An algebraic solution of driven single band tight binding dynamics

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Abstract

The dynamics of the driven single band tight binding model for Wannier–Stark systems is formulated and solved using a dynamical algebra. This Lie algebraic approach is very convenient for evaluating matrix elements and expectation values. A classicalization of the tight binding model is discussed as well as some illustrating examples of Bloch oscillations and dynamical localization effects. It is also shown that a dynamical invariant can be constructed.

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1. Introduction

The celebrated single band tight binding system

\[ H = -\frac{\Delta}{4} \sum_{n=-\infty}^{+\infty} (|n\rangle\langle n+1| + |n+1\rangle\langle n|) \]

\[ + dF \sum_{n=-\infty}^{+\infty} n|n\rangle\langle n| \] (1)

models a space periodic system with period \(d\) in a (possibly time dependent) linear field. Here, \(n\) numbers the sites and \(|n\rangle\) are the Wannier states with \(\langle n|n'\rangle = \delta_{nn'}\). In (1) only nearest neighbor interactions are taken into account. In this model, the periodic field free system has only a single band with dispersion relation

\[ E(\kappa) = -\frac{\Delta}{2} \cos(\kappa d), \] (2)

where \(\kappa\) is the Bloch index and \(\Delta\) is the band width.

In the simplest case, the field \(F\) is constant, a dc-field. More complicated is the combined ac–dc-system with time periodic driving; an often considered case is the harmonic driving, \(F(t) = F_0 - F_1 \cos(\omega t)\).

The dynamics of the driven tight binding system is quite involved and, despite of the large number of previous studies, of increasing interest, in particular in view of the recent progress in studies of the dynamics of ultracold atoms in standing wave laser fields. For more information, see [1,2] and the references given there. It is well known that the tight binding system allows an analytic treatment and various approaches have been proposed (for early studies see [3–5]). Quite generally, however, the derivations are quite tedious. Here, we recommend a treatment based on the dynamical Lie algebra [6–8] which appears to be
favorable because of its generality and simplicity. This approach allows a straightforward evaluation of the time evolution operator, matrix elements, expectation values and dynamical invariants by purely algebraic operations.

2. The algebra

The three operators $\hat{N}, \hat{K}, \hat{K}^\dagger$ where $\hat{N}$ is Hermitian and $\hat{K}$ unitary with commutation relations

$$\begin{align*}
[\hat{K}, \hat{N}] &= \hat{K}, \\
[\hat{K}^\dagger, \hat{N}] &= -\hat{K}^\dagger,
\end{align*}$$

and

$$[\hat{K}, \hat{K}^\dagger] = 0$$

(3)

form a closed Lie algebra $\mathcal{L}$. This shift-operator algebra [9] is obviously different from the ubiquitous oscillator algebra $[\hat{n}, \hat{a}, \hat{a}^\dagger]$ , but some features are similar (see also [10] for a discussion of the more general quantum boson algebra which contains both algebras as limiting cases).

The dynamics generated by the Hermitian Hamiltonian

$$\hat{H} = G(t)(\hat{K} + \hat{K}^\dagger) + F(t)\hat{N},$$

(4)

with real valued, possibly time dependent functions $F$ and $G$ can be conveniently studied by algebraic techniques.

A realization is the tight binding model (1) with

$$\hat{N} = \sum_{n=-\infty}^{+\infty} n|n\rangle\langle n|, \quad \hat{K} = \sum_{n=-\infty}^{+\infty} |n\rangle\langle n+1|,$$

$$\hat{K}^\dagger = \sum_{n=-\infty}^{+\infty} |n+1\rangle\langle n|.$$ (5)

It should be noted, however, that this algebra appears also in different context [9] and therefore some general considerations seem to be appropriate. First, one can easily show that $\hat{K}$ and $\hat{K}^\dagger$ act on the eigenstates of $\hat{N}, \hat{N}|n\rangle = n|n\rangle$, as shift- or ladder-operators:

$$\hat{K}|n\rangle = |n-1\rangle, \quad \hat{K}^\dagger|n\rangle = |n+1\rangle,$$ (6)

which fixes the eigenvalues of $\hat{N}$ at $n_0 + n$ with $n \in \mathbb{Z}$ up to an arbitrary value of $n_0$ in the unit interval. This value can be fixed if one considers the algebra as a subalgebra of a bigger one by adding an antiunitary operator representing time inversion. This leads to the two possible cases of $n_0 = 0$ (bosonic) or $n_0 = 1/2$ (fermionic). See [11] and references given there for more details. Here we are interested in the bosonic case, i.e.,

$$\hat{N}|n\rangle = n|n\rangle, \quad n \in \mathbb{Z}.$$ (7)

In context of the tight binding system, $\hat{N}$ is a ‘position operator’: the expectation value $\langle N \rangle = \langle \psi | \hat{N} | \psi \rangle$ is the mean position on the lattice and $p_n = |\langle n | \psi \rangle|^2$ is the population probability of the ‘lattice site’ at position $n$. This is the physical system we have in mind. It should be noted, however, that the same algebra appears in different contexts as, e.g., for the plane rotor $[J_+, J_-] = \pm J_z, [J_+, J_-] = 0$.

