

# Notes on Classical Floquet Theory

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2020 April 12

## 1: Bloch's Theorem

As always, the simplest place is to start with what we know well, which in this case is nonrelativistic quantum mechanics. In particular, we'll start with the proof of Bloch's theorem for periodic potentials, and then examine how this generalizes to the classical Floquet theory for ordinary differential equations.

### 1.1: Bravais Lattice Vectors

We start with the single-electron Schrödinger equation in a lattice. The underlying structure of the lattice is defined by the *Bravais lattice vectors*  $\{R^\mu\} \subset \mathbb{R}^m$ , which are the set of vectors from the origin that define the entire lattice. We can define the  $\{R^\mu\}$ s in terms of a set of *primitive basis vectors*  $\{a_i^\mu\} \subset \mathbb{R}^m$ :

$$R^\mu = \sum_i n_i a_i^\mu \quad (1)$$

Here,  $n_i \in \mathbb{Z}$ . The primitive basis vectors are a set of vectors in  $\mathbb{R}^m$  where at least two of the vectors are not coplanar. Unsurprisingly, this is just a new basis for m-dimensional space; all points in space can be reached by some linear combination of the  $a_i^\mu$ s. This basis ultimately lets us define the primitive cell of the lattice, and the goal here will be to distinguish intra-cell dynamics, useful because of the periodicity of most of the dynamics.

(This is the goal of most of the times we use the lattice; although the primitive cell the  $\{a_i^\mu\}$ s define isn't unique, because the periodicity is an inter-cell property, we can define our cell and then examine intra-cell dynamics. If we're pressed for uniqueness, we can always use the locus of points closer to a given lattice point than any other lattice points: this is the *Wigner-Seitz cell*, which is unique.)

We can further define the *reciprocal lattice* as the set of the wave vectors  $K_\mu$  that satisfy  $e^{iK_\mu R^\mu} = 1$ . The set of  $K_\mu$  that satisfy this relation forms its own Bravais lattice in momentum space; naturally, this lattice is the dual lattice to the original lattice. Unsurprisingly, the double dual (i.e. the dual of the reciprocal lattice) is just the original lattice again. In terms of the Bravais lattice basis vectors  $a_i^\mu$ , we have the reciprocal lattice basis vectors  $b_{i\mu}$  as:

$$b_{1\mu} = 2\pi \frac{a_2^\nu a_3^\sigma \epsilon_{\mu\nu\sigma}}{a_1^\rho a_2^\nu a_3^\sigma \epsilon_{\nu\sigma\rho}}, \quad b_{2\mu} = 2\pi \frac{a_3^\nu a_1^\sigma \epsilon_{\mu\nu\sigma}}{a_1^\rho a_2^\nu a_3^\sigma \epsilon_{\nu\sigma\rho}}, \quad b_{3\mu} = 2\pi \frac{a_1^\nu a_2^\sigma \epsilon_{\mu\nu\sigma}}{a_1^\rho a_2^\nu a_3^\sigma \epsilon_{\nu\sigma\rho}} \quad (2)$$

Particularly notable is that the  $a_i^\mu$ s and  $b_{i\mu}$ s satisfy:

$$b_{i\mu} a_j^\mu = 2\pi \delta_{ij} \quad (3)$$

## 1.2: Properties of Translation Operators

Before we rederive Bloch's theorem, we also need to use the properties of translation operators, which we'll list and prove here. We'll start with the general translation operator  $\hat{T}(r^\mu)$ , defined by  $\hat{T}(r^\mu)\{f(x^\mu)\} := f(x^\mu + r^\mu)$ , as well as the definition of the momentum operator as the generator of translations:

$$\hat{p}_\mu = i\hbar \left( \partial_\mu \hat{T}(r^\mu) \right)_{r^\mu=0^\mu} = i\hbar \frac{r^\mu}{\|r^\mu\|} \lim_{\epsilon \rightarrow 0} \frac{\hat{T}(\epsilon r^\mu) - 1}{\epsilon} \quad (4)$$

The properties of translation operators, with brief proofs, are:

1.)  $\hat{T}(0^\mu) = 1$ .

– Pf.: Applying  $\hat{T}(0^\mu)$  to a position eigenstate  $|q^\mu\rangle$  gives:  $\hat{T}(0^\mu)|q^\mu\rangle = |q^\mu + 0^\mu\rangle = |q^\mu\rangle = 1|q^\mu\rangle$ . //

2.)  $\hat{T}(r^\mu)\hat{T}(s^\mu) = \hat{T}(r^\mu + s^\mu)$ .

– Pf.: Applying  $\hat{T}(r^\mu)\hat{T}(s^\mu)$  to  $|q^\mu\rangle$  gives:

$$\begin{aligned} \hat{T}(r^\mu)\hat{T}(s^\mu)|q^\mu\rangle &= \hat{T}(r^\mu)|q^\mu + s^\mu\rangle = |q^\mu + s^\mu + r^\mu\rangle \\ \hat{T}(r^\mu)\hat{T}(s^\mu)|q^\mu\rangle &= |q^\mu + (r^\mu + s^\mu)\rangle = \hat{T}(r^\mu + s^\mu)|q^\mu\rangle. // \end{aligned}$$

3.)  $\left(\hat{T}(r^\mu)\right)^{-1} = \hat{T}(-r^\mu)$ .

– Pf.:  $1 = \hat{T}(0^\mu) = \hat{T}(r^\mu - r^\mu) = \hat{T}(r^\mu)\hat{T}(-r^\mu)$ . //

4.)  $\hat{T}(r^\mu)$  is unitary.

– Pf.: In position space,  $\langle\phi(x^\mu)|\psi(x^\mu)\rangle$  is given by:

$$\langle\phi(x^\mu)|\psi(x^\mu)\rangle = \int d^k x^\mu \phi^*(x^\mu) \psi(x^\mu) \quad (5)$$

Meanwhile,  $\langle\hat{T}(r^\mu)\{\phi(x^\mu)\}|\hat{T}(r^\mu)\{\psi(x^\mu)\}\rangle$  is given by:

$$\langle\hat{T}(r^\mu)\{\phi(x^\mu)\}|\hat{T}(r^\mu)\{\psi(x^\mu)\}\rangle = \langle\phi(x^\mu + r^\mu)|\psi(x^\mu + r^\mu)\rangle = \int d^k x^\mu \phi^*(x^\mu + r^\mu) \psi(x^\mu + r^\mu)$$

Under the change of variables  $x^\mu \mapsto y^\mu := x^\mu + r^\mu$ , we have  $dy^\mu = d[x^\mu + r^\mu] = dx^\mu + d\cancel{r^\mu} = dx^\mu$ , giving:

$$\langle\hat{T}(r^\mu)\{\phi(x^\mu)\}|\hat{T}(r^\mu)\{\psi(x^\mu)\}\rangle = \int d^k x^\mu \phi^*(x^\mu + r^\mu) \psi(x^\mu + r^\mu) = \int d^k y^\mu \phi^*(y^\mu) \psi(y^\mu)$$

Since this is the exact same expression as we had with  $\langle\phi(x^\mu)|\psi(x^\mu)\rangle$ , this gives:

$$\langle\hat{T}(r^\mu)\{\phi(x^\mu)\}|\hat{T}(r^\mu)\{\psi(x^\mu)\}\rangle = \langle\phi(x^\mu)|\psi(x^\mu)\rangle$$

Thus,  $\hat{T}^\dagger = \hat{T}^{-1}$ . //

5.)  $[\hat{T}(r^\mu), \hat{T}(s^\mu)] = 0$ .

– Pf.:  $\hat{T}(r^\mu) \hat{T}(s^\mu) = \hat{T}(r^\mu + s^\mu) = \hat{T}(s^\mu + r^\mu) = \hat{T}(r^\mu) \hat{T}(s^\mu).$

6.)  $[\hat{q}^\mu, \hat{T}(r^\mu)] = r^\mu \hat{T}(r^\mu).$

– Pf.: Applying  $[\hat{q}^\mu, \hat{T}(r^\mu)]$  to  $|q^\mu\rangle$  gives:

$$[\hat{q}^\mu, \hat{T}(r^\mu)]|q^\mu\rangle = \hat{q}^\mu \hat{T}(r^\mu)|q^\mu\rangle - \hat{T}(r^\mu) \hat{q}^\mu|q^\mu\rangle = \hat{q}^\mu|q^\mu + r^\mu\rangle - q^\mu \hat{T}(r^\mu)|q^\mu\rangle$$

$$[\hat{q}^\mu, \hat{T}(r^\mu)]|q^\mu\rangle = (q^\mu + r^\mu)|q^\mu + r^\mu\rangle - q^\mu|q^\mu + r^\mu\rangle = r^\mu|q^\mu + r^\mu\rangle$$

As an operator, this is just a translation operator times the translation scale factor:

$$[\hat{q}^\mu, \hat{T}(r^\mu)]|q^\mu\rangle = r^\mu|q^\mu + r^\mu\rangle = r^\mu \hat{T}(r^\mu)|q^\mu\rangle.$$

7.)  $[\hat{p}_\mu, \hat{T}(x^\mu)] = 0.$

– Pf.: We start again with the definition of momentum in terms of the translation operator:

$$\hat{p}_\mu = i\hbar \left( \partial_\mu \hat{T}(r^\mu) \right)_{r^\mu=0^\mu} = i\hbar \frac{r^\mu}{\|r^\mu\|} \lim_{\epsilon \rightarrow 0} \frac{\hat{T}(\epsilon r^\mu) - \mathbb{1}}{\epsilon} = i\hbar \frac{r^\mu}{\|r^\mu\|} \lim_{\epsilon \rightarrow 0} \frac{\hat{T}(\epsilon r^\mu) - \hat{T}(0^\mu)}{\epsilon}$$

