established the required properties to write the eigenvalue equation

$$\hat{\mathcal{T}}_{\mathcal{R}}|\psi_{\mathbf{k}}(\mathbf{r})\rangle = e^{i\mathbf{k}\cdot\mathcal{R}}|\psi_{\mathbf{k}}(\mathbf{r})\rangle \tag{6.16}$$

with $\mathbf{k}$ restricted to magnetic brillouin zone $k_x \in [0, 2\pi/qd)$, $k_y \in [0, 2\pi/d)$. Inspired from bloch theory, we can write

$$|\psi_{\mathbf{k}}(\mathbf{r})\rangle = e^{i\mathbf{k}\cdot\mathbf{r}}|u_{\mathbf{k}}(\mathbf{r})\rangle \tag{6.17}$$

However, $|u_{\mathbf{k}}(\mathbf{r}+\mathcal{R})\rangle \neq |u_{\mathbf{k}}(\mathbf{r})\rangle$. This relationship can be determined by applying the definition of magnetic translation operator on Eq. (6.16).

$$|u_{\mathbf{k}}(\mathbf{r}+\mathcal{R})\rangle = e^{-i2\pi\frac{e}{h}Bqmdy}|u_{\mathbf{k}}(\mathbf{r})\rangle \tag{6.18}$$

This is called the *Generalized bloch condition*.

6.2   Tight-Binding Hamiltonian

To write the hamiltonian under the tight-binding approximation, the wavefunction is expanded as a linear combination of a set of localized states [34, 35]. In the absence of magnetic field, the wavefunction is written in terms of the wannier states/single atom states as[1]

$$|\psi(\mathbf{r})\rangle = \sum_{\mathbf{R}} a_{\mathbf{R}}|\phi_{\mathbf{R}}(\mathbf{r})\rangle$$

where the wannier states $|\phi_{\mathbf{R}}\rangle$ are localized at their corresponding lattice sites $\mathbf{R}$. The overlap integral of wannier states localized at different sites is zero.

$$\langle\phi_{\mathbf{R}'}|\phi_{\mathbf{R}}\rangle = \delta_{m'm}\delta_{n'n} \tag{6.19}$$

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[1]With this method, we obtain one band structure of the hamiltonian as we are accounting for contributions from a single state at each lattice site. Two band tight-binding model is described in [42]

The tight-binding approximation for the zero-magnetic field case is obtained by plugging the above expansion into the eigenvalue equation

$$\left(\frac{1}{2m}\mathbf{p}^2 + \hat{V}(\mathbf{r}) \right) \sum_{\mathbf{R}} a_{\mathbf{R}} \, |\phi_{\mathbf{R}}(\mathbf{r})\rangle = E \sum_{\mathbf{R}} a_{\mathbf{R}} \, |\phi_{\mathbf{R}}(\mathbf{r})\rangle$$

$$\sum_{m,n} \hat{H}_0 a_{m,n} |\phi_{m,n}(\mathbf{r})\rangle = \sum_{m,n} E a_{m,n} |\phi_{m,n}(\mathbf{r})\rangle$$

$$\sum_{k,l} |\phi_{k,l}\rangle \langle\phi_{k,l}| \sum_{m,n} \hat{H}_0 a_{m,n} |\phi_{m,n}\rangle = \sum_{k,l} |\phi_{k,l}\rangle \langle\phi_{k,l}| \sum_{m,n} E a_{m,n} |\phi_{m,n}\rangle$$

Switching dummy indices on the left

$$\sum_{m,n} |\phi_{m,n}\rangle \langle\phi_{m,n}| \sum_{k,l} \hat{H}_0 a_{k,l} |\phi_{k,l}\rangle = \sum_{k,l} |\phi_{k,l}\rangle \langle\phi_{k,l}| \sum_{m,n} E a_{m,n} |\phi_{m,n}\rangle$$

$$\sum_{m,n,k,l} a_{k,l} \langle\phi_{m,n}|\hat{H}_0|\phi_{k,l}\rangle \, |\phi_{m,n}\rangle = \sum_{k,l,m,n} E a_{m,n} \langle\phi_{k,l}|\phi_{m,n}\rangle \, |\phi_{m,n}\rangle$$

$$\sum_{m,n} \sum_{k,l} a_{k,l} \langle\phi_{m,n}|\hat{H}_0|\phi_{k,l}\rangle \, |\phi_{m,n}\rangle = \sum_{k,l,m,n} E a_{m,n} \delta_{k,m} \delta_{l,n} \, |\phi_{m,n}\rangle$$

$$\sum_{m,n} \sum_{k,l} a_{k,l} \langle\phi_{m,n}|\hat{H}_0|\phi_{k,l}\rangle \, |\phi_{m,n}\rangle = \sum_{m,n} E a_{m,n} \, |\phi_{m,n}\rangle$$

Comparing coefficients of $|\phi_{m,m}\rangle$

$$\sum_{k,l} a_{k,l} \langle\phi_{m,n}|\hat{H}_0|\phi_{k,l}\rangle = E a_{m,n}$$

$$\sum_{k\neq m, l\neq n} a_{k,l} \langle\phi_{m,n}|\hat{H}_0|\phi_{k,l}\rangle + a_{m,n} \langle\phi_{m,n}|\hat{H}_0|\phi_{m,n}\rangle = E a_{m,n} \qquad (6.20)$$

$\langle\phi_{m,n}|\hat{H}_0|\phi_{m,n}\rangle$ is independent of indices m, n due to translation invariance of $\hat{H}_0$. This is set to zero, as this is equivalent to shifting the energy scale. Translational symmetry also means that

$$\langle\phi_{m,n}|\hat{H}_0|\phi_{k,l}\rangle = \langle\phi_{m-k,n-l}|\hat{H}_0|\phi_{0,0}\rangle$$

Using the above properties, the above equation can be written as

$$\sum_{k\neq 0, l\neq 0} a_{m+k,n+l} \langle\phi_{0,0}|\hat{H}_0|\phi_{k,l}\rangle = E a_{m,n}$$

Designating $W_{k,l} = \langle\phi_{0,0}|\hat{H}_0|\phi_{k,l}\rangle$ Tight-binding approximation entails assuming that the wannier functions are well localized and the overlap between far-off wannier states is approximately zero. Therefore, only interactions between the nearest neighbors is significant in the summation defined above. We also expect $W_{1,0} = W_{-1,0}$ and $W_{0,1} = W_{0,-1}$ as justified in [43]. With these assumptions, the tight-binding equation is written as

$$W_{1,0}(a_{m+1,n} + a_{m-1,n}) + W_{0,1}(a_{m,n+1} + a_{m,n-1}) = E a_{m,n} \qquad (6.21)$$

In matrix form, the hamiltonian is written as

$$\hat{H}_0 = \sum_{m,n} W_{1,0} \, |m+1, n\rangle \langle m, n| + W_{0,1} \, |m, n+1\rangle \langle m, n| + h.c. \qquad (6.22)$$

This expression is succinctly expressed in terms of the translation operators

$$\hat{H}_0 = W_{1,0}\hat{T}_x + W_{0,1}\hat{T}_y + h.c. \qquad (6.23)$$

When the magnetic field is non-zero, the expansion is written as [39, 43–45]

$$|\psi(\mathbf{r})\rangle = \sum_{\mathbf{R}} a_{\mathbf{R}} e^{2\pi \frac{ie}{h} \int_{\mathbf{R}}^{\mathbf{r}} \mathbf{A} \cdot d\mathbf{r}'} |\phi_{\mathbf{R}}(\mathbf{r})\rangle \tag{6.24}$$

The line integral in the exponent is taken along the straight line path between the two points. We have used a local gauge transformation of the wannier states in the above expansion. This is equivalent to the choice of gauge in writing the electromagnetic potential [10, 22, 46]. This transformation is done is the same spirit as the one we did when we defined the magnetic translation operators in Eq. (6.10). As shown in [44], the following property holds under the approximation of slowly varying magnetic field

$$\hat{H} e^{2\pi \frac{ie}{h} \int_{\mathbf{R}}^{\mathbf{r}} \mathbf{A} \cdot d\mathbf{r}'} |\phi_{\mathbf{R}}\rangle = e^{2\pi \frac{ie}{h} \int_{\mathbf{R}}^{\mathbf{r}} \mathbf{A} \cdot d\mathbf{r}'} \hat{H}_0 |\phi_{\mathbf{R}}\rangle \tag{6.25}$$

and for slowly varying magnetic field, the hopping integrals modify as

$$\langle\phi_{\mathbf{R}}| e^{-2\pi \frac{ie}{h} \int_{\mathbf{R}}^{\mathbf{r}} \mathbf{A} \cdot d\mathbf{r}'} \hat{H} e^{2\pi \frac{ie}{h} \int_{\mathbf{R}'}^{\mathbf{r}} \mathbf{A} \cdot d\mathbf{r}'} |\phi_{\mathbf{R}'}\rangle = e^{2\pi \frac{ie}{h} \int_{\mathbf{R}}^{\mathbf{R}'} \mathbf{A} \cdot d\mathbf{r}'} \langle\phi_{\mathbf{R}}|\hat{H}_0|\phi_{\mathbf{R}'}\rangle \tag{6.26}$$

