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Calculation of Wannier-Bloch and Wannier-Stark states

M. Glück[1], A. R. Kolovsky[1], H. J. Korsch[1], and and N. Moiseyev[2]

[1] Fachbereich Physik, Universität Kaiserslautern, D-67653 Kaiserslautern, Germany

[2] Department of Chemistry and Minerva Center for Non Linear Physics of Complex Systems, Technion – Israel Institute of Technology, Haifa 32000, Israel

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Abstract. The paper discusses the metastable states of a quantum particle in a periodic potential under a constant force (the model of a crystal electron in a homogeneous electric field), which are known as the Wannier-Stark ladder of resonances. An efficient procedure to find the positions and widths of resonances is suggested and illustrated by numerical calculation for a cosine potential.

PACS. 03.65.-w Quantum mechanics – 73.40Gk Tunneling – 73.20Dx Electron states in low-dimensional structures

1 Introduction

The problem of the quantum states of crystal electrons in a homogeneous electric field had been of fundamental interest since the early Bloch paper of 1929 [1]. Being of very physical importance this problem, however, meets certain mathematical difficulties, which interfere obtaining an exact analytical solution even in 1-dimensional case. In 1960 Wannier [2] took an attempt to overcome them by introducing the Wannier states. His paper (partially wrong) initiated a long discussion on the subject, which continued more than 20 years. (For a historical review of this discussion we refer the reader to the introductory section of paper [3] as well as the more recent review [4].) During this discussion an understanding was achieved that the states of an electron in a homogeneous field, important from the physical point of view, are a sequence of resonances separated by equal energy intervals (the so-called Wannier-Stark ladder of resonances [5,4]).

Recently the interest in the problem of Wannier states was renewed by the experiments with semiconductor superlattices [6] and optical lattices [7,8] (in optical lattices a neutral atom plays the role of an electron). These new experimental objects offer a number of unique possibilities and will definitely initiate a further progress in the theory. In view of this growing interest it would be useful to have an efficient procedure for the numerical calculation of Wannier states. In this paper we suggest such a procedure. It is based on the presentation of a Wannier state as a Floquet state, where the time period is given by the Bloch period. The proposed method proves to be very simple, accurate and fast.

The paper is organized as a sequence of short subsections, discussing a particular problem. In the introductory subsections A and B we briefly review the theory of Bloch and Wannier states. Section C and D describe the analytical approach, which makes the basis for our numerical calculation of Wannier-Bloch and Wannier-Stark states. (We distinguish Wannier-Bloch and Wannier-Stark states - the former is a continuous set of Bloch-like functions, while the latter form a discrete set of localized states.) This analytical approach based, as mentioned above, on the Floquet formalism also suggests a simple proof of the existence of the "energy" (i.e. time-independent) Wannier states. Although the energy states exist, we can not find them numerically and we explain the reason in subsection E. Fortunately this is not the case for the metastable states or resonances. The results of a numerical calculation of the metastable Wannier-Bloch and Wannier-Stark states are presented in subsection F. In subsection G we compare the results with resonances calculated by using the method of complex scaling. Finally, in the concluding section we sum up the results obtained and compare our method with the most commonly used analytical and numerical approaches to the problem.

2 Wannier states

We are interested in the states of a quantum particle in a periodic potential plus constant force (a model of an electron in a crystal lattice under the influence of an external electric field):

$$\widehat{H} = \widehat{H}_0 + Fx \ , \tag{1}$$

$$\widehat{H}_0 = \frac{\widehat{p}^2}{2} + V(x) \ , \quad V(x+2\pi) = V(x) \ . \tag{2}$$

In what follows the analytical expressions are presented for a general form of the potential, in the numerical calculation we choose $V(x) = \cos x$.

