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2002 J. Phys. A: Math. Gen. 35 L105

(http://iopscience.iop.org/0305-4470/35/9/101)

INSTITUTE OF PHYSICS PUBLISHING JOURNAL OF PHYSICS A: MATHEMATICAL AND GENERAL

J. Phys. A: Math. Gen. **35** (2002) L105–L116 PII: S0305-4470(02)32130-9

LETTER TO THE EDITOR

Infinite-variable Bessel functions in two-dimensional Wannier–Stark systems

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Received 17 December 2001
Published 22 February 2002
Online at stacks.iop.org/JPhysA/35/L105

Abstract

We discuss the spectrum and the eigenfunctions of a 2D Wannier–Stark system in both the tight-binding and single-band approximations. We show that the unfamiliar infinite-variable Bessel functions play a crucial role in these considerations. Furthermore, a closed formula for the eigenfunction for an arbitrary tight-binding ansatz in terms of an expansion in Wannier states is derived. Finally we give a closed form solution for the Wannier–Stark states in the scope of the single-band approximation.

PACS numbers: 02.30.Gp, 05.50.+q, 31.10.+z, 73.21.Cd

1. Introduction

The tight-binding model for the discussion of Wannier–Stark systems (i.e. spatial periodic structures affected by a constant or time-periodic external force) has always provided an easy approach and a playground for the description of a multitude of physical phenomena. The work in this area covers such different applications or effects as ac-field controlled Anderson localization in disordered superlattices [Hol95], the description of Rabi oscillations between different Bloch bands [Zha96] or the discussion of carrier dynamics in semiconductor superlattices [Rot95]. For a review on the whole subject, see [Glü01b]. Depending on the strength of the field applied, the interaction between different bands can be neglected and the description can be restricted to the so-called single-band approximation. All these publications deal with a 1D Wannier–Stark system. Recently, a new theoretical and numerical approach to 2D Wannier–Stark systems was successfully applied [Glü01a], but not in the scope of a tight-binding approximation. This motivated a discussion of the analogue tight-binding system. For first steps in this direction, see the works of Nakanish *et al* [Nak93, Nak95].

In this work, we discuss the properties of a 2D Wannier–Stark system in both the tight-binding and the single-band approximations. By solving the appropriate Schrödinger equation in closed form, we derive the Wannier–Stark spectrum of the system independently of the field applied. Furthermore, it is shown that the usage of the infinite-variable Bessel functions [Lor95] allows the solution of nearly every possible tight-binding model in a straightforward manner.

2. 2D Bloch system

Let us briefly recapitulate the properties of a Bloch system which will be needed in the following discussion. The typical 2D Bloch Hamiltonian reads

$$H_0 = \frac{\boldsymbol{p}^2}{2m} + V(\boldsymbol{r}) \tag{1}$$

where $V(\boldsymbol{r})$ is a periodic potential with the two periods a_x and a_y in the x- and y-directions in cartesian coordinates $\boldsymbol{r} = (x, y)$. The simultaneous eigenstates of this Hamiltonian H_0 and the translation over one period in each direction $T_{1,1}$ are called Bloch states $|\Phi_{\boldsymbol{\kappa}}\rangle$:

$$H_0|\Phi_{\boldsymbol{\kappa}}\rangle = E(\boldsymbol{\kappa})|\Phi_{\boldsymbol{\kappa}}\rangle \qquad T_{1,1}|\Phi_{\boldsymbol{\kappa}}\rangle = \exp(\mathrm{i}\boldsymbol{r}_{1,1}\cdot\boldsymbol{\kappa})\,|\Phi_{\boldsymbol{\kappa}}\rangle. \tag{2}$$

Here we use the abbreviation $\boldsymbol{r}_{1,1} = (a_x, a_y)$. Because the Bloch states are periodic in $\boldsymbol{\kappa}$, they can be expanded in a Fourier series:

$$|\Phi_{\boldsymbol{\kappa}}\rangle = \sum_{m,n\in\mathbb{Z}} \exp(\mathrm{i}\boldsymbol{r}_{m,n}\cdot\boldsymbol{\kappa})\,|m,n\rangle \qquad \text{where} \quad \boldsymbol{r}_{m,n} = \begin{pmatrix} ma_x \\ na_y \end{pmatrix}. \tag{3}$$

The states $|m, n\rangle$ introduced in this expansion are the so-called Wannier states. They are—in contrast to the extended Bloch states—exponentially localized in the unitary cell at position (m, n) of the system and provide therefore the ideal orthogonal basis set for the tight-binding approximations. Note that they are neither eigenstates of H_0 nor $T_{1,1}$. The different Wannier states can be generated by

$$|m, n\rangle = T_{m,n}|0, 0\rangle \tag{4}$$

where $T_{m,n} = \exp\left(\mathrm{i}\boldsymbol{p}\cdot\boldsymbol{r}_{m,n}/\hbar\right)$ is the translational operator which shifts the state $|0, 0\rangle$ to the cell at position (m, n).