This gives the commutator as:

$$[\hat{p}_\mu, \hat{T}(r^\mu)] = \left[ i\hbar \frac{r^\mu}{\|r^\mu\|} \lim_{\epsilon \rightarrow 0} \frac{\hat{T}(\epsilon r^\mu) - \hat{T}(0^\mu)}{\epsilon}, \hat{T}(x^\mu) \right]$$

$$[\hat{p}_\mu, \hat{T}(r^\mu)] = i\hbar \frac{r^\mu}{\|r^\mu\|} \lim_{\epsilon \rightarrow 0} \frac{1}{\epsilon} ([\hat{T}(\epsilon r^\mu), \hat{T}(x^\mu)] - [\hat{T}(0^\mu), \hat{T}(x^\mu)])$$

As shown earlier,  $[\hat{T}(r^\mu), \hat{T}(s^\mu)] = 0$ , so both of these commutators vanish, and  $[\hat{p}_\mu, \hat{T}(r^\mu)] = 0.$

Before moving on, it's worth noting that the set of all translation operators forms a continuous Abelian group (unsurprisingly called the translation group,  $T(m)$ ). If we consider the group of all of the transformations that preserve distances in  $\mathbb{R}^m$  (i.e. the translations, rotations, and reflections), called the Euclidean group  $E(m)$ . Then,  $T(m)$  is the quotient group  $T(m) = E(m)/O(m)$ , where  $O(m)$  is the orthogonal group.

### 1.3: Bloch's Theorem

Now, finally, with the Bravais lattice vectors and the properties of translation operators in hand, we can examine the one-electron Schrödinger equation:

$$\hat{H}|\Psi\rangle = \left( -\frac{\hbar^2 \partial_\mu \partial^\mu}{2m} + \hat{U}(r^\mu) \right) |\Psi\rangle = \left( \frac{\hat{p}_\mu^2}{2m} + \hat{U}(r^\mu) \right) |\Psi\rangle = E|\Psi\rangle \quad (6)$$

Here, we enforce that  $\hat{U}(r^\mu)$  is a periodic potential; i.e. for all  $R^\mu$ , we have  $\hat{U}(r^\mu + R^\mu) = \hat{U}(r^\mu)$ . With this, we have Bloch's theorem<sup>[1]</sup> as:

## Bloch's Theorem Claim

The eigenstates  $\{|\psi_{k,n}\rangle\}$  of a Hamiltonian with a periodic potential  $\hat{U}(r^\mu + R^\mu) = \hat{U}(r^\mu)$  have the form  $\{|\psi_{k,n}\rangle\} = e^{ik_\mu r^\mu} \{|u_{k,n}(r^\mu)\rangle\}$ , where  $|u_{k,n}(r^\mu + R^\mu)\rangle = |u_{k,n}(r^\mu)\rangle$  for all Bravais lattice vectors  $R^\mu$  and some  $k_\mu$ .

## Bloch's Theorem Proof

For the Bravais lattice vectors  $R^\mu$ , we define the translation operator  $\hat{T}_R$  as  $\hat{T}_R f(r^\mu) := f(r^\mu + R^\mu)$ . The set of all  $\{\hat{T}_R\}$ s form a (normal Abelian) group; it's actually this set that *defines* the Bravais lattice properly.

We can immediately note that  $\hat{T}(R^\mu)$  for a generic lattice vector  $R^\mu$  commutes with  $\hat{H}$ . Starting with  $[\hat{T}_R, \hat{H}]$ , we have:

$$[\hat{T}_R, \hat{H}] = \left[ \hat{T}_R, \frac{\hat{p}_\mu^2}{2m} + \hat{U}(r^\mu) \right] = \left[ \hat{T}_R, \frac{\hat{p}_\mu^2}{2m} \right] + [\hat{T}_R, \hat{U}(r^\mu)]$$

We get  $[\hat{T}_R, \hat{U}(r^\mu)] = 0$  when examining the action on a generic state  $|\Psi(r^\mu)\rangle$ :

$$\begin{aligned} [\hat{T}_R, \hat{U}(r^\mu)]|\Psi(r^\mu)\rangle &= \hat{T}_R \{ \hat{U}(r^\mu) |\Psi(r^\mu)\rangle \} - \hat{U}(r^\mu) \{ \hat{T}_R |\Psi(r^\mu)\rangle \} \\ [\hat{T}_R, \hat{U}(r^\mu)]|\Psi(r^\mu)\rangle &= \hat{U}(r^\mu + R^\mu) |\Psi(r^\mu + R^\mu)\rangle - \hat{U}(r^\mu) |\Psi(r^\mu + R^\mu)\rangle \\ [\hat{T}_R, \hat{U}(r^\mu)]|\Psi(r^\mu)\rangle &= \hat{U}(r^\mu + R^\mu) |\Psi(r^\mu + R^\mu)\rangle - \hat{U}(r^\mu) |\Psi(r^\mu + R^\mu)\rangle = 0 \end{aligned} \quad (7)$$

Additionally, since all of the  $\{\hat{T}_R\}$ s commute with each other, we have  $\{\hat{H}, \hat{T}_R\}$  as a set of commuting operators (not a *complete* set yet, though!), and thus we can simultaneously diagonalize them. For the eigenstates  $|\psi\rangle$  of  $\hat{H}$  with eigenvalue  $E_n$ , we have:

$$\hat{H}|\psi(r^\mu)\rangle = E_n |\psi(r^\mu)\rangle; \quad \hat{T}_R |\psi(r^\mu)\rangle = c(R^\mu) |\psi(r^\mu)\rangle \quad (8)$$

(Here, the  $c(R^\mu)$ s are just the eigenvalues of the translation operator.) However, due to the composition property  $\hat{T}_R \hat{T}_S = \hat{T}_{R+S}$  of translation vectors, the  $c(R^\mu)$ s are related with each other. Applying this property to the eigenvalues:

$$\begin{aligned} \hat{T}_R \hat{T}_S |\psi(r^\mu)\rangle &= c(R^\mu) c(S^\mu) |\psi(r^\mu)\rangle; \quad \hat{T}_{R+S} |\psi(r^\mu)\rangle = c(R^\mu + S^\mu) |\psi(r^\mu)\rangle \\ c(R^\mu) c(S^\mu) &= c(R^\mu + S^\mu) \end{aligned} \quad (9)$$

Heuristically, this implies that  $c(R^\mu)$  will be an exponential. Thus, as a function of the Bravais lattice vector,  $c(R^\mu)$  will look something like  $c(R^\mu) = e^{\mathcal{P}_\mu R^\mu}$  or  $c(R^\mu) = e^{g_{\mu\nu} v^\mu R^\nu}$  for some appropriate  $v^\mu$  or  $\mathcal{P}_\mu$ . (I think this can be formally proved, but I don't really have the time or the motivation; heuristic is good enough.) As a scalar, this is just a complex exponential:  $c(R^\mu) = e^\omega$  for some  $\omega \in \mathbb{C}$ .

We'll set the eigenvalue of  $\hat{T}_{a_i}$  as  $\hat{T}_{a_i}|\psi(r^\mu)\rangle = e^{2\pi i\theta_i}|\psi(r^\mu)\rangle$ , and deal entirely with the  $\{\theta_i\}$ s now. (The extra factor of  $2\pi i$  will help later.) Since the  $\{a_i^\mu\}$ s formed a basis for every  $R^\mu$ , we had  $R^\mu = \sum_i n_i a_i^\mu$ , so  $\hat{T}_R = \hat{T}_{\sum_i n_i a_i}$ . Using the composition property  $\hat{T}_R \hat{T}_S = \hat{T}_{R+S}$ , this gives an expression for  $c(R^\mu)$  in terms of the  $\{\theta_i\}$ s:

$$\begin{aligned}\hat{T}_R|\psi(r^\mu)\rangle &= \hat{T}_{\sum_i n_i a_i}|\psi(r^\mu)\rangle = \prod_i \hat{T}_{n_i a_i}|\psi(r^\mu)\rangle = \prod_i \hat{T}_{\sum_{j=1}^{n_i} a_i}|\psi(r^\mu)\rangle = \prod_i \prod_{j=1}^{n_i} \hat{T}_{a_i}|\psi(r^\mu)\rangle \\ \hat{T}_R|\psi(r^\mu)\rangle &= \prod_i (\hat{T}_{a_i})^{n_i}|\psi(r^\mu)\rangle = \prod_i (e^{2\pi i\theta_i})^{n_i}|\psi(r^\mu)\rangle = \prod_i e^{2\pi i n_i \theta_i}|\psi(r^\mu)\rangle\end{aligned}\quad (10)$$

(Explicitly, we have  $c(R^\mu) = \prod_i e^{2\pi i n_i \theta_i}$ .) Now, we can finally prove Bloch's theorem: defining  $k_\mu := \sum_j \theta_j b_{j\mu}$ , where the  $\{\theta_j\}$ s are the *same* as the  $\{\theta_i\}$ s in the eigenvalues  $e^{2\pi i\theta_i}$  of the  $\{a_i\}$ s, we can define the function  $|u(r^\mu)\rangle := e^{-ik_\mu r^\mu}|\psi(r^\mu)\rangle$ . Then, the action of  $\hat{T}_R$  on  $|u(r^\mu)\rangle$  gives:

$$\begin{aligned}\hat{T}_R|u(r^\mu)\rangle &= \hat{T}_R\{e^{-ik_\mu r^\mu}|\psi(r^\mu)\rangle\} = e^{-ik_\mu(r^\mu+R^\mu)}(\hat{T}_R|\psi(r^\mu)\rangle) = e^{-ik_\mu r^\mu} e^{-ik_\mu R^\mu} \left(\prod_i e^{2\pi i n_i \theta_i}\right)|\psi(r^\mu)\rangle \\ \hat{T}_R|u(r^\mu)\rangle &= e^{-ik_\mu r^\mu} \left(\exp\left\{-i \sum_{i,j} (\theta_j b_{j\mu})(n_i a_i^\mu)\right\}\right) \left(\prod_i e^{2\pi i n_i \theta_i}\right)|\psi(r^\mu)\rangle\end{aligned}$$