2.1 Bloch states

First we discuss the Bloch states of a quantum particle with the Hamiltonian $\widehat{H}_0$. The Bloch states are known to be the eigenfunctions of the Hamiltonian (2),

$$\widehat{H}_0 \phi_{l,k}(x) = \epsilon_l(k) \phi_{l,k}(x) \ , \tag{3}$$

and are periodic in the quasimomentum k, $-1/2 < k < 1/2$. In addition to the periodicity we also request that the $\phi_{l,k}(x)$ are analytic functions of k. This imposes some restriction on a k-specific phase prefactor, up to which the Bloch states are defined. It is also worthwhile to recall that the $\phi_{l,k}(x)$ can be written as

$$\phi_{l,k}(x) = \exp(ikx) \chi_{l,k}(x) \ , \tag{4}$$

where $\chi_{l,k}(x)$ is a periodic function in x satisfying the equation

$$\widehat{H}_0^{(k)} \chi_{l,k}(x) = \epsilon_l(k) \chi_{l,k}(x) \ , \quad \widehat{H}_0^{(k)} = \frac{(\widehat{p} + \hbar k)^2}{2} + V(x) \ , \tag{5}$$

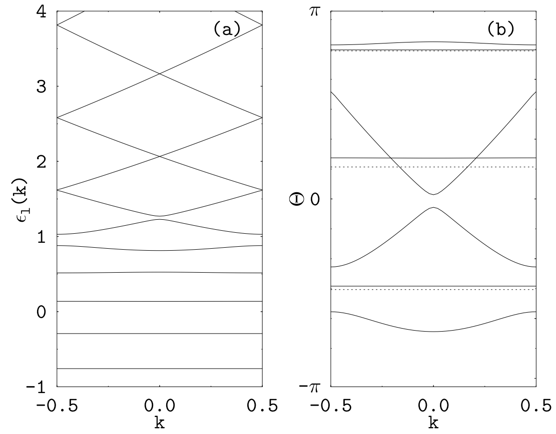

Fig. 1. (a) Spectrum of the Bloch functions for the scaled Planck constant $\hbar = 0.5$. (b) First seven bands folded into the interval $-\pi\hbar/T_B < \epsilon_l(k) < \pi\hbar/T_B$, $T_B = 2.5$. The dotted lines indicate the positions (shifted by 3.04) of the first three most stable resonances for $F = 0.2$.

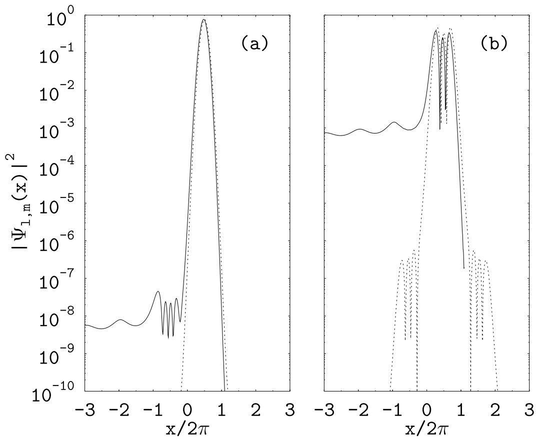

Fig. 2. Dashed line – the localized quasistationary states $\Phi_{l,m}(x)$ constructed from the Bloch states with $l = 0$ (a) and $l = 2$ (b), the cell index is $m = 0$. Solid line – the ground and second excited metastable Wannier-Stark states.

$$\chi_{l,k}(x) = \frac{1}{\sqrt{2\pi}} \sum_n c_n^{(l,k)} \exp(inx) \ .$$

We display Eq. (5) because it makes the basis for the numerical solution of the eigenvalue problem (3). In fact, using the representation of the periodic function $|n\rangle = (2\pi)^{-1/2}\exp(inx)$, we reduce the problem to diagonalizing the real symmetric matrices $H_0^{(k)}(n', n)$. We note that the routine supplies us with a set of *real* k-specific eigenvectors. Then, to insure the analyticity of the Bloch function in k, we multiply every eigenvector by the phase factor $\exp(i\pi k)$.