3. Tight-binding Hamiltonian for a Wannier–Stark system

A Wannier–Stark system is obtained when one adds an external force $\boldsymbol{F}(t)$ to the Hamiltonian (1). For our discussion we restrict ourselves to the case of a constant (i.e. time-independent) field described by the Hamiltonian

$$H = H_0 + \boldsymbol{F}\cdot\boldsymbol{r}. \tag{5}$$

As mentioned above, we use the Wannier states of the field-independent case as a basis to evaluate the Hamiltonian. In the tight-binding approximation only the interaction in the so-called von Neumann neighbourhood is taken into account which leads to the tight-binding Hamiltonian H_{tb}

$$\begin{aligned} H \approx H_{\mathrm{tb}} = \sum_{m,n} &\left(E + F_x a_x m + F_y a_y n\right)|m,n\rangle\langle m,n| \\ &+ \frac{\Delta_x}{4}\left(|m+1,n\rangle\langle m,n| + |m,n\rangle\langle m+1,n|\right) \\ &+ \frac{\Delta_y}{4}\left(|m,n+1\rangle\langle m,n| + |m,n\rangle\langle m,n+1|\right). \end{aligned} \tag{6}$$

Here, E is given by $E = \langle 0,0|H_0|0,0\rangle$ and Δ_x and Δ_y are the band widths along the two axes for H_0. The term proportional to $F_x a_x m + F_y a_y n$ results from the expectation value $\langle m, n|\boldsymbol{F}\cdot\boldsymbol{r}|m'n'\rangle$, which—using the orthogonality of the Wannier states and the relation (4)—equals $\boldsymbol{F}\cdot\boldsymbol{r}_{m,n}\delta_{m,m'}\delta_{n,n'}$. To derive the energy spectrum of the system, we have to discuss the Schrödinger equation

$$H_{\mathrm{tb}}|\Psi\rangle = E_k|\Psi\rangle. \tag{7}$$

We expand the wavefunction $|\Psi\rangle$ using the Wannier states $|m, n\rangle$

$$|\Psi\rangle = \sum_{m,n} c_{m,n}|m, n\rangle. \tag{8}$$

Inserting this into equation (7) leads to a recursion relation for the coefficients $c_{m,n}$

$$(E + F_x a_x m + F_y a_y n)c_{m,n} + \frac{\Delta_x}{4}(c_{m-1,n} + c_{m+1,n}) + \frac{\Delta_y}{4}(c_{m,n-1} + c_{m,n+1}) = E_k c_{m,n} \tag{9}$$

or

$$(E_k - E - F_x a_x m - F_y a_y n)c_{m,n} = \frac{\Delta_x}{4}(c_{m-1,n} + c_{m+1,n}) + \frac{\Delta_y}{4}(c_{m,n-1} + c_{m,n+1}). \tag{10}$$

For this first discussion we will restrict ourselves to 'rational' directions of the field strength

$$\boldsymbol{F} = \frac{F}{\sqrt{q^2 + r^2}} \begin{pmatrix} q \\ r \end{pmatrix} \qquad q, r \in \mathbb{Z} \tag{11}$$

where q and r are coprime integers ($\gcd(q, r) = 1$). Furthermore, we will consider the special case $a_x = a_y = a$ which simplifies the notation. Under these preconditions, there exists a common integer multiple of the two one-dimensional Bloch times associated with the two directions of periodicity. Only in this case can we expect to find a non-continuous, structured energy spectrum [Glü01a]. This was already pointed out in [Fuk73]. With these assumptions, the recursion relation reads

$$\frac{aF}{\sqrt{q^2 + r^2}} \left(\sqrt{q^2 + r^2}\, \frac{E_k - E}{aF} - mq - nr \right) c_{m,n} = \frac{\Delta_x}{4}(c_{m-1,n} + c_{m+1,n}) + \frac{\Delta_y}{4}(c_{m,n-1} + c_{m,n+1}). \tag{12}$$

To solve this recurrence relation we consider the infinite-variable Bessel functions (IVBs)

$$J_s(\{\beta_m\}) = \frac{1}{\pi} \int_0^\pi \cos\left(s\theta - \sum_m \beta_m \sin(m\theta) \right) \mathrm{d}\theta \tag{13}$$

with $s \in \mathbb{Z}$, $m \in \mathbb{N}$ and $\sum_1^\infty |\beta_m| < \infty$. The IVBs are a straightforward extension of the usual Bessel functions with integer index to multiple or even infinitely many variables. (IVBs were first used by Pérès and Appell [P15, App15]. For a well written introduction to IVBs, see [Lor95]; for another physical application, see [Dat92].) For $\{\beta_m\} = \{\beta, 0, 0, \ldots\}$ we rediscover the ordinary Bessel functions $J_s(\beta)$. The IVBs satisfy the recursion relation

$$2s J_s(\{\beta_m\}) = \sum_m m\beta_m \left(J_{s-m}(\{\beta_m\}) + J_{s+m}(\{\beta_m\}) \right) \qquad s \in \mathbb{Z} \tag{14}$$

if the series $\sum_m m|\beta_m|$ is convergent. First assume $q \neq r$ (the other case $q = r = 1$ will be discussed later). With the abbreviations

$$\begin{aligned} s &= \sqrt{q^2 + r^2}\, \frac{E_k - E}{aF} - mq - nr \\ \beta_q &= 2\frac{\Delta_x}{4} \frac{\sqrt{q^2 + r^2}}{aFq} = \frac{\Delta_x}{2aF_x} \\ \beta_r &= 2\frac{\Delta_y}{4} \frac{\sqrt{q^2 + r^2}}{aFr} = \frac{\Delta_y}{2aF_y} \end{aligned} \tag{15}$$

it is straightforward to check that the $J_s(\beta_q, \beta_r)$ (all other β_i are set to zero) fulfil the recursion relation (12) provided that s is integer, which leads to the condition

$$\sqrt{q^2 + r^2}\, \frac{E_k - E}{aF} \in \mathbb{Z} \tag{16}$$

or

$$E_k = E + k\,\frac{aF}{\sqrt{q^2+r^2}} \qquad \text{with} \quad k \in \mathbb{Z}. \tag{17}$$

This is exactly the same result that was obtained in [Glü01a] using a full quantum computation and diagonalizing the time evolution operator over the Bloch time T_B. The energy $aF/\sqrt{q^2+r^2}$ is equal to the energy splitting between two neighbouring subbands.