Equation (3) gave us  $b_{j\mu} a_i^\mu = 2\pi\delta_{ij}$ , so this simplifies to:

$$\begin{aligned}\hat{T}_R|u(r^\mu)\rangle &= e^{-ik_\mu r^\mu} \left(\exp\left\{-2\pi i \sum_{i,j} \theta_j n_i \delta_{ij}\right\}\right) \left(\prod_i e^{2\pi i n_i \theta_i}\right)|\psi(r^\mu)\rangle \\ \hat{T}_R|u(r^\mu)\rangle &= e^{-ik_\mu r^\mu} e^{-2\pi i \sum_i n_i \theta_i} \left(\prod_i e^{2\pi i n_i \theta_i}\right)|\psi(r^\mu)\rangle = e^{-ik_\mu r^\mu} \left(\prod_i e^{-2\pi i n_i \theta_i}\right) \left(\prod_i e^{2\pi i n_i \theta_i}\right)|\psi(r^\mu)\rangle \\ \hat{T}_R|u(r^\mu)\rangle &= |u(r^\mu + R^\mu)\rangle = e^{-ik_\mu r^\mu}|\psi(r^\mu)\rangle = |u(r^\mu)\rangle\end{aligned}\quad (11)$$

Thus,  $|u(r^\mu)\rangle$  has the same periodicity as the potential (i.e.  $|u(r^\mu + R^\mu)\rangle = |u(r^\mu)\rangle$ ), and the eigenstates  $|\psi(r^\mu)\rangle$  of the Hamiltonian with this periodic potential can be expressed as  $|\psi(r^\mu)\rangle = e^{ik_\mu r^\mu}|u(r^\mu)\rangle$ .

## 1.4: Crystal Momentum

The  $k_\mu$  covectors that we used to derive Bloch's theorem have some extremely interesting properties, which are worth looking at to understand things we'll see later in Floquet theory as well as to understand some properties of electron dynamics in lattices.

First, we note that the  $k_\mu$ s are a conserved quantity and are observable (e.g. in ARPES experiments), and are Fourier dual to the  $r^\mu$ . This makes them very momentum-like, which is the motivation for us to define the *crystal momentum*  $p_{c\mu} := \hbar k_\mu$ . Notably, the crystal momentum is generally *not* equal to (or even proportional to) the momentum.

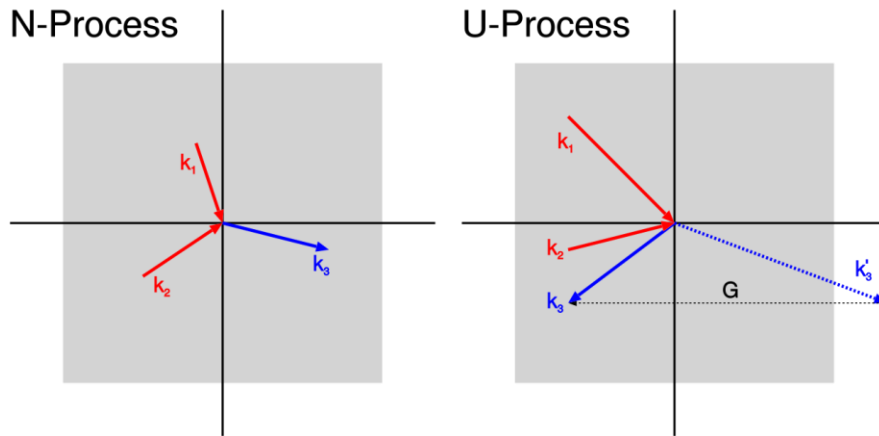
From a group theoretic perspective, we note that  $\hat{H}$  is *not* invariant under the entire translation group, but is instead invariant under the (discrete) lattice subgroup. Since  $\hat{p}_\mu$  is the generator of the *entire* translation group,  $[\hat{H}, \hat{p}_\mu] \neq 0$ , and thus they're not generally simultaneously diagonalizable. Instead, we can recognize the operator corresponding to the crystal momentum,  $\hat{p}_{c\mu}$ , as the generator of the discrete lattice translations  $\{\hat{T}_R\}$ . We can verify this through direct calculation, too, applying  $\hat{p}_\mu$  to the Bloch decomposition  $|\psi_{k,n}\rangle = e^{ik_\mu r^\mu} |u_{k,n}(r^\mu)\rangle$ :

$$\begin{aligned}\hat{p}_\mu |\psi_{k,n}\rangle &= -i\hbar \hat{\partial}_\mu |\psi_{k,n}\rangle = -i\hbar \hat{\partial}_\mu \{e^{ik_\mu r^\mu} |u_{k,n}(r^\mu)\rangle\} = \hbar k_\mu e^{ik_\mu r^\mu} |u_{k,n}(r^\mu)\rangle - i\hbar e^{ik_\mu r^\mu} \hat{\partial}_\mu |u_{k,n}(r^\mu)\rangle \\ \hat{p}_\mu |\psi_{k,n}\rangle &= \hbar k_\mu |u_{k,n}(r^\mu)\rangle - i\hbar e^{ik_\mu r^\mu} \hat{\partial}_\mu |u_{k,n}(r^\mu)\rangle\end{aligned}\quad (12)$$

In general, the second term doesn't vanish, so  $|\psi_{k,n}\rangle$  isn't generally an eigenstate of  $\hat{p}_\mu$ .

Applying the Bloch decomposition to the periodic boundary condition  $f(r^\mu + R^\mu) = f(r^\mu)$  gives two crucial additional pieces of information. First, this periodic boundary condition yields a periodic boundary condition on functions of the reciprocal lattice:  $g(k_\mu + K_\mu) = g(k_\mu)$ . This means, importantly, that crystal momentum is only conserved to *within a reciprocal lattice cell*: we can't distinguish between any given value of the crystal momentum and values of the crystal momentum that we get by adding any reciprocal lattice vector.

This is a really important feature for understanding Floquet theory, since this property shows up for the so-called *Floquet exponents*. Additionally, it gives some interesting physical effects. In *umklapp scattering*, if two particles scatter in such a way that the resulting momentum is outside the lattice, the momentum appears to be pointing in the opposite direction. Diagrammatically, this appears as:



(Diagram courtesy of Daniel Schwen<sup>[2]</sup>.) Here, the N-process is a “normal” process, whereas the U-process is the umklapp process.

## 1.5: Lessons from Bloch's Theorem

What was the point of all of this, aside from being a cute derivation in its own right? The key aspect of Bloch's theorem is the decomposition of  $|\psi(r^\mu)\rangle$  into  $e^{ik_\mu r^\mu}$  and  $|u(r^\mu)\rangle$ . The eigenstates of the total system Hamiltonian end up being decomposed into plane waves over the entire space we're considering (here, the first Brillouin zone), and a function that has the same periodicity as the potential. This decomposition is the key to

Bloch's theorem, and Floquet theory generally: for any periodic differential equation (whether in space or time), the solutions will have the form  $e^{\lambda_\mu x^\mu} f(x^\mu)$  for some  $\lambda_\mu \in \mathbb{C}^m$ . The exponential prefactor  $e^{\lambda_\mu x^\mu}$  could in principle be a decay, a plane wave, a spiraling decay, or even a spiraling growth; determining which one it is is the subject of *Floquet-Lyapunov theory*. Since everything we'll encounter physically will be plane waves, I won't touch that.

Another notable point is that we weren't free in our choice of  $k_\mu$ ; rather, the form of  $k_\mu$  was dictated by the eigenvalues  $e^{2\pi i \theta_i}$ . Additionally, we saw that the  $k_\mu$  were only uniquely specified up to the reciprocal unit cell; i.e. we had  $k_\mu + K_\mu = k_\mu$ . These properties will be relevant later on when we talk about Floquet modes, since these will be reflected in the properties of the so-called Floquet exponents. For now, we'll keep in mind the fact that although  $|\psi(r^\mu)\rangle$  can be decomposed into the periodic piece  $|u(r^\mu)\rangle$  and the plane wave piece  $e^{ik_\mu r^\mu}$ , the eigenvalues of the primitive lattice vectors (which in turn depend on the shape of the lattice) dictate the kinds of plane waves we encounter.

## 2: Floquet's Theorem

### 2.1: Fundamental Matrices and the Abel-Jacobi-Liouville Identity

Mathematicians often call Bloch's theorem a generalized version of Floquet's theorem, since it deals with functions in  $L^2(\mathbb{R}^3; \mathbb{C}^6)$  rather than simply  $L^2(\mathbb{R})$ . Still, it's worth seeing the expression of Floquet's theorem and its proof, since there's some additional information that a standard presentation of Bloch's theorem doesn't include. A fully rigorous proof from the point of view of function spaces is in [3].