Figure 1(a) shows the spectrum $\epsilon_l(k)$ for the dimensionless Planck constant $\hbar = 0.5$. The first 5 bands are associated with classically bounded motion and are flat. Their widths are (starting from the ground band) $6.7 \cdot 10^{-7}$, $3.6 \cdot 10^{-5}$, $8.3 \cdot 10^{-4}$, $1.0 \cdot 10^{-2}$, and $6.6 \cdot 10^{-2}$. We note that the widths of the low-lying bands are extremely small. This allows one to construct from the extended Bloch states the localized and almost nondispersive (i.e., quasistationary) states

$$\Phi_{l,m}(x) = \int_{-1/2}^{1/2} \mathrm{d}k \exp(i2\pi mk)\phi_{l,k}(x) \ . \qquad (6)$$

These states are well localized within the m-th cell of the lattice and resemble very much the states of a quantum particle in the "bounded" potential $\cos x$, $0 < x < 2\pi$. Figure 2 (dashed line) shows two states, $\Phi_{0,0}(x)$ and $\Phi_{2,0}(x)$, in the configuration space. In addition, for future use, Fig. 3 shows these states in the momentum representation. (Numerically we first construct the localized states in the momentum representation and then find them in the configuration space by Fourier transformation.)

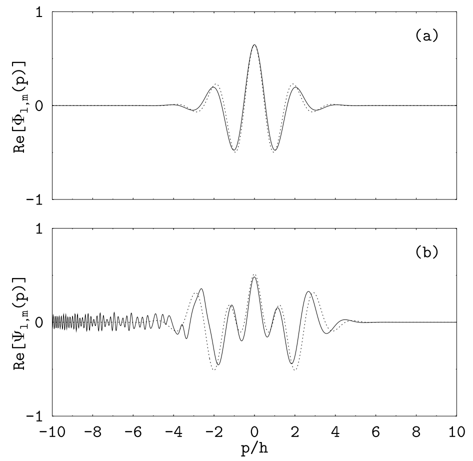

Fig. 3. The same function as in Fig. 2 but in the momentum representation. Only the real part of the functions is shown, the imaginary part looks similar.

2.2 Wannier-Bloch states

We proceed with the case $F \neq 0$. In this subsection we discuss the Wannier-Bloch states of the Hamiltonian (1) as they were introduced by Wannier in 1960 [2]. According to the cited paper these states are a Bloch-like solution of the following equation

$$\left[\frac{\widehat{p}^2}{2} + \cos x + F\left(x + i\frac{\partial}{\partial k}\right)\right]\psi_{l,k}(x) = \varepsilon_l(k)\psi_{l,k}(x) \ . \tag{7}$$

To prove the existence of such a solution Wannier used an iterative procedure in powers of F beginning from the Bloch state $\phi_{l,k}(x)$ of the Hamiltonian $\widehat{H}_0$. In the other words, a solution was assumed to have the form

$$\psi_{l,k}(x) = \psi_{l,k}^{(0)}(x) + F\psi_{l,k}^{(1)}(x) + F^2\psi_{l,k}^{(2)}(x) + \dots \ ,$$
$$\psi_{l,k}^{(0)}(x) = \phi_{l,k}(x) \ . \tag{8}$$

The use of the states (7) is to "decouple" (no interband transition) the Bloch bands. In particular, provided the functions $\psi_{l,k}(x)$ exist, one can then construct the time-dependent Houston-like functions

$$\psi_l(x,t) = \psi_{l,k-Ft/\hbar}(x)\exp\left[-\frac{i}{\hbar}\int_0^t \varepsilon_l\left(k - \frac{F}{\hbar}t'\right)\mathrm{d}t'\right] \ , \tag{9}$$

which satisfy the Schrödinger equation $i\hbar\partial\psi_l(x,t)\partial t = \widehat{H}\psi_l(x,t)$ exactly. The functions (9) in zero order of F coincide with the Houston functions [9], which are known to be only an approximate solution of the time-dependent Schrödinger equation neglecting interband transitions.

Three remarks on the Wannier states (8) should be done. First, these states originate from the Bloch states, which are not proper Hilbert space basis functions for the unbounded operator $\widehat{x}$. Second, the "energy" $\varepsilon_l(k)$ is not unique – by multiplication of the states $\psi_{l,k}(x)$ by a phase factor $\exp[if(k)]$, where $f(k)$ is an arbitrary analytic periodic function, the energy $\varepsilon_l(k)$ gains an additive term $(F/\hbar)\partial f/\partial k$. Third, there is no proof for convergence of the functional series (8). The mentioned drawbacks make the theory of Wannier-Bloch states somehow controversial and have caused a long discussion on the subject [3]. In the next subsection we shall show that many of the debatable problems can be avoided just by introducing the Wannier-Bloch states in a different way.