Let us write down again the expansion coefficients $c_{m,n}$:

$$c_{m,n} = J_s(\beta_q, \beta_r) = J_{k-(mq+nr)}(\beta_q, \beta_r) \tag{18}$$

or

$$c_{m,n} = \frac{1}{\pi}\int_0^\pi \cos\Big(s\theta - \beta_q \sin(q\theta) - \beta_r \sin(r\theta)\Big)\,\mathrm{d}\theta. \tag{19}$$

Inserting this into (8) gives

$$|\Psi_k\rangle = \sum_{m,n} c_{m,n}|m,n\rangle = \sum_{m,n} J_{k-(mq+rn)}(\beta_q, \beta_r)|m,n\rangle. \tag{20}$$

Therefore each Wannier state $|m,n\rangle$ which satisfies the condition $mq+nr =$ constant has the same prefactor and gives the same contribution. In configuration space all these states lie on a line perpendicular to the direction of the field. This leads to the expected symmetry properties of $|\Psi_k\rangle$ which are discussed below.

But first let us briefly consider the case $q = r = 1$ which we skipped before. Here (12) reduces to

$$\frac{aF}{\sqrt{2}}\left(\sqrt{2}\,\frac{E_k - E}{aF} - m - n\right) c_{m,n} = \frac{\Delta_x}{4}(c_{m-1,n} + c_{m+1,n}) + \frac{\Delta_y}{4}(c_{m,n-1} + c_{m,n+1}). \tag{21}$$

The solution to this equation is the usual Bessel function

$$c_{m,n} = J_s\left(\frac{\Delta_x + \Delta_y}{\sqrt{2}aF}\right) \tag{22}$$

with $s = \sqrt{2}(E_k - E)/(aF) - (m+n)$. The wavefunction is given by

$$|\Psi_k\rangle = \sum_{m,n} c_{m,n}|m,n\rangle = \sum_{m,n} J_{k-(m+n)}\left(\frac{\Delta_x + \Delta_y}{\sqrt{2}aF}\right)|m,n\rangle \tag{23}$$

with the expected energy splitting $\Delta E = aF/\sqrt{2}$ between two neighbouring subbands.

Let us return to the case $q \neq r$. As we have seen, the condition that two Wannier states $|m,n\rangle$ and $|\tilde{m},\tilde{n}\rangle$ contribute with equal weight to the expansion (8), i.e. $c_{m,n} = c_{\tilde{m},\tilde{n}}$, reads

$$mq + nr = \tilde{m}q + \tilde{n}r \tag{24}$$

or

$$(m - \tilde{m})q = (\tilde{n} - n)r. \tag{25}$$

Because q and r are coprime integers, this equation can only be satisfied if we have

$$m - \tilde{m} = gr \qquad \tilde{n} - n = gq \qquad g \in \mathbb{N} \tag{26}$$

which yields a condition for the energy of these states. Computing the energy expectation values

$$\begin{aligned}\langle m,n|H_0 + \boldsymbol{F}\cdot\boldsymbol{r}|m,n\rangle &= \langle 0,0|H_0 + \boldsymbol{F}\cdot\boldsymbol{r}|0,0\rangle + mF_x a + nF_y a \\ &= \langle 0,0|H_0 + \boldsymbol{F}\cdot\boldsymbol{r}|0,0\rangle + \tilde{m}F_x a + \tilde{n}F_y a \\ &= \langle \tilde{m},\tilde{n}|H_0 + \boldsymbol{F}\cdot\boldsymbol{r}|\tilde{m},\tilde{n}\rangle\end{aligned} \tag{27}$$

we see that the two states $|m,n\rangle$ and $|\tilde{m},\tilde{n}\rangle$ have the same energy expectation value.

3.1. Symmetries of $\Psi_k(\boldsymbol{r})$

To derive the symmetry properties of the wavefunction, we use the coordinate shift operator $T_{m,n}$,

$$T_{m,n}\boldsymbol{r} = \boldsymbol{r} + a\begin{pmatrix} m \\ n \end{pmatrix} \qquad \text{i.e.} \quad T_{m,n} = \exp\left(\frac{\mathrm{i}}{\hbar}\,\boldsymbol{p}\cdot\boldsymbol{r}_{m,n}\right). \tag{28}$$

When we shift the argument of the wavefunction $\Psi_k(\boldsymbol{r}) = \langle \boldsymbol{r}|\Psi_k(\boldsymbol{r})\rangle$ in a direction orthogonal to the field by multiples of the potential period a, i.e.