Before getting to Floquet's theorem, we'll briefly define the *fundamental matrix*, which has some useful properties that don't show up in the proof of Bloch's theorem. We start with the system of  $m$  differential equations, expressed in vector form by:

$$\frac{dx^\mu(t)}{dt} = A_v^\mu(t) x^\nu(t) \quad (13)$$

(Here,  $x^\mu(t) \in \mathbb{C}^m$ , and  $A_v^\mu(t)$  is the coefficient matrix.) If we have  $\{x_a^\mu\}_{a=1}^m$  as the solutions to this equation, we can define a matrix  $X_v^\mu$  in terms of these solutions:

$$X_v^\mu(t) := \begin{bmatrix} | & \cdots & | \\ x_1^\mu(t) & \cdots & x_m^\mu(t) \\ | & \cdots & | \end{bmatrix} \quad (14)$$

If  $X_v^\mu(t)$  is invertible (i.e.  $\det X_v^\mu \neq 0$ ),  $X_v^\mu(t)$  is the *fundamental matrix*. By construction, this  $X_v^\mu(t)$  is the matrix solution to the same type of differential equation:

$$\frac{dX_v^\mu(t)}{dt} = A_\sigma^\mu(t) X_v^\sigma(t) \quad (15)$$

The fundamental matrix  $X_v^\mu(t)$  characterizes the set of all possible time evolutions that the system can take under the dynamics dictated by  $A_\sigma^\mu(t)$ ; the differential equation for  $x^\nu(t)$  then corresponds to a specific case. (An

important point to note that  $X_v^\mu(t)$  isn't unique: we can interchange the columns, scale the matrix, or do both by multiplying  $X_v^\mu(t)$  by a time-independent invertible matrix. The properties we'll use, however, are true for all possible fundamental matrices.)

The formal solution to this is familiar to us from quantum many-body theory<sup>[4]</sup>:

$$X_v^\mu(t) = U_\sigma^\mu(t, t_0) X_v^\sigma(t_0); \quad U_v^\mu(t, t_0) = \mathcal{T} \left\{ \exp \left\{ \int_{t_0}^t d\tau \operatorname{Tr} A(\tau) \right\} \right\} \quad (16)$$

Usually, we can solve this perturbatively. However, because of the periodicity of  $A_v^\mu$ , we have  $[A_v^\mu(t + nT), A_v^\mu(t + mT)] = 0$  for  $n, m \in \mathbb{Z}$ , so the Floquet property can help us avoid all of the complications of time ordering and perturbation. This holds just as true for classical Floquet theory as it does for quantum Floquet theory, as we'll see right now.

Starting with general properties, an extremely important property of *general*  $X_v^\mu$ s (including the ones solved in equation (15)) is the *Abel-Jacobi-Liouville identity*, which gives the time evolution of the determinant:

$$\det X(t) = \det X(t_0) \exp \left\{ \int_{t_0}^t d\tau \operatorname{Tr} A(\tau) \right\} \quad (17)$$

(Although for the most part I'm using Einstein convention, I find  $\operatorname{Tr} A(\tau)$  clearer than  $A_\rho^\rho(\tau)$  and  $\det X$  way clearer than  $\varepsilon_{ij\dots k} X_{1i} X_{2j} \dots X_{Nk}$ , so I'll just use these. For completeness, in Einstein convention, this would appear as:

$$\varepsilon_{ij\dots k} X_{1i} X_{2j} \dots X_{Nk}(t) = \varepsilon_{ij\dots k} X_{1i} X_{2j} \dots X_{Nk}(t_0) \exp \left\{ \int_{t_0}^t d\tau A_\rho^\rho(\tau) \right\} \quad (18)$$

This can be derived to first order using the Taylor expansion, and to all orders using the Leibniz formula for determinants. I find the Taylor expansion technique a lot clearer than the Leibniz formula; the fact that the Leibniz formula version exists implies that an all-orders Taylor expansion derivation should exist as well. I'll rederive it when time permits.

Considering the Taylor expansion of  $X_v^\mu(t)$ , we have:

$$X_v^\mu(t) = \sum_{n=0}^{\infty} \frac{d^n X_v^\mu(t)}{dt^n} \Big|_{t=t_0} (t - t_0)^n = X_v^\mu(t_0) + \frac{dX_v^\mu(t)}{dt} \Big|_{t=t_0} (t - t_0) + \mathcal{O}(t^2) \quad (19)$$

Applying  $dX_v^\mu/dt = A_\sigma^\mu X_v^\sigma$ , this gives:

$$X_v^\mu(t) \approx X_v^\mu(t_0) + (t - t_0) A_\sigma^\mu(t_0) X_v^\sigma(t_0) + \mathcal{O}(t^2) = X_v^\sigma(t_0) \left( \mathbb{1}_\sigma^\mu + (t - t_0) A_\sigma^\mu(t_0) \right) + \mathcal{O}(t^2)$$

Taking the determinant of both sides:

$$\det X(t) \approx \det \{ X(t_0) (\mathbb{1} + (t - t_0) A(t_0)) \} + \mathcal{O}(t^2) = \det X(t_0) \det \{ \mathbb{1} + (t - t_0) A(t_0) \}$$

At lowest order, we have an expansion of the determinant given by:



$$\det\{\mathbb{1} + \varepsilon T\} \approx 1 + \varepsilon \text{Tr} T + \mathcal{O}(\varepsilon^2) \quad (20)$$

Since we're taking the Taylor expansion around  $(t - t_0)$  to lowest order in  $t$ , this expansion can apply. This gives:

$$\det X(t) = \det X(t_0) \det\{\mathbb{1} + (t - t_0) A(t_0)\} = \det X(t_0) (1 + (t - t_0) \text{Tr} A(t_0)) + \mathcal{O}(t^2)$$

$$\det X(t) = \det X(t_0) + (t - t_0) \det X(t_0) \text{Tr} A(t_0) + \mathcal{O}(t^2)$$

Comparing this term-by-term with the Taylor expansion of  $\det X(t)$  around  $(t - t_0)$ :

$$\det X(t) = \sum_{n=0}^{\infty} \frac{d^n[\det X(t)]}{dt^n} \Big|_{t=t_0} (t - t_0)^n = \det X(t_0) + (t - t_0) \frac{d[\det X(t)]}{dt} \Big|_{t=t_0} + \mathcal{O}(t^2) \quad (21)$$

Matching terms between the Taylor expansion and the earlier expansion, the first-order terms give:

$$\frac{d[\det X(t)]}{dt} \Big|_{t=t_0} = \det X(t_0) \text{Tr} A(t_0) \quad (22)$$

Since this holds for *arbitrary*  $t_0$ , this gives the differential equation:

$$\frac{d}{dt} [\det X(t)] = \text{Tr} A(t) \det X(t) \quad (23)$$

These are all scalars, so this can be directly solved by integrating:

$$\begin{aligned} \frac{d[\det X(t)]}{\det X(t)} &= \text{Tr} A(t) dt \\ \int_{\det X(t_0)}^{\det X(t)} \frac{d[\det X(\tau)]}{\det X(\tau)} &= \int_{t_0}^t d\tau \text{Tr} A(\tau) \\ \ln \det X(t) - \ln \det X(t_0) &= \ln \frac{\det X(t)}{\det X(t_0)} = \int_{t_0}^t d\tau \text{Tr} A(\tau) \\ \frac{\det X(t)}{\det X(t_0)} &= \exp \left\{ \int_{t_0}^t d\tau \text{Tr} A(\tau) \right\} \end{aligned}$$

Thus, we have equation (14):

$$\det X(t) = \det X(t_0) \exp \left\{ \int_{t_0}^t d\tau \text{Tr} A(\tau) \right\}$$

(Since these are scalars, this is guaranteed to converge<sup>[4]</sup>; furthermore, we have  $[\text{Tr} A(t_1), \text{Tr} A(t_2)] = 0$ , so we don't need to worry about time ordering<sup>[5]</sup>.)

## 2.2: Fundamental Matrices in a Periodic System

We still need to show a couple of stepping-stone properties before we can get to Floquet's theorem itself; these will help us derive Floquet's theorem and some of the properties we're after. Now that we have  $X_v^\mu(t)$ , we can examine its properties when subject to a periodic driving or implemented in a periodic system. We start again with the differential equation given by equation (13), but now imposing periodicity:

$$\frac{dX_v^\mu(t)}{dt} = A_v^\mu(t) X_v^\sigma(t); \quad A_v^\mu(t+T) = A_v^\mu(t) \quad (24)$$

The periodicity of the system is represented in the coefficient matrix, by the condition  $A_v^\mu(t+T) = A_v^\mu(t)$ . [3] and [6] rigorously prove some key properties that we'll just take for granted, since they're decent assumptions for a physical system: existence and uniqueness of solutions, and the property that  $X_v^\mu(t)$  is a fundamental matrix (i.e.  $\det X(t) \neq 0$ ) at all times, including  $t+T$ .

Existence and uniqueness have the same interpretations physically that they do mathematically; uniqueness is the assumption that we don't have any multi-valued differential equations. The assumption that  $X_v^\mu(t)$  is a fundamental matrix at all times corresponds physically to the idea that the time evolution of every specific case  $x^v(t)$  will be well-defined at all times.