2.3 Wannier state as a Floquet state

In the following subsection we adopt the formalism of Floquet states developed earlier for studying quantum systems under time-periodic perturbation [10] to find the states of the system (1).

Let us introduce the unitary operator $\widehat{U}$ of the system evolution over the time interval $0 < t < T_B$, where $T_B = \hbar/F$ is the so-called Bloch period [11]

$$\widehat{U} = \exp\left(-\frac{i}{\hbar}\int_0^{T_B} \widehat{H}\mathrm{d}t\right) . \qquad (10)$$

We define the Wannier-Bloch states as the eigenfunction of the operator (10)

$$\widehat{U}\psi_{l,k}(x) = \exp\left[-\frac{i}{\hbar}E_l(k)T_B\right]\psi_{l,k}(x) . \qquad (11)$$

It is shown below that, unlike the definition (7) given by Wannier, this definition is correct in the mathematical sense. We shall give a proof for a more general case of the Hamiltonian

$$\widehat{H} = \frac{\widehat{p}^2}{2} + V(x,t) + Fx , \qquad (12)$$

where $V(x,t)$ is periodic in time with a period T rational to the Bloch period T_B:

$$V(x,t+T) = V(x,t) , \quad T = \frac{r}{q}T_B . \qquad (13)$$

(This complication actually facilitates the understanding.) It is obvious that the case $V(x,t) = V(x)$ is included here and corresponds to an arbitrary choice of the integers r and q. For the sake of simplicity we shall assume $r = 1$.

We look for the solution of the Schrödinger equation $i\hbar\partial\psi(x,t)/\partial t = \widehat{H}\psi(x,t)$ in the form

$$\psi(x,t) = \exp(-iFtx/\hbar)\widetilde{\psi}(x,t) . \qquad (14)$$

The substitution (14) eliminates the Stark term Fx and leads to the Schrödinger equation with the Hamiltonian $\widetilde{H}(t)$, which is just the original Hamiltonian $\widehat{H}_0$ with the momenta shifted by Ft:

$$i\hbar\frac{\partial\widetilde{\psi}(x,t)}{\partial t} = \widetilde{H}(t)\widetilde{\psi}(x,t) , \quad \widetilde{H}(t) = \frac{(\widehat{p}-Ft)^2}{2} + V(x,t) . \qquad (15)$$

We note, that because the Bloch period is assumed to be a multiple of the time period of the potential $V(x,t)$, the Hamiltonian (15) possesses a "symmetry"

$$\widetilde{H}(t+T_B) = e^{+ix}\widetilde{H}(t)e^{-ix} . \qquad (16)$$

Now we introduce the unitary operator $\widetilde{U}(t,0)$ of the evolution of the system (15) over the time interval $(0,t)$

$$\widetilde{U}(t,0) = \widehat{\exp}\left(-\frac{i}{\hbar}\int_0^t \widetilde{H}(t)\mathrm{d}t\right) \qquad (17)$$

(the hat over the exponential function denotes time ordering). Let us prove the following intermediate relation, which is just a consequence of the symmetry (16),

$$\widetilde{U}(t+T_B,T_B) = e^{+ix}\widetilde{U}(t,0)e^{-ix} . \qquad (18)$$

In fact, Eq. (18) holds for $t = 0$, when both sides of the equation are the identity operators. To show that it also holds for other times one should compare the derivatives with respect to t from both sides of the equation. Using the operator Schrödinger equation $i\hbar\partial\widetilde{U}(t,0)/\partial t = \widetilde{H}(t)\widetilde{U}(t,0)$ and the property (16) it is easy to check that the derivatives do coincide, which proves Eq. (18) for arbitrary t.

