Chapter 3

Floquet Formalism

Floquet theory is both an analytical and numerical formalism used to solve systems of ordinary differential equations subject to periodic time conditions. Its central element is Floquet's theorem, proposed by Gaston Floquet in 1883, which provides the general form of the solutions of the system [47]. In this chapter, Floquet's theorem is first stated, highlighting its main conditions and consequences. Subsequently, it is shown how Floquet's theorem can be understood as the temporal counterpart of Bloch's theorem, referring to the quantities that are discretized in both cases: the quasimomentum and the quasienergies for Bloch and Floquet, respectively. Consequently, the different numerical approaches that Floquet's theorem can take to solve an arbitrary system are formulated, focusing mainly on the extended Hilbert space approach and the expansion in discrete Fourier series. Finally, the problem of the spin-1 Bose-Hubbard Hamiltonian for a single particle in two sites is addressed through Floquet's theorem. These results are compared with those obtained from analytical solutions in momentum space, thus corroborating the validity of the technique to be used in the complete one- and two-particle systems that are analyzed in last chapter.

3.1 Floquet's Theorem

The Floquet's theorem in quantum mechanics can be enunciated in several ways, one of them focuses on the form of the time evolution operator $\hat{U}(t, t_0)$ and its properties at any time and during periodic jumps, emphasizing the Heisenberg picture [76]. The other approach is to use that operator on an arbitrary initial state, providing a general form for the solutions of the system's Hamiltonian, emphasizing the Schrödinger picture [46]. Considering the convenience of using the numerical approach, we express it in the latter form as follows:

Consider a quantum system whose dynamics is governed by a time-periodic Hamiltonian:

$$\hat{H}(t + T) = \hat{H}(t),$$

with driving period T.

The system's evolution state $|\psi_n(t)\rangle$ can be expanded in a complete basis of orthonormal quasi-

stationary states called "*Floquet states*":

$$|\psi_n(t)\rangle = e^{-\frac{i}{\hbar}\varepsilon_n(t-t_0)}|u_n(t)\rangle, \tag{3.1}$$

where the states $|u_n(t)\rangle$ are called the "*Floquet modes*" and satisfy $|u_n(t+T)\rangle = |u_n(t)\rangle$. The parameter ε_n is called the "*quasienergy*" and n labels the different eigenstates, reflecting the analogy with the quasimomentum k characteristic of Bloch's theorem in the solid state physics (see Appendix B for supplementary material that deepens Floquet's theory).

3.1.1 Consequences of Floquet's Theorem

Floquet's theorem presents a scenario in which, independent of the Hamiltonian, if it is periodic, a general expression can be given for the evolution of the state $|\psi(t)\rangle$ at any time $t > 0$. This provides a basis to write any initial state $|\psi(0)\rangle$ that subsequently evolves using the time evolution operator. This basis is clearly given by the Floquet modes, which fulfill the typical completeness relation at an arbitrary time, let's say $t_0 = 0$:

$$\sum_n |u_n(0)\rangle\langle u_n(0)| = \hat{I}, \tag{3.2}$$

Then, we can write any initial state as a superposition of this basis,

$$\begin{aligned} \hat{I}|\psi(0)\rangle &= \sum_n |u_n(0)\rangle \underbrace{\langle u_n(0)|\psi(0)\rangle}_{\equiv c_n}, \\ |\psi(0)\rangle &= \sum_n c_n |u_n(0)\rangle. \end{aligned}$$

Therefore, the state at later times is given by

$$\begin{aligned} |\psi(t)\rangle &= \hat{U}(t,0)|\psi(0)\rangle, \\ &= \sum_n c_n \hat{U}(t,0)|u_n(0)\rangle, \\ &= \sum_n c_n |\psi_n(t)\rangle, \\ |\psi(t)\rangle &= \sum_n c_n e^{-\frac{i}{\hbar}\varepsilon_n t}|u_n(t)\rangle. \end{aligned} \tag{3.3}$$

We can see that in this superposition, the coefficients c_n don't depend on time, carrying all dynamics in the Floquet modes $|u_n(t)\rangle$ and the "*Floquet multipliers*", $e^{-\frac{i}{\hbar}\varepsilon_n t}$. This implies that occupancy probabilities $|c_n|^2$ can be assigned to states that are conserved despite the periodic influence of time, allowing various concepts and techniques used for time-independent quantum systems to be applied to periodically time-dependent systems [56].

In fact, the factor $e^{-\frac{i}{\hbar}\varepsilon_n t}$ in Eq. (3.3) resembles the factors $e^{-\frac{i}{\hbar}E_n t}$ that appear in the temporal evolution of the eigenstates of time-independent Hamiltonians, with E_n being the eigenenergies of the system itself, i.e. resembles to stationary states [77]. Therefore, the quantity ε_n is similar to the energy of the system and were aptly named quasi-energy by physicists Yakov Borisovich Zel'dovich [78] and Vladimir Ivanovich Ritus [79] in 1966, referring also to the aforementioned Bloch theorem.

Now, the problem is to find the respective eigenvalue equation that satisfies the Floquet modes, thus also allowing us to find the quasienergies. This enables us to determine the superposition of the Eq. (3.1) and construct the evolved state at any time t. To achieve this, we start with the time-dependent Schrödinger equation and apply Floquet's theorem.

$$\begin{aligned} i\hbar\frac{d}{dt}|\psi(t)\rangle &= \hat{H}(t)|\psi(t)\rangle, \\ i\hbar\frac{d}{dt}\left[e^{-\frac{i}{\hbar}\varepsilon_n t}|u_n(t)\rangle\right] &= e^{-\frac{i}{\hbar}\varepsilon_n t}\hat{H}(t)|u_n(t)\rangle, \\ \left[\hat{H}(t) - i\hbar\frac{d}{dt}\right]|u_n(t)\rangle &= \varepsilon_n|u_n(t)\rangle, \\ \hat{H}_F(t)|u_n(t)\rangle &= \varepsilon_n|u_n(t)\rangle, \end{aligned} \tag{3.4}$$

where $\hat{H}_F(t) = \hat{H}(t) - i\hbar\frac{d}{dt}$ is the Hamiltonian that satisfies the eigenvalue equation for the Floquet modes, and is called the "*Floquet Hamiltonian*". Note that the eigenvalue equation in Eq. (3.4) resembles a typical time-independent eigenvalue equation; however, both the Floquet Hamiltonian and the Floquet modes depend on time. This implies that the state does evolve over time, despite not having the typical form of the Schrödinger equation. Nevertheless to solve it, we need a specific representation, and due to the form of the Floquet Hamiltonian, its matrix representation loses meaning, requiring additional elements to solve and find the respective Floquet modes and their quasienergies. These elements are discussed in subsequent sections, delving into one of the numerical approaches to Floquet's formalism.

Another consequence of Floquet's theorem, as seen in Eq. (3.4), is that the Floquet modes can be

expressed with an additional phase that has a certain driving frequency ω. Specifically,

$$|u_{n,m}(t)\rangle = e^{im\omega t}|u_n(t)\rangle, \tag{3.5}$$

where m is an integer $m = 0, \pm 1, \pm 2$, and $\omega = 2\pi/T$. This new form of Floquet modes yields the same eigenvalue equation (3.4), but with a shifted quasienergy:

$$\varepsilon_n \to \varepsilon_{n,m} = \varepsilon_n + m\hbar\omega. \tag{3.6}$$

Therefore, this implies that the quasienergies ε_n can be mapped into a zone that contains independent information and is not affected by the multi-evaluation of the complex exponential function. This zone is called the first "*Floquet-Brillouin zone*" [46], alluding again to a concept from solid-state physics, the Brillouin zone. By convention, it is given for $m = 0$ and includes the interval $-\hbar\omega/2 < \varepsilon < \hbar\omega/2$, which can be shifted in multiples of $\hbar\omega$ for the convenience of each system.

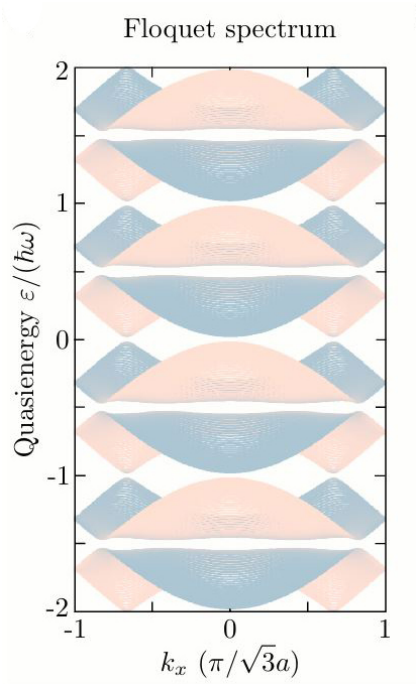

Figure 3.1: The Floquet (quasienergy) spectrum, obtained by diagonalizing the Floquet Hamiltonian $\hat{H}_F$, is periodic with a Floquet-Brillouin zone of width equal to the driving field energy, $\hbar\omega$[46].