From this, we define the matrix  $B_v^\sigma(t)$ , which will be critically important for Floquet's theorem:

$$B_v^\sigma(t) := \left(X_v^\mu(t)\right)^{-1} X_v^\mu(t+T) \quad (25)$$

$B_v^\sigma(t)$  is the propagator from  $t$  to  $t+T$ , which will help us understand the time evolution of the system. First, we can derive the *Wronskian*,  $\det B(t)$ . Since  $X_v^\mu(t+T) = X_v^\mu(t) B_v^\sigma(t)$  by definition, and  $X_v^\mu(t+T)$  is a fundamental matrix,  $X_v^\mu(t+T)$  must have evolved from  $X_v^\mu(t)$  via the Abel-Jacobi-Liouville identity:

$$\det X(t+T) = \det X(t) \exp \left\{ \int_t^{t+T} d\tau \operatorname{Tr} B(\tau) \right\}$$

However, from the periodicity  $A_v^\mu(\tau+T) = A_v^\mu(\tau)$ , the integral over  $[t, t+T]$  is the same as the integral over  $[0, T]$ , so we have:

$$\det X(t+T) = \det X(t) \exp \left\{ \int_0^T d\tau \operatorname{Tr} A(\tau) \right\}$$

The second term is completely independent of  $t$ , so  $\det B_v^\sigma(t)$  must be time-independent:

$$\det B(t) = \exp \left\{ \int_0^T d\tau \operatorname{Tr} A(\tau) \right\} \quad (26)$$

It turns out that  $B_v^\sigma$  itself is time-independent, which we'll derive now. First, we define the matrix  $\mathcal{B}_v^\sigma$  as the matrix of numbers that we get by evaluating  $B_v^\sigma$  at  $t = t_0$ :

$$\mathcal{B}_v^\sigma := B_v^\sigma(t_0) = \left(X_\sigma^\mu(t_0)\right)^{-1} X_v^\mu(t_0 + T) \quad (27)$$

Since  $\mathcal{B}_v^\sigma$  is a matrix of numbers, by construction it's time independent. Additionally, since we're assuming that  $X_v^\mu(t)$  is a fundamental matrix at all times, by construction it's invertible at all times, so  $\left(X_\sigma^\mu(t_0)\right)^{-1} X_v^\sigma(t_0 + T)$  must be invertible as well. Thus,  $\mathcal{B}_v^\sigma$  is a time-independent invertible matrix. Since any rescaling of a fundamental matrix by a time-independent invertible matrix is *also* a fundamental matrix,  $X_v^\mu(t) \mathcal{B}_v^\sigma$  must be a fundamental matrix as well.

We can then compare the time evolved expressions for  $X_\sigma^\mu(t) B_v^\sigma(t)$  and  $X_v^\mu(t) \mathcal{B}_v^\sigma$ :

$$X_\sigma^\mu(t) B_v^\sigma(t) = X_v^\mu(t) \left(X_\sigma^\sigma(t)\right)^{-1} X_v^\sigma(t + T)$$

vs.

$$X_v^\mu(t) \mathcal{B}_v^\sigma = X_v^\mu(t) \left(X_\sigma^\sigma(t_0)\right)^{-1} X_v^\sigma(t_0 + T)$$

Both  $X_\sigma^\mu(t) B_v^\sigma(t)$  and  $X_v^\mu(t) \mathcal{B}_v^\sigma$  solve the differential equation we're interested in (i.e.  $dX_v^\mu/dt = A_\sigma^\mu X_v^\sigma$  with  $A_\sigma^\mu$  being  $T$ -periodic). Additionally,  $X_\sigma^\mu(t) B_v^\sigma(t)$  and  $X_v^\mu(t) \mathcal{B}_v^\sigma$  coincide at the initial condition  $t_0$ . From the uniqueness of solutions, then,  $\mathcal{B}_v^\sigma = B_v^\sigma(t)$  at *all* times  $t$ :  $\mathcal{B}_v^\sigma$  itself is a time-independent invertible matrix.

### 2.3: Floquet Exponents and Floquet's Theorem

We set up  $B_v^\sigma$  the way we did because its properties are actually incredibly important for Floquet's theorem. Since it's invertible, it has  $k$  eigenvalues (although multiplicity is allowed), which we'll label  $\{\rho_a\}_{a=1}^m$ . These eigenvalues are called the *characteristic multipliers*.

From these, we get the *Floquet exponents*  $\{\omega_a\}_{a=1}^m$  with  $\omega_a \in \mathbb{C}$  by the relation:

$$\rho_a = e^{\omega_a T} \quad (28)$$

Notably, the Floquet exponents are *not* unique, since they're  $2\pi i/T$ -periodic:

$$\rho_a = e^{\omega_a T} = e^{(\omega_a + 2\pi i/T)T} \quad (29)$$

Particularly notable is the relationship between the Floquet exponents and the Wronskian (and thus the coefficient matrix  $A_\sigma^\mu(\mathbf{r})$ ). Combining equation (16) and the fact that the determinant is just the product of the eigenvalues, we have:

$$\det B = \det \left\{ \left(X(t_0)\right)^{-1} X(t_0 + T) \right\} = \prod_{a=1}^m \rho_a = \prod_{a=1}^m e^{\omega_a T} = \exp \left\{ \int_0^T d\mathbf{r} \operatorname{Tr} A(\mathbf{r}) \right\} \quad (30)$$

The trace of  $B_v^\sigma$  is, as always, the sum of the eigenvalues:

$$\operatorname{Tr} B = \operatorname{Tr} \left\{ \left(X(t_0)\right)^{-1} X(t_0 + T) \right\} = \sum_{a=1}^m \rho_a = \sum_{a=1}^m e^{\omega_a T} \quad (31)$$

Finally, we note that the Floquet exponents don't depend on the specific fundamental matrix we're considering, but rather depend entirely on the periodic system (encoded in  $A_\sigma^\mu$ ). This is proven in [6]; I might prove this later. Instead, we can now directly go to Floquet's theorem:

## Floquet's Theorem Claim

Suppose we have a periodic differential equation, given by:

$$\frac{dx^\mu(t)}{dt} = A_\nu^\mu(t) x^\nu(t); \quad A_\nu^\mu(t+T) = A_\nu^\mu(t) \quad (32)$$

Solutions to this differential equation have the form:

$$x_a^\mu(t) = e^{\omega_a t} p_a^\mu(t) \quad (33)$$

Here,  $p_a^\mu(t+T) = p_a^\mu(t)$  has the same periodicity as  $A_\nu^\mu(t)$ :  $p_a^\mu(t+T) = p_a^\mu(t)$ .

## Floquet's Theorem Proof

We'll start again with the fundamental matrix  $X_\nu^\mu$ , which is a solution to the matrix version of the differential equation we're interested in:

$$\frac{dX_\nu^\mu(t)}{dt} = A_\sigma^\mu(t) X_\nu^\sigma(t); \quad A_\nu^\mu(t+T) = A_\nu^\mu(t)$$

(This is just equation (15) again.) Since  $X_\nu^\mu(t)$  solves this equation for all times, this equation holds for  $X_\nu^\mu(t+T) = X_\sigma^\mu(t) B_\nu^\sigma(t)$  as well:

$$\frac{dX_\nu^\mu(t+T)}{dt} = A_\sigma^\mu(t) X_\nu^\mu(t+T); \quad A_\nu^\mu(t+T) = A_\nu^\mu(t) \quad (34)$$

$$\frac{d[X_\sigma^\mu(t) B_\nu^\sigma]}{dt} = A_\sigma^\mu(t) X_\lambda^\sigma(t) B_\nu^\lambda; \quad A_\nu^\mu(t+T) = A_\nu^\mu(t) \quad (35)$$

Additionally, since  $B_\nu^\sigma$  is time-independent, its eigenvalues and eigenvectors are as well. Thus, if we take the eigenvalue  $\rho_i$  and corresponding eigenvector  $b^\sigma$ , the vector  $x^\nu := X_\sigma^\nu(t) b^\sigma$  will be a solution to the differential equation (equation (22)) we're interested in:

$$\frac{dx^\mu(t)}{dt} = A_\nu^\mu(t) x^\nu(t); \quad A_\nu^\mu(t+T) = A_\nu^\mu(t)$$

(We can see this most directly again from the fact that  $X_\nu^\mu(t+T)$  solves equation (15).) Then, examining  $x^\mu(t+T)$ , we get:

$$x_a^\mu(t+T) = X_\nu^\mu(t+T) b_a^\nu = (X_\sigma^\mu(t) B_\nu^\sigma) b_a^\nu = X_\sigma^\mu(t) B_\nu^\sigma b_a^\nu = \rho_a X_\sigma^\mu(t) b_a^\sigma = e^{\omega_a T} x_a^\mu(t) \quad (36)$$

From here, we do the same thing as with Bloch's theorem: defining  $p_a^\mu(t) := e^{-\omega_a t} x_a^\mu(t)$  and examining  $p_a^\mu(t+T)$ , we get:

$$p_a^\mu(t+T) = e^{-\omega_a(t+T)} x_a^\mu(t+T) = e^{-\omega_a(t+T)} e^{\omega_a T} x_a^\mu(t) = e^{-\omega_a t} x_a^\mu(t) = p_a^\mu(t) \quad (37)$$

Thus, we have  $p_a^\mu(t+T) = p_a^\mu(t)$ , and  $x_a^\mu(t) = e^{\omega_a t} p_a^\mu(t)$ . //

## Matrix Formulation of Floquet's Theorem

Before going on, we note that some textbooks and papers refer to the matrix form of Floquet's theorem, relying on the fundamental matrix version of the equation (i.e. equation (15) once again):

$$\frac{dX_v^\mu(t)}{dt} = A_v^\mu(t) X_v^\mu(t); \quad A_v^\mu(t+T) = A_v^\mu(t)$$