The above result is known as *Peirels substitution*. Therefore, the tight-binding hamiltonian in the presence of magnetic field is written as [38, 39, 47]

$$\hat{H} = \sum_{m,n} W_{1,0} e^{2\pi \frac{ie}{h} \int_{md}^{(m+1)d} \mathbf{A} \cdot d\mathbf{x}} |m+1, n\rangle \langle m, n| + W_{0,1} e^{2\pi \frac{ie}{h} \int_{nd}^{(n+1)d} \mathbf{A} \cdot d\mathbf{y}} |m, n+1\rangle \langle m, n| + h.c. \tag{6.27}$$

In Landau gauge

$$\hat{H} = \sum_{m,n} W_{1,0} |m+1, n\rangle \langle m, n| + W_{0,1} e^{2\pi i\alpha m} |m, n+1\rangle \langle m, n| + h.c. \tag{6.28}$$

where α is the magnetic flux through an unit cell

$$\alpha = \frac{eBd^2}{h} \tag{6.29}$$

In terms of the lattice translation operators as

$$\hat{H} = W_{1,0} \hat{T}_x + W_{0,1} e^{2\pi i\alpha m} \hat{T}_y + h.c. \tag{6.30}$$

$$= W_{1,0} \hat{\mathcal{T}}_x + W_{0,1} \hat{\mathcal{T}}_y + h.c. \tag{6.31}$$

The eigenvalue equation is written as

$$W_{1,0}(a_{m+1,n} + a_{m-1,n}) + W_{0,1}(e^{2\pi i\alpha m} a_{m,n+1} + e^{-2\pi i\alpha m} a_{m,n-1}) = E a_{m,n} \tag{6.32}$$

Coefficients in the above equation, involve only m and do not depend on n. We therefore assume plane wave behaviour along y-direction and assume $a_{mn} = e^{in\theta} a_m$, where $\theta = k_y d$ [43, 47]. This is also clear from the generalized bloch condition derived in the previous section - $|u\rangle$ is periodic under translation along the y-axis by a unit cell. On substitution, we obtain the harper equation [43, 47–49]

$$a_{m+1} + a_{m-1} + \lambda \cos(2\pi m\alpha + \theta) a_m = E a_m \tag{6.33}$$

The harper equation is a recurrence relation involving coefficients $a_0, a_1, \ldots$. This recurrence relationship is best expressed in terms of a transfer matrix

$$\begin{bmatrix} a_{m+1} \\ a_m \end{bmatrix} = \begin{bmatrix} E - \cos(2\pi m\alpha + \theta) & -1 \\ 1 & 0 \end{bmatrix} \begin{bmatrix} a_m \\ a_{m-1} \end{bmatrix} = \mathbf{T}(m) \begin{bmatrix} a_m \\ a_{m-1} \end{bmatrix} \tag{6.34}$$

In terms of the transfer matrix, we can write

$$\begin{bmatrix} a_{m+1} \\ a_m \end{bmatrix} = \left(\prod_{j=1}^{m} \mathbf{T}(j) \right) \begin{bmatrix} a_1 \\ a_0 \end{bmatrix} = \mathbf{Q}^m \begin{bmatrix} a_1 \\ a_0 \end{bmatrix} \tag{6.35}$$

We have not considered the possibility of this recursion blowing up as $m \to \infty$ i.e., $a_m \to \infty$ as $m \to \infty$. This represents an unphysical situation that must not be allowed. Under the assumption of rationality of α, periodicity of $\cos(2\pi m\alpha + \theta)$ implies that $\mathbf{T}(q+1) = \mathbf{T}(1)$ and $\mathbf{T}(q)\mathbf{T}(q-1)\ldots\mathbf{T}(1) = \mathbf{T}(nq)\mathbf{T}(nq-1)\ldots\mathbf{T}((n-1)q+1) = \mathbf{Q}^q$. The matrix $\mathbf{Q}^q$ is a function of E and θ. The condition that the coefficients must be bounded translates to a condition on $\mathbf{Q}^q$

$$|tr(\mathbf{Q}^q)| \leq 4 \tag{6.36}$$

The trace of $\mathbf{Q}^q$ is q-degree polynomial known as the harper polynomial [42, 47, 50] and the energy values that satisfy the above equation occur in q distinct energy bands. Thus, the spectrum of the hamiltonian has q-subbands[2]. A physical explanation in terms of there being q potential wells inside each magnetic unit cell is conceivable. But, a rigorous mathematical explanation is far more satisfying as much of the content presented in this thesis is beyond the reach of intuition.

6.3 Hamiltonian in Momentum Space

Expanding the lattice localized states in terms of states localized in crystal momentum space $|k_x, k_y\rangle$ using fourier transform

$$|m, n\rangle = \int_{-\pi}^{\pi} \int_{-\pi}^{\pi} \frac{dk_x}{2\pi} \frac{dk_y}{2\pi} e^{ik_x m + ik_y n} |k_x, k_y\rangle \tag{6.37}$$

$$\langle m, n| = \int_{-\pi}^{\pi} \int_{-\pi}^{\pi} \frac{dk_x}{2\pi} \frac{dk_y}{2\pi} e^{-ik_x m - ik_y n} \langle k_x, k_y| \tag{6.38}$$

where $-\pi \leq k_x, k_y < \pi$ and $|k_x + 2\pi a, k_y + 2\pi b\rangle = |k_x, k_y\rangle$ where $a, b \in \mathbb{Z}$.

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[2]This is not true for even values of q as the middle bands touch. This is described as the "kiss" in [47, 50]

Consider[3]

$$W_{1,0} \sum_{m,n} |m+1,n\rangle \langle m,n| + |m-1,n\rangle \langle m,n|$$

$$= \frac{W_{1,0}}{(2\pi)^4} \sum_{m,n} \iiiint dk_x dk_y dk_x' dk_y' (e^{ik_x(m+1)+ik_y n} e^{-ik_x' m - ik_y' n} + e^{ik_x(m-1)+ik_y n} e^{-ik_x' m - ik_y' n}) |k_x, k_y\rangle \langle k_x', k_y'|$$

$$= \frac{W_{1,0}}{(2\pi)^4} \iiiint dk_x dk_y dk_x' dk_y' \sum_{m,n} (e^{ik_x} e^{i(k_x-k_x')m} e^{i(k_y-k_y')n} + e^{-ik_x} e^{i(k_x-k_x')m} e^{i(k_y-k_y')n}) |k_x, k_y\rangle \langle k_x', k_y'|$$

$$= \frac{W_{1,0}}{(2\pi)^2} \iiiint dk_x dk_y dk_x' dk_y' (e^{ik_x} + e^{-ik_x}) \delta(k_x - k_x') \delta(k_y - k_y') |k_x, k_y\rangle \langle k_x', k_y'|$$

$$= \frac{2W_{1,0}}{(2\pi)^2} \iint dk_x dk_y \cos(k_x) |k_x, k_y\rangle \langle k_x, k_y|$$

$$W_{0,1} \sum_{m,n} |m, n+1\rangle \langle m,n| e^{i2\pi\alpha m}$$

$$= \frac{W_{1,0}}{(2\pi)^4} \sum_{m,n} \iiiint dk_x dk_y dk_x' dk_y' e^{ik_x m + ik_y(n+1)} e^{-ik_x' m - ik_y' n} e^{i2\pi\alpha m} |k_x, k_y\rangle \langle k_x', k_y'|$$

$$= \frac{W_{1,0}}{(2\pi)^4} \iiiint dk_x dk_y dk_x' dk_y' \sum_{m,n} e^{i(k_x-k_x'+2\pi\alpha)m} e^{i(k_y-k_y')n} e^{ik_y} |k_x, k_y\rangle \langle k_x', k_y'|$$

$$= \frac{W_{1,0}}{(2\pi)^2} \iiiint dk_x dk_y dk_x' dk_y' e^{ik_y} \delta(k_x + 2\pi\alpha - k_x') \delta(k_y - k_y') |k_x, k_y\rangle \langle k_x', k_y'|$$

$$= \frac{W_{1,0}}{(2\pi)^2} \iint dk_x dk_y e^{ik_y} |k_x + 2\pi\alpha, k_y\rangle \langle k_x, k_y|$$