Thus, any solution to the Eq. (3.4) with quasienergies outside the first Floquet-Brillouin zone, contains physical information identical to a corresponding one inside the first Floquet-Brillouin

zone. Consequently, as illustrated in Fig. (3.1), the spectrum of $\hat{H}_F$ consists of an infinite number of copies of the Floquet spectrum, that is, the information within the first Floquet-Brillouin zone, shifted up and down by integer multiples of $\hbar\omega$.

Now, what type of information about the system do quasienergies offer? We know that because the Hamiltonian depends on time, the energy is no longer conserved, and its expected value loses meaning. However, it can be shown that, under certain conditions, the quasienergies and Floquet states can be seen as approximations to the eigenenergies and eigenstates of the time-independent system [54], thereby providing insights into the system's behavior across different regimes with or without periodic driving. Nevertheless, although quasienergies can provide us with important information about the system, they are not analyzed in this document due to the initially proposed objectives. Thus, quasienergies are utilized solely for constructing the evolved state, as shown in Eq. (3.3) and from it extract information about the observables raised in the Chapter 2. Then, before addressing the time-dependent problem, let's briefly review the theory that describes the spatially periodic but yet temporally static system, Bloch's theorem and its similarities with the Floquet theorem.

3.1.2 Analogies between Bloch's Theorem and Floquet's Theorem

The Bloch theorem is the spatial counterpart of Floquet's theorem, and like it, it provides the general form of the solutions for a system that is periodic, but in space [80].

This theorem is used when solving the stationary Schrödinger equation for a Hamiltonian with a spatially periodic potential, i.e., $\mathcal{H}(x) = \mathcal{H}_0(x) + \mathcal{V}(x)$ with $\mathcal{V}(x) = \mathcal{V}(x+R)$, where R is the lattice spacing. Bloch's theorem tells us that the solutions to the system are given by $\psi_n(x,k) = e^{ikx}\phi_n(x,k)$ with $\phi_n(x,k) = \phi_n(x+R,k)$, where $\phi_n(x,k)$ are the Bloch functions and k is called quasimomentum.

The crucial advantage of the Bloch functions is their spatial periodicity, which allows us to expand them into position-independent Fourier coefficients $a_{n,j}(k)$:

$$\phi_n(x,k) = \sum_{j=-\infty}^{\infty} a_{n,j}(k) e^{i\frac{2\pi}{R}jx}. \tag{3.7}$$

This expansion is not limited to functions or states with spatial periodicities but can be applied to any function or state with a parameter that meets the same periodicity conditions. In this

way, Floquet states can also be expanded into a discrete Fourier series, enabling advantages in the harmonic Fourier space, as discussed in the following section.

So, in spatially discrete lattice systems, the continuous momentum p loses its meaning and is replaced by $\hbar k$, the *quasimomentum*, defined within the first Brillouin zone $-\pi/R < k < \pi/R$ and the Bloch's theorem helps us describe such systems more adequately. Conversely, in Floquet theory, due to the periodicity in time, energy becomes undefined and must be replaced by *quasienergy*, defined within the first Floquet-Brillouin zone $-\hbar\omega/2 < \varepsilon < \hbar\omega/2$. In both theories, a given quantity of the system is replaced due to the discretization of one of its parameters. In Bloch's theorem, space discretization replaces momentum with quasimomentum, and in Floquet's theorem, time discretization (or periodic time jumps T) replaces energy with quasienergy. This illustrates the clear relationship between space-momentum and energy-time, as pairs of canonically conjugated variables that are inherently closely related, exemplifying basic principles of quantum mechanics such as the the canonical commutation relations or the Heisenberg uncertainty principle [77]. However, the analogies between Bloch and Floquet theories hold only to a certain extent and should not be overstretched, as the two descriptions address different problems and time cannot be associated as eigenvalue to any operator.

Given this context, we see the importance of both tools for the problem posed in this work. Bloch's theorem helps us lay the foundations for writing and understanding our initial Hamiltonian, which is inherently periodic in space. On the other hand, Floquet's theorem provides a method to tackle the system's dynamics, considering its all degrees of freedom (spin, quadrupole and charge) in a simple and practical manner, provided the condition of temporal periodicity is also met. This condition was introduced in Chapter 2 through external fields, constituting the periodic driving. With this in mind, we are now ready to demonstrate how the Floquet eigenvalue equation proposed in Eq. (3.1) can be solved numerically to analyze the dynamics of the proposed system, which is the main objective of this work.

3.2 Numerically solving the Floquet problem

To solve the Floquet problem numerically, that is, to find a solution to the Floquet modes and quasienergies, there are several approaches focuses in the time evolution operator [76]. However, another common option is to further exploit the periodicity property by expanding the Floquet modes and the Hamiltonian of the system into discrete Fourier series, as we saw can be done in the previous section. This approach transfers the system to harmonic Fourier space, where Eq.

(3.4) can be diagonalized directly. This method is known as extended Hilbert space [46] and is the method used to solve the system under study in this Thesis. .

3.2.1 The Extended Hilbert Space

The extended Hilbert space method [46] uses, as mentioned, the fact that the Floquet modes meet the periodic condition $|u_n(t+T)\rangle = |u_n(t)\rangle$, in such a way that they can be expanded into discrete Fourier series in terms of their harmonics and the drive frequency $\omega = 2\pi/T$,

$$|u_n(t)\rangle = \sum_{m=-\infty}^{\infty} e^{-im\omega t}|\nu_n^{(m)}\rangle, \tag{3.8}$$

where $|\nu_n^{(m)}\rangle$ is the m-th Fourier coefficient. Note that the Fourier coefficients $|\nu_n^{(m)}\rangle$ are not normalized, i.e., generically $\langle\nu_n^{(m)}|\nu_n^{(m)}\rangle < 1$ and there is not a simple orthogonality relation between different Fourier coefficients $|\nu_n^{(m)}\rangle$ and $|\nu_n^{(m')}\rangle$, apart from the (nontrivial) fact that they must add up to produce orthogonal Floquet states $|\psi_n(t))\rangle$ at every time t. Now, the Hamiltonian of the system $\hat{H}(t)$ for the same reasons, also can be expressed as,

$$\hat{H}(t) = \sum_{m=-\infty}^{\infty} e^{-im\omega t}\hat{H}^{(m)}. \tag{3.9}$$

Then taking into a account de Fourier decomposition of Floquet modes Eq. (3.8) and the Hamiltonian (3.9) the eigenvalue equation (3.4) can be express in terms of the Fourier coefficients as follows,

$$\left(\sum_{m'} \hat{H}^{(m-m')} - m\hbar\omega\right)|\nu_n^{(m)}\rangle = \varepsilon_n|\nu_n^{(m)}\rangle, \tag{3.10}$$

where

$$\hat{H}^{(m-m')} = \frac{1}{T}\int_0^T dt\hat{H}(t)e^{-i\omega(m-m')t}. \tag{3.11}$$

Note that the Eq. (3.10) takes the form of a typically eigenvalue equation in the Fourier harmonic space. Specifically, we can create a vector $\vec{\varphi}_n$ by "stacking up" the Fourier coefficients $\{|\nu_n^{(m)}\rangle\}$, and rearrange the coefficients $\hat{H}^{(m-m')}$ into a matrix $\mathcal{H}$ acting on vectors in this space, namely the Eq. (3.10) can be represented as:

$$\mathcal{H}\vec{\varphi}_n = \varepsilon_n \vec{\varphi}_n \ , \tag{3.12}$$

with

$$\mathcal{H} = \begin{pmatrix} \ddots & \hat{H}^{(-1)} & \hat{H}^{(-2)} & \\ \hat{H}^{(1)} & \hat{H}^{(0)} - m\hbar\omega & \hat{H}^{(-1)} & \hat{H}^{(-2)} \\ \hat{H}^{(2)} & \hat{H}^{(1)} & \hat{H}^{(0)} - (m+1)\hbar\omega & \hat{H}^{(-1)} \\ & \hat{H}^{(2)} & \hat{H}^{(2)} & \ddots \end{pmatrix}, \quad \vec{\varphi}_n = \begin{pmatrix} \vdots \\ |\nu_n^{(m)}\rangle \\ |\nu_n^{(m+1)}\rangle \\ \vdots \end{pmatrix}, \tag{3.13}$$

where

$$\hat{H}^{(0)} = \frac{1}{T}\int_0^T dt \hat{H}(t) \ , \tag{3.14}$$

is the time-average Hamiltonian. Note that the matrix $\mathcal{H}$, known as the *Floquet Matrix*, in Eq. (3.13) has a block structure: each block is of size d, where d is the dimension of the Hilbert space of the local system, i.e., the dimension of $\hat{H}(t)$. The number of blocks, labeled by Fourier harmonic indices, is formally infinite since the sum over m in Eq. (3.8) and (3.9) ranges over all integers.