Equation (18) leads to the following useful relation

$$\widetilde{U}(nT_B,0) = e^{+inx}\left[e^{-ix}\widetilde{U}(T_B,0)\right]^n , \qquad (19)$$

which can be proved also by induction. On the basis of this equation and using Eq. (14) we conclude that the evolution of the original wave function $\psi(x,t)$ can be described in terms of Floquet-like theory

$$\psi(x,nT_B) = \widehat{U}^n\psi(x,0) , \qquad (20)$$

where the operator $\widehat{U}$ is the product of the momentum shift operator $\exp(-ix)$ and the unitary operator $\widetilde{U}(T_B, 0)$

$$\widehat{U} = e^{-ix}\widehat{\exp}\left(-\frac{i}{\hbar}\int_0^{T_B} \widetilde{H}(t')\mathrm{d}t'\right) . \tag{21}$$

We also display another representation of the operator $\widehat{U}$

$$\widehat{U} = \widehat{U}_T^q; \quad \widehat{U}_T = e^{-ix/q}\widehat{\exp}\left(-\frac{i}{\hbar}\int_0^{T} \widetilde{H}(t')\mathrm{d}t'\right) , \tag{22}$$

which can be deduced from the Hamiltonian symmetry

$$\widetilde{H}(t+T) = \exp(ix/q)\widetilde{H}(t)\exp(-ix/q) \tag{23}$$

[compare with Eq. (16)] in the way described above.

The key point of the analysis is that for a spatially periodic potential $V(x+2\pi, t) = V(x,t)$ the operator $\widehat{U}$ commutes with the translation operator over the lattice period, $\widehat{a} = \exp(2\pi\partial/\partial x)$, and, therefore, the formalism of the quasimomentum can be employed. Then, after introducing the periodic function $\chi_{l,k}(x)$,

$$\psi_{l,k}(x) = \exp(ikx)\chi_{l,k}(x) , \quad \chi_{l,k}(x+2\pi) = \chi_{l,k}(x) , \tag{24}$$

the eigenvalue problem (11) takes the form

$$\widehat{U}^{(k)}\chi_{l,k}(x) = \exp\left[-\frac{i}{\hbar}E_l(k)T_B\right]\chi_{l,k}(x) , \tag{25}$$

$$\widehat{U}^{(k)} = e^{-ix}\widetilde{U}^{(k)} , \tag{26}$$
$$\widetilde{U}^{(k)} = \widehat{\exp}\left\{-\frac{i}{\hbar}\int_0^{T_B}\left[\frac{(\widehat{p}+\hbar k - Ft)^2}{2} + V(x,t)\right]\mathrm{d}t\right\} .$$

Equations (25) and (26) are mathematically well defined and, therefore, the Wannier states do exist. In Subsection F we use these equations to calculate the metastable Wannier-Bloch states numerically.

2.4 Spectrum of the Wannier-Bloch states and Wannier-Stark states

So far we made no difference between the case of a time-periodic potential $V(x, t+T) = V(x,t)$ and a time-independent potential $V(x)$. This difference appears when we discuss the (quasi-)energy spectrum $E_l(k)$. It is possible to show that in the case of time-periodic potentials (we recall that $T = T_B/q$) the operators $\widehat{U}^{(k)}$ and $\widehat{U}^{(k+1/q)}$ are unitary equivalent and, therefore, the spectrum is q-fold degenerate [12]. The q-fold degeneracy can also be proved by using Eq. (22). In fact, the function $\psi'(x) = \widehat{U}_T\psi_{l,k}(x)$ has the Bloch index $k' = k + 1/q$ but corresponds to the same value of the quasienergy: $\widehat{U}\psi'(x) = \widehat{U}_T^q\widehat{U}_T\psi_{l,k}(x) = \exp[-iE_l(k)T_B/\hbar]\,\psi'(x)$. In the case of a time independent potential the integer q can be chosen arbitrarily and, therefore, the spectrum is completely degenerate, i.e. $E_l(k) = E_l$. This also implies the continuous time evolution of the Wannier-Bloch functions in the form

$$\psi_{l,k}(x,t) = e^{-iE_lt/\hbar}\psi_{l,k-Ft/\hbar}(x) . \tag{27}$$

We note that Eq. (27) has the typical structure of a quasienergy function. This justifies the use of the term "quasienergy" for E_l also in the case of time-independent potentials, where the Bloch period T_B should be considered as some intrinsic time-period of the system.