Similarly,

$$W_{0,1} \sum_{m,n} |m, n-1\rangle \langle m,n| e^{-i2\pi\alpha m} = \frac{W_{1,0}}{(2\pi)^2} \iint dk_x dk_y e^{-ik_y} |k_x - 2\pi\alpha, k_y\rangle \langle k_x, k_y|$$

The hamiltonian in the momentum space is

$$\hat{H} = \int_{-\pi}^{\pi} \int_{-\pi}^{\pi} \frac{dk_x}{2\pi} \frac{dk_y}{2\pi} \left[2W_{1,0} \cos(k_x) |k_x, k_y\rangle \langle k_x, k_y| + W_{1,0} e^{ik_y} |k_x + 2\pi\alpha, k_y\rangle \langle k_x, k_y| + h.c. \right] \tag{6.39}$$

The hamiltonian has hopping terms mixing (k_x, k_y) with $(k_x + 2\pi\alpha, k_y)$. We can sector the brillouin zone into q zones of $2\pi/q$ size each. This partitioning is guided by our insight that two wavevectors in the same sector do not mix with each other. This enables us to write the hamiltonian as [39]

$$H = \frac{1}{(2\pi)^2} \int_{\frac{-\pi}{q}}^{\frac{\pi}{q}} \int_{-\pi}^{\pi} dk_x^0 dk_y \hat{H}_{k_x^0, k_y} \tag{6.40}$$

$$\hat{H}_{k_x^0, k_y} = \sum_{n=0}^{q-1} [-2W_{1,0} \cos(k_x^0 + 2\pi\alpha n) |k_x^0 + 2\pi\alpha, k_y\rangle \langle k_x^0 + 2\pi\alpha, k_y|$$

$$- W_{0,1}(e^{ik_y} |k_x^0 + 2\pi\alpha(n+1), k_y\rangle \langle k_x^0 + 2\pi\alpha n, k_y|$$

$$+ e^{-ik_y} |k_x^0 + 2\pi\alpha(n-1), k_y\rangle \langle k_x^0 + 2\pi\alpha n, k_y|)] \tag{6.41}$$

---

[3]Limits of integration are not written for typesetting convenience

Our new momentum variable k_x^0 lies in the magnetic brillouin zone $[-\pi/q, \pi/q]$.

We shall expand the q-site hamiltonian $\hat{H}_{k_x^0, k_y}$ as an eigenvalue equation. With $|\psi\rangle = \sum_{n=0}^{q-1} a_n |k_x^0 + 2\pi\alpha n, k_y\rangle$, the eigenvalue equation is

$$2W_{1,0}\cos(k_x^0 + 2\pi\alpha n)a_n + W_{0,1}(e^{ik_y}a_{n+1} + e^{-ik_y}a_{n-1}) = E_{k_x^0, k_y}a_n \tag{6.42}$$

with the periodicity condition $a_n = a_{n+q}$. However, the hamiltonian written in this form is not periodic in k_x^0, k_y. We seek this property as it is necessary when calculating topological invariants - called chern numbers - intimately related to the concept of geometric phase. We make use of a linear transformation, known as the duality transformation [51] to obtain such a hamiltonian

$$a_n = \sum_{m=1}^{q} e^{i2\pi\alpha mn}x_m \tag{6.43}$$

In terms of x_m we obtain

$$2W_{1,0}\cos(k_y + 2\pi\alpha m)x_m + W_{0,1}(e^{-ik_x^0}x_{m-1} + e^{ik_x^0}x_{m+1}) = E_{k_x^0, k_y}x_m \tag{6.44}$$

This transformation has the effect of switching the roles of k_x^0 and k_y. We can push the k_x^0 dependence to the corners from the upper/lower diagonal terms by $x_m = e^{-ik_x^0 m}b_m$

$$2W_{1,0}\cos(k_y + 2\pi\alpha m)e^{-ik_x^0 m}b_m + W_{0,1}(e^{-ik_x^0}e^{-ik_x^0(m-1)}b_m + e^{ik_x^0}e^{-ik_x^0(m+1)}b_m) = E_{k_x^0, k_y}e^{-ik_x^0 m}b_m$$
$$2W_{1,0}\cos(k_y + 2\pi\alpha m)b_m + W_{0,1}(b_{m-1} + b_{m+1}) = E_{k_x^0, k_y}b_m \tag{6.45}$$

The requirement that $x_{m+q} = x_m$ translates to

$$x_{m+q} = x_m$$
$$e^{-ik_x^0(m+q)}b_{m+q} = e^{-ik_x^0 m}b_m$$
$$b_{m+q} = e^{ik_x^0 q}b_m \tag{6.46}$$

The above hamiltonian written in matrix form is

$$H_{ij} = 2W_{1,0}\cos(k_y + 2\pi\alpha m)\delta ij + W_{0,1}(\delta_{i+1,j} + \delta_{i,j+1}) + W_{0,1}\delta_{i,q}\delta_{j,1}e^{ik_x^0 q} + W_{0,1}\delta_{i,1}\delta_{j,q}e^{-ik_x^0 q} \tag{6.47}$$

In the above form the hamiltonian satisfies

$$\hat{H}(k_x^0, k_y) = \hat{H}(k_x^0 + 2\pi/q, k_y) \tag{6.48}$$
$$\hat{H}(k_x^0, k_y) = \hat{H}(k_x^0, k_y + 2\pi) \tag{6.49}$$

The parametric dependence of $\hat{H}$ on k_x^0, k_y is described by a torus.

6.4   Spectrum

The above Hamiltonian is called the Harper model when $\lambda = W_{1,0}/W_{0,1} = 1$. The general model is called the Aubry-Andre model. When the energy spectrum of the Harper Hamiltonian is plotted against α, the famous Hofstadter butterfly is revealed [47]. One of the remarkable aspects of the energy spectrum is that, it splits into q unique subbands for

$\alpha = p/q$. This is confounding, because even a slight variation in α causes q to change rapidly. Infact, the number of real values between any two real numbers is uncountably infinite. As a result, a rich pattern resembling a butterfly is obtained as the plot. Some characterisitics displayed by the plot are [47, 50, 52, 53]

1. α and $N + \alpha$ produce the same spectrum. α may be restricted to $[0, 1]$ for this reason.

2. The energy eigenvalues are symmteric with respect to zero. i.e., if $\epsilon \in spectrum(\alpha)$, then $-\epsilon \in spectrum(\alpha)$.

3. $|\epsilon| \leq 4$. This is a consequence of the boundedness of the wavefunction discussed earlier.