By diagonalizing Eq. (3.12), we can obtain the stack of Fourier coefficients and their respective quasienergies, thus providing the necessary superposition to reconstruct the Floquet states and subsequently the state at any time t:

$$|\psi(t)\rangle = \sum_n c_n e^{-\frac{i}{\hbar}\varepsilon_n t}|u_n(t)\rangle = \sum_n c_n e^{-\frac{i}{\hbar}\varepsilon_n t}\left(\sum_{m=-\infty}^{\infty} e^{-im\omega t}|\nu_n^{(m)}\rangle\right). \tag{3.15}$$

However, the extended Hilbert space method has a significant challenge. As seen in Eq. (3.13), we have transitioned from a problem with a matrix of finite dimensions to one requiring the diagonalization of an infinite-dimensional matrix, since the Fourier expansion includes all possible integer harmonics to reconstruct the state. Numerically, this makes it impossible to completely reconstructed the state. Nevertheless, it is important to consider that, as is known, not all coefficients in a Fourier expansion are significant, allowing for the truncation of the matrix in Eq. (3.13). This truncation depends on the regime being studied, as discussed in the following section.

3.2.2 Truncation of the harmonic Fourier space

The problem of dimensionality in the extended Hilbert space can be managed by truncating the Fourier expansion, that is, truncating the matrix of Eq. (3.13), at a certain harmonic m', such that the sum over the harmonics is within the interval $m \in [-m', m']$. This approach increases the dimensionality of the original system's matrix $\hat{H}(t)$ from d to $d(2m'+1)$, making it numerically solvable. However, the question arises: Is it possible to truncate the matrix $\mathcal{H}$ without losing relevant system information? To answer this, it is convenient to analyze the structure of the matrix $\mathcal{H}$ given a certain periodic drive, which is commonly cosine-shaped. Let's consider the following time-dependent Hamiltonian:

$$\hat{H}(t) = \hat{H}_0 + \hat{V}(t), \quad \hat{V}(t) = \hat{V}e^{i\omega t} + \hat{V}^\dagger e^{-i\omega t}, \tag{3.16}$$

the corresponding extended-zone of the Floquet Hamiltonian, $\mathcal{H}$ then takes the form in Eq. (3.13) with $\hat{H}^{(1)} = \hat{V}$, $\hat{H}^{(-1)} = \hat{V}^\dagger$, and $\hat{H}^{(\Delta m)} = 0$ for $|\Delta m| > 1$. In this case, $\mathcal{H}$ has a block-tridiagonal form, with the non-driven Hamiltonian $\hat{H}_0$ (shifted by multiples of $\hbar\omega$) repeated along the diagonal blocks, and the drive coupling $\hat{V}$ ($\hat{V}^\dagger$) placed in the blocks above (below) the diagonal:

$$\mathcal{H} = \begin{pmatrix} \ddots & \hat{V} & 0 & & \\ \hat{V}^\dagger & \hat{H}_0 + \hbar\omega & \hat{V} & 0 & \\ 0 & \hat{V}^\dagger & \hat{H}_0 & \hat{V} & 0 \\ & 0 & \hat{V}^\dagger & \hat{H}_0 - \hbar\omega & \hat{V} \\ & & 0 & \hat{V}^\dagger & \ddots \end{pmatrix}. \tag{3.17}$$

Importantly, the (block) tridiagonal structure of $\mathcal{H}$ is closely analogous to a tight-binding lattice with nearest-neighbor hopping and a linear potential, i.e., to the problem of a particle in a one-dimensional lattice with a uniform electric field, but in this case it would be in a harmonic Fourier space or in a "*Floquet lattice*", as can be seen in the Fig. (3.2). By making analogies to Bloch oscillations [81] and to the Wannier-Stark ladder [82], we may gain important insight into the nature of the Floquet states encoded in the solutions to Eq. (3.13). These insights furthermore shed light on the utility of this approach as a numerical method for obtaining Floquet states.

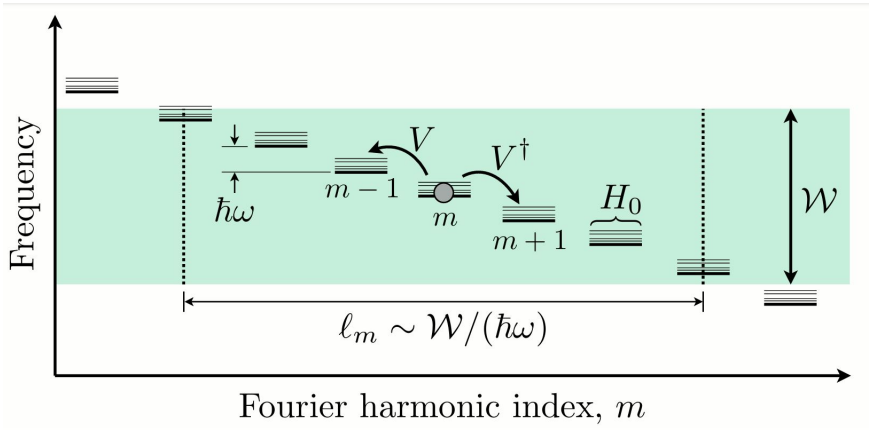

Figure 3.2: The extended-zone of the Floquet Hamiltonian, Eq. (3.17), can be interpreted as describing the one-dimensional tight-binding dynamics of an effective "particle" hopping in Fourier harmonic space [46].

So, as we can see, the extended Hamiltonian in the Fourier harmonic space can be interpreted as the dynamics of an effective "particle" that jumps between sites of a one-dimensional lattice, the Floquet lattice. Each unit cell is represented by a harmonic m and is described by the time-averaged Hamiltonian $\hat{H}_0$. The linear driving term induces "jumps" between neighbors in the different lattice sites of the Fourier space, making the harmonic index m change by one, and the energies at the sites vary linearly with m due to the terms $-m\hbar\omega$ in the diagonal blocks of Eqs. (3.14), which can be interpreted as a "linear potential" analogous to applying a uniform field in a classical system. In the absence of this potential, the eigenstates of the system can be understood as "Bloch functions" in Fourier space with a corresponding bandwidth $\mathcal{W} \sim \{\langle\hat{V}\rangle, \langle\hat{H}_0\rangle\}$, being strongly delocalized. However, by including the "linear potential" $(-m\hbar\omega)$, it acts as a uniform electric field on the particle, meaning that from a semiclassical point of view, the effective particle can only explore a range of harmonics $\ell_m \sim \mathcal{W}/(\hbar\omega)$, and therefore the Floquet states represent "Wannier functions", implying they are strongly localized in the Fourier harmonic space. Consequently, the infinite dimensional matrices of Eqs. (3.13) and (3.14) can be safely truncated up to the most relevant harmonics [46].

But how can we truncate this matrix up to the most relevant harmonics? Here, we have to distinguish two regimes. In the "*weak-driving*" regime, i.e. $\hbar\omega \gg \langle\hat{V}\rangle$, which is also known as the high-frequency regime [83], only one block of the Floquet matrix is relevant, namely,

$$\mathcal{H} = \begin{pmatrix} \hat{H}_0 + \hbar\omega & \hat{V} \\ \hat{V}^\dagger & \hat{H}_0 \end{pmatrix}, \tag{3.18}$$

in which it recognize in the context of quantum optics as the rotating-wave approximation [84]. If instead the driving frequency is on the same order as the periodic driving $\hbar\omega \sim \langle \hat{V} \rangle$, we reach the "*strong-driving*" regime in which many blocks of the Floquet matrix have to be taken into account [85]. One way to know how many blocks or harmonics are enough to completely reconstruct the state is to consider the completeness of the Floquet modes. Since unitary evolutions are always being considered, the norm of the state must be preserved (Eq. 3.15), and therefore, the sum of the square modulus of the superposition coefficients must be exactly equal to 1, at every instant of time t, $\sum_n |c_n|^2 = 1$. If this sum is greater or less, it means that not enough harmonics are being considered and therefore they must be increased, or, alternatively, the period of the driving must be decreases to be closer to the high-frequency regime.

Having explained the technique and numerical method to be used, the implementation of Floquet's Theorem and the extended Hilbert space for the case of a single particle in a two-site lattice is shown below, in addition to the exact analytical calculation that can be developed. This comparison between the numerical technique and the exact solution demonstrates the validity of the method for its subsequent use in the complete system described in Chapter 2.