$$\begin{aligned}\Psi_k\left(\boldsymbol{r}+\boldsymbol{r}_{r,-q}\right) &= T_{r,-q}\Psi_k(\boldsymbol{r}) = \sum_{m,n} c_{m,n}\langle \boldsymbol{r}+\boldsymbol{r}_{r,-q}|m,n\rangle \\ &= \sum_{m,n} c_{m,n}\langle \boldsymbol{r}|m-r,n+q\rangle \\ &= \sum_{m,n} c_{m-r,n+q}\langle \boldsymbol{r}|m-r,n+q\rangle \\ &= \Psi_k(\boldsymbol{r})\end{aligned} \tag{29}$$

we see that the wavefunction is invariant under this translation. Therefore $\Psi_k(\boldsymbol{r})$ is periodic in the direction orthogonal to the field with period $a\sqrt{q^2+r^2}$. One can derive this result directly from the Schrödinger equation. Starting with its representation in configuration space

$$H(\boldsymbol{r})\Psi_k(\boldsymbol{r}) = E_k\Psi_k(\boldsymbol{r}) \tag{30}$$

we apply the translation $T_{r,-q}$ perpendicular to the field ($T_{r,-q}$ commutes with H because $\boldsymbol{F}\cdot\boldsymbol{r}_{r,-q} = 0$):

$$T_{r,-q}H(\boldsymbol{r})\Psi_k(\boldsymbol{r}) = H(\boldsymbol{r})\Psi_k(\boldsymbol{r}+\boldsymbol{r}_{r,-q}) = E_k\Psi_k(\boldsymbol{r}+\boldsymbol{r}_{r,-q}). \tag{31}$$

Therefore $\Psi_k(\boldsymbol{r})$ and $\Psi_k(\boldsymbol{r}+\boldsymbol{r}_{r,-q})$ fulfil the same equation, i.e. $\Psi_k(\boldsymbol{r}) = \Psi_k(\boldsymbol{r}+\boldsymbol{r}_{r,-q})$ as above.

3.2. The 1D case as a special case of the 2D problem

In this subsection we will briefly discuss the connection of 1D and 2D Wannier–Stark systems. Let therefore $\boldsymbol{F}$ be given by $\boldsymbol{F} = F\boldsymbol{E}_x$, where $\boldsymbol{E}_x$ is the unit vector in the x-direction. The Bloch time T_B is then given by $T_\mathrm{B} = 2\pi\hbar/(aF)$. Inserting this into equation (9) leads to

$$aF\left(\frac{E_k - E}{aF} - m\right)c_{m,n} = \frac{\Delta_x}{4}(c_{m-1,n} + c_{m+1,n}) + \frac{\Delta_y}{4}(c_{m,n-1} + c_{m,n+1}). \tag{32}$$

The prefactor of the left hand side is independent of n and—with the ansatz $c_{m,n} = g_m f_n$—the contributions to m and n are separable and

$$aF\left(\frac{E_k - E}{aF} - m\right) - \frac{\Delta_x}{4g_m}(g_{m-1} + g_{m+1}) = K = \frac{\Delta_y}{4f_n}(f_{n-1} + f_{n+1}) \tag{33}$$

where K is a constant whose value and significance will be determined later. Let us first consider the right-hand side of this equation:

$$\frac{4K}{\Delta_y}f_n = f_{n-1} + f_{n+1}. \tag{34}$$

The solution of this equation is $f_n = f\exp(\mathrm{i}n\alpha)$, i.e. a periodic function of the site index n. Therefore we have a periodic solution orthogonal to the field with the period $2\pi/\alpha$.

Now let us identify the constant K. We consider a translation of the eigenfunction $\Psi_k(\boldsymbol{r})$ orthogonal to the field:

$$\begin{aligned}\Psi_k(\boldsymbol{r}+a\boldsymbol{e}_y) &= T_{0,1}\Psi_k(\boldsymbol{r}) = \sum_{m,n} c_{m,n}\langle \boldsymbol{r}+a\boldsymbol{e}_y|m,n\rangle \\ &= \sum_{m,n} c_{m,n}\langle \boldsymbol{r}|m,n-1\rangle = \sum_{m,n} g_m f\exp(\mathrm{i}n\alpha)\boldsymbol{r}|m,n-1\rangle \\ &= \exp(\mathrm{i}\alpha)\Psi_k(\boldsymbol{r}). \end{aligned} \tag{35}$$

The eigenfunction $\Psi_k(\boldsymbol{r})$ is therefore also an eigenfunction of the translation operator over one period in the y-direction

$$T_{0,1}\Psi_k(\boldsymbol{r}) = \exp(\mathrm{i}\alpha)\Psi_k(\boldsymbol{r}) \tag{36}$$

as expected from the Bloch theorem. Writing the parameter α in the form $\alpha = \kappa_y a$ and substituting this into equation (34) determines the constant K:

$$K = \frac{\Delta_y}{2}\cos(\alpha) = \frac{\Delta_y}{2}\cos(\kappa_y a). \tag{37}$$

Now let us return to the recursion equation for g_m

$$\frac{4aF}{\Delta_y}\left(\frac{E_k - E - K}{aF} - m\right) = g_{m-1} + g_{m+1}. \tag{38}$$

Introducing the variables

$$s = \frac{E_k - E - K}{aF} - m \in \mathbb{Z} \qquad z = \frac{\Delta_x}{2aF} \tag{39}$$

we see that the solution of equation (38) is given by $g_m = J_s(z)$, where J_s is an ordinary Bessel function. Therefore the dispersion relation reads

$$E_k = E + K + kaF = E + \frac{\Delta_y}{2}\cos(\kappa_y a) + kaF \qquad k \in \mathbb{Z} \tag{40}$$

which is independent of κ_x and periodic in κ_y with amplitude Δ_y. Not surprisingly, this result resembles the one obtained for a one-dimensional Wannier–Stark system interacting with a time-dependent field.