The eigenvectors of $\hat{K}$ with eigenvalues $e^{\pm \kappa}$ are $|\kappa\rangle = \frac{1}{\sqrt{2\pi}} \sum_{n=-\infty}^{+\infty} e^{i\kappa n}|n\rangle$;

$$\hat{K} |\kappa\rangle = \frac{1}{\sqrt{2\pi}} \sum_{n=-\infty}^{+\infty} e^{i\kappa n} |n-1\rangle$$

$$= \frac{1}{\sqrt{2\pi}} e^{i\kappa} \sum_{m=-\infty}^{+\infty} e^{i\kappa m} |m\rangle = e^{i\kappa} |\kappa\rangle.$$ (8)

These ‘Bloch states’ are $2\pi$ periodic and normalized as

$$|\kappa |\kappa'\rangle = \sum_{n=-\infty}^{+\infty} \delta (\kappa - \kappa' - 2\pi n) = \delta_{2\pi} (\kappa - \kappa'),$$ (9)

where $\delta_{2\pi}$ is the $2\pi$-periodic comb function.

The representation of the operator $\hat{N}$ in this basis is

$$\langle \kappa | \hat{N} | \kappa' \rangle = \delta_{2\pi} (\kappa - \kappa') \frac{d}{d\kappa},$$ (10)

The algebra $\mathcal{L} = \{\hat{K}, \hat{K}^\dagger, \hat{N}\}$ has the radical $\mathcal{R} = \{\hat{K}, \hat{K}^\dagger\}$, the simple part $\mathcal{S} = \{\hat{N}\}$, and can be decomposed into the semidirect sum $\mathcal{L} = \mathcal{R} \ltimes \mathcal{S}$ as, e.g., described in [8]. For a Hamiltonian $\hat{H} = \hat{H}_S + \hat{H}_R$ with $\hat{H}_R \in \mathcal{R}$ and $\hat{H}_S \in \mathcal{S}$, the time evolution operator can be factorized:

$$\hat{U} = \hat{U}_S \hat{U}_R,$$ (11)

with

$$i\hbar \frac{d\hat{U}_S}{dt} = \hat{H}_S \hat{U}_S, \quad i\hbar \frac{d\hat{U}_R}{dt} = (\hat{U}_S^{-1} \hat{H}_R \hat{U}_S) \hat{U}_R.$$ (12)

(Moreover, $U_S$ can be factorized into simple parts if $\mathcal{S}$ is only semisimple; for more details see [8].)
This product decomposition has several advantages in comparison with the pure exponential solution, in particular it provides a global solution [12,13] and the calculation of expectation values and matrix elements is simplified as will become clear later on.

The initial step of any application is the evaluation of all necessary $\hat{F}$-evolved operators $\hat{A}$ of interest, i.e.,

$$e^{\varepsilon \hat{F}} \hat{A} := e^{\hat{F}} \hat{A} e^{-\hat{F}}$$

$$= \hat{A} + z[\hat{F}, \hat{A}] + \frac{z^2}{2!} [\hat{F}, [\hat{F}, \hat{A}]] + \cdots ,$$

with $z \in \mathbb{C}$ for all $\Gamma \in \mathcal{L}$. Trivially we have $e^{\varepsilon \hat{F}} \hat{F} = \hat{F}$. Here we certainly need the evolved operators of our algebra $\mathcal{L} = \{\hat{K}, \hat{K}^\dagger, \hat{N}\}$. Because $\hat{K}$ and $\hat{K}^\dagger$ commute, we have

$$e^{\varepsilon \hat{K}} \hat{K} = F(\hat{K}^\dagger), \quad e^{\varepsilon \hat{K}^\dagger} F(\hat{K}) = F(\hat{K})$$

and the non-trivial expressions are

$$e^{\varepsilon \hat{K}} \hat{N} = \hat{N} + \varepsilon \hat{K}, \quad e^{\varepsilon \hat{N}} \hat{K} = e^{-\varepsilon \hat{K}},$$

$$e^{\varepsilon \hat{K}^\dagger} \hat{N} = \hat{N} - \varepsilon \hat{K}^\dagger, \quad e^{\varepsilon \hat{N}} \hat{K}^\dagger = e^{+\varepsilon \hat{K}^\dagger}$$

(15)

which can be easily obtained from (13) using (3).

### 3. Time evolution operator

For the tight binding Hamiltonian (4), where for simplicity we introduce the notation $g_t = G(t)/\hbar$, $f_t = F(t)/\hbar$, the simple part of the time evolution is $i\dot{U}_S = f_t \hat{N} \hat{U}_S$ with solution

$$\dot{U}_S(t) = e^{-in\hat{N}}, \quad n_t = \int_0^t f_t \, d\tau$$

(16)

and the remaining equation of motion $i\dot{U}_R = (\dot{U}_S^{-1} \times \hat{H}_R \dot{U}_S)\dot{U}_R$ for the radical part can be solved in a second step. Using the relation (15) we find

$$\dot{U}_S^{-1} \hat{H}_R \dot{U}_S = e^{in \hat{N}} \hat{H}_R$$

= $\hbar g_t (e^{-in\hat{K}} + e^{+in\hat{K}^\dagger})$

(17)

and therefore

$$\hat{U}_R(t) = e^{-i(\chi_t \hat{K} + \chi_t^\dagger \hat{K}^\dagger)}, \quad \chi_t = \int_0^t g_\tau e^{-in_\tau} \, d\tau$$

(18)

and finally

$$\dot{U}(t) = \dot{U}_S(t) \hat{U}_R(t) = e^{-in_\eta \hat{N}} e^{-i\chi_t \hat{K}} e^{-i\chi_t^\dagger \hat{K}^\dagger},$$

(19)

the Wei–Norman product form of the time evolution operator [8,12,13] which is, in fact, a version of the so-called momentum gauge in this case.