4. The energy eigenvalues of irrational α is homeomorphic to a cantor set.

5. The graph has a recursive structure.

Figure 6.1: Hofstadter butterfly.
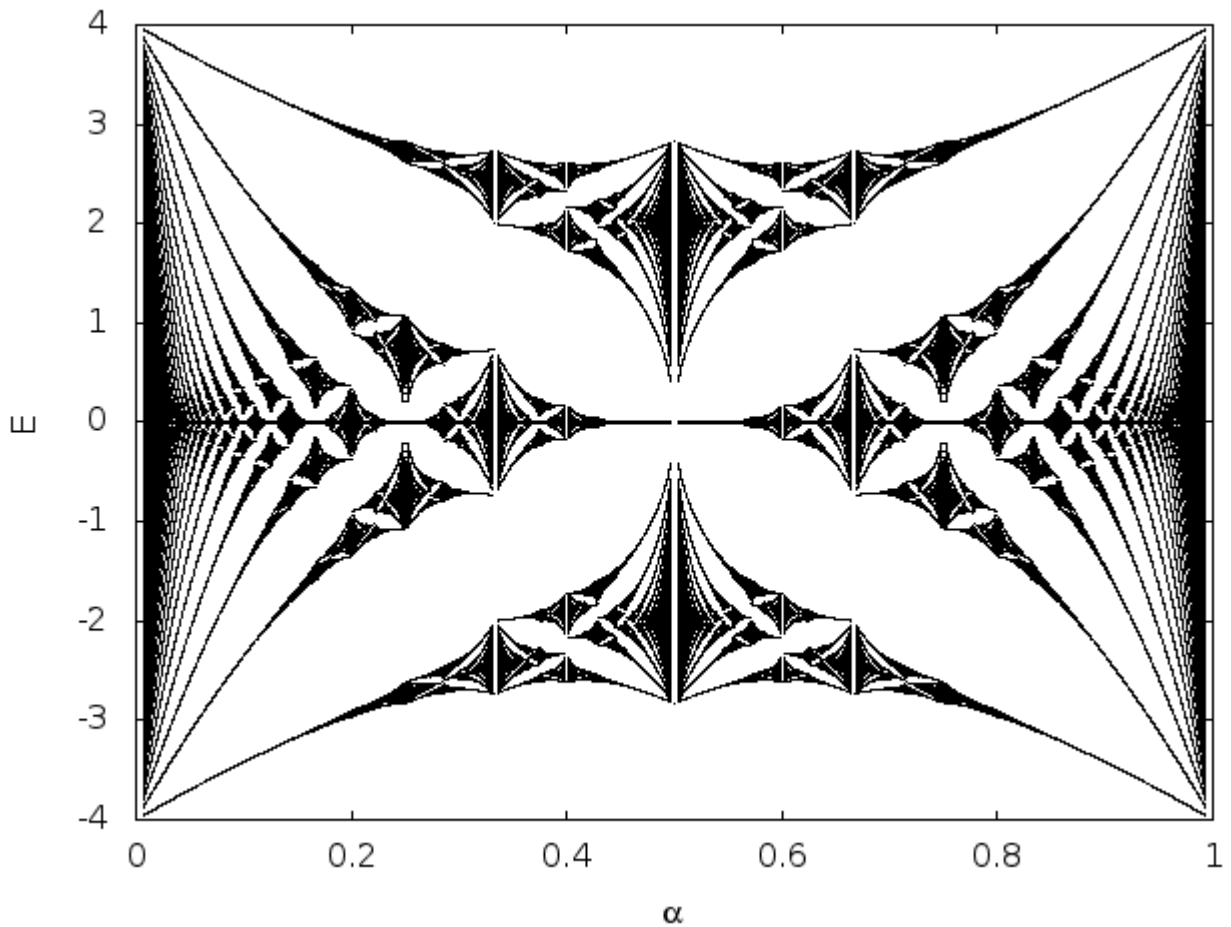
6.5   Metal-Insulator phase transition

The Aubry-Andre model exhibits a phase transition from localized to delocalized behaviour at $\lambda = 2$ for Diophantine irrational numbers [51, 54, 55]. Localization means that the wavefunctions are concentrated at certain lattice sites. Delocalized wavefunctions are roughly uniformly distributed at all lattice sites. Localized wavefunctions have insulator like properties with no effective contribution to transport of charge, whereas the delocalized wavefunctions contribute to metallic behaviour. The quantitative measure of localization is called as the Inverse Participation Ratio (IPR). It is defined as

$$IPR = \frac{\sum_{n=1}^{L} |a_n|^4}{(\sum_{n=1}^{L} |a_n|^2)^2} \tag{6.50}$$

where an are the expansion coefficients of the energy eigenstates in a local discrete-site basis and L is the number of lattice sites [51, 54, 56]. IPR lies in the range 1 to $1/L$, where 1 indicates a perfectly localized state and $1/L$ indicates a perfectly delocalized state.

Figure 6.2: The metal-to-insulator transition of the AAH Hamiltonian for the systems ground state. Plot (a) shows the IPR versus V0 or λ in real space for L = 144, 1597 and 10 946 (top to bottom) with $\alpha_0 = (\sqrt{5} - 1)/2$ (inverse of golden ratio). The inset shows the variation of D2 with V0 which also exhibits a transition. Plot (b) exhibits the mirror behavior in the dual space
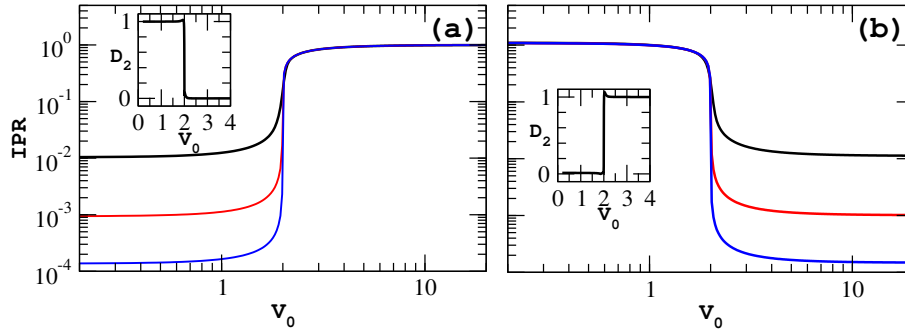
AAH model has a duality transformation of the form [51, 54, 56]

$$|m\rangle = \frac{1}{\sqrt{L}} \sum_n e^{-i2\pi\alpha_0 mn} |n\rangle \tag{6.51}$$

The effect of this transformation is to switch to a momentum space like representation. Wavefunctions localized in real space is delocalized in the dual space and vice versa. AAH model is an exactly self-dual model i.e., the hamiltonian retains its tri-diagonal form under the duality transformation, and the IPR plot in the dual space is an exact mirror image of the IPR plot in the real space. We also seek a relationship between IPR and L of the form $IPR \propto L^{-D_2}$. The sharp transition of D_2 to 0 at $V_0 = 2$ indicates that this metal-insulator transition is independent of length and true even under the limit of $L \to \infty$.

We shall use the IPR measure to evaluate the metal insulator phase transitions in the variants of the AAH model we study in this thesis.

6.6 Hall Conductivity and Chern numbers

As already mentioned in Chapter 3, the Hall conductivity is a topological invariant. In fact, the harper model was the first problem for which this result was established [18]. An interesting discussion on chern numbers and their physical interpretation as applied to this problem can be found in [57]. Another statement that chern numbers are the only topological invariants associated with energy bands is also shown using topological arguments [58]. Hall conductivity can be calculated both numerically - using the berry connection, and analytically - using the Streda formula.

Conductivity represents a linear relationship between the current density and the electric field. This is written as

$$J_i = \sum_j \sigma_{ij} E_j \tag{6.52}$$

The off-diagonal term of the conductivity matrix is the hall conductivity.

$$J_i = \sigma_H \epsilon_{ij} E_j \tag{6.53}$$

ϵ_{ij} is the levi-cevita symbol. The local charge conservation of electromagnetism is represented by the continuity equation

$$\nabla \cdot \mathbf{J} = -\frac{\partial \rho}{\partial t} \tag{6.54}$$

Therefore, for this problem we write

$$\frac{\partial \rho}{\partial t} = -\nabla \cdot \mathbf{J}$$
$$= -(\partial_x J_x + \partial_y J_y)$$
$$= -(\partial_x(\sigma_h E_y) + \partial_y(-\sigma_h E_x))$$
$$= -\sigma_H(\partial_x E_y - \partial_y E_x)$$

Using Maxwell's equation $\tag{6.55}$

$$= -\sigma_H \frac{\partial B}{\partial t}$$

Therefore $\tag{6.56}$

$$\sigma_H = \frac{\partial \rho}{\partial B} \tag{6.57}$$

This is known as the Streda formula [39, 59]. ρ used in the above equation is the charge density. If the magnetic flux through an unit cell is a rational number p/q, then the charge density can be expressed in terms of numbers of filled bands (bands below the fermi energy) r, as $e\frac{1}{V}\frac{r}{q}$ [39, 60], V is the unit cell area. Any three integers p, q and r can be related by the diophantine equation as

$$r = qs_r + pt_r$$

where $s_r, t_r \in \mathbb{Z}$ and $|t_r| \leq q/2$, $0 \leq r \leq q$. Implies that

$$\frac{r}{q} = s_r + \frac{p}{q} t_r = s_r + \frac{e}{h} BV t_r$$

41

Therefore the Hall conductance when fermi level is in the rth gap is [4]

$$\sigma_H = \frac{e^2}{h} t_r$$

The Hall conductivity can be calculated numerically by simply performing the integral of the Berry curvature over the Brillouin zone torus. This is conveniently done using the four-point Bargmann invariant formulation discussed in Chapter 2. The validity of this approach for discretized Brillouin zone has been established using lattice gauge theory [8, 62–64]. The algorithm for the non-abelian case (works even in the presence of degeneracies) is presented step by step below. We intend to calculate chern number for the rth gap.