In this form, Floquet's theorem states that solutions have the form:

$$X_v^\mu = P_v^\mu(t) (B_v^\mu)^{t/T} \quad (38)$$

Here,  $P_v^\mu(t+T) = P_v^\mu(t)$  has the same periodicity as  $A_v^\mu(t)$ . The links between the vector formulation and the matrix formulation are given by the fact that  $\{e^{\omega_a t}\}$  are the eigenvalues of  $B_v^\mu$ , and that  $X_v^\mu$  and  $P_v^\mu$  are expressed in terms of  $\{x_a^\mu(t)\}$  and  $\{p_a^\mu(t)\} = \{e^{\omega_a t} x_a^\mu(t)\}$  by:

$$X_v^\mu(t) := \begin{bmatrix} | & \cdots & | \\ x_1^\mu(t) & \cdots & x_m^\mu(t) \\ | & \cdots & | \end{bmatrix} \quad P_v^\mu(t) := \begin{bmatrix} | & \cdots & | \\ p_1^\mu(t) & \cdots & p_m^\mu(t) \\ | & \cdots & | \end{bmatrix} \quad (39)$$

## 2.4: Lyapunov Exponents and Mathieu's Equation

The Floquet solutions  $x_a^\mu(t) = e^{\omega_a t} p_a^\mu(t)$  have some important properties that are worth knowing about. First, as with Bloch's theorem, we note that the essential aspect of Floquet's theorem is that the solutions are broken up into a periodic piece (the Floquet modes)  $p_a^\mu(t)$  and an exponential piece  $e^{\omega_a t}$ . Since the  $\omega_a$  in the Floquet exponents were only unique up to  $2\pi i/T$ , the mapping  $\omega_a \mapsto \omega_a + 2\pi i/T$  changes  $x_a^\mu(t) = e^{\omega_a t} p_a^\mu(t)$  as well:

$$e^{\omega_a t} p_a^\mu(t) \mapsto e^{(\omega_a + 2\pi i/T)t} p_a^\mu(t) \quad (40)$$

However, the overall function  $e^{(\omega_a + 2\pi i/T)t} p_a^\mu(t)$  is still  $T$ -periodic, so the essential idea of breaking up  $x_a^\mu(t)$  into an exponential piece and a  $T$ -periodic piece is still maintained.

In Bloch's theorem, the exponential piece was plane waves. Conversely, here, they could be either plane waves, exponential decay, or inspiralling decays. This is the subject of Floquet-Lyapunov theory<sup>[7]</sup>, which we'll just briefly touch on here. Since we have  $x_a^\mu(t+T) = e^{\omega_a T} x_a^\mu(t)$ , we have  $x_a^\mu(t+nT) = e^{\omega_a nT} x_a^\mu(t)$ . For the  $t \rightarrow \infty$  limit, we get three distinct cases:

- For  $|e^{\omega_a T}| < 1$  (which corresponds to  $\Re\{\omega_a\} < 0$ ), we get  $\lim_{t \rightarrow \infty} x_a^\mu(t) = 0$ .
- For  $|e^{\omega_a T}| = 1$  (which corresponds to  $\Re\{\omega_a\} = 0$ ), we get plane waves, and  $x_a^\mu(t)$  is pseudo-periodic.
  - When  $e^{\omega_a T} = \pm 1$ ,  $x_a^\mu(t)$  is properly periodic.
- For  $|e^{\omega_a T}| > 1$  (which corresponds to  $\Re\{\omega_a\} > 0$ ), we get  $\lim_{t \rightarrow \infty} x_a^\mu(t) \rightarrow \infty$ .

The  $t \rightarrow \infty$  properties of  $x_a^\mu(t)$  depend on  $\Re\{\omega_a\}$ ; this is called the *Lyapunov exponent*<sup>[7]</sup>, which shows up in analysis of nonlinear and chaotic systems. If all of the  $\omega_a$  satisfy  $|e^{\omega_a T}| \leq 1$ ,  $x_a^\mu(t)$  is called *Lyapunov stable*.

As a specific example of using Floquet's theorem to help find the solutions to a differential equation, we'll examine Mathieu's equation<sup>[8]</sup>, which come up for 3D Laplace problems and 2D or 3D Helmholtz problems in elliptic coordinates. (One such example would be the scattering of electromagnetic waves off elliptic cylinders, or wave propagation in elliptic waveguides.) Mathieu's equation is given by:

$$\frac{d^2 x}{dt^2} + (a - 2q \cos 2t)x = 0 \quad (41)$$

Here,  $a, q \in \mathbb{R}$ . Since  $L[x] = D_x^2 + (a - 2q \cos 2t)$  is a linear differential operator, it has full rank. This means that there exist two solutions to this equation (which I'll label  $s_1$  and  $s_2$ ), and the remaining solutions are linear combinations of these (via the superposition principle). Using symmetry principles and Floquet's theorem, we can try to find the functional form of  $s_1$  and  $s_2$ .

As usual, we can convert a second order ODE into a first-order matrix ODE by defining the column vector:

$$\begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} x \\ \frac{dx}{dt} \end{bmatrix} \quad (42)$$

Then, solutions to Mathieu's equation satisfy:

$$\frac{d}{dt} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \frac{d}{dt} \begin{bmatrix} x \\ dx/dt \end{bmatrix} = \begin{bmatrix} 0 & 1 \\ -a + 2q \cos 2t & 0 \end{bmatrix} \quad (43)$$

Then, we want to construct a fundamental solution matrix out of the vectors  $s_1^\mu$  and  $s_2^\mu$ , defined by:

$$s_1^\mu(t) := \begin{bmatrix} s_1(t) \\ ds_1(t)/dt \end{bmatrix} \quad s_2^\mu(t) := \begin{bmatrix} s_2(t) \\ ds_2(t)/dt \end{bmatrix} \quad (44)$$

Additionally, we can impose the initial conditions:

$$X_\sigma^\mu(0) = \begin{bmatrix} s_1(0) & s_2(0) \\ ds_1(0)/dt & ds_2(0)/dt \end{bmatrix} = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} \quad (45)$$

Now, we can use some of the results that we derived earlier from Floquet's theorem. From the initial conditions,  $B_v^\mu$  is given by:

$$B_v^\mu = \left(X_\sigma^\mu(0)\right)^{-1} X_v^\mu(0 + T) = \left(\begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}\right)^{-1} \begin{bmatrix} s_1(T) & s_2(T) \\ ds_1(T)/dt & ds_2(T)/dt \end{bmatrix} = \begin{bmatrix} s_1(T) & s_2(T) \\ ds_1(T)/dt & ds_2(T)/dt \end{bmatrix}$$

As before,  $B_v^\mu$  is time-invariant. Thus, the Wronskian  $\det B_v^\mu$  is also time-invariant. In terms of  $s_1$  and  $s_2$ , the Wronskian is given by:

$$\det B = \begin{vmatrix} s_1(T) & s_2(T) \\ d s_1(T)/dt & d s_2(T)/dt \end{vmatrix} = s_1(T) \frac{d s_2(T)}{dt} - s_2(T) \frac{d s_1(T)}{dt}$$

However, since the Wronskian is time-invariant, this is going to be the same as the Wronskian at  $t = 0$ :

$$\det B = \begin{vmatrix} s_1(0) & s_2(0) \\ d s_1(0)/dt & d s_2(0)/dt \end{vmatrix} = \begin{vmatrix} 1 & 0 \\ 0 & 1 \end{vmatrix} = 1$$

(As a sanity check, this is the same thing we'd get if we explicitly used equation (24): since  $\text{Tr } A(\tau) = 0$  in equation (41), we get  $\det B = \exp\{\int d\tau 0\} = e^0 = 1$ .) So, the two solutions we can get will be linearly independent.

The equation has two notable symmetries: invariance under time reversal ( $t \mapsto -t$ ) and the periodicity we're interested in ( $t \mapsto t \pm \pi$ ). From invariance under time reversal and the form of the differential operator, we get one even and one odd solution. Then, from the periodicity, we can guess that the solutions will have cos-like and sin-like addition formulae at  $t \pm \pi$ . WLOG we can set  $s_1$  as the even function and  $s_2$  as the odd function. This then gives the addition formulae at  $t \pm \pi$  as:

$$s_1(t \pm \pi) = s_1(\pi) s_1(t) \pm \frac{d s_1(\pi)}{dt} s_2(t) \quad s_2(t \pm \pi) = \pm s_2(\pi) s_1(t) \pm \frac{d s_2(\pi)}{dt} s_2(t) \quad (46)$$

Additionally, from the linear independence of the solutions and the cos-like and sin-like property at  $t = \pi$  (and the periodicity around  $\pi$ ), we get:

$$s_1(\pi) = \frac{d s_2(\pi)}{dt} \quad (47)$$

Finally, from Floquet's theorem, we have the familiar shape of  $s_1(t)$  and  $s_2(t)$ :

$$s_1(t) = e^{\omega_1 t} p_1(t) \quad s_2(t) = e^{\omega_2 t} p_2(t) \quad (48)$$

So, finding solutions to Mathieu's equation reduces to finding expressions for  $\omega_1, \omega_2, p_1(t)$ , and  $p_2(t)$ . Unfortunately, this is all we can do: Floquet's theorem can't give us any more insights into the values of  $\omega_1$  and  $\omega_2$ , nor the functional forms of  $p_1(t)$  or  $p_2(t)$ . (The NIST Handbook of Mathematical Functions lists<sup>[9]</sup> an extra symmetry of the differential operator,  $\{t \mapsto t \pm \pi/2, q \mapsto -q\}$ , but I wasn't considering the possibility of changing one of the parameters. Similarly, it lists four extra relations, likely derived from this symmetry in conjunction with the  $t \mapsto t \pm \pi$  symmetry, but I wasn't quite sure how to derive them.) From here on out, we'll have to use a standard technique like trying to convert it to Sturm-Liouville form.