3.3 Implementation of the Floquet's Theorem

To show the comparison between the numerical implementation of Floquet's theorem and the exact calculation provided for a single-particle system, let us start with the analytical solution which involves a typical diagonalization with Fourier transforms.

3.3.1 Exact Solution

To solve the single-particle system described in chapter 2, we start with the Hamiltonian given in Eq. (2.20), which is:

$$\hat{H}(t) = -J \sum_{i,\sigma} \left(\hat{b}^\dagger_{i,\sigma} \hat{b}_{i+1,\sigma} + \hat{b}^\dagger_{i+1,\sigma} \hat{b}_{i,\sigma} \right) - \mu \sum_{i,\sigma} \hat{n}_{i,\sigma} + D_0 \cos^2(\omega t) \sum_{i,\sigma} \sigma \hat{n}_{i,\sigma}. \tag{3.19}$$

As mentioned, this Hamiltonian describes a single spin-1 particle in a one-dimensional optical lattice under the influence of a periodic driving, let's consider the linear Zeeman field, but one can equally apply a quadratic Zeeman field. The analytical solution for this system is obtained through a Fourier transform of the Hamiltonian, which allows it to be expressed in momentum space,

$$\hat{b}_{j,\sigma} = \frac{1}{\sqrt{L}} \sum_{k=1}^{L} e^{-i\frac{2\pi}{L}jk} \hat{c}_{k,\sigma}, \quad \hat{c}_{k,\sigma} = \frac{1}{\sqrt{L}} \sum_{j=1}^{L} e^{i\frac{2\pi}{L}jk} \hat{b}_{j,\sigma}, \tag{3.20}$$

then, the Hamiltonian in momentum space takes the form:

$$\hat{H}(t) = -2J \sum_{k,\sigma} \cos\left(\frac{2\pi}{L}k\right) \hat{n}_{k,\sigma} - \mu \sum_{k,\sigma} \hat{n}_{k,\sigma} + D_0 \cos^2(\omega t) \sum_{k,\sigma} \sigma \hat{n}_{k,\sigma}, \tag{3.21}$$

which is diagonal in momentum space. Note that the temporal dependency of the Hamiltonian in Eq. (2.20) was introduced as an amplitude of a specific operator, in this case $\hat{S}^z$. This indicates that the commutation relations between the operators that make up the Hamiltonian do not change over time, ensuring that the Hamiltonian commutes at different times, i.e., $[\hat{H}(t_1), \hat{H}(t_2)] = 0$. Consequently, the time evolution operator can be calculated in the usual form:

$$\hat{U}(t) = \exp\left\{-\frac{i}{\hbar}\int_0^t \hat{H}(t')dt'\right\}, \tag{3.22}$$

therefore, integrating the Hamiltonian, we obtain

$$\int_0^t \hat{H}(t')dt' = \sum_{k,\sigma} \left(-2J\cos\left(\frac{2\pi}{L}k\right) - \mu\right) t\hat{n}_{k,\sigma} + D_0 \frac{\sin(2\omega t) + 2\omega t}{4\omega} \sum_{k,\sigma} \sigma \hat{n}_{k,\sigma}, \tag{3.23}$$

and finally, the time-evolution operator is given by

$$\hat{U}(t) = \exp\left\{\frac{i}{\hbar} \sum_{k,\sigma} \left(\epsilon_{k,L}t - g(t)\sigma\right) \hat{n}_{k,\sigma}\right\}, \tag{3.24}$$

where we define $\epsilon_{k,L} = 2J\cos\left(\frac{2\pi}{L}k\right) + \mu$ and $g(t) = D_0\frac{\sin(2\omega t)+2\omega t}{4\omega}$. Now, the choice of basis is clearly the eigenbasis of the number operator $\{|n_1, n_{-1}, n_0\rangle\}$, which tells us the number of particles with a momentum k (site i) in a specific magnetic projection σ, namely,

Position space	**Momentum space**
$\cdots \lvert n_1, n_{-1}, n_0\rangle_i \lvert n_1, n_{-1}, n_0\rangle_{i+1} \cdots$	$\cdots \lvert n_1, n_{-1}, n_0\rangle_k \lvert n_1, n_{-1}, n_0\rangle_{k+1} \cdots$

(3.25)

Then, since we want to describe a single spin-1 particle in the entire lattice, the only possible states are of the type $\{|1,0,0\rangle_1|\varnothing\rangle\cdots, |0,1,0\rangle_1|\varnothing\rangle\cdots, |0,0,1\rangle_1|\varnothing\rangle\cdots, |\varnothing\rangle|1,0,0\rangle_2|\varnothing\rangle\cdots, \cdots\}$, i.e., one particle in the magnetic projection $1, -1$, or 0 with a momentum (site) 1 and vacuum in the other sites, or one particle in the magnetic projection $1, -1$, or 0 with a momentum (site) 2 and vacuum in the other sites, and so on. Note that the time evolution operator of Eq. (3.24) evolves any initial state for any number of sites. However, determining the evolved state for any number of initial states and calculating all observables for those different initial states becomes impractical, thus the implementation of a numerical technique (Floquet) to speed up this process becomes more striking. Therefore, for comparison, let us consider only two sites $L = 2$. The matrix representation for the two-site time evolution operator is given by

$\mathcal{U} =$

(k)	$\lvert\varnothing\rangle$	$\lvert1,0,0\rangle\lvert\varnothing\rangle$	$\lvert0,1,0\rangle\lvert\varnothing\rangle$	$\lvert0,0,1\rangle\lvert\varnothing\rangle$	$\lvert\varnothing\rangle\lvert1,0,0\rangle$	$\lvert\varnothing\rangle\lvert0,1,0\rangle$	$\lvert\varnothing\rangle\lvert0,0,1\rangle$
$\langle\varnothing\rvert$	1	0	0	0	0	0	0
$\langle\varnothing\rvert\langle1,0,0\rvert$	0	$e^{\frac{i}{\hbar}(\epsilon_{1,2}t-g(t))}$	0	0	0	0	0
$\langle\varnothing\rvert\langle0,1,0\rvert$	0	0	$e^{\frac{i}{\hbar}(\epsilon_{1,2}t+g(t))}$	0	0	0	0
$\langle\varnothing\rvert\langle0,0,1\rvert$	0	0	0	$e^{\frac{i}{\hbar}\epsilon_{1,2}t}$	0	0	0
$\langle1,0,0\rvert\langle\varnothing\rvert$	0	0	0	0	$e^{\frac{i}{\hbar}(\epsilon_{2,2}t-g(t))}$	0	0
$\langle0,1,0\rvert\langle\varnothing\rvert$	0	0	0	0	0	$e^{\frac{i}{\hbar}(\epsilon_{2,2}t+g(t))}$	0
$\langle0,0,1\rvert\langle\varnothing\rvert$	0	0	0	0	0	0	$e^{\frac{i}{\hbar}\epsilon_{2,2}t}$

where the matrix representation is given in the momentum basis (k). We can see that the vacuum state $|\varnothing\rangle$ has been included in the basis, due to the importance of the vacuum state in this type of lattice systems, where jumps between sites only occur if there is a vacuum in the consecutive sites. Without the vacuum state, the description of the system in Hilbert space would be incomplete, meaning that some physically possible configurations of the system would be inaccessible in the mathematical formulation. Furthermore, the vacuum state plays a crucial role in modeling phase transitions, such as the Superfluid-Mott Insulator transition in the spinless model [86]. Thus, only the initial conditions $|\psi(0)\rangle$ are needed to calculate the state at any time $|\psi(t)\rangle = \hat{U}(t)|\psi(0)\rangle$.

3.3.2 Numerical implementation

For the numerical implementation of Floquet's Theorem and the extended Hilbert space approach in the spin-1 Bose-Hubbard model, the following steps are followed (for further details see appendix C):

1. **Set the initial parameters:** For both of our considered systems defined by the Eqs. (2.20) and (2.24), we set the number of sites L, the hopping rate J, the chemical potential μ, the interaction strengths U_2 and U_0 (which vanish for the one particle system), the Linear Zeeman Strength D_0 (or quadratic Zeeman strength Q_0), the driving frequency ω, which is set to $\omega \gg D_0$ ($\hbar$ is fixed to 1) for the high-frequency regime or $\omega \sim D_0$ for the strong-driving regime, and the number of harmonics m, which are determined depending on the regime used, and is equivalent to $2m+1$ blocks of the Floquet matrix.

2. **Generate the local and non-local matrix of the Hamiltonian:** With the parameters defined previously, we generate the local matrix of each operator of the Hamiltonian in the position basis, i.e., the matrix of each operator of only one site (two sites in the case of the hopping term): the hopping term, the chemical potential $\hat{n}_{i,\sigma}$, the charge scattering $\hat{n}_{i,\sigma}(\hat{n}_{i,\sigma}-1)$, the spin scattering $\hat{\boldsymbol{F}}_i^2$, and the linear Zeeman field $\sigma\hat{n}_{i,\sigma}$ (or quadratic Zeeman field $\sigma^2\hat{n}_{i,\sigma}$). Then, we generate the non-local matrices from the local ones using Kronecker products, i.e., we generate the matrices for L sites.