1. Write the Hamiltonian as a periodic function of k_x and k_y. This was achieved in the previous section.

2. Discretize the Brillouin zone. The discrete values of k_x and k_y are given by $k_x[j] = \frac{2\pi}{qN_x}j$ where $j = 0, 1 \ldots N_x - 1$ and $k_y[j] = \frac{2\pi}{N_y}j$ where $j = 0, 1 \ldots N_y - 1$. Roughly choose $N_y \sim qN_x$ [5].

3. For each point on the discrete Brillouin zone, diagonalize the Hamiltonian. $\psi[k, i, j]$ denotes the kth eigenvector (eigenvectors ordered in ascending order of corresponding eigenvalues) of Hamiltonian at $k_x[i]$ and $k_y[j]$.

4. For each point (i, j) on the lattice, calculate $r \times r$ matrices $\mathbf{U}^x$ and $\mathbf{U}^y$. $U^x_{[a,b]} = \langle \psi[a, i, j] | \psi[b, (i+1) \bmod N_x, j] \rangle$ and $U^y_[a, b] = \langle \psi[a, i, j] | \psi[b, i, (j+1) \bmod N_y] \rangle$, where $1 \leq a, b \leq r$. We denote the $U_x[i, j] = \det(\mathbf{U}^x)$ and $U_y[i, j] = \det(\mathbf{U}^y)$.

5. The four-point Bargmann invariant (equivalently the Berry curvature times the area) is calculated for each point as

$$F[i, j] = U_x[i, j] U_y[(i+1) \bmod N_x, j] U_x^*[(i+1) \bmod N_x, (j+1) \bmod N_y] U_y^*[i, (j+1) \bmod N_y]$$

6. The chern number is then calculated by summing up the berry curvature values $C = \frac{1}{2\pi i} \sum_{i,j} F[i, j]$.

The chern numbers for the Harper-Hofstadter problem were successfully calculated using this method. Both methods, of course give the same results!

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[4]Admittedly, this proof is not rigorous. Refer to [61] for a discussion in terms of Landau levels. Also, the TKNN paper also has a different way to arrive at the diophantine equation [18].

[5]Using Landau gauge. However, this method is applicable for all gauge choices. Suitable modifications are required for symmetric gauge.
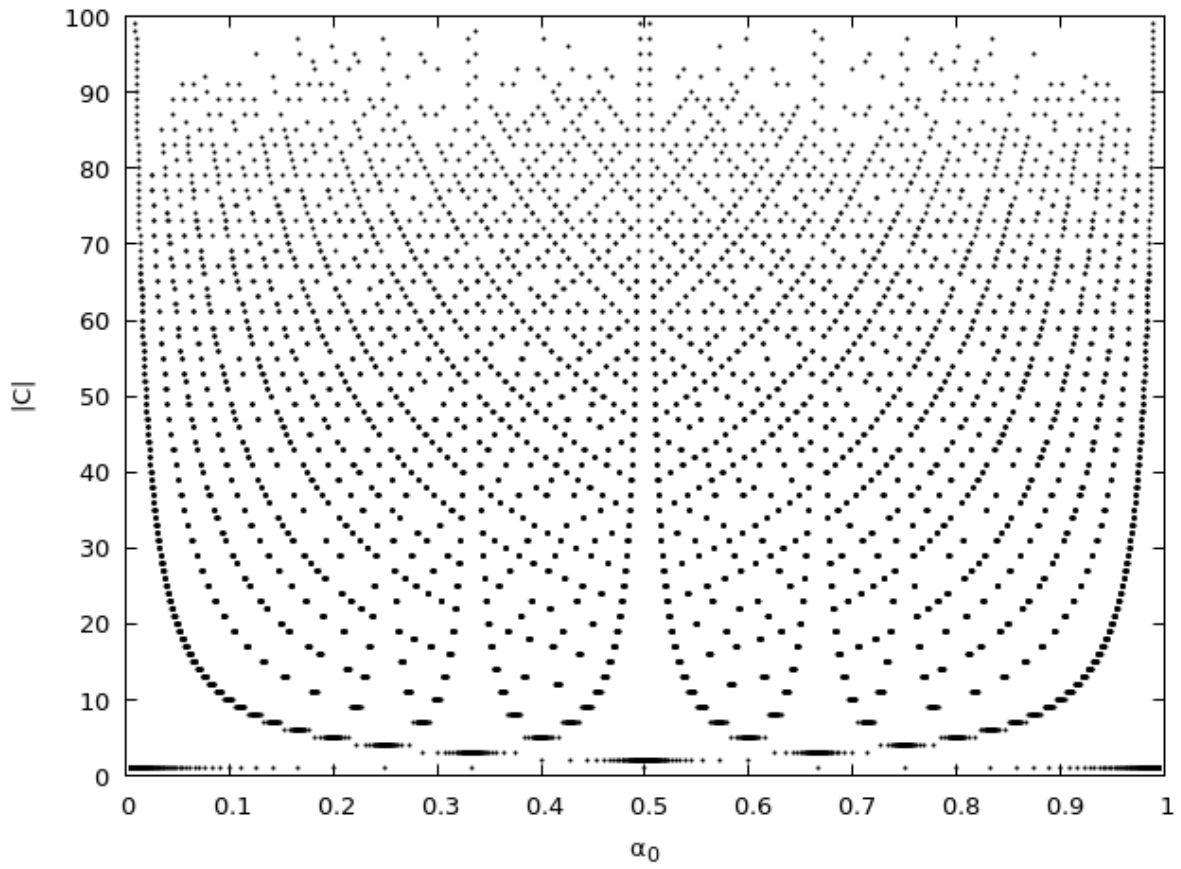
Figure 6.3: Absolute value of Chern number $|C|$ of the lowest energy eigenstate as a function of magnetic flux α_0.

Part II

Study of driven AAH models

Chapter 7

AAH model with Oscillating Magnetic Field

Driving in this model is introduced in the form of a rapidly oscillating magnetic field perpendicular to the 2D lattice plane. This is a notoriously hard problem because as magnetic flux varies with time, the q-subband structure is no longer present. In fact, q is an extremely discontinuous function of time and of course it cannot be ascribed a closed form description. This variant of the AAH model was absent in scientific literature until our recent publication [56]. We deal with this problem using the time-independent effective Hamiltonian picture presented in Chapter 5.

7.1   Effective Hamiltonian

Magnetic vector potential $\mathbf{A}(t)$ (written in Landau gauge) is

$$\mathbf{A}(t) = Bx \cos(\omega t)\hat{\mathbf{y}} \tag{7.1}$$

where ω is the driving frequency, and it is assumed to be very high. The Hamiltonian in the tight-binding form is

$$\hat{H} = \sum_n |n\rangle \langle n+1| + |n\rangle \langle n-1| + V_0 \cos(2\pi\alpha_0 n \cos(\omega t) + \theta) |n\rangle \langle n| \tag{7.2}$$

The effective Hamiltonian up to order $\mathcal{O}(\frac{1}{\omega^3})$ is

$$\begin{aligned}
\hat{H}_{eff} = &\sum_n |n\rangle \langle n+1| + |n\rangle \langle n-1| + V_0 \cos(\theta) \sum_n \mathcal{J}_0(2\pi\alpha_0 n) |n\rangle \langle n| \\
&- \frac{1}{2\omega^2} V_0^2 \cos^2(\theta) \sum_n \sum_{j=1} (\mathcal{J}_{2j}(2\pi\alpha_0(n+1)) - \mathcal{J}_{2j}(2\pi\alpha_0 n))^2 |n\rangle \langle n+1| \\
&- \frac{1}{2\omega^2} V_0^2 \sin^2(\theta) \sum_n \sum_{j=1} (\mathcal{J}_{2j-1}(2\pi\alpha_0(n+1)) - \mathcal{J}_{2j-1}(2\pi\alpha_0 n))^2 |n\rangle \langle n+1| \\
&+ h.c.
\end{aligned} \tag{7.3}$$

Effective Hamiltonian is found to have retained the tri-diagonal structure in position space.

7.2   Metal-Insulator transition

This model also displays a sharp metal-insulator transition like the AAH model. However, it is not self-dual. A detailed discussion can be found in [56].