Until now we have restricted ourselves to the case $a_x = a_y = a$. Let us now extend the discussion to the case $a_x/a_y = q_l/r_l$, i.e. a_x and a_y are integer multiples of a fundamental lattice length scale a, $a_x = q_l a$ and $a_y = r_l a$. As before we will consider fields of the form

$$\boldsymbol{F} = \frac{F}{\sqrt{{q_f}^2 + {r_f}^2}}\begin{pmatrix} q_f \\ r_f \end{pmatrix} \qquad q_f, r_f \in \mathbb{Z} \tag{41}$$

because otherwise the two Bloch times in the two directions are incommensurable. The two directional Bloch times are

$$\begin{aligned} T_x &= \frac{2\pi\hbar}{a_x F_x} = \frac{2\pi\hbar}{aq_l q_f F}\sqrt{{q_f}^2 + {r_f}^2} \\ T_y &= \frac{2\pi\hbar}{a_y F_y} = \frac{2\pi\hbar}{ar_l r_f F}\sqrt{{q_f}^2 + {r_f}^2} \end{aligned} \tag{42}$$

and the common Bloch time is defined by

$$T_{\mathrm{B}} = qT_x = rT_y \qquad \text{with} \qquad q = \frac{q_l q_f}{kl} \quad r = \frac{r_l r_f}{kl} \tag{43}$$

with $k = \gcd(q_l, r_f)$ and $l = \gcd(r_l, q_f)$. Inserting this into equation (9) gives

$$\frac{aFkl}{\sqrt{{q_f}^2 + {r_f}^2}} \left(\frac{E_k - E}{aFkl} \sqrt{{q_f}^2 + {r_f}^2} - qm - rn \right) c_{m,n} = \frac{\Delta_x}{4}(c_{m-1,n} + c_{m+1,n}) + \frac{\Delta_y}{4}(c_{m,n-1} + c_{m,n+1}) \tag{44}$$

and, similar to the derivation above, we obtain the energy spectrum

$$E_n = E + n \frac{aFkl}{\sqrt{{q_f}^2 + {r_f}^2}}. \tag{45}$$

The splitting between two levels in the case $a_x = a_y = a$ is therefore enlarged by a factor kl. The same result can be obtained when we consider the following simplistic model. Given the period of the potential both parallel and orthogonal to the field direction, one can determine the number of initial Wannier states located in a Wigner–Seitz cell. This number is equal to the number of subbands that are contained in one fundamental energy interval of the system. The latter is given by the strength of the field multiplied by the period of the potential in the field direction. Because of symmetry, the splitting between two arbitrary adjacent subbands is constant. Let us check this more carefully, as follows.

The period a_p of the potential parallel to the field direction is given by

$$a_\mathrm{p} = s_\mathrm{p} a \sqrt{{q_f}^2 + {r_f}^2} \qquad s_\mathrm{p} = \frac{q_l r_l}{\gcd(q_f r_l, q_l r_f)} \tag{46}$$

and the period a_o orthogonal to the field reads

$$a_\mathrm{o} = s_\mathrm{o} a \sqrt{{q_f}^2 + {r_f}^2} \qquad s_\mathrm{o} = \frac{q_l r_l}{\gcd(q_f q_l, r_f r_l)}. \tag{47}$$

The size of the Wigner–Seitz cell is $a_\mathrm{p} a_\mathrm{o}$ and the main part of each inital Wannier state occupies approximately the area $a_x a_y = q_l r_l a^2$. Therefore we have

$$N = \frac{a_\mathrm{p} a_\mathrm{o}}{a_x a_y} = \frac{s_\mathrm{p} s_\mathrm{o} ({q_f}^2 + {r_f}^2)}{q_l r_l} \tag{48}$$

states in this area. With the fundamental energy interval $\Delta E_f = a_\mathrm{p} F$, we get the splitting between two adjacent subbands:

$$\begin{aligned} \Delta E = \frac{\Delta E_f}{N} &= \frac{aF\sqrt{{q_f}^2 + {r_f}^2}}{s_\mathrm{o}({q_f}^2 + {r_f}^2)} q_l r_l \\ &= \frac{aF}{\sqrt{{q_f}^2 + {r_f}^2}} \gcd(q_f q_l, r_f r_l) \\ &= \frac{aF}{\sqrt{{q_f}^2 + {r_f}^2}} \gcd(q_f, r_l) \gcd(q_l, r_f) \\ &= \frac{aFkl}{\sqrt{{q_f}^2 + {r_f}^2}}. \end{aligned} \tag{49}$$

The factorization of $\gcd(q_f q_l, r_f r_l)$ in the form used above is only possible because $\gcd(q_f, r_f) = \gcd(q_l, r_l) = 1$. Note that the result obtained in this simple way is equivalent to that in equation (45).

3.3. One step beyond the tight-binding approximation

So far we have only considered the most simple tight-binding approximation, i.e. we have only taken into account the interaction between two neighbouring Wannier states. But we will see that we can quite easily drop this restriction and still arrive at similar results as before.

For simplicity, we restrict ourselves to the case where the two periods of the potential are the same, i.e. $a_x = a_y = a$. In the previous sections, we worked with a tight-binding Hamiltonian which includes only the von Neumann neighbourhood between interacting states. The next logical step is to choose the Moore neighbourhood which also takes into account the neighbouring states along the diagonals. This leads to the tight-binding Hamiltonian

$$\begin{aligned} H_{\mathrm{tb}} = \sum_{m,n} \big(E + F_x a_x m + F_y a_y n\big)\,|m,n\rangle\langle m,n| + \frac{\Delta_x}{4}\big(|m+1,n\rangle\langle m,n| + |m,n\rangle\langle m+1,n|\big) \\ + \frac{\Delta_y}{4}\big(|m,n+1\rangle\langle m,n| + |m,n\rangle\langle m,n+1|\big) \\ + \frac{\Delta_{xy}}{4}\big(|m+1,n+1\rangle\langle m,n| + |m,n\rangle\langle m+1,n+1| \\ + |m+1,n-1\rangle\langle m,n| + |m,n\rangle\langle m+1,n-1|\big). \end{aligned} \tag{50}$$