Degeneracy of the spectrum in the case of a time independent potential allows one to introduce instead of the continuous set of functions $\psi_{l,k}(x)$ a discrete set of eigenfunctions

$$\Psi_{l,m}(x) = \int_{-1/2}^{1/2} \mathrm{d}k \exp(i2\pi mk)\psi_{l,k}(x) \ . \qquad (28)$$

[compare with Eq. (6)]. By construction the functions (28) are stationary functions, i.e., their continuous time evolution has the form $\Psi_{l,m}(x,t) = \exp[-i(E_l + 2\pi mF)t/\hbar]$ $\Psi_{l,m}(x)$. Referring to the Hamiltonian (1) these states are associated with a set of discrete levels $E_m^{(l)} = E_l + 2\pi Fm$ and form the famous Wannier-Stark ladder (note that using the definition $T_B = \hbar/F$ the Wannier-Stark ladder coincides with the Floquet quasienergy ladder $E_m^{(l)} = E_l + \hbar 2\pi/T_B$). In the further proceeding we will consider only the case of time independent potentials.

2.5 Numerical solution using Floquet theory

Since we have an explicit expression (26) for the unitary operator $\widehat{U}^{(k)}$ defining the Wannier-Bloch states, we can try to find them numerically. However, seeking for the numerical solution of the eigenvalue problem (25) meets problems related to the truncation procedure.

First we discuss the case $F = 0$. Figure 1(b) shows the band structure of the system (2) obtained by diagonalizing the unitary operators $\widehat{U}^{(k)} = \exp(-i\widehat{H}_0^{(k)}T_B/\hbar)$, where we set $T_B = 2.5$. Because the matrix $U^{(k)}(n',n)$ tends asymptotically ($|n'|,|n| \to \infty$) to a diagonal one, the truncation of it causes no problem. It is also possible to truncate first the Hamiltonian and then calculate the evolution operator by taking the operator exponent, what was actually done in our calculations. (In the case of the Hamiltonian $\widetilde{H}^{(k)}(t)$ operator $\widetilde{U}^{(k)}$ is calculated using the formula

$$\widetilde{U}^{(k)} = \prod_{j=0}^{M-1} \exp\left[-\frac{i}{\hbar}\widetilde{H}^{(k)}(j\Delta t)\Delta t\right] \ , \qquad (29)$$

where $\Delta t = T_B/M$, $M \gg 1$.) This procedure has the advantage that the obtained matrix is strictly unitary. The first seven bands are shown in Fig. 1(b), which can be easily identified with the corresponding bands in Fig. 1(a). Calculation of higher bands brings additional dispersion curves without disturbing the curves already found. Unfortunately this is not the case for the operator (26).

In fact, we should truncate both the matrix $\widetilde{U}^{(k)}(n',n)$ and the matrix

$$S(n',n) = \langle n'|\exp(ix)|n\rangle = \delta_{n',n+1} \ . \qquad (30)$$

By the reason indicated above the truncation ($|n'|,|n| \le N$) of the matrix $\widetilde{U}^{(k)}(n',n)$ is a harmless procedure, but the truncation of the matrix (30) explicitly violates the unitarity of the operator. One can recover the unitarity of $S(n',n)$ by putting a unit in the lower corner of the matrix. However, this would mean that we impose a periodic boundary condition on the momentum and the problem becomes only loosely related to the initial eigenvalue problem. As an example Fig. 4 shows the spectrum of the truncated and "unitarized" operator (26) for two different dimensions $2N+1$ of the matrices ($N = 10$ and $N = 20$). It is seen that the details of the spectrum depend on N. The quasicrossing of the bands is also an artifact of the truncation.