Furthermore, a series expansion in powers of the ladder operator will be useful, which can be obtained by means of the generating function for the Bessel functions

$$e^{\alpha (\hat{b} - \hat{b}^{-1})} = \sum_{n=-\infty}^{+\infty} J_n(2u) \hat{B}^n.$$  

(20)

Identifying $\hat{B} = e^{-i(\phi + \pi/2)} \hat{K}$ where $\chi_t = |\chi_t| e^{-i\phi_t}$, Eq. (18) can be rewritten as

$$\hat{U}_R(t) = \sum_{n=-\infty}^{+\infty} J_n(2|\chi_t|) e^{-in(\phi_t + \pi/2)} \hat{K}^n.$$  

(21)

In various applications, matrix elements of the time evolution operator are required. Making use of

$$\langle \kappa | e^{-iu \hat{N}} | \kappa' \rangle = \sum_n \langle \kappa | n \rangle e^{-in \eta} | n | \kappa' \rangle$$

$$= \frac{1}{2\pi} \sum_n e^{in(\kappa - \kappa - u)} = \delta_{2n} (\kappa' - \kappa - u).$$

(22)

the matrix elements in the Bloch wave basis can be directly read off from (19):

$$\langle \kappa | \dot{U}(t) | \kappa' \rangle = \delta_{2n} (\kappa' - \kappa - \eta_t) e^{-2i|\chi_t| \cos(\kappa' - \phi_t)}.$$  

(23)

Matrix elements of the propagator (19) in the basis $|n\rangle$ follow immediately from (21) and the ladder property $\hat{K}^n |n'\rangle = |n' - n\rangle$:

$$U_{nn'}(t) = e^{-i(n' - n)(\phi_t + \pi/2) - in_\eta t} J_{n'-n}(2|\chi_t|)$$

(24)

which coincides, of course, with the result derived many years ago by Dunlap and Kenkre [4].

For completeness, we should also state the explicit results for the most frequently studied cases:
(1) For time independent functions $g_t = g_0$ and $f_t = f_0$ the integrals in (16) and (18) yield
\[
\eta_t = f_0 t, \quad X_t = \frac{2g_0}{f_0} e^{-if_0t/2} \sin(f_0t/2).
\] (25)

Note that at time $t = T_B = 2\pi/f_0$ the evolution operator is equal to the identity
\[
\hat{U}(T_B) = e^{-i2\pi \hat{N}} = \hat{I}
\] (26)
because of $e^{-i2\pi \hat{N} |n\rangle} = e^{-i2\pi n |n\rangle} = |n\rangle$. Therefore the dynamics is periodic with the Bloch period $T_B$ and Bloch frequency $\omega_B = f_0$. It is also of interest to compare the product form (19) of the propagator with the pure exponential one which is trivial in this case, namely
\[
\hat{U}(t) = e^{-iHt/b} = e^{-i(g_0\hat{K} + g_0\hat{K} + f_0\hat{N})t}.
\] (27)
The non-obvious identity between (27) and (19) becomes clear in view of the generalized Baker–Campbell–Hausdorff formula [9]
\[
e^{a(b+c)} = e^b e^a e^{b(a^{-1} - c)}
\] (28)
for shift-operators $\hat{X}$, $\hat{Y}$ with commutator $[\hat{X}, \hat{Y}] = \hat{Y}$.

(2) For harmonic driving,
\[
f_t = f_0 - f_1 \cos(\omega t), \quad g_t = g_0.
\] (29)
we have
\[
\eta_t = f_0 t - f_1 \sin(\omega t)
\] (30)
and, using again the Bessel expansion (20):
\[
X_t = g_0 \int_0^t dx \ e^{-if_1x + if_0 x} \sin(\omega x) = g_0 \sum_{\nu = -\infty}^{\infty} J_{\nu} f_0 \frac{1}{\omega} \int_0^t e^{-i\omega\nu x} dx
\]
\[
= 2g_0 \sum_{\nu = -\infty}^{\infty} J_{\nu} f_0 \frac{1}{\omega} \ e^{-i\omega\nu t/2} \sin(\omega_\nu t/2),
\]
\[
\omega_\nu = \omega_B - \nu \omega \neq 0.
\] (31)

This is an oscillating function of time. For resonant driving,
\[
\omega_B = n\omega, \quad n = 1, 2, \ldots,
\] (32)
the integration of the $n$th term in the sum (31) yields a linearly growing term, which dominates the oscillating rest of the sum for long times, i.e., we have
\[
X_t \approx \gamma_n t/2, \quad \gamma_n = 2g_0 J_0 \left( \frac{f_1}{\omega} \right).
\] (33)
Later on, in Section 8, some consequences of this resonant behaviour will be discussed.