In this formula, Δ_{xy} determines the interaction strength along the diagonals. Performing the same steps as before, we arrive at the recursion relation

$$\begin{aligned} \frac{aF}{\sqrt{q^2+r^2}}\left(\sqrt{q^2+r^2}\,\frac{E_k - E}{aF} - mq - nr\right) c_{m,n} \\ = \frac{\Delta_x}{4}(c_{m-1,n} + c_{m+1,n}) + \frac{\Delta_y}{4}(c_{m,n-1} + c_{m,n+1}) \\ + \frac{\Delta_{xy}}{4}(c_{m+1,n+1} + c_{m+1,n-1} + c_{m-1,n+1} + c_{m-1,n-1}). \end{aligned} \tag{51}$$

It is easy to check that the coefficient $c_{m,n}$ is again proportional to J_s, where s is given by $s = \sqrt{q^2+r^2}(E_k - E)/(aF) - mq - nr$, and therefore the energy spectrum does not change. But now, due to the new terms in the rescursion relation, J_s depends not only on β_q and β_r, but also on β_{q+r} and $\beta_{|q-r|}$, where the last two are given by

$$\beta_{q+r} = 2\frac{\Delta_{xy}}{4}\frac{\sqrt{q^2+r^2}}{aF(q+r)} \qquad \beta_{|q-r|} = 2\frac{\Delta_{xy}}{4}\frac{\sqrt{q^2+r^2}}{aF|q-r|}. \tag{52}$$

Therefore the absolute value of the coefficients $c_{m,n}$ do change when we discuss another neighbourhood—which is no surprise—but the energy spectrum and the symmetry properties of the eigenfunctions stay the same. It is remarkable that using the generalized Bessel functions, we can express the solution of nearly every possible 2D Wannier–Stark tight-binding Hamiltonian in closed form.

4. Time evolution of a 2D Floquet–Bloch state in the single-band approximation

The last section of this paper deals with the time evolution of a 2D Floquet–Bloch state in the single-band approximation for the case $a_x = a_y = a$. A Floquet–Bloch state is an eigenstate of the time evolution operator over one Bloch period which reproduces itself up to a phase factor. When using the single-band approximation, i.e. by neglecting the interaction between different bands, the Floquet–Bloch state can be approximated by propagating an arbitrary Bloch state of the field-independent Hamiltonian over one Bloch period and collecting the phase it gathers

during this process. The time evolution of a Floquet–Bloch state can therefore be approximated by the Houston-like formula [Hou40]

$$\begin{aligned}\phi_{\boldsymbol{\kappa}_0} &= \exp\left(-\frac{\mathrm{i}}{\hbar}\int_0^t E\left(\boldsymbol{\kappa}_0 - \frac{\boldsymbol{F}t'}{\hbar}\right)\mathrm{d}t'\right)\phi_{\boldsymbol{\kappa}_0-\boldsymbol{F}t/\hbar} \\ &= \exp\left(-\frac{\mathrm{i}}{F}\int_\gamma E(\boldsymbol{\kappa})\,\mathrm{d}\kappa\right)\phi_{\boldsymbol{\kappa}} \end{aligned} \tag{53}$$

where $\gamma = [0,t] \to [\boldsymbol{\kappa}_0 - \boldsymbol{F}t/\hbar, \boldsymbol{\kappa}_0]$, $\boldsymbol{\kappa}(t') = \boldsymbol{\kappa}_0 - \boldsymbol{F}(t-t')/\hbar$ is a path in quasi-momentum space and $\phi_{\boldsymbol{\kappa}}$ is the Bloch state with quasi-momentum $\boldsymbol{\kappa}$ in the field-free case. $E(\boldsymbol{\kappa})$ consists of the dispersion relation of the field-free case plus a field-dependent term. It is a periodic function in $\boldsymbol{\kappa}$ and can therefore be written as

$$E(\boldsymbol{\kappa}) = \sum_{m,n} E_{m,n}\mathrm{e}^{\mathrm{i}ma\kappa_x + \mathrm{i}na\kappa_y} \tag{54}$$

where the expansion coefficients $E_{m,n}$ are given by $E_{m,n} = \langle 0,0|H_0 + \boldsymbol{F}\cdot\boldsymbol{r}|m,n\rangle$. The Wannier states can be chosen to be real [Koh72] and therefore the $E_{m,n}$ are also real. Because $E_{\pm m,\pm n} = E_{m,n}$ is independent of the individual signs of m and n, we can write $E(\boldsymbol{\kappa})$ in the form

$$E(\boldsymbol{\kappa}) = \sum_{m,n} E_{m,n}\cos(ma\kappa_x + na\kappa_y). \tag{55}$$