3. **Generate the Floquet Matrix:** Once the Hamiltonian matrix for L sites is defined, we generate the Floquet matrix from Eq. (3.13), calculating each Fourier coefficient of the Hamiltonian as specified by Eq. (3.11), integrating with the Trapezoidal Quadrature, given by the C++ Boost-Math library and only up to the number of harmonics m specified.

4. **Diagonalization and reconstruction of the state:** Given the previously calculated Floquet matrix, we proceed to diagonalize it with the help of the LAPACK library, thereby finding the quasienergies and the determined Floquet modes to reconstruct the state given by Eq. (3.15), taking into account the previous calculation of the coefficients c_n defining the initial state $|\psi(0)\rangle$.

5. **Measurement of observables:** Once the state $|\psi(t)\rangle$ has been reconstructed for any time t, we measure the observables described in chapter 2, the number of atoms per lattice site in each spin component $\langle\hat{n}_{i,\sigma}\rangle$, the magnetic density $\langle\hat{S}_i^z\rangle$, the quadrupolar density $\langle\hat{Q}_i^d\rangle$, and the total transverse magnetization, $|\langle\hat{F}_i^x\rangle|^2$, analyzing their behavior over time.

3.3.3 Comparison between analytical and numerical solutions

To compare the numerical technique with the exact analytical solution, we established the two-site single-particle model. The analytically evolved state is obtained by applying the time evolution operator given by Eq. (3.24), and the numerically evolved state is obtained by following the steps described above. Note that the matrix of the two-site system is expressed as follows:

$$\mathbf{H} = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & -\mu + D_0 & 0 & 0 & -2J & 0 & 0 \\ 0 & 0 & -\mu - D_0 & 0 & 0 & -2J & 0 \\ 0 & 0 & 0 & -\mu & 0 & 0 & -2J \\ 0 & -2J & 0 & 0 & -\mu + D_0 & 0 & 0 \\ 0 & 0 & -2J & 0 & 0 & -\mu - D_0 & 0 \\ 0 & 0 & 0 & -2J & 0 & 0 & -\mu \end{pmatrix}. \tag{3.26}$$

To simplify both analytical and numerical calculations, we set the following values for the system parameters, taking into account that the hopping rate is our energy unit: $J = \mu = D_0 = 1$ and $\omega = 2\pi/T$ with $T = 0.01$ s. This places us in the high-frequency regime, where only one harmonic $m = 1$ is sufficient to consider. Once the parameters are established, we choose an arbitrary initial state; in this case, $|\psi(0)\rangle = |1,0,0\rangle^{(1)}|\varnothing\rangle$, i.e., the initial state is given by a particle with magnetic projection 1 at site $i = 1$.

It must be noted that the numerical method is given in the position basis, while the analytical solution is in the momentum basis. To ensure that the same initial state is evolving, it must be written $|\psi(0)\rangle$ in the momentum basis using Eq. (3.20),

$$|\psi(0)\rangle = |1,0,0\rangle^{(i)}|\varnothing\rangle = -\frac{1}{\sqrt{2}}|1,0,0\rangle^{(k)}|\varnothing\rangle + \frac{1}{\sqrt{2}}|\varnothing\rangle|1,0,0\rangle^{(k)}, \tag{3.27}$$

where the superscript i (k) indicates the state in the position (momentum) basis. Therefore, using the time-evolution operator of Eq. (3.24) and noting that with the parameters given above $\epsilon_{1,2} = -1$, $\epsilon_{2,2} = 3$, and $g(t)$ results in a global phase, the evolved state in the momentum basis is given by

$$|\psi(t)\rangle = -\frac{e^{-2it}}{\sqrt{2}}|1,0,0\rangle^{(k)}|\varnothing\rangle + \frac{e^{2it}}{\sqrt{2}}|\varnothing\rangle|1,0,0\rangle^{(k)}, \tag{3.28}$$

or in the position basis using again Eq. (3.20) as

$$|\psi(t)\rangle = \cos(2t)|1,0,0\rangle^{(i)}|\varnothing\rangle + i\sin(2t)|\varnothing\rangle|1,0,0\rangle^{(i)}. \tag{3.29}$$

This allows us to measure the observables mentioned in the previous section over time. For comparison purposes, a clear behavior of the evolution of the state can be seen if we project it onto its initial state $|\psi(0)\rangle$,

$$|\langle\psi(0)|\psi(t)\rangle|^2 = \cos^2(2t), \tag{3.30}$$

which can also be seen numerically in Fig 3.3.

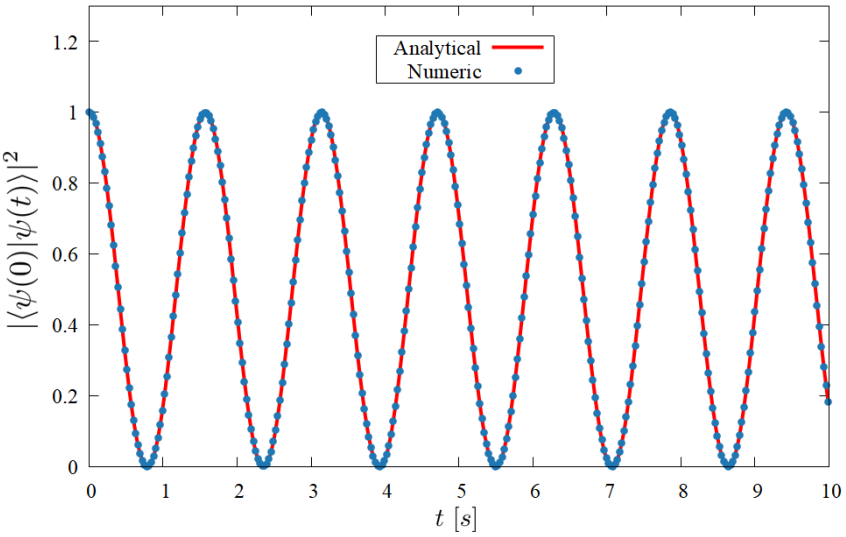

Figure 3.3: Probability that the evolved state $|\psi(t)\rangle$ returns to its initial state $|\psi(0)\rangle = |1,0,0\rangle^{(i)}|\varnothing\rangle$, calculated exactly Eq. (3.30) and numerically through Floquet's theory, for $L = 2$, $J = \mu = D_0 = 1$ and $T = 0.01$ s.

Then, we can see that the numerical implementation matches perfectly with the exact analytical solution, showing in both cases a clear transition between the states $|1,0,0\rangle|\varnothing\rangle \to |\varnothing\rangle|1,0,0\rangle$, i.e., a jump of a particle from site 1 to site 2, then from site 2 to site 1 again, and so on in time, always preserving the same initial magnetic projection (i.e., σ=1) due to the absence of interactions.

We can also compare the behavior of the observables described in Chapter 2. However, due to the lack of interactions and the polarized initial state, it can be easily shown that the quadrupolar density, magnetic density, and transverse magnetization remain constant over time: $\langle\hat{Q}_i^d\rangle_t = \frac{1}{\sqrt{3}}$, $\langle\hat{S}_i^z\rangle_t = 1$, $|\langle\hat{S}_i^x\rangle_t|^2 = 0$, as corroborated by Fig 3.4.

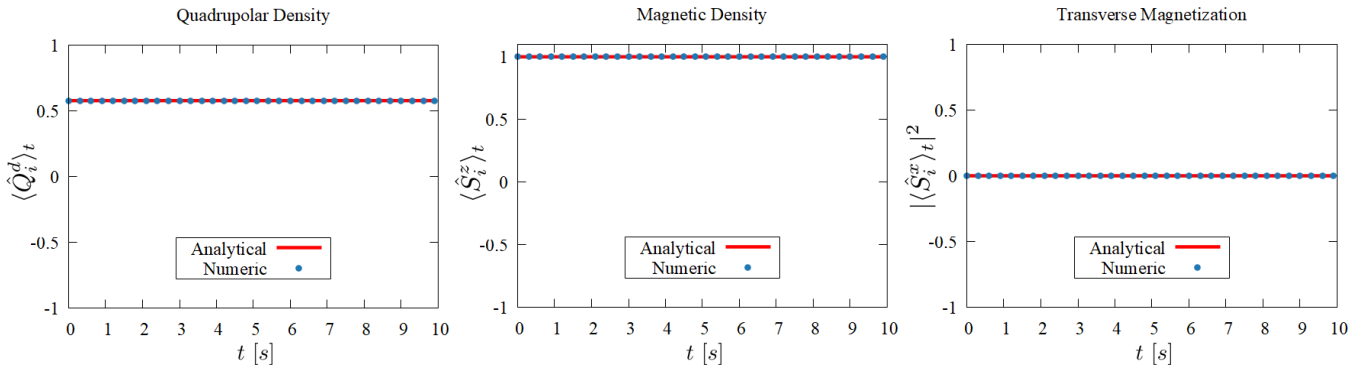

Figure 3.4: The expected value in time for the quadrupolar density $\hat{Q}_i^d$, the magnetic density $\hat{S}_i^z$ and the transverse magnetization $\hat{S}_i^x$ given the initial state $|\psi(0)\rangle = |1,0,0\rangle^{(i)}|\varnothing\rangle$.