What was the point of Floquet's theorem, then, if it can't get us to an actual answer? It turns out that while Floquet couldn't help us finding the exact form of  $s_1(t)$  or  $s_2(t)$ , it gives us something even better: a new basis for  $L^2(\mathbb{R})$  from which to expand the solutions we're interested in. Just as with any other basis of  $L^2(\mathbb{R})$  we deal with, we can treat this basis (appropriately called the Floquet basis) as the eigenbasis from which to expand solutions to Floquet problems. In this sense, we can think of Floquet's theorem as the theorem that tells us that the Floquet basis is the appropriate one whenever we have a periodic system.

(Incidentally, we shouldn't be particularly dismayed that we couldn't get a closed-form solution; a general closed form solution doesn't really exist. People seem content to write down special function solutions which are then simply expressed in terms of the Floquet basis, or use Floquet's theorem and Floquet-Lyapunov theory to examine the infinite-time properties of solutions, or examine special cases by picking specific values of  $a$  and  $q$  that make the equation solvable. A closed-form analytic solution to a linearized version of the Mathieu equation was found<sup>[10]</sup>, but it doesn't seem to have been accepted at any journals or cited anywhere.)

### 3: Floquet Basis

#### 3.1: Floquet Basis from Fourier Basis

Floquet's theorem offers us a new basis from which to examine problems (the Floquet basis), which is very much the natural basis from which to expand Floquet problems. It turns out that we can get these directly from our familiar Fourier basis. I'll provide the results but not the derivations, since I assume we're already familiar with these derivations.

As a reminder, we can construct the Fourier basis from the generalized Stone-Weierstrass theorem, which just says that we can expand a function over  $\mathbb{R}^m$  or  $\mathbb{C}^m$  in polynomials<sup>[11]</sup>, where each dimension gets its own polynomial basis. Fourier series specifically can be constructed by examining a function over  $\mathbb{R}^2$  in polar, and setting  $r = 1$  at the end:

$$f(x, y)|_{r=1} = f(r \cos \theta, r \sin \theta)|_{r=1} = \sum_{j, \ell=-\infty}^{\infty} a_{\ell n} r^{j+\ell} \cos^j \theta \sin^\ell \theta \Big|_{r=1} = \sum_{n=-\infty}^{\infty} f_n e^{in\theta} \quad (49)$$

Already by construction, we're putting the problem on a circle, so  $f(\theta)$  has a  $2\pi$  periodicity, and  $\{e^{in\theta}\}_{n=-\infty}^{\infty}$  is a basis for  $L^2(-\pi, \pi)$ . It's already orthogonal; the orthonormalized version is  $\{e^{in\theta}/\sqrt{2\pi}\}_{n=-\infty}^{\infty}$ . This basis is Cauchy-complete for continuous and piecewise  $L^2$  continuous functions on  $(-\pi, \pi)$ . The Fourier coefficients  $f_n$  are given by the Fourier transform:

$$f_n = \int_{-\pi}^{\pi} \frac{d\theta}{\sqrt{2\pi}} e^{-in\theta} f(\theta) \quad (50)$$

The transformation  $\theta \mapsto x = L\theta/2\pi + a + L/2$  gives a periodic function  $f(x)$  defined over  $(a, a + L)$  and with period  $L$ :

$$f(x) = \frac{1}{\sqrt{L}} \sum_{n=-\infty}^{\infty} F_n e^{2\pi i n x / L}; \quad F_n = \int_a^{a+L} \frac{dx}{\sqrt{L}} e^{-2\pi i n x / L} f(x) \quad (51)$$

Now, our orthonormal basis for continuous and piecewise continuous  $L^2$  functions over  $(a, a + L)$  is given by  $\{e^{2\pi i n x / L}\}_{n=-\infty}^{\infty}$ .



We want to apply Fourier analysis to Floquet's theorem, and the presence of the  $e^{\omega_a t}$  term in the Floquet solutions gives us a hint on how to do this. As before, we start with the differential equation given by equation (31):

$$\frac{dx^\mu(t)}{dt} = A_v^\mu(t) x^\nu(t); \quad A_v^\mu(t+T) = A_v^\mu(t)$$

From here, Floquet's theorem gives us the solutions  $x_a^\mu(t) = e^{\omega_a t} p_a^\mu(t) = \rho_a p_a^\mu(t)$  with  $p_a^\mu(t+T) = p_a^\mu(t)$  and  $\omega_a, \rho_a \in \mathbb{C}$ . For convenience, we'll define  $\varphi_a = -i\omega_a$ , so that the solutions are now:  $x_a^\mu(t) = e^{i\varphi_a t} p_a^\mu(t)$  with  $\varphi_a \in \mathbb{C}$ . Expanding  $p_a^\mu(t)$  in a Fourier series, we get:

$$p_a^\mu(t) = \sum_{n=-\infty}^{\infty} \frac{b_{n,a}}{\sqrt{T}} e^{2\pi i n t / T} \quad (52)$$

However, since  $x_a^\mu(t) = e^{i\varphi_a t} p_a^\mu(t)$ , the corresponding Fourier expansion of  $x_a^\mu(t)$  is given by:

$$x_a^\mu(t) = \sum_{n=-\infty}^{\infty} e^{i\varphi_a t} \frac{b_{n,a}}{\sqrt{T}} e^{2\pi i n t / T} = \sum_{n=-\infty}^{\infty} \frac{b_{n,a}}{\sqrt{T}} e^{i(\varphi_a + 2\pi n / T)t} \quad (53)$$

For the  $n$ th Fourier mode, the corresponding Floquet mode is  $b_{n,a} e^{i\varphi_a t}$ , and the corresponding Floquet phase is  $e^{2\pi i n t / T}$ .

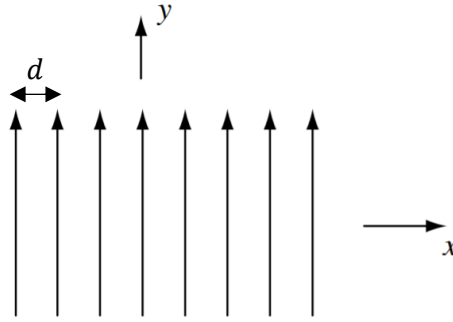
The elementary basis functions for  $L^2(a, b)$  are now given by  $\{e^{i(\varphi_a + 2\pi n / T)t}\}_{n=-\infty}^{\infty} = \{e^{i\varphi_a t} e^{2\pi i n t / T}\}_{n=-\infty}^{\infty}$ . This changes the Fourier coefficients slightly, since the Fourier transform is taken with respect to a new set of Fourier basis functions (but *not* with respect to a different  $dt$ <sup>[12]</sup>):

$$b_{n,a} = \int_{-\pi}^{\pi} \frac{dt}{\sqrt{T}} e^{-i(\varphi_a + 2\pi n / T)t} x_a^\mu(t) \quad (54)$$

When expanding something in a Fourier series, we assume that the magnitude and phase have the same periodicity. One of the biggest advantages of the Floquet basis, conversely, is that it allows us to deal with problems where the magnitude and phase have *different* periodicity<sup>[12]</sup>: if we tried expanding this in a Fourier basis, we'd have to use the periodicity given by the least common multiple of their individual periodicities, which might be unduly large (or even inapplicable entirely, if they're irrational multiples of each other).

### 3.2: Example of the Floquet Basis: Infinite Array of Parallel Wires

To illustrate how the Floquet basis can be used, we'll look at an example drawn from electromagnetism, of the electric and magnetic fields induced by a synchronized set of oscillating currents on a grid of infinite parallel wires:



Since we have a synchronized set of oscillating currents, the overall effect is that of a uniform wave along the  $x$ -direction, propagating in the  $y$ -direction. Here,  $d$  is the distance between wires. We'll examine the  $x$ -component specifically of the electric field at a point  $(y, z)$  above the  $xy$ -plane. If the current in the 0<sup>th</sup> wire (the wire located at the  $y$ -axis) is given by  $I_0$ , then the current in the  $n$ th wire is given by Floquet's theorem<sup>[13]</sup>:

$$I_n = I_0 e^{-in\varphi d} \quad (55)$$

(The currents and fields are completely independent of  $x$  in this setup, so we can safely ignore the  $x$  direction.) The electric field in the  $x$ -direction due to the  $n$ th wire is given by<sup>[14]</sup>:

$$E_{x,n}(y, z) = -\frac{\mu_0 \omega}{4} I_n H_0^{(2)} \left( \omega \sqrt{\epsilon_0 \mu_0} \sqrt{z^2 + (nd - y)^2} \right) = -\frac{k}{4} \sqrt{\frac{\mu_0}{\epsilon_0}} I_0 e^{-in\varphi d} H_0^{(2)} \left( k \sqrt{z^2 + (nd - y)^2} \right) \quad (56)$$

(The derivation of this is straightforward but very lengthy; I'll reproduce it when I have the time.)  $k = \omega \sqrt{\epsilon_0 \mu_0}$  is the wave number and  $H_0^{(2)}$  is the 0<sup>th</sup>-order second-kind Hankel function, defined as a linear combination of the first-kind and second-kind Bessel functions:

$$H_\alpha^{(2)}(x) := J_\alpha(x) - iY_\alpha(x) \quad (57)$$

From the Floquet series expression in (52), the total  $x$ -component of the electric field is just given by the sum of these:

$$E_x(y, z) = -\frac{k}{4} \sqrt{\frac{\mu_0}{\epsilon_0}} I_0 \sum_{n=-\infty}^{\infty} e^{-in\varphi d} H_0^{(2)} \left( k \sqrt{z^2 + (nd - y)^2} \right) \quad (58)$$