We use this formula to compute the integral in the exponent of equation (53):

$$\begin{aligned}\int_0^t E\left(\boldsymbol{\kappa}_0 - \frac{\boldsymbol{F}t'}{\hbar}\right)\mathrm{d}t' &= \sum_{m,n} E_{m,n}\int_0^t \cos\left(\alpha_{m,n} - \frac{maF_x t'}{\hbar} - \frac{naF_y t'}{\hbar}\right)\mathrm{d}t' \\ &= \sum_{m,n} E_{m,n}\int_0^t \cos\left(\alpha_{m,n} - 2\pi\frac{t'}{T_\mathrm{B}}(q_f m + r_f n)\right)\mathrm{d}t' \\ &= \sum_{q_f m + r_f n = 0} E_{m,n}\cos(\alpha_{m,n})\,t + \frac{T_\mathrm{B}}{2\pi}\sum_{q_f m + r_f n \neq 0}\frac{E_{m,n}}{q_f m + r_f n} \\ &\quad\times\left\{\sin\left(\alpha_{m,n} - 2\pi\frac{t}{T_\mathrm{B}}(q_f m + r_f n)\right) - \sin\alpha_{m,n}\right\}. \end{aligned} \tag{56}$$

Here, $\alpha_{m,n}$ is an abbreviation for $ma\kappa_{x,0} + na\kappa_{y,0}$. The quasi-energy is defined by the phase the state gathers while being propagated over one Bloch period. By inserting the Bloch time T_B in the equation above we get the quasi-energy

$$\begin{aligned}\bar{E}(\boldsymbol{\kappa}_0) &= \sum_{q_f m + r_f n = 0} E_{m,n}\cos(\alpha_{m,n}) \\ &= \sum_{q_f m + r_f n = 0} \langle 0,0|H_0 + \boldsymbol{F}\cdot\boldsymbol{r}|m,n\rangle\cos(\alpha_{m,n}). \end{aligned} \tag{57}$$

Therefore only those matrix elements contribute whose associated Wannier states lie on a line perpendicular to the direction of the field. Taking into account that the phase in equation (53) is only determined up to multiples of 2π, we get the Wannier–Stark ladder

$$E_k = \bar{E}(\boldsymbol{\kappa}) + k\frac{aF}{\sqrt{q_f^2 + r_f^2}}. \tag{58}$$

Note that due to the summation condition $q_f m + r_f n = 0$, the quasi-energy (57) does not change when we shift its argument $\boldsymbol{\kappa}$ along the direction of the field.

The Wannier–Stark states of the system are given by the following integral:

$$\begin{aligned}\Psi(\boldsymbol{r},0) &= \frac{1}{T_{\mathrm{B}}}\int_0^{T_{\mathrm{B}}} \mathrm{d}t \exp\left(\frac{\mathrm{i}}{\hbar}\bar{E}t\right) U(t)\phi_{\boldsymbol{\kappa}_0}(\boldsymbol{r},0) \\ &= \frac{1}{T_{\mathrm{B}}}\int_0^{T_{\mathrm{B}}} \mathrm{d}t \exp\left(\frac{\mathrm{i}}{\hbar}\bar{E}t\right) \exp\left(-\frac{\mathrm{i}}{\hbar}\int_0^t E\left(\boldsymbol{\kappa}_0 - \frac{\boldsymbol{F}t'}{\hbar}\right)\mathrm{d}t'\right)\phi_{\boldsymbol{\kappa}_0-\boldsymbol{F}t/\hbar}(\boldsymbol{r},0).\end{aligned} \tag{59}$$

To simplify the notation we choose $\boldsymbol{\kappa}_0 = 0$. Inserting (56) into (59) we arrive at

$$\Psi(\boldsymbol{r},0) = \frac{1}{T_{\mathrm{B}}}\int_0^{T_{\mathrm{B}}} \mathrm{d}t \exp\left(-\frac{\mathrm{i}}{\hbar}\frac{T_{\mathrm{B}}}{2\pi}\sum_{\neq 0}\frac{E_{m,n}}{q_f m + r_f n}\sin\left(\frac{2\pi t}{T_{\mathrm{B}}}(q_f m + r_f n)\right)\right)\phi_{-\boldsymbol{F}t/\hbar}(\boldsymbol{r},0) \tag{60}$$

where $\neq 0$ abbreviates the expression $q_f m + r_f n \neq 0$. Representing the Bloch state $\phi_{\boldsymbol{\kappa}}(\boldsymbol{r},0)$ in terms of Wannier functions $\langle \boldsymbol{r}|m,n\rangle$

$$\phi_{\boldsymbol{\kappa}}(\boldsymbol{r},0) = \sum_{\tilde{m},\tilde{n}} \exp\left(\mathrm{i}a\kappa_x\tilde{m} + \mathrm{i}a\kappa_y\tilde{n}\right)\langle \boldsymbol{r}|\tilde{m},\tilde{n}\rangle \tag{61}$$

and inserting this into equation (60) leads to

$$\begin{aligned}\Psi(\boldsymbol{r},0) &= \frac{1}{T_{\mathrm{B}}}\int_0^{T_{\mathrm{B}}} \mathrm{d}t \sum_{\tilde{m},\tilde{n}} \exp\left(-\frac{\mathrm{i}}{\hbar}\frac{T_{\mathrm{B}}}{2\pi}\sum_{\neq 0}\frac{E_{m,n}}{q_f m + r_f n}\sin\left(\frac{2\pi t}{T_{\mathrm{B}}}(q_f m + r_f n)\right)\right) \\ &\quad \times \exp\left(-\mathrm{i}\frac{2\pi t}{T_{\mathrm{B}}}(q_f\tilde{m} + r_f\tilde{n})\right)\langle \boldsymbol{r}|\tilde{m},\tilde{n}\rangle \\ &= \sum_{\tilde{m},\tilde{n}} c_{\tilde{m},\tilde{n}}\langle \boldsymbol{r}|\tilde{m},\tilde{n}\rangle\end{aligned} \tag{62}$$

where $c_{\tilde{m},\tilde{n}}$ is given by

$$\begin{aligned}c_{\tilde{m},\tilde{n}} = \frac{1}{T_{\mathrm{B}}}\int_0^{T_{\mathrm{B}}} \mathrm{d}t \exp\Bigg(&-\mathrm{i}\frac{2\pi t}{T_{\mathrm{B}}}(q_f\tilde{m} + r_f\tilde{n}) \\ &-\frac{\mathrm{i}}{\hbar}\frac{T_{\mathrm{B}}}{2\pi}\sum_{\neq 0}\frac{E_{m,n}}{q_f m + r_f n}\sin\left(\frac{2\pi t}{T_{\mathrm{B}}}(q_f m + r_f n)\right)\Bigg)\end{aligned} \tag{63}$$