Note that for this specific initial state, the contribution of the Zeeman field results in a global phase, so the imposed driving does not affect the system, and its behavior depends exclusively on the hopping term and the chemical potential. However, this is due exclusively to the initial condition, and by exploring different initial states, the effect of the driving and its different regimes on the system can be better analyzed, both for linear and quadratic Zeeman fields, as discussed in depth in the following chapter.

Although the above description for the implementation of Floquet's theorem was given for a particular physical system with an exact analytical solution, it is easy to modify all parameters to work with more sites, different initial states, include interactions, among other modifications which make the system more complex and therefore analytically unsolvable, but numerically plausible and flexible. Whether for one or two particles, the method requires following the steps provided in this section. Likewise, if two-dimensional or three-dimensional lattices are considered, it is possible to apply Floquet's technique by adjusting the Hamiltonian of the system accordingly, just as with any other numerical method that works with lattice systems. In Appendix C, we provide a more in-depth explanation of the implementation of Floquet's theorem in the C++ language, mentioning the libraries used, specifications in the integration method, and other details introduced to make the calculations more efficient.

With the construction of our Numerical Floquet Theorem, we proceed to use it to study the dynamics of one and two spin-1 lattice bosons in the presence of external magnetic fields, focusing mainly on the behavior of spinorial and quadrupolar dynamics and the effects of driving on this type of system.

Appendix B

Supplementary Material on Floquet Theory

Since Floquet theory encompasses many analytical and numerical approaches, this appendix provides supplementary material to delve deeper into the formalism used. First, the most common proof of Floquet's theorem is provided, emphasizing the properties of the time evolution operator. Then, other types of numerical solutions to Floquet's problem are covered. Finally, the different concepts and definitions established in Floquet's formalism are summarized, highlighting its analogies with Bloch's theorem.

B.1 Proof of Floquet theorem

As mentioned in chapter 3 there are several ways to express Floquet's theorem, for its demonstration it is easier to state it in such a way that it focuses on the properties of the time evolution operator, which due to the periodicity of the Hamiltonian satisfies:

$$\hat{U}(t+nT,t_0) = \hat{U}(t,t_0)\left[\hat{U}(t_0+T,t_0)\right]^n. \tag{B.1}$$

This proof is a simplified form of the typical proof basing in the time evolution operator, emphasizing in the more relevant points [76].

Then, in principle, the whole dynamics is captured by the unitary time-evolution operator $\hat{U}(t,t_0)$, which evolve the state in the common way

$$|\psi(t)\rangle = \hat{U}(t,t_0)|\psi(t_0)\rangle, \quad \text{with} \quad \hat{U}(t,t_0) = \mathcal{T}\exp\left\{-\frac{i}{\hbar}\int_{t_0}^{t}\hat{H}(t')dt'\right\}, \tag{B.2}$$

where $\mathcal{T}$ denotes the time-ordering. Now, evidently this time evolution operator satisfy the following property

$$\hat{U}(t_2,t_0) = \hat{U}(t_2,t_1)\hat{U}(t_1,t_0), \tag{B.3}$$

with this in mind consider the time-evolution operator from initial time t_0 to some final time $t+T$

$$\begin{aligned}\hat{U}(t+T,t_0) &= \hat{U}(t+T,t_0+T)\hat{U}(t_0+T,t_0),\\ &= \hat{U}(t,t_0)\hat{U}(t_0+T,t_0).\end{aligned}$$

We knowing that any time-evolution operator $\hat{U}(t_2,t_1)$ must be unitary (i.e. $\hat{U}^\dagger\hat{U}=\mathbb{1}$), therefore we are able to write the second part of our time-evolution operator as

$$\hat{U}(t_0+T,t_0) = e^{-\frac{i}{\hbar}\hat{H}_F T}, \tag{B.4}$$

where $\hat{H}_F$ is called the "*Floquet Hamiltonian*" and its exponential is the "*Floquet Operator*", the "*Floquet Propagator*" or the "*slow-motion operator*", and as $\hat{H}_F$ is a hermitian operator ($\hat{H}_F^\dagger = \hat{H}_F$) using this, we can rewrite the time-evolution operator of the whole system as

$$\hat{U}(t,t_0) = \underbrace{\hat{U}(t,t_0)e^{\frac{i}{\hbar}\hat{H}_F\times(t-t_0)}}_{\hat{P}(t,t_0)} e^{-\frac{i}{\hbar}\hat{H}_F\times(t-t_0)},$$

$$\hat{U}(t,t_0) = \hat{P}(t,t_0)e^{-\frac{i}{\hbar}\hat{H}_F\times(t-t_0)},$$

and now again due the unitarity $\hat{P}(t,t_0)$ must be

$$\hat{P}(t,t_0) = \hat{U}(t,t_0)e^{\frac{i}{\hbar}\hat{H}_F\times(t-t_0)} = e^{-i\hat{K}_F(t)}, \tag{B.5}$$

where $\hat{K}_F(t)$ is called the "*stroboscopic kick operator*" and its exponential the "*fast-motion operator*", that obeys $e^{-i\hat{K}_F(t+T)} = e^{-i\hat{K}_F(t)}$

This means that the kick operator describes the motion within one period T but does change from one period to the next(it just depends on the global choice of starting time t_0). This allows us to directly write down Floquet's theorem for periodically modulated hamiltonians, which states that given a Hamiltonian that satisfies $\hat{H}(t) = \hat{H}(t+T)$ then its time-evolution operator is given by

$$\hat{U}(t,t_0) = e^{-i\hat{K}_F(t)}e^{-\frac{i}{\hbar}\hat{H}_F\times(t-t_0)}, \tag{B.6}$$

where

$$e^{-i\hat{K}_F(t)} : \text{Fast-motion operator}, \qquad e^{-\frac{i}{\hbar}\hat{H}_F\times(t-t_0)} : \text{Slow-motion operator}.$$

This result is the mathematical way of separating the slow dynamics $\left(\text{governed by } \hat{H}_F\right)$ from the fast-motion during one period T $\left(\text{governed by } e^{-i\hat{K}_F(t)}\right)$, as illustrated in the Figs B.1 and B.2.

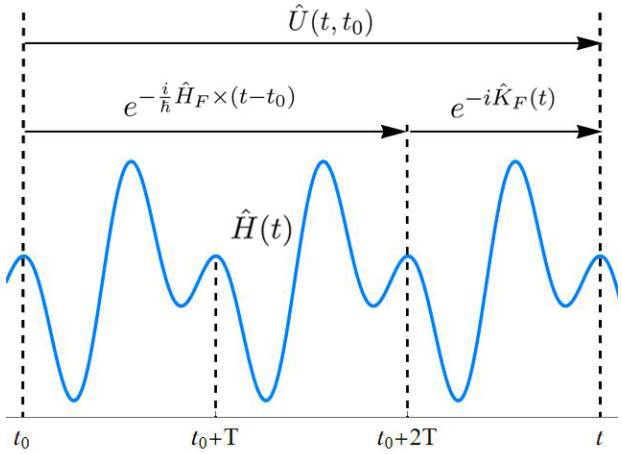

Figure B.1: Floquet's theorem illustrated. The slow dynamics (from one period T to the next) is captured by Floquet Hamiltonian $\hat{H}_F$, whereas the fast "micromotion" within a period is governed by the fast motion operator $e^{-i\hat{K}_F(t)}$.