(3) The general case of a combined dc–ac-system can be treated in a similar manner. Let us consider the case
\[
f_t = f_0 + f_1, \quad g_t = g_0, \quad T = nT_B,
\] (34)
with $f_0$ chosen according to $\int_0^T f_1 dt = 0$. Again we consider the case of resonant driving, $T = nT_B$, with $T_B = 2\pi/\omega_B$, $\omega_B = f_0$. Fourier expansion of the periodic part of the force
\[
\tilde{f}_t = \sum_{\nu = -\infty}^{\infty} b_\nu e^{i\omega\nu t}, \quad b_0 = 0,
\] (35)
with $\omega = 2\pi/T$ yields
\[
\eta_t = f_0 t + \sum_{\nu \neq 0} b_\nu \int_0^T e^{i\omega\nu t - i\nu t} dt = \omega_B t + \tilde{\eta}_t,
\] (36)
where $\tilde{\eta}_t$ is $T$-periodic. A second Fourier expansion
\[
g_t e^{-i\eta t} = \sum_{\nu = -\infty}^{\infty} a_\nu e^{i\omega\nu t},
\]
\[
a_\nu = \frac{1}{2\pi} \int_0^T g_t e^{i\omega\nu t - i\nu t} dt,
\] (37)
allows the evaluation of $X_t$:
\[
X_t = \int_0^T g_t e^{-i\eta t} dt = \int_0^T g_t e^{-i\omega_B t - i\nu t} dt
\]
\[
= a_\nu t + \sum_{\nu \neq 0} \frac{d_\nu}{\nu \omega\nu} \left[ 1 - e^{-i\omega_B t} \right],
\] (38)
with
\[
\omega_\nu = \omega_B - \nu \omega.
\] (39)
Note that this is again a sum of a linear growing and a $T$-periodic part:
\[
X_t = a_\nu t + \tilde{X}_t, \quad \tilde{X}_{t+T} = \tilde{X}_t.
\] (40)
The coefficients of two Fourier expansions (35) and (37) are, of course, not unrelated for constant \(g_0\). Let us confine ourselves here for simplicity to the case of a symmetric resonant driving:

\[
f_t = f_0 + \sum_{m=1}^{\infty} f_m \cos(m \omega t), \quad \omega_B = n \omega,
\]

which commutes with \(\hat{K}\) and allows the construction of simultaneous eigenstates

\[
\hat{K} |\psi_k(T)\rangle = e^{i\kappa} |\psi_k(T)\rangle, \quad \kappa = \kappa_t = \kappa - \eta_t
\]

with \(\eta_t = \omega_B t + \sum_{m=1}^{\infty} \beta_m \sin(mt), \quad \beta_m = f_m / m \omega\). (42)

Using now the generating function for the infinite-variable Bessel functions \([14]\) (for a recent application of these little known functions to a two-dimensional tight binding system see \([15]\)),

\[
\exp\left(\sum_{m=1}^{\infty} \beta_m \sin(m \omega t)\right) \sim \sum_{\nu=-\infty}^{\infty} J_{\nu}(\beta_m)e^{i\nu \mu}, \quad \mu = \omega t/2.
\]

The quasienergies \(\varepsilon_k\) are identified as

\[
\varepsilon_k = a_n e^{+i \kappa} + a_n^* e^{-i \kappa} = 2|a_n| \cos(\kappa + \varphi),
\]

the dispersion relation for the quasienergy. Here \(4|a_n|\) is the width of the quasienergy band and \(\varphi\), the phase of the Fourier coefficient \(a_n = |a_n| e^{i \varphi}\), is zero if \(g_t\) and \(f_t\) are symmetric in time.

It is also of interest to construct explicitly the time dependent quasienergy (or Floquet) states. As can be easily seen, the states

\[
|\psi_k(t)\rangle = \hat{U}(t) |\psi_k(T)\rangle = \frac{1}{\sqrt{2\pi}} \sum_n e^{i n \kappa t} e^{i (\varepsilon_k T + \varepsilon^*_{k} T^{-1}) n} |n\rangle,
\]

\[\kappa_t = \kappa - \eta_t\]

are solutions of the time dependent Schrödinger equation

\[
\left(\frac{\partial}{\partial t} - \frac{1}{\hbar} \hat{H}\right) |\psi_k(t)\rangle = 0
\]

\[\kappa \frac{\partial}{\partial t} - \frac{1}{\hbar} \hat{H} |\psi_k(t)\rangle = 0\]

and, simultaneously, eigenstates of \(\hat{K}\):

\[
\hat{K} |\psi_k(t)\rangle = e^{i \kappa} |\psi_k(t)\rangle,
\]

the so-called Houston states. Using again (36) and (40), we have

\[
|\psi_k(t + T)\rangle = \frac{1}{\sqrt{2\pi}} \sum_n e^{i n (\kappa - \eta_t + T)} e^{i (\varepsilon_k T + \varepsilon^*_{k} T^{-1}) n} |n\rangle
\]

\[= e^{-i \omega T} e^{i \varphi T} |\psi_k(T)\rangle = e^{-i \varepsilon_{k} T} |\psi_k(t)\rangle.\]

Therefore the state

\[
|u_k(t)\rangle = e^{+i \varepsilon_{k} t} |\psi_k(t)\rangle,
\]

with \(\varepsilon_{k}\) given in (48) is \(T\)-periodic, \(|u_k(t + T)\rangle = |u_k(t)\rangle\) and solves

\[
\left(\frac{\partial}{\partial t} - \frac{1}{\hbar} \hat{H}\right) |u_k(t)\rangle = \varepsilon |u_k(t)\rangle,
\]

\[= e^{-i \varepsilon_{k} T} |\psi_k(t)\rangle.\]
i.e., it is a quasienergy state and $ε$ is the quasienergy. From (49) we see that the Floquet states extend over the whole lattice. As a final remark, we also note the obvious identity $|u_κ(T)⟩ = |κ⟩$.