One should not be disappointed by the failure to find the (quasi-)energies of the Wannier-Bloch states. In fact, for the classical counterpart of the system (1) bounded

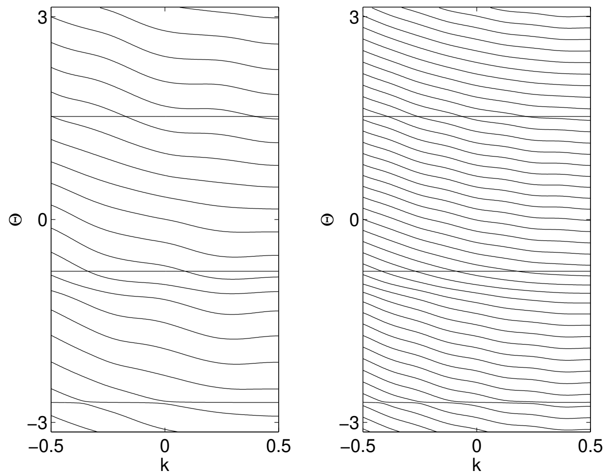

Fig. 4. "Energy spectrum" of the Wannier-Bloch states for two dimensions of the truncated and "unitarized" matrix $\widehat{U}^{(k)}$. The locations of the resonance energies appear as (almost) horizontal lines.

motion coexists with unbounded motion. For such a system the notion of metastable states or resonances proves to be more appropriate than the notion of the energy states. We discuss the metastable states of the system (1) in the next subsection. It is, however, worthwhile to point out that the location of the resonances manifest themselves in the "energy spectrum" of the Wannier-Bloch states in Fig. 4 by the (almost) horizontal lines at the phases $\Theta = ET_B/\hbar \approx -0.765, +1.53$ and -2.70, which get more pronounced with increasing N. This behavior closely resembles the one observed when resonances are computed by the method of box-quantization (see, e.g. [13]).

2.6 Metastable states

Two definitions of a metastable state or resonance are mainly in use: a "rigorous" one which defines the resonances as the poles of the scattering matrix; and an "intuitive" one which assumes the metastable state to be a "stationary" solution of the Schrödinger equation with constant rate of probability leaking. The simplest example of a metastable state is the quasibound state of a quantum particle in a potential like $V(x) = x^2 \exp(-x)$, $x \geq 0$ [14]. Being considered in the finite interval $0 \leq x < x_{max}$ (x_{max} essentially exceeds the width of the potential well), this system has a solution of the form

$$\psi_l(x,t) = \exp(-\Gamma_l t/2\hbar)\exp(-iE_l t/\hbar)\psi_l(x) \,, \qquad (31)$$

where E_l approximately coincides with the spectrum of a particle in the well for a non-penetrable potential barrier, and $\Gamma_l/2$ is related to the probability of tunneling through the barrier. We would like to stress that the "intuitive" definition of metastable states implicitly assumes a truncation of the coordinate.

In this paper we use the "intuitive" definition. To find the metastable Wannier-Bloch states one should follow the prescription outlined above with the only difference that the truncation of the coordinate is substituted by a truncation of the momentum. In other words we define the metastable Wannier-Bloch state as a state satisfying the equation

$$\widehat{W}^{(k)}\chi_{l,k}(x) = \exp[-\Gamma_l(k)T_B/2\hbar] \exp[-iE_l(k)T_B/\hbar]\chi_{l,k}(x) \,, \qquad (32)$$

where $\widehat{W}^{(k)}$ is the operator (21) truncated in momentum space. In a numerical calculation we find these states by diagonalizing the nonunitary matrices $W^{(k)}(n', n)$. The key point is that the spectrum of the metastable states, unlike the Wannier energy spectrum (but similar to the Bloch energy spectrum) discussed in the preceding subsection, is *insensitive* to the dimension of the matrix $W^{(k)}(n', n)$.