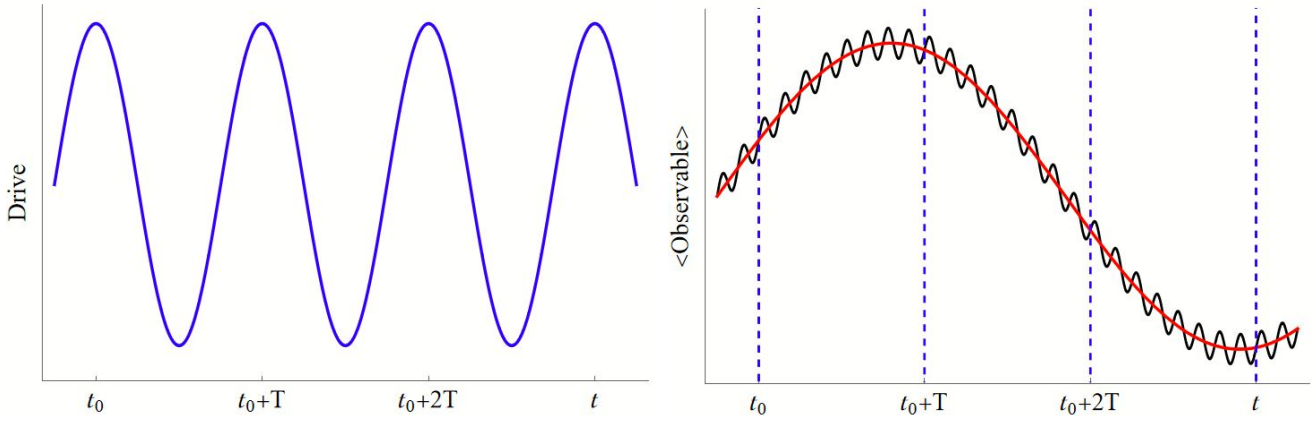

Figure B.2: The action of a periodic drive (left panel) on the time-evolution of a quantum system. The slow dynamics of an observable (red line) is captured by the Floquet Hamiltonian $\hat{H}_F$ whereas the exact dynamics (black line) is composed of fast dynamics (micromotion) and slow dynamics. The micromotion is described by the kick operators $e^{-i\hat{K}_F(t)}$ and vanishes at stroboscopic times $t_0, t_0 + T$, etc.

Now, the Floquet operator, being unitary can be in principle diagonalised, it means that a complete

set of eigenstates exist, let us indicate them by $|u_n(t_0)\rangle$, such that

$$e^{-\frac{i}{\hbar}\hat{H}_F\times(t-t_0)}|u_n(t_0)\rangle = e^{-\frac{i}{\hbar}\varepsilon_n\times(t-t_0)}|u_n(t_0)\rangle, \tag{B.7}$$

where, these eigenvalues $e^{-\frac{i}{\hbar}\varepsilon_n\times(t-t_0)}$ are called the "*Floquet multipliers*". Remember ε_n is a real parameter called quasienergy being unique up to multiples of $\hbar\omega$, $\omega = \frac{2\pi}{T}$. Taking the multivaluedness of the energies ε_n into account, we can also directly get the eigenstates and eigenvalues via

$$\hat{H}_F|u_n(t_0)\rangle = \varepsilon_n|u_n(t_0)\rangle, \tag{B.8}$$

where the eigenstates $|u_n(t_0)\rangle$ are called the "Floquet Modes". Now we expand an arbitrary initial state $|\psi(t_0)\rangle$ in eigenbasis of Floquet hamiltonian

$$\begin{aligned}|\psi(t_0)\rangle &= \sum_n |u_n(t_0)\rangle \underbrace{\langle u_n(t_0)|\psi(t_0)\rangle}_{\equiv c_n},\\ &= \sum_n c_n|u_n(t_0)\rangle.\end{aligned}$$

Then, the state at later times is expressed as

$$\begin{aligned}|\psi(t)\rangle &= \hat{U}(t,t_0)|\psi(t_0)\rangle,\\ &= \sum_n c_n e^{-i\hat{K}_F(t)}e^{-\frac{i}{\hbar}\hat{H}_F\times(t-t_0)}|u_n(t_0)\rangle,\\ &= \sum_n c_n e^{-\frac{i}{\hbar}\varepsilon_n\times(t-t_0)}e^{-i\hat{K}_F(t)}|u_n(t_0)\rangle,\\ &= \sum_n c_n e^{-\frac{i}{\hbar}\varepsilon_n\times(t-t_0)}|u_n(t)\rangle,\end{aligned} \tag{B.9}$$

where $|u_n(t)\rangle = e^{-i\hat{K}_F(t)}|u_n(t_0)\rangle$ with $|u_n(t)\rangle = |u_n(t+T)\rangle$, and in the literature the states

$$|\psi_n(t)\rangle = e^{-\frac{i}{\hbar}\varepsilon_n\times(t-t_0)}|u_n(t)\rangle, \tag{B.10}$$

are often called "Floquet states" in analogy with the Bloch theorem.

B.2 Alternative Approaches to Numerical Solutions

In the following subsections, we explore additional methods for numerically solving the Floquet problem, either directly or through approximations of the time evolution operator $\hat{U}(t_0+T, t_0)$.

B.2.1 Exact Time-Evolution of $\hat{U}(t_0 + T, t_0)$

If the Hilbert space of $\hat{H}(t)$ is not excessively large and its analytical form is not overly complex, it is possible to obtain $\hat{U}(t_0 + T, t_0)$ by integrating the time-dependent Schrödinger equation over one period, i.e., by solving the Schrödinger equation in the standard manner. First, the initial state is expanded in the Floquet modes:

$$|\psi(t_0)\rangle = \sum_n c_n(t_0)|u_n(t_0)\rangle. \tag{B.11}$$

The state $|\psi(t_0)\rangle$ is then evolved over one period according to the time-dependent Schrödinger equation:

$$i\hbar\frac{d}{dt}c_n(t) = \sum_m H_{nm}(t)c_m(t). \tag{B.12}$$

This results in a set of n coupled differential equations for each coefficient $c_n(t_0)$ from t_0 to $t_0 + T$. The solutions to this set of differential equations provide the time-evolved vectors $\{c_n(t_0 + T)\}$, which are directly related to the columns of $\hat{U}(t_0 + T, t_0)$. Diagonalizing this matrix yields the Floquet multipliers $\left\{e^{-\frac{i}{\hbar}\varepsilon_n T}\right\}$, thereby providing all the necessary components to reconstruct the state at any time t.

Clearly, solving a set of n coupled differential equations is not a trivial numerical task. Therefore, this approach is recommended only for cases where the dimension of the Hamiltonian is relatively small (which is not the our case) and the functional form of the Hamiltonian is not overly complex.

B.2.2 Trotter Decomposition of $\hat{U}(t_0 + T, t_0)$

If the Hilbert space is too large, a direct numerical integration of Eq. (B.12) can become impractical. In such cases, an alternative approach is the Trotter decomposition of the time-evolution operator [94], which involves dividing the timespan $[t_0, t_0 + T]$ into N segments $t_i = t_0 + i\Delta t$ with $\Delta t = \frac{T}{N}$ (see Fig B.3). The time-evolution operator can then be approximated as follows:

$$\begin{aligned}\hat{U}(t_0+T,t_0) &= \mathcal{T}\exp\left(-\frac{i}{\hbar}\int_{t_0}^{t_0+T}\hat{H}(t)dt\right),\\ &\approx \exp\left(-\frac{i}{\hbar}\sum_{i=0}^{N-1}\hat{H}(t_i)\Delta t\right),\\ &\approx \prod_{i=0}^{N-1}\exp\left(-\frac{i}{\hbar}\hat{H}(t_i)\Delta t\right)+\mathcal{O}(\Delta t^2).\end{aligned} \tag{B.13}$$

Here, $\mathcal{T}$ denotes time-ordering, and the third line represents the Trotter decomposition, i.e., transitioning from the exponential of a sum to the product of exponentials. This can be challenging because Hamiltonians at different times generally do not commute, i.e., $[\hat{H}(t_1),\hat{H}(t_2)]\neq 0$. The Trotter decomposition ensures that the error introduced by ignoring the commutators is only $\mathcal{O}(\Delta t^2)$, meaning it decreases quadratically with the duration of each time-step. During each time-step, the Hamiltonian $\hat{H}(t_i)$ is assumed to be constant, thereby reducing the time-ordered integral to a product of exponentiated matrices. As before, diagonalizing $\hat{U}(t_0+T,t_0)$ yields the Floquet multipliers $\left\{e^{-\frac{i}{\hbar}\varepsilon_n T}\right\}$, providing all the necessary components to reconstruct the state at any time t.