5. Expectation values

The time dependence of expectation values follows immediately [8] from the relations (14) and (15):

$$\hat{K}(t) = \hat{U}^{-1}(t)\hat{K}\hat{U}(t) = e^{i\chi_t\hat{K}^\dagger}e^{i\chi_t\hat{K}}\hat{N}e^{-i\chi_t\hat{K}^\dagger}e^{-i\chi_t\hat{K}}$$

$$= e^{i\chi_t\hat{K}^\dagger}e^{i\chi_t\hat{K}}e^{-i\chi_t\hat{K}^\dagger}e^{-i\chi_t\hat{K}}$$

$$= e^{-i\mu_κ\hat{K}}$$

and therefore

$$⟨\hat{K}⟩_t = e^{-i\mu_κ}⟨\hat{K}⟩_0 = e^{i(e-n)\mu_κ}$$

with $⟨\hat{K}⟩_0 = K = |K|e^{iκ}$. From

$$\hat{K}^2(t) = e^{-2i\mu_κ}K^2$$

and

$$⟨\hat{K}^2⟩_t = e^{-2i\mu_κ}⟨\hat{K}^2⟩_0$$

we see that, up to a phase factor, the variance is constant:

$$Δ^2_κ(t) = |⟨\hat{K}⟩_t|^2 - |⟨\hat{K}⟩_0|^2 = Δ^2_κ(0).$$

The time dependence of the position operator is a bit more interesting:

$$\hat{N}(t) = e^{i\chi_t\hat{K}^\dagger}e^{i\chi_t\hat{K}}\hat{N}e^{-i\chi_t\hat{K}^\dagger}e^{-i\chi_t\hat{K}}$$

$$= e^{i\chi_t\hat{K}^\dagger}(\hat{N} + i\chi_t\hat{K})e^{-i\chi_t\hat{K}^\dagger}e^{-i\chi_t\hat{K}}$$

$$= \hat{N} + i(\chi_t\hat{K} - \chi_t^*\hat{K}^\dagger)$$

and therefore, using $\chi_t = |χ_t|e^{-iκ}$,

$$⟨\hat{N}⟩_t = ⟨\hat{N}⟩_0 + i(⟨\chi_t|\hat{K}⟩_0 - ⟨\chi_t^*|\hat{K}^\dagger⟩_0)$$

$$= ⟨\hat{N}⟩_0 + 2|K||χ_t|\sin(κ - κ).$$

Introducing the anti-commutator $\hat{J} = \hat{N}\hat{K} + \hat{K}\hat{N}$, the evolution of $\hat{N}$ is

$$\hat{N}^2(t) = (\hat{N} + i(\chi_t\hat{K} - \chi_t^*\hat{K}^\dagger))^2$$

$$= \hat{N}^2 + i(\chi_t\hat{J} - \chi_t^*\hat{J}^\dagger)$$

$$- \chi_t^2\hat{K}^2 - \chi_t^2\hat{K}^2 + 2|\chi_t|^2$$

and, with

$$⟨\hat{J}⟩_0 = J = |J|e^{iκ}, \quad ⟨\hat{K}⟩_0 = L = |L|e^{iκ},$$

the expectation value evolves as

$$[\hat{N}^2]_t = [\hat{N}^2]_0 + 2J|χ_t|\sin(κ - μ)$$

$$+ 2|χ_t|^2(1 - |L|\cos(2κ - ν)).$$

Finally, the time evolution of the variance is given by

$$Δ^2_κ(t) = |⟨\hat{N}⟩_t|^2 - |⟨\hat{N}⟩_0|^2$$

$$= Δ^2_κ(0) + 2|χ_t|^2\left[1 - |L|\cos(2κ - ν) - 2|K|^2\sin^2(κ - κ)\right]$$

$$+ 2|χ_t|^2\left[2[⟨\hat{N}⟩_0]|K|\sin(κ - κ) + |J|\sin(κ - μ)\right].$$

The dynamics of the expectation values therefore depends on three complex coherence parameters which are explicitly

$$K = \sum_n c_n^*c_n,$$

$$J = \sum_n (2n - 1)c_n^*c_n,$$

$$L = \sum_n c_{n-2}^*c_n$$

if the initial normalized state is specified as $|ψ⟩ = \sum_n c_n|n⟩$.