(interchanging integration and summation is justified because the series is uniformly convergent). To simplify this expression, we use the Jacobi–Anger equation (see equation (2.3) in [Lor95]) for the IVBs

$$\exp\left(\mathrm{i}\sum_{m=1}^{\infty}\beta_m\sin(m\theta)\right) = \sum_{n=-\infty}^{\infty} J_n(\{\beta_m\})\exp(\mathrm{i}n\theta)\,. \tag{64}$$

The right-hand side of this equation is also uniformly convergent. Therefore:

$$\begin{aligned}&\exp\left(-\frac{\mathrm{i}}{\hbar}\sum_{\neq 0}\frac{E_{m,n}}{q_f m + r_f m}\sin\left(\frac{2\pi t'}{T_{\mathrm{B}}}(q_f m + r_f n)\right)\right) \\ &\quad = \exp\left(-\mathrm{i}\sum_{\neq 0}\sum_{k=1}^{\infty}\frac{2E_{m,n}T_{\mathrm{B}}}{2\pi\hbar k}\sin\left(\frac{2\pi t'}{T_{\mathrm{B}}}k\right)\delta_{k,q_f m+r_f n}\right) \\ &\quad = \exp\left(-\mathrm{i}\sum_{k=1}^{\infty}\delta_{k,q_f m+r_f n}\sum_{\neq 0}\frac{2E_{m,n}T_{\mathrm{B}}}{2\pi\hbar k}\sin(k\theta)\right) \\ &\quad = \sum_{l=-\infty}^{\infty} J_{-l}(\{\beta_k\})\exp(\mathrm{i}l\theta)\,.\end{aligned} \tag{65}$$

Above we have introduced the abbreviation $\theta = 2\pi t/T_B$ and the variables

$$\beta_k = \sum_{\neq 0} \delta_{k,q_f m + r_f n} \frac{2E_{m,n} T_B}{2\pi\hbar k}. \tag{66}$$

We use this to continue with our computation of $c_{\tilde{m},\tilde{n}}$:

$$\begin{aligned} c_{\tilde{m},\tilde{n}} &= \frac{1}{T_B} \int_0^{T_B} \mathrm{d}t \sum_{l=-\infty}^{\infty} J_{-l}(\{\beta_k\}) \exp\left(-\mathrm{i}\frac{2\pi t}{T_B}(\tilde{m}q_f + \tilde{n}r_f - l)\right) \\ &= \sum_{l=-\infty}^{\infty} J_{-l}(\{\beta_k\})\, \delta_{l,\tilde{m}q_f+\tilde{n}r_f} = J_{-(\tilde{m}q_f+\tilde{n}r_f)}(\{\beta_k\}). \end{aligned} \tag{67}$$

Therefore the expansion coefficient $c_{\tilde{m},\tilde{n}}$ is given solely by the IVB $J_{-(\tilde{m}q_f+\tilde{n}r_f)}(\{\beta_k\})$.

Let us compare this to the tight-binding result that we got before. In the tight-binding case, we can simplify the variables (66) because the number of interactions which are taken into account is limited. In the von Neumann neighbourhood only the combinations $m = \pm 1, n = 0$ and $m = 0, n = \pm 1$ are possible, and therefore only two variables β_k are different from zero, namely

$$\beta_{q_f} = \frac{2E_{1,0}T_B}{2\pi\hbar q_f} = \frac{2E_{1,0}}{F_x a} \qquad \beta_{r_f} = \frac{2E_{0,1}T_B}{2\pi\hbar r_f} = \frac{2E_{0,1}}{F_y a} \tag{68}$$

and the result (15) is recovered. The same holds if we consider the Moore neighbourhood which adds the possible combinations $m = \pm 1, n = \pm 1$. Here we get the same formulae as in section 3.3.

5. Conclusion

In this paper, the spectrum and the eigenfunctions of a 2D Wannier–Stark system in both the tight-binding and single-band approximations are discussed. In the case of rational direction of the field, the spectrum consists of a set of equally spaced energy ladders, the Wannier–Stark ladders. The splitting between two energy levels depends *strongly* on the direction of the field as does the number of levels in one fundamental energy interval. For the special case where the field was aligned along one of the axes, the energy relation $E(\boldsymbol{\kappa})$ is independent of shifts along the field direction and is periodic orthogonal to it. Using the infinite-variable Bessel functions, a closed solution for the eigenfunction of an arbitrary 2D Wannier–Stark tight-binding Hamiltonian is obtained and for two special neighbourhoods (von Neumann, Moore) the results are given in explicit form. The generalization to Hamiltonians which include interactions with sites farther apart is straightforward. Finally, the Wannier–Stark states in the scope of the single-band approximation are derived using a basis of Wannier functions. The results obtained give a promising start for the generalization of 1D results and effects to 2D systems which are now experimentally accessible.

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