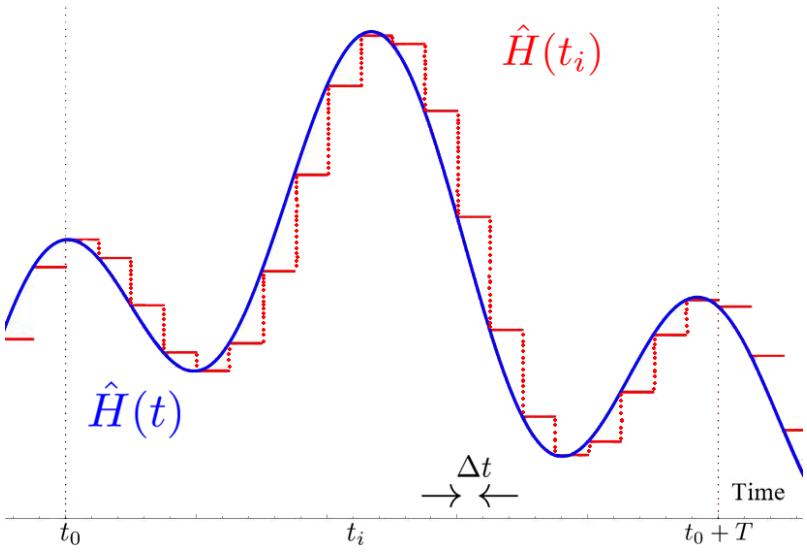

Figure B.3: Trotter decomposition of the time-evolution operator $\hat{U}(t_0+T,t_0)$. The time-axis is discretized in units of Δt , taking the Hamiltonian $\hat{H}(t_i)$ to be constant at each instant.

B.3 Summary of important definitions

Name(s)	Definition	Expression
Floquet Hamiltonian	A Hermitian operator that extends the concept of the Hamiltonian to include the effects of periodic variations in a quantum system.	$\hat{H}_F = \hat{H}(t) - i\hbar\frac{d}{dt}$
Floquet modes	The eigenstates of the Floquet Hamiltonian, which define the basis of the system.	$\|u_n(t_0)\rangle$
Quasienergies	The eigenvalues of the Floquet Hamiltonian, serving as the replacement for energy in the system. The term originates from the analogy with quasimomentum in Bloch's theorem.	$\varepsilon_n \sim \hbar\omega$
Floquet operator\ Floquet propagator\ Slow-motion operator	A time-evolution operator that governs the "slow dynamics," i.e., the dynamics from one interval to another in the system. Its respective generator is the Floquet Hamiltonian.	$e^{-\frac{i}{\hbar}\hat{H}_F\times(t-t_0)}$
Floquet multipliers	The exponentials of the quasienergies and the corresponding eigenvalues of the Floquet operator.	$e^{-\frac{i}{\hbar}\varepsilon_n\times(t-t_0)}$
Stroboscopic kick operator	An operator that describes how the state of a quantum system changes after one complete cycle of the periodic perturbation.	$\hat{K}_F(t)$
Fast-motion operator	A time-evolution operator that governs the "fast dynamics," i.e., the dynamics within an interval in the system. Its respective generator is the Stroboscopic operator.	$e^{-\frac{i}{\hbar}\hat{K}_F(t)}$
Floquet states	The solutions of the time-dependent Schrödinger equation, expanded in terms of Floquet modes and Floquet multipliers. The term draws an analogy with Bloch states in Bloch's theorem.	$\|\psi_n(t)\rangle = e^{-\frac{i}{\hbar}\varepsilon_n t}\|u_n(t)\rangle$
Floquet-Brillouin zone	The zone that, in analogy with solid state theory, contains all distinct Floquet state solutions to the Schrödinger equation.	$\varepsilon_{min} < \varepsilon_n < \varepsilon_{min} + \hbar\omega$

Table B.1: Summary of important concepts discussed in this document.

Appendix C

Floquet's Implementation in C/C++

This appendix provides more detailed information about the numerical implementation used in this work. It serves as a guide for implementing the extended Hilbert space method of Floquet theory in other physical systems or as an instruction manual for further research into the spin-1 Bose-Hubbard model. It includes the names of the essential libraries and programs required for implementing the numerical technique. As well as a description of how to create the Hamiltonian of the system from the local operators of the basis.

C.0 Numerical Implementation Details

The first observation to note is that the numerical implementation of the extended Hilbert space method, as described by Floquet theory, is carried out in C/C++. This language is chosen for its efficiency in controlling system resources and its ability to compile directly to machine code, which enables significantly faster execution compared to interpreted or bytecode-compiled languages such as Python. Additionally, C/C++ allows the use of robust and well-optimized libraries in the field of linear algebra. Given the requirements of the method, the resources employed are as follows:

1. **Linear Algebra Handling:** The extended Hilbert space method and state reconstruction are managed using a matrix representation of the system. All operations involving matrices, vectors, tensors, and basic linear algebra routines are handled with the Boost library, specifically the uBLAS module. This module facilitates the manipulation, operation, and measurement of various observables and necessary states (for more information, see `https://www.boost.org/doc/libs/1_85_0/libs/numeric/ublas/doc/index.html`). Additionally, standard C/C++ libraries are utilized to handle arrays for matrix and vector blocks, as used in the Floquet matrix.

2. **Numerical Integration:** As discussed in Chapter 3, the extended Hilbert space method requires the calculation of various Fourier coefficients, as expressed in Eq. (3.11), which necessitates numerical integration. This integration is performed using the trapezoidal quadrature method, implemented via the Math module of the Boost library. This module

includes a variety of mathematical tools such as constants, special functions, interpolation, differentiation, and numerical integration, among others (for more information, see https://www.boost.org/doc/libs/1_85_0/libs/math/doc/html/index.html). The trapezoidal quadrature method is chosen for its simplicity and efficiency in integrating periodic functions both rapidly and accurately [95].

3. **Diagonalization:** As noted in Chapter 3, the extended Hilbert space method requires diagonalization of the Floquet matrix. This process is accomplished using a static library provided by the Solid State Physics Theory research group of the Physics Department, which employs the LAPACK subroutine "*zheev*." This subroutine returns the eigenvalues and eigenvectors of a Hermitian matrix.

4. **Compilation and Plotting:** It is advisable to include flags during the command or compilation of the code to identify potential errors. Since repeating this process can be uncomfortable, we utilize the make program and create a Makefile to register all necessary flags and commands for compilation and execution. Once the code is compiled and executed, the measured observables are plotted using .dat files with the assistance of the Gnuplot program.

It is also important to note that the numerical implementation of the system, from coding the local matrices, integration, and diagonalization to state reconstruction and measurement of observables, is conducted within a single .cpp file. This approach allows for direct modification of system parameters within the source code, which is then compiled, executed, and plotted for each variation. Despite this setup, and considering the cases addressed in Chapter 4, the numerical implementation of the extended Hilbert space method under Floquet's theorem proves to be both efficient and practical for periodic systems.

C.0 Construction of the Hamiltonian

To generate the matrices for the entire system and therefore the complete Hamiltonian, we employ the standard construction of non-local matrices in a lattice from the local ones using the Kronecker product. Let $\hat{O}_i$ be a local operator at site i with dimension $n_l \times n_l$. To generate the operator that acts on a state of the complete lattice with L sites, we construct it as follows:

$$\hat{O} = \hat{O}_1 \otimes \underbrace{\hat{I}_v \otimes \cdots \otimes \hat{I}_v}_{L-1} + \hat{I}_v \otimes \hat{O}_2 \otimes \underbrace{\hat{I}_v \otimes \cdots \otimes \hat{I}_v}_{L-2} + \cdots + \underbrace{\hat{I}_v \otimes \cdots \otimes \hat{I}_v}_{L-1} \otimes \hat{O}_L$$

$$\hat{O} = \sum_{i=0}^{L-1} \hat{I}_v^{\otimes i} \otimes \hat{O}_{i+1} \otimes \hat{I}_v^{\otimes (L-1-i)}, \tag{C.1}$$

where $\otimes$ represents the tensor product or Kronecker product, and $\hat{I}_v$ is the vacuum identity operator, which has a 1 in the vacuum state and 0 in the other local states, namely:

$$I_v = \underbrace{\begin{pmatrix} 1 & 0 & \cdots & 0 \\ 0 & 0 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & 0 \end{pmatrix}}_{n_l}. \tag{C.2}$$

This matrix represents the addition of an empty site in the lattice, and $\hat{I}_v^{\otimes n}$ represents the tensor product of the vacuum identity operator with itself n times, i.e., $\hat{I}_v^{\otimes 0} = 1$, $\hat{I}_v^{\otimes 1} = \hat{I}_v$, $\hat{I}_v^{\otimes 2} = \hat{I}_v \otimes \hat{I}_v$, and so on.

This construction is used to generate the matrices of the entire system from the local ones. If the local operator is defined over two or more sites (such as the hopping term), the sum must be adjusted to consider the tensor product with the remaining sites. Note also that, in our system, the tensor product is performed with the vacuum identity operator, thereby adding only sites and not particles. If we wish to add more sites that can also host particles, we must use the standard identity operator.

This method was implemented only for the two-particle system, as the one-particle system allows for the matrices of the entire system to be easily constructed by considering only the effective states. The Kronecker product generates a matrix with all mathematically possible states; however, since only empty sites are added and not all of them are physically relevant, considering all states results in $(n_l)^L$ states, significantly increasing computational cost.

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