Sometimes it may be more convenient to replace the unitary shift operators $\hat{K}$ and $\hat{K}^\dagger$ by the Hermitian operators $\hat{C}$ and $\hat{S}$,

$$\hat{K} = \hat{C} + i\hat{S}, \quad \hat{K}^\dagger = \hat{C} - i\hat{S},$$

whose expectation values allow a direct interpretation. Clearly, also these operators commute and the commutators with the position operator are

$$[\hat{C}, \hat{N}] = i\hat{S}, \quad [\hat{S}, \hat{N}] = -i\hat{C}.$$
and, with $\hat{J} = [\hat{N}, \hat{C}]_+ + i[\hat{N}, \hat{S}]_+$, the time evolution of $\hat{N}$ in (61) and (63) is rewritten as
\[
\dot{\hat{N}}^2 = \hat{N}^2 + v_i [\hat{N}, \hat{C}]_+ - u_i [\hat{N}, \hat{S}]_+ + v_i^2 \hat{C}^2 + u_i^2 \hat{S}^2 - 2u_i v_i \hat{C}\hat{S},
\] (71)
\[
[\hat{N}]_0 = \{ [\hat{N}], [\hat{C}]_+ \}_0 - u_i [\{ \hat{N}, \hat{S} \}, 0] + v_i^2 \{ \hat{C}^2 \}_0 + u_i^2 \{ \hat{S}^2 \}_0 - 2u_i v_i \{ \hat{C}\hat{S} \}_0,
\] (72)
with $\{ \hat{C}^2 \}_0 + \{ \hat{S}^2 \}_0 = 1$. The time evolution of the variance of the position $N$ can then be formulated in the convenient form
\[
\Delta^2_N(t) = \Delta^2_N(0) + 2v_i \Delta^2_{CN} - 2u_i \Delta^2_{SN} + v_i^2 \Delta^2_{CC} + u_i^2 \Delta^2_{SS} - 2u_i v_i \Delta^2_{CS},
\] (73)
where $\Delta^2_{AB}$ is the covariance of the expectation values of the operators $\hat{A}$ and $\hat{B}$ at time $t = 0$:
\[
\Delta^2_{AB} = \left\{ \frac{1}{2} \{ \hat{A}, \hat{B} \}_+ \right\}_0 = \left\{ \hat{A} \right\}_0 \left\{ \hat{B} \right\}_0.
\] (74)
Note that the relations for the expectation values derived above are valid for pure states as well as for mixed states (see [16–19] for an application of the tight binding system using density matrices).

6. Classicalization

Recently, a classicalization of the tight binding model with Hamiltonian
\[ H = 2G(t) \cos(p\delta) + F(t)q/d, \] (75)
has been discussed [2, 22]; related observations can also be found in [18, 23]. In this classicalization, the operators $\hat{N}$ and $\hat{C} = (\hat{K} + \hat{K})^1/2$ are replaced by phase space functions. The parameter $\delta = d/h$ depends explicitly on $h$ which implies, of course, that this ‘classicalization’ differs from the usual classical limit of quantum dynamics. It has been observed that the classical dynamics generated by (75),
\[
\dot{\hat{p}} = -\frac{\partial H}{\partial q} = -\frac{F}{d},
\]
\[
\dot{\hat{q}} = \frac{\partial H}{\partial p} = -2G\delta \sin(p\delta),
\] (76)
show a surprising agreement with the quantum one. Here we will analyze this correspondence from an algebraic point of view.

First, we can again generalize and consider a classical Hamiltonian (75) with time dependent coefficients. Introducing the dimensionless phase space functions $C(p) = \cos(p\delta), S(p) = \sin(p\delta)$ and $N(q) = q/d$, with Poisson brackets
\[
\{ C, N \} = \frac{1}{h} S(p), \quad \{ S, N \} = -\frac{1}{h} C(p),
\] (77)
the set $\{ N, C, S \}$ forms a closed Lie algebra with Lie bracket $[ , ]$ and therefore the dynamics induced by the Hamiltonian $H(p, q, t) = G(t)C(p) + F(t)N(q)$ can be evaluated again by purely algebraic techniques.

Moreover, the classical algebra and the quantum algebra studied above are isomorphic in the present case which is evident from the mapping
\[
\hat{N} \leftrightarrow N, \quad \hat{C} \leftrightarrow C, \quad \hat{S} \leftrightarrow S,
\] (78)
where the operators $\hat{C}$ and $\hat{S}$ are defined in (66) (the Lie brackets map according to $[ , ] \leftrightarrow \frac{1}{i\hbar} [ , ]$). This implies the equality of the dynamical evolution of quantum operators and classical phase space functions in this case. In particular, the evolution of the expectation values agrees. There are, however, some differences, e.g., for the initial conditions. Whereas there is no limitation in the classical case, the quantum covariances are limited by uncertainty relations.

Furthermore, the equations of motion
\[
\dot{\hat{C}} = fS, \quad \dot{\hat{S}} = -fC, \quad \dot{\hat{N}} = -gS,
\] (79)
with $f = F/h, g = G/h$, are linear which implies that the classical dynamics is regular, i.e., not chaotic.

7. The dynamical invariant

The driven tight binding system (4) possesses a dynamical invariant, very similar to the harmonic oscillator with time dependent frequency, where the so-called Lewis invariant $\hat{I}$ [20, 21], a time dependent constant of motion,
\[
\frac{d\hat{I}}{dt} = \frac{1}{i\hbar} [\hat{I}, \hat{H}] + \frac{\partial \hat{I}}{\partial t} = 0,
\] (80)
plays an important role.

The dynamical algebra offers a convenient technique for constructing such an invariant [6, 7]. Writing the invariant as a linear combination of the basis of
the algebra, \( \hat{I} = \sum_j \lambda_j \hat{\gamma}_j \), as well as the Hamiltonian and inserting these expressions into Eq. (80) using the commutator relations, one obtains a set of linear first order differential equations for the coefficients \( \lambda_j(t) \).