Figure 7.1: The metal-to-insulator transition of the Effective Hamiltonian for the systems ground state. Plots (c) and (d) are the real- and dual-space plots for the ground state with phase $\theta = 0$.
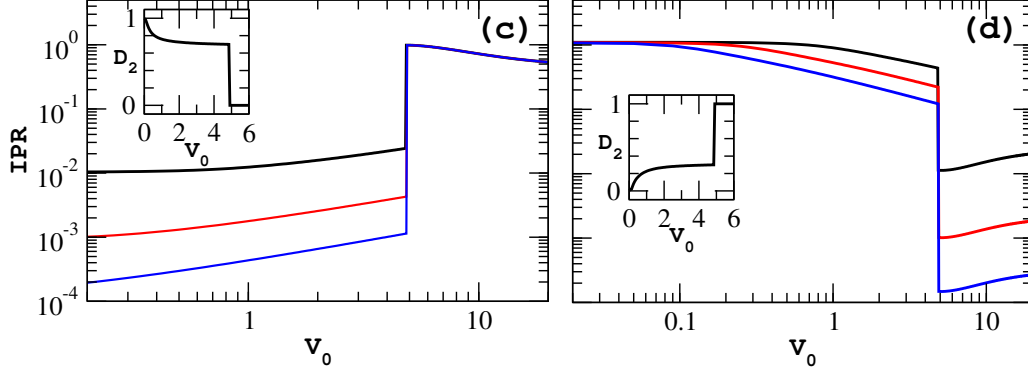
7.3   Spectrum

The striking feature of the spectrum is the presence of energy-dependent mobility edge, an edge that splits the spectrum into two regions, one containing localized states and other containing delocalized states. This is a significant result as the mobility edge is atypical of 1-dimensional models [56].

In order to qualitatively analyze some of our results we consider a simplified model comprising of a trivial constant hopping term and an on-site potential T which is aperiodic or quasi-periodic. The Schrödinger equation is given by

$$a_{n+1} + a_{n-1} + \Lambda T(\alpha_0 n + \phi)a_n = E a_n \tag{7.4}$$

where, Λ is the strength of on-site energy and E are the energy eigenvalues. One can go to the dual space for the above system by defining an expansion, as follows

$$a_n = \frac{e^{ikn}}{\sqrt{L}} \sum_m \tilde{a}_m e^{i m(\alpha_0 n + \phi)} \tag{7.5}$$

where, the $\tilde{a}_m$'s are the dual space amplitudes, and k is a wave vector from the Bloch wave expansion ansatz. This allows T to be expressed as

$$T(\alpha_0 n + \phi) = \frac{1}{\sqrt{L}} \sum_{\acute{m}} \mathcal{T}_{\acute{m}} e^{i \acute{m}(\alpha_0 n + \phi)}. \tag{7.6}$$

Equations (7.5) and (7.6) yield an on-site term in the dual space from the the hopping terms of Eq.(7.4) as

$$a_{n-1} + a_{n+1} = \frac{e^{ikn}}{\sqrt{L}} \sum_m \tilde{a}_m e^{i m(\alpha_0 n + \phi)} \cos(\alpha_0 m + k) \tag{7.7}$$

46

with a cosine modulation of the on-site energy (as seen in the Aubry and André model). Interestingly, the real space on-site energy term transforms as

$$\Lambda T(\alpha_0 n + \phi) a_n = \frac{\Lambda e^{ikn}}{L} \sum_{\acute{m}} \sum_{m} \mathcal{T}_{\acute{m}} \tilde{a}_m e^{i(m+\acute{m})(\alpha_0 n + \phi)}. \tag{7.8}$$

The RHS can be slightly rearranged to give

$$\frac{\Lambda e^{ikn}}{L} \sum_{\acute{m} \neq \pm 1} \sum_{m} \mathcal{T}_{\acute{m}} \tilde{a}_{m+\acute{m}} e^{im(\alpha_0 n + \phi)} +$$

$$\frac{\Lambda e^{ikn}}{L} \sum_{m} (\mathcal{T}_1 \tilde{a}_{m-1} + \mathcal{T}_{-1} \tilde{a}_{m+1}) e^{im(\alpha_0 n + \phi)} \tag{7.9}$$

In the above form, the second term clearly indicates the apparent nearest neighbor hopping terms in the dual space whose strength is modulated by the Fourier components of T. It is the first term in the above expression which explicitly breaks the exact duality. The form of $\mathcal{T}_{\acute{m}}$ determines the extent to which different m values in the dual space are coupled. It is well known that for decaying oscillatory functions like Sinc and Bessel function of the zeroth order $\mathcal{T}_{\acute{m}}$ is a rectangular function, with possibly a $\acute{m}$ dependent modulation, symmetric about the origin. Thus, in our case, we expect a truncation effect in dual space which restricts the range of couplings. This deviation from exact duality is expected to have some impact on the probability of an "analytic accident" along the lines of [51]. The appearance of localized states (real eigenfunctions) happens when there are superpositions of counter-propagating plane waves with wave vectors of near-commensurate magnitude. This would mean, in our model, some harmonics from the expansion of T shall scatter the wave with wave vector k by an amount commensurate with $2n\pi$. This has to be considered together with the fact that for a rational approximation of α_0 as a ratio of two large successive Fibonacci numbers, the true momentum(Fourier) space eigenvalues κ are related to m as $\kappa = mF_{i-1} \mathrm{mod} F_i$, where F_{i-1} and F_i are successive Fibonacci numbers [54, 65]. Thus, what appear to be close neighbors in m could possibly be well separated in the actual wave vector space. Further, the range of m values that shall remain coupled in the dual space will be dictated by the extent of T in the real lattice for example the first zero in the Bessel function. The set of m's which conspires with a given k value to yield a localized state shall be dictated by V_0 and $E(k)$. This explains the energy dependent mobility edge in Fig.7.2.

In the dual space, where k acts as a phase (see Eq.(7.7)), a state localized at few m values could be shifted by large amounts for a small change in k. This allows for the interpretation that a small change in ϕ could in effect cause a state localized around some lattice site to localize about a far off site. In terms of symmetry, the absence of translational invariance in Euclidean space of quasi-periodic structures with two incommensurate periodicities can be restored in an extended space using the ϕ dimension [66, 67]. This effect of ϕ on localization properties leads to the differences between the three plots in Fig.7.2.
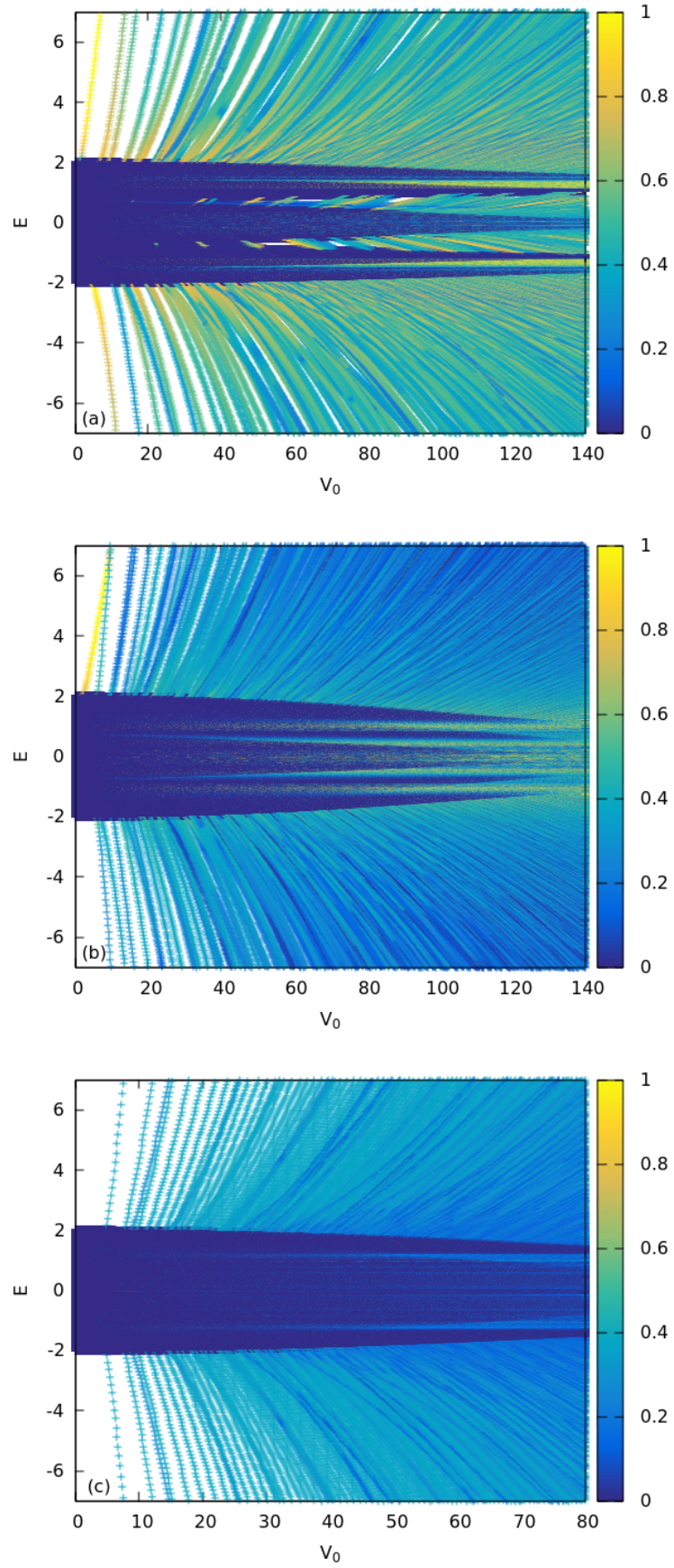
Figure 7.2: The localization phase diagram with IPR in the (E,V_0) phase plane, for lattice size L = 4181 and three values of the variable θ: (a) $\theta = 0$, (b) $\theta = \pi/4$, (c) $\theta = \pi/2$