We can convert this sum into something more familiar by using the Poisson summation formula<sup>[15]</sup>:

$$\sum_{n=-\infty}^{\infty} f(x + nL) = \frac{1}{L} \sum_{v=-\infty}^{\infty} e^{2\pi i v x / L} \tilde{f}\left(\frac{v}{L}\right) \quad (59)$$

In this formula, the Fourier conjugate pair variables are  $nd$  and  $n/d$ , with  $L \mapsto d$ . Applying this to the sum we're interested in, the left-hand side is  $f(x + nL) \mapsto e^{-in\varphi d} H_0^{(2)} \left( k \sqrt{z^2 + (nd - y)^2} \right)$ , with  $x \mapsto -y$ . For the right-hand side, we have  $\tilde{f}(v/L) \mapsto \mathcal{F} \left\{ e^{-in\varphi d} H_0^{(2)} \left( k \sqrt{z^2 + (nd - y)^2} \right) \right\}$ . We can calculate this transform via the convolution theorem:

$$\mathcal{F}\{f(x) \cdot g(y)\} = \mathcal{F}\{f(x)\} * \mathcal{F}\{g(y)\} = \int_{-\infty}^{\infty} d\xi \tilde{f}(\xi) \tilde{g}(\xi - \nu) \quad (60)$$

So, for the right-hand side of the Poisson sum, we need to evaluate  $\mathcal{F}\{H_0^{(2)}(k\sqrt{z^2 + (nd - y)^2})\}$ . The Fourier transform of  $H_0^{(2)}$  is given by<sup>[16]</sup>:

$$\int_{-\infty}^{\infty} dp e^{-ipx} H_0^{(2)}(\alpha\sqrt{p^2 + m^2}) = \frac{2e^{-i|m|\sqrt{\alpha^2 - x^2}}}{\sqrt{\alpha^2 - x^2}} \quad (61)$$

(As before, this derivation is straightforward (via the integral representation of the Hankel function) but extremely lengthy; I'll deal with this later.) Applying this to  $H_0^{(2)}(k\sqrt{z^2 + (nd - y)^2})$ , we have  $x \mapsto \nu/d$ ,  $\alpha \mapsto k$ ,  $m \mapsto z$ , and  $p \mapsto (nd - y)$  with  $dp \mapsto d(nd)$ . This then gives  $\mathcal{F}\{e^{-in\varphi d} H_0^{(2)}(k\sqrt{z^2 + (nd - y)^2})\}$  as:

$$\begin{aligned} \mathcal{F}\{e^{-in\varphi d} H_0^{(2)}(k\sqrt{z^2 + (nd - y)^2})\} &= \mathcal{F}\{e^{-in\varphi d}\} * \mathcal{F}\{H_0^{(2)}(k\sqrt{z^2 + (nd - y)^2})\} \\ \mathcal{F}\{e^{-in\varphi d} H_0^{(2)}(k\sqrt{z^2 + (nd - y)^2})\} &= \delta(\varphi - \xi) * \frac{2 \exp\{-i|z|\sqrt{k^2 - (\xi + 2\pi\nu/d)^2}\}}{\sqrt{k^2 - (\xi + 2\pi\nu/d)^2}} \end{aligned} \quad (62)$$

(Here,  $\xi$  is the convolution variable in equation (59).) The convolution just gives the second function evaluated at  $\xi = \varphi$ :

$$\int_{-\infty}^{\infty} d\xi \delta(\varphi - \xi) \frac{2 \exp\{-i|z|\sqrt{k^2 - (\xi + 2\pi\nu/d)^2}\}}{\sqrt{k^2 - (\xi + 2\pi\nu/d)^2}} = \frac{2 \exp\left\{-i|z|\sqrt{k^2 - \left(\varphi + \frac{2\pi\nu}{d}\right)^2}\right\}}{\sqrt{k^2 - \left(\varphi + \frac{2\pi\nu}{d}\right)^2}}$$

This then gives the full series as:

$$\begin{aligned} E_x(y, z) &= -\frac{kI_0}{4} \sqrt{\frac{\mu_0}{\epsilon_0}} \sum_{n=-\infty}^{\infty} e^{-in\varphi d} H_0^{(2)}(k\sqrt{z^2 + (nd - y)^2}) \\ &= -\frac{kI_0}{2d} \sqrt{\frac{\mu_0}{\epsilon_0}} \sum_{\nu=-\infty}^{\infty} e^{-2\pi i \nu y/d} \frac{\exp\left\{-i|z|\sqrt{k^2 - \left(\varphi + \frac{2\pi\nu}{d}\right)^2}\right\}}{\sqrt{k^2 - \left(\varphi + \frac{2\pi\nu}{d}\right)^2}} \end{aligned}$$

Separating the  $\nu = 0$  term condenses this into a much more familiar form:

$$E_x(y, z) = -\frac{kI_0}{2d} \sqrt{\frac{\mu_0}{\epsilon_0}} \frac{e^{-i|z|\sqrt{k^2 - \varphi^2}}}{\sqrt{k^2 - \varphi^2}} - \frac{kI_0}{2d} \sqrt{\frac{\mu_0}{\epsilon_0}} \sum_{\nu \in \mathbb{Z} \setminus \{0\}} e^{-2\pi i \nu y/d} \frac{\exp\left\{-i|z|\sqrt{k^2 - \left(\varphi + \frac{2\pi\nu}{d}\right)^2}\right\}}{\sqrt{k^2 - \left(\varphi + \frac{2\pi\nu}{d}\right)^2}}$$

Expressing  $\exp\{\dots\}/\sqrt{\dots}$  as  $f(z, \varphi)$  for a second, we get:

$$E_x(y, z) = -\frac{kI_0}{2d} \sqrt{\frac{\mu_0}{\epsilon_0}} \frac{e^{-i|z|\sqrt{k^2 - \varphi^2}}}{\sqrt{k^2 - \varphi^2}} - \frac{kI_0}{2d} \sqrt{\frac{\mu_0}{\epsilon_0}} \sum_{\nu \in \mathbb{Z} \setminus 0} e^{-2\pi i \nu y/d} f(z, \varphi)$$

$$E_x(y, z) = -\frac{kI_0}{2d} \sqrt{\frac{\mu_0}{\epsilon_0}} \frac{e^{-i|z|\sqrt{k^2 - \varphi^2}}}{\sqrt{k^2 - \varphi^2}} - \frac{kI_0}{d} \sqrt{\frac{\mu_0}{\epsilon_0}} \left( \sum_{\nu=1}^{\infty} e^{-2\pi i \nu y/d} f(z, \varphi) + \sum_{\nu=-\infty}^{-1} e^{-2\pi i \nu y/d} f(z, \varphi) \right)$$

Taking  $\nu \mapsto -\nu$  in the second sum and bringing the factor of 2 inside:

$$E_x(y, z) = -\frac{kI_0}{2d} \sqrt{\frac{\mu_0}{\epsilon_0}} \frac{e^{-i|z|\sqrt{k^2 - \varphi^2}}}{\sqrt{k^2 - \varphi^2}} - \frac{kI_0}{d} \sqrt{\frac{\mu_0}{\epsilon_0}} \sum_{\nu=1}^{\infty} \frac{(e^{-2\pi i \nu y/d} + e^{2\pi i \nu y/d})}{2} f(z, \varphi)$$

Thus, this gives:

$$E_x(y, z) = -\frac{kI_0}{2d} \sqrt{\frac{\mu_0}{\epsilon_0}} \frac{e^{-i|z|\sqrt{k^2 - \varphi^2}}}{\sqrt{k^2 - \varphi^2}} - \frac{kI_0}{d} \sqrt{\frac{\mu_0}{\epsilon_0}} \sum_{\nu=1}^{\infty} \cos\left(\frac{2\pi \nu y}{d}\right) \frac{\exp\left\{-i|z|\sqrt{k^2 - \left(\varphi + \frac{2\pi \nu}{d}\right)^2}\right\}}{\sqrt{k^2 - \left(\varphi + \frac{2\pi \nu}{d}\right)^2}} \quad (62)$$

This expression gives us a concrete understanding of the series expansion given by equation (57) (and is why we spent all of this time dealing with these transformations): the electric field is a bunch of different waves along the  $z$ -direction, each propagating as  $\varphi + 2\pi \nu/d$ . Each member of the series (including the  $\nu = 0$  term) is an individual *Floquet mode* (a.k.a. *Floquet harmonic*); the  $\nu > 0$  terms are the *higher-order Floquet modes*.

This expansion also gives us some interesting properties, which we probably wouldn't have seen without the Floquet decomposition. The Floquet modes are waves along the  $z$ -direction, with a group velocity given by:

$$v_g = \frac{\partial \omega}{\partial \left(\varphi + \frac{2\pi \nu}{d}\right)} \quad (63)$$

Since the only difference between the modes is the  $2\pi \nu/d$  term, which is independent of  $\omega$ , the Floquet modes have the *same* group velocity! Conversely, the modes have different phase velocities:

$$v_p = \frac{\omega}{\varphi + \frac{2\pi \nu}{d}} \quad (64)$$

### 3.3: Conclusion

The series expansion given by equation (57) is the strength of the Floquet technique. Here, we see that a lot of the complications of having multiple wires are taken care of entirely by the  $e^{-in\varphi d}$  term. Despite how complicated this series of steps was, it would have been even *more* complicated if we tried to expand this in a normal Fourier series. Even more importantly, the physical understanding that we got from a lot of the transformations we did would have been lost on us. Thus, the strength of the Floquet technique lies in providing us with a natural basis for problems characterized by the periodicity we've been dealing with.

# Notes and References

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