In the present case, we write

\[
\dot{I} = \gamma \hat{N} + i \lambda \hat{K} + \lambda^* \hat{K}^\dagger,
\]

with \( \gamma \in \mathbb{R} \) because the invariant can be chosen to be Hermitian. The procedure described above \([6,7]\) leads directly to the differential equations

\[
\dot{\lambda} = i (f_j \lambda - g_j \gamma), \quad \dot{\gamma} = 0,
\]

i.e., \( \gamma \) is an arbitrary scaling constant which can be chosen as \( \gamma = 1 \) and the solution for \( \gamma \) is

\[
\lambda = -ie^{\eta t} \chi_t, \quad (82)
\]

were \( \eta \) and \( \chi \) are defined in Eqs. (16) and (18). The full expression for the invariant is therefore

\[
\dot{I}(t) = \dot{\hat{N}}(t) + i \lambda \dot{\hat{K}}(t) + \lambda^* \dot{\hat{K}}^\dagger(t) = \dot{\hat{I}}(0) = \hat{N}, \quad (84)
\]

where the time evolved operators \( \hat{K}(t) \) and \( \hat{N}(t) \) have already been calculated in Eqs. (55) and (59). The time evolution conserves the commutator relations \((3)\) and therefore \( \dot{\hat{K}}(t) \) and \( \dot{\hat{K}}^\dagger(t) \) are still acting as ladder operators on the time dependent eigenstates \( |n, t \rangle \) of \( \hat{N}(t) \) with the (time independent) eigenvalues \( n \in \mathbb{Z} \). Following Lewis and Riesenfeld [21], one can also construct the general time evolution from the eigenstates of the invariant.

In view of the classical version of the tight binding model in the preceding section, we will also express the dynamical invariant in terms of the Hermitian operators \( \hat{C} \) and \( \hat{S} \) given in (66) which yields after some algebra

\[
\dot{\hat{I}}(t) = \dot{\hat{N}}(t) + (u_t \sin \eta_t - v_t \cos \eta_t) \hat{C}(t) + (u_t \cos \eta_t + v_t \sin \eta_t) \dot{\hat{S}}(t). \quad (85)
\]

In the classical version (78), the invariant is the phase space function

\[
I(p, q, t) = \frac{q}{d} + (u_t \sin \eta_t - v_t \cos \eta_t) \cos(p \delta) + (u_t \cos \eta_t + v_t \sin \eta_t) \sin(p \delta), \quad (86)
\]

where \( p = p_0 \) and \( q = q_0 \) evolve under the Hamiltonian equations of motion (76) and

\[
I(p, q, t) = I(p_0, q_0, 0) = \frac{q_0}{d} \quad (87)
\]

is a constant of motion.

8. Oscillating versus breathing modes and dynamic localization

Despite of the algebraic simplicity, the tight binding dynamics shows some non-intuitive features, even in the case where the Hamiltonian does not explicitly depend on time, where the famous Bloch oscillations are observed. Much more phenomena can be found for driven system, as for instance dynamical localization effects \([1,4,23]\). A discussion of these phenomena is far beyond the scope of the present Letter. Some quite general features, however, can be directly seen from the dynamics of the expectation values for the position operator and its variance. For simplicity we will use the classical description of the tight binding dynamics outlined in the preceding section. To avoid misinterpretations, it should be recalled that the Bloch oscillation remains, of course, a pure quantum phenomenon because the ‘classical’ system is \( h \)-dependent.

First, the general dynamical behaviour is strongly influenced by the initial distribution, more precisely by the expectation values of \( C(p) = \cos(p \delta) \), \( C^2(p) = \cos^2(p \delta) \) \ldots \) which satisfy the obvious bounds \( -1 \leq \langle C \rangle, \langle S \rangle \leq +1 \) and \( 0 \leq \langle C^2 \rangle, \langle S^2 \rangle \leq +1 \). We will assume in the following that the initial classical phase space distribution is symmetric in the position \( q \), which implies \( \langle N \rangle_0 = 0 \) and \( \Delta_{CN}^2 = \Delta_{SN}^2 = 0 \), i.e., Eqs. (70) and (73) read

\[
\left[ \hat{N} \right]_t = v_t (\hat{C})_0 - u_t (\hat{S})_0, \quad (88)
\]

\[
\Delta_{CN}^2(t) = \Delta_{SN}^2(t) = \Delta_{C}^2(0) + v_t^2 \Delta_{CC}^2 + u_t^2 \Delta_{SS}^2 - 2u_t v_t \Delta_{CS}^2. \quad (89)
\]

Now the dynamics is most strongly influenced by the localization properties in the momentum. Let us distinguish two extreme cases:

(1) If the initial distribution is sharply localized in the vicinity of momentum \( p_0 \), we have \( \langle C \rangle_0 \approx \cos(p_0 \delta), \langle S \rangle_0 \approx \sin(p_0 \delta) \) and \( \Delta_{CC}^2 \approx \Delta_{SS}^2 \approx \Delta_{CS}^2 \approx 0 \) and therefore

\[
\left[ \hat{N} \right]_t \approx v_t \sin(p_0 \delta) - u_t \sin(p_0 \delta), \quad (90)
\]

\[
\Delta_{CN}^2(t) \approx \Delta_{SN}^2(t) \approx \Delta_{C}^2(0), \quad (91)
\]

and the distribution moves in space with constant width. This is an oscillatory mode.