Chapter 8

AAH model driven by Linearly Polarized Light

Chapter 9

AAH model driven by Circularly Polarized Light

Part III

Appendices

Chapter J

Effective Hamiltonian – perturbative expansion

[1] As derived in Chapter 5, we are looking to perturbatively expand the equation

$$\hat{H}_{eff} = e^{i\hat{F}(t)}\hat{H}e^{-i\hat{F}(t)} + i\frac{\partial}{\partial t}\left(e^{i\hat{F}(t)}\right)e^{-i\hat{F}(t)} \tag{J.1}$$

The entire solution is divided into

1. Initial Kick ($e^{i\hat{F}(t_i)}$)

2. Evolution under a time-independent Hamiltonian $\hat{H}_{eff}(e^{-i\hat{H}_{eff}(t_f-ti)})$

3. Final Kick ($e^{-i\hat{F}(t_i)}$)

Consider periodic potentials

$$\hat{V}(t) = \hat{V}(t+T)$$

assume T to be small and $\omega = \frac{2\pi}{T}$ to be large. Except for special cases $\hat{H}_{eff}$ cannot be obtained from (5) in a closed form.

Let us make a perturbation ansatz.

$$\hat{H}_{eff} = \sum_{0 \leq n < \infty} \frac{1}{\omega^n}\hat{H}^{(n)} \tag{J.2}$$

$$\hat{F} = \sum_{1 \leq n < \infty} \frac{1}{\omega^n}\hat{F}^{(n)} \tag{J.3}$$

Convergence is not guaranteed.

The prescription is

1. Write Eqn. (J.1) for $\hat{H}_{eff}$ as an expanded perturbation series in ($\frac{1}{\omega}$).

2. At each order of perturbation, which corresponds to a specific power of ($\frac{1}{\omega}$) retain the time-independent average in $\hat{H}_{eff}$ and adjust $\hat{F}$ to annhilate any time dependence.

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[1]This chapter was wholly borrowed from Tridev Mishra, Ph.D Student, Department of Physics, BITS Pilani. (tridevmishra@gmail.com)

3. Repeat the procedure at each order in perturbation.

We use the following identities:

$$e^{i\hat{F}}\hat{H}e^{-i\hat{F}} = \hat{H} + i[\hat{F},\hat{H}] - \frac{1}{2}\left[\hat{F},[\hat{F}'\hat{H}]\right] - \frac{i}{6}\left[\hat{F},[\hat{F},[\hat{F},\hat{H}]]\right] + \dots \qquad (J.4)$$

$$\left(\frac{\partial}{\partial t}e^{\hat{F}}\right)e^{-i\hat{F}} = i\frac{\partial\hat{F}}{\partial t} - \frac{1}{2}[\hat{F},\frac{\partial\hat{F}}{\partial t}] - \frac{i}{6}\left[\hat{F},[\hat{F},\frac{\partial\hat{F}}{\partial t}]\right] + \dots \qquad (J.5)$$

Substituting $\hat{H}_{eff} = \sum_{0 \leq n < \infty} \frac{1}{\omega^n}\hat{H}^{(n)}$ and $\hat{F} = \sum_{1 \leq n < \infty} \frac{1}{\omega^n}\hat{F}^{(n)}$ in Eqn. (J.1) and only retaining upto $\mathcal{O}\left(\frac{1}{\omega^2}\right)$ we have

$$\hat{H}_{eff} = \hat{H}_o + \hat{V}(t) + i\left[\frac{\hat{F}^{(1)}}{\omega},\hat{H}\right] + i\left[\frac{\hat{F}^{(2)}}{\omega^2},\hat{H}\right] - \frac{1}{2}\left[\frac{\hat{F}^{(1)}}{\omega},\left[\frac{\hat{F}^{(1)}}{\omega},\hat{H}\right]\right] - \frac{1}{\omega}\frac{\partial\hat{F}^{(1)}}{\partial t} - \frac{1}{\omega^2}\frac{\partial\hat{F}^{(2)}}{\partial t}$$

$$- \frac{1}{\omega^3}\frac{\partial\hat{F}^{(2)}}{\partial t} - \frac{i}{2}\left[\frac{\hat{F}^{(1)}}{\omega} + \frac{\hat{F}^{(2)}}{\omega^2}, \frac{1}{\omega}\frac{\partial\hat{F}^{(1)}}{\partial t} + \frac{1}{\omega^2}\frac{\partial\hat{F}^{(2)}}{\partial t}\right] + \frac{1}{6}\left[\frac{\hat{F}^{(1)}}{\omega},\left[\frac{\hat{F}^{(1)}}{\omega},\frac{1}{\omega}\frac{\partial\hat{F}^{(1)}}{\partial t}\right]\right]$$

The operator $\hat{F}$ is periodic with period T and has zero mean.

$$\Rightarrow \frac{1}{T}\int_0^T \hat{F}dt = 0$$

$\Rightarrow \hat{F}^{(n)}$ are all periodic and have zero mean or

$$\langle\hat{F}^{(n)}\rangle = 0$$
$$\hat{F}^{(n)}(t+T) = \hat{F}^{(n)}(t)$$

At each order in perturbation, the time independent average is retained in $\hat{H}_{eff}$ and $\hat{F}$ is used to nullify the time dependent part.

ORDER ω^0 :

$$\hat{H}_0 + \hat{V}(t) - \frac{1}{\omega}\frac{\partial\hat{F}^{(1)}}{\partial t}$$

$$H_{eff}^{(0)} = \left\langle \hat{H}_0 + \hat{V}(t) - \frac{1}{\omega}\frac{\partial\hat{F}^{(1)}}{\partial t}\right\rangle$$

$$= \langle\hat{H}_0\rangle + \langle\hat{V}(t)\rangle - \frac{1}{\omega}\left\langle\frac{\partial\hat{F}^{(1)}}{\partial t}\right\rangle$$

$$= \frac{\hat{H}_0}{T}\int_0^T dt + \frac{1}{T}\int_0^T \hat{V}(t)dt - \frac{1}{\omega T}\int_0^T \frac{\partial\hat{F}^{(1)}}{\partial t}dt$$

$$\hat{V}(t) = \hat{V}(t + T)$$

$\hat{V}(t)$ may be expanded in a Fourier series as

$$\hat{V}(t) = \hat{V}_0 + \sum_{1 \leq n < \infty} \hat{V}_n e^{in\omega t} + \sum_{1 \leq n < \infty} \hat{V}_{-n} e^{-in\omega t}$$

$\hat{F}^{(1)}$ can be expanded similarly but $\hat{F}^{(1)}$ has zero mean. So $\frac{\partial \hat{F}^{(1)}}{\partial t}$ also has zero mean.

$$H_{eff}^{(0)} = \hat{H}_0 + \hat{V}_0 \qquad \hat{V}_0 = \frac{1}{T} \int_{0 \leq t \leq T} \hat{V}(t) dt$$

The time dependent part is

$$\hat{H}_0 + \hat{V}(t) - \frac{1}{\omega} \frac{\partial \hat{F}^{(1)}}{\partial t} - \left\langle \hat{H}_0 + \hat{V}(t) - \frac{1}{\omega} \frac{\partial \hat{F}^{(1)}}{\partial t} \right\rangle$$

$$\Rightarrow \hat{V}(t) - \hat{V}_0 - \frac{1}{\omega} \frac{\partial \hat{F}^{(1)}}{\partial t}$$