(2) If the momentum distribution is broad and approximately constant over a period of \( \cos(p \delta) \), we
have \( \langle C \rangle \approx \langle S \rangle \approx 0 \) and \( \Delta_{CC}^2 \approx \Delta_{SS}^2 \approx 1/2 \) and \( \Delta_{CS} \approx 0 \) and therefore

\[
\langle \hat{N} \rangle_t \approx 0, \quad (92)
\]

\[
\Delta_N^2(t) = \Delta_N^2(0) + \frac{1}{2}(v_t^2 + u_t^2) \quad (93)
\]

and the distribution is frozen in space with a time dependent width. This is a breathing mode. (Alternatively, Eq. (93) can be derived directly from (24) for an initial distribution localized on site \( n \).)

9. Single band model

The single band model is an extension of the tight binding model by replacing the cosine dispersion relation (2) by a more realistic periodic function \( E(\kappa) \).

Instead of the Hamiltonian (4) one considers the generalization

\[
\hat{H} = \hbar \sum_{m=0}^{\infty} (g_m(t) \hat{K}^m + g_m^*(t) \hat{K}^m) + F(t) \hat{N}
\]

\[
= \hat{H}_R + F(t) \hat{N}. \quad (96)
\]

Here, the algebra is extended to the set \( \mathcal{L} = \{ \hat{K}^m, \hat{K}^m \} \) with radical \( \mathcal{R} = \{ \hat{K}^m, \hat{K}^m, m \in \mathbb{N} \} \). The subsequent analysis follows exactly the same lines as in the tight binding model. By means of the auxiliary relations \( \langle \hat{K}^m, \hat{N} \rangle = 2^{m-1} \hat{K}^m \) and \( \langle \hat{K}^m, \hat{N} \rangle = -2^{m-1} \hat{K}^m \) one obtains

\[
\hat{U}_S^{-1} \hat{H} \hat{U}_S = \sum_{m=0}^{\infty} (g_m(t) e^{-i2m-1\eta t} \hat{K}^m + g_m^*(t) e^{i2m-1\eta t} \hat{K}^m) \quad (97)
\]

and the time evolution of the radical part of the algebra is given by

\[
\hat{U}_R(t) = \exp \left( -i \sum_{m=0}^{\infty} (\chi_m(t) \hat{K}^m + \chi_m^*(t) \hat{K}^m) \right) \quad (98)
\]

with

\[
\chi_m(t) = \int_0^t d\tau \ g_m(\tau) e^{-i2m-1\eta \tau}. \quad (99)
\]

The full time evolution operator is again \( \hat{U}(t) = \hat{U}_S(t) \hat{U}_R(t) \), where \( \hat{U}_S(t) \) is still given by (16).

For most applications, however, the coefficients \( g_m \) will be independent of time. In such a case, the dispersion relation is given by the Fourier series

\[
E(\kappa) = \hbar \sum_{m=0}^{\infty} (g_me^{im\kappa} + g_m^*e^{-im\kappa}). \quad (100)
\]

Matrix elements of \( \hat{U}(t) \) in the Bloch basis are similar to (23):

\[
\langle \kappa | \hat{U}^m(t) | \kappa' \rangle = \delta_{\kappa\kappa'} \delta_{m\eta}(\kappa - \kappa' - \eta) e^{-i(f(\kappa,t) + f^*(\kappa',t))}, \quad (101)
\]

with \( f(\kappa,t) = \sum_{m} \chi_m(t)e^{im\kappa} \). The matrix elements in the \( |n\rangle \) basis are, however, more complicated than the tight binding expression (24).
The time evolution of the ladder operator $\hat{K}(t)$ is still given by (55) and, using
\begin{equation}
e^{z \hat{a} \hat{d}^{\dagger}} \hat{N} = \hat{N} + z 2^{m-1} \hat{K}^m,
\end{equation}
the evolution of the position operator is
\begin{equation}
\hat{N}(t) = \hat{N} + i \sum_{m=0}^{\infty} 2^{m-1} \left( \chi_m(t) \hat{K}^m - \chi_m^*(t) \hat{K}^m \right),
\end{equation}
with expectation value
\begin{equation}
\langle \hat{N} \rangle_t = \langle \hat{N} \rangle_0 + i \sum_{m=0}^{\infty} 2^{m-1} \left( \chi_m(t) \langle \hat{K}^m \rangle - \chi_m^*(t) \langle \hat{K}^m \rangle \right).
\end{equation}
Finally it should be noted that also in this case a classicalization is possible with classical Hamiltonian
\begin{equation}
H(p, q, t) = E(p\delta) + Fq
\end{equation}
as discussed above for the tight binding model.

10. Concluding remarks

The driven tight binding system is in many aspects very similar to the driven harmonic oscillator. It can be treated algebraically by means of ladder operators, there exists a dynamical invariant, and one observes a close correspondence between quantum and classical time evolution. Some of these features of the tight binding dynamics have been discussed in the present Letter. There are, of course, still a number of interesting questions to be answered as for instance the role of the coherent states [11,24,25] and the relation between the invariant and the quasienegries for a periodically driven system [26,27]. Moreover, an extension of the algebraic technique to treat Bloch–Zener oscillations in doubly periodic structures [22] or the recently investigated two-dimensional case [15,22,28,29]. Work in these directions is in progress.

References