(equating this to zero)

or

$$\sum_{1 \leq n < \infty} \hat{V}_n e^{in\omega t} + \sum_{1 \leq n < \infty} \hat{V}_{-n} e^{-in\omega t} = \frac{1}{\omega} \frac{\partial \hat{F}^{(1)}}{\partial t}$$

$$\Rightarrow \hat{F}^{(1)} = \omega \int_0^t \left(\sum_{1 \leq n < \infty} \hat{V}_n e^{in\omega t'} + \sum_{1 \leq n < \infty} \hat{V}_{-n} e^{-in\omega t'} \right) dt'$$

$$\Rightarrow \frac{1}{i} \sum_{1 \leq n < \infty} \frac{1}{n} \left(\hat{V}_n e^{in\omega t} - \hat{V}_{-n} e^{-in\omega t} \right)$$

or   at order ω_0

$$H_{eff}^{(0)} = \hat{H}_0 + \hat{V}_0$$

$$\hat{F}^{(1)} = \frac{1}{i} \sum_n \frac{1}{n} \left(\hat{V}_n e^{in\omega t} - \hat{V}_{-n} e^{-in\omega t} \right)$$

ORDER ω^{-1}

$$i \left[\frac{\hat{F}^{(1)}}{\omega}, \hat{H} \right] - \frac{1}{\omega^2} \frac{\partial \hat{F}^{(2)}}{\partial t} - \frac{i}{2} \left[\frac{\hat{F}^{(1)}}{\omega}, \frac{1}{\omega} \frac{\partial \hat{F}^{(1)}}{\partial t} \right]$$

$$H_{eff}^{(1)} = \left\langle i \left[\frac{\hat{F}^{(1)}}{\omega}, \hat{H} \right] \right\rangle - \left\langle \frac{1}{\omega^2} \frac{\partial \hat{F}^{(2)}}{\partial t} \right\rangle - \frac{i}{2} \left\langle \left[\frac{\hat{F}^{(1)}}{\omega}, \frac{1}{\omega} \frac{\partial \hat{F}^{(1)}}{\partial t} \right] \right\rangle$$

The second bracket in the above expression is put to zero.Hence

$$H_{eff}^{(1)} = i\left\langle\left[\frac{\hat{F}^{(1)}}{\omega}, \hat{H}\right]\right\rangle - \frac{i}{2}\left\langle\left[\frac{\hat{F}^{(1)}}{\omega}, \frac{1}{\omega}\frac{\partial\hat{F}^{(1)}}{\partial t}\right]\right\rangle$$

$$= i\left\langle\left[\frac{\hat{F}^{(1)}}{\omega}, (\hat{V}(t) - \hat{V}_0)\right]\right\rangle - \frac{i}{2}\left\langle\left[\frac{\hat{F}^{(1)}}{\omega}, (\hat{V}(t) - \hat{V}_0)\right]\right\rangle$$

$$= \frac{i}{2}\left\langle\left[\frac{\hat{F}^{(1)}}{\omega}, (\hat{V}(t) - \hat{V}_0)\right]\right\rangle$$

$$\hat{V}(t) - \hat{V}_0 = \sum_n \frac{1}{n}\left(\hat{V}_n e^{in\omega t} - \sum_n \hat{V}_{-n}e^{-in\omega t}\right)$$

$$\hat{F}^{(1)} = \int^t (\hat{V}(\acute{t}) - \hat{V}_0)d\acute{t}$$

$$\frac{\hat{F}^{(1)}}{\omega} = \sum_n\left(\frac{\hat{V}_n e^{in\omega t}}{in\omega} - \frac{\hat{V}_{-n}e^{-in\omega t}}{in\omega}\right)$$

$$\left\langle\frac{\hat{F}^{(1)}}{\omega}(\hat{V}(t) - \hat{V}_0)\right\rangle = \frac{1}{T}\int_0^t \sum_{n,m}\left(\frac{\hat{V}_n e^{in\omega\acute{t}}}{in\omega} - \frac{\hat{V}_{-n}e^{-in\omega\acute{t}}}{in\omega}\right)\left(\hat{V}_m e^{im\omega\acute{t}} + \hat{V}_{-m}e^{-im\omega\acute{t}}\right)$$

$$= \frac{1}{T}\int_0^T d\acute{t} \sum_{m,n}\frac{\hat{V}_n\hat{V}_m}{in\omega}e^{i(n+m)\omega\acute{t}} + \frac{\hat{V}_n\hat{V}_{-m}}{in\omega}e^{i(n-m)\omega\acute{t}} - \frac{\hat{V}_{-n}\hat{V}_m}{in\omega}e^{-i(n-m)\omega\acute{t}} - \frac{\hat{V}_{-n}\hat{V}_{-m}}{in\omega}e^{-i(n+m)\omega\acute{t}}$$

$$= \sum_n \frac{\hat{V}_n\hat{V}_{-n}}{in\omega} - \frac{\hat{V}_{-n}\hat{V}_n}{in\omega} \tag{J.6}$$

$$\left\langle(\hat{V}(t) - \hat{V}_0)\frac{\hat{F}^{(1)}}{\omega}\right\rangle = \sum_n \frac{\hat{V}_{-n}\hat{V}_n}{in\omega} - \frac{\hat{V}_n\hat{V}_{-n}}{in\omega} = \sum_n \frac{2}{in\omega}[\hat{V}_n, \hat{V}_{-n}] \tag{J.7}$$

or

$$H_{eff} = \frac{i}{2}\sum_n \frac{2}{in\omega}[\hat{V}_n, \hat{V}_{-n}]$$

$$= \sum_n \frac{1}{n\omega}[\hat{V}_n, \hat{V}_{-n}]$$

$$i\left[\frac{\hat{F}^{(1)}}{\omega}, \hat{H}\right] - \frac{1}{\omega^2}\frac{\partial \hat{F}^{(2)}}{\partial t} - \frac{i}{2}\left[\hat{F}^{(1)}, \frac{\partial \hat{F}^{(1)}}{\partial t}\right] - \sum_n \frac{1}{n\omega}[\hat{V}_n, \hat{V}_{-n}] = 0$$

$$\Rightarrow \hat{F}^{(2)} = \frac{1}{i}\sum_n \frac{1}{n^2}\left([\hat{V}_n, \hat{H}_0 + \hat{V}_0]e^{in\omega t} - h.c.\right) + \frac{1}{2i}\sum_{n,m=1}^{\infty} \frac{1}{n(n+m)}\left([\hat{V}_n, \hat{V}_m]e^{i(n+m)\omega t} + h.c.\right)$$

$$+ \frac{1}{2i}\sum_{n\neq m=1}^{\infty} \frac{1}{n(n+m)}\left([\hat{V}_n, \hat{V}_{-m}]e^{i(n-m)\omega t} + h.c.\right)$$

Finally, we have in the same manner

$$\hat{H}_{eff} = \hat{H}_0 + \hat{V}_0 + \frac{1}{\omega}\sum_{n=1}^{\infty}\frac{1}{n}[\hat{V}_n, \hat{V}_{-n}] + \frac{1}{2\omega^2}\sum_{n=1}^{\infty}\frac{1}{n^2}\left(\left[[\hat{V}_n, \hat{H}_0], \hat{V}_{-n}\right] + h.c.\right)$$

$$+ \frac{1}{3\omega^2}\sum_{n,m=1}^{\infty}\frac{1}{nm}\left(\left[\hat{V}_n, [\hat{V}_m, \hat{V}_{-(n+m)}]\right] - 2\left[\hat{V}_n, [\hat{V}_{-n}, \hat{V}_{(n-m)}]\right] + h.c.\right)$$

and

$$\hat{F}(t) = \frac{1}{i\omega}\sum_{n=1}^{\infty}\frac{1}{n}\left(\hat{V}_n e^{in\omega t} - \hat{V}_{-n}e^{-in\omega t}\right) + \frac{1}{i\omega^2}\sum_{n=1}^{\infty}\frac{1}{n^2}\left([\hat{V}_n, \hat{H}_0 + \hat{V}_0]e^{in\omega t} - h.c.\right)$$

$$+ \frac{1}{2i\omega^2}\sum_{n,m=1}^{\infty}\frac{1}{n(n+m)}\left([\hat{V}_n, \hat{V}_m]e^{i(n+m)\omega t} - h.c.\right) + \frac{1}{2i\omega^2}\sum_{n\neq m=1}^{\infty}\frac{1}{n(n-m)}\left([\hat{V}_n, \hat{V}_{-m}]e^{i(n-m)\omega t} - h.c.\right)$$

Proof not shown here but the prescription is as before.

Chapter K

Brillouin-Wigner Effective Hamiltonian

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