As an example, we calculate the complex energy spectrum $\mathcal{E} = E - \mathrm{i}\Gamma/2$ of the metastable states for $F = 0.2$ and $\hbar = 0.5$. The Bloch period is $T_B = 2.5$, the dimension of the matrix is taken to be $2N + 1 = 41$. Within numerical accuracy the "bands" are degenerate. The locations of the first three most stable bands are $E_0 = -0.153$, $E_1 = 0.305$, $E_2 = 0.716$ or — written in terms of phases $\Theta = ET_B/\hbar \bmod 2\pi$ — -0.765, $+1.53$, -2.70 in agreement with the position of the horizontal lines in Fig 4. In comparison with the field-free case $F = 0$, the most important modification is a shift in energy because of a change in the potential minima, corresponding to a shift of 3.04 in the phase Θ for $F = 0.2$ [see the dotted lines in Fig. 1(b)]. The obtained values of the imaginary parts, i. e. of the decay coefficients, are $\Gamma_0/2 = 3.24 \cdot 10^{-9}$, $\Gamma_1/2 = 2.36 \cdot 10^{-6}$, and $\Gamma_2/2 = 6.05 \cdot 10^{-4}$. The next state has the value $\Gamma_3/2 = 2.47 \cdot 10^{-2}$ and should be considered as very unstable.

We also calculated the eigenfunctions $\chi_{l,k}(x)$ of the operator $\widehat{W}^{(k)}$. Figure 5 shows $\chi_{l,k}(x)$ for $l = 0, 2$ and $k = 0$ in the momentum representation and Fig. 6 shows the ground state ($l = 0$) as a function of k. The absolute squares of the expansion coefficients $c_n^{(l,k)}$ [see Eq. (5)] are plotted on a logarithmic scale and connected by lines. As expected, the metastable states are extended in the negative n-direction. If we ignore this negative tail, the depicted functions well coincide with the corresponding Bloch functions (dashed lines).

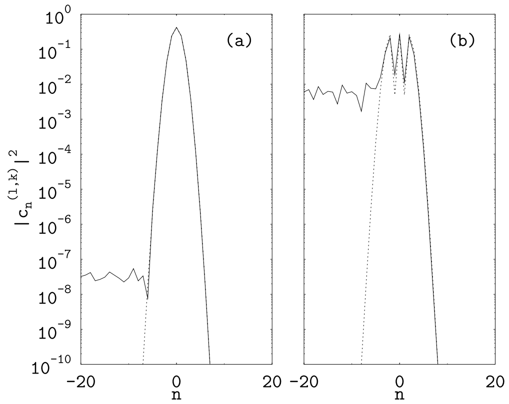

Fig. 5. Expansion coefficients for the periodic part of the metastable Wannier-Bloch (solid line) and Bloch (dashed line) functions for $l = 0$ (a) and $l = 2$ (b), quasimomentum $k = 0$.

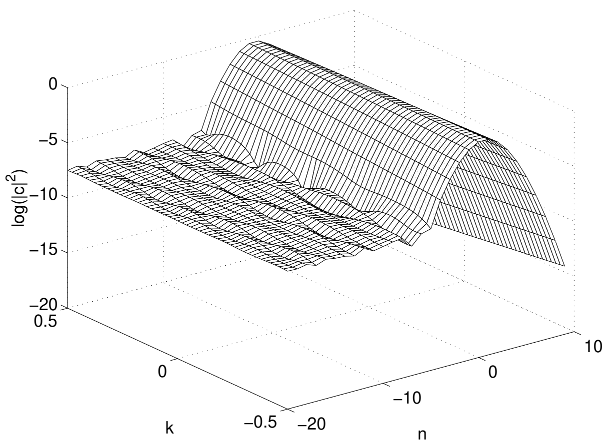

Fig. 6. Expansion coefficients for the ground metastable Wannier-Bloch state ($l = 0$) as a function of k.

We proceed with the Wannier-Stark states. Similar to the case of energy states we can construct a set of localized metastable states by using Eq. (28). Figure 3 shows the ground ($l = 0$) and second excited ($l = 2$) localized states $\Psi_{l,m}(p)$ with index $m = 0$ in the momentum representation. It is seen that for $F \neq 0$ there is a finite probability to find a particle with an arbitrary negative momentum. The increasing frequency of oscillation of the tail indicates just the fact, that a particle can be found arbitrarily far from the origin $x = 0$. The family of states $\Psi_{l,m}(p)$ with the same l forms the Wannier-Stark ladder associated with the l-th band. By Fourier transforming $\Psi_{l,m}(p)$ we obtain the metastable Wannier-Stark states in configuration space (see Fig. 2, solid line). It is worthwhile to note that neither the Wannier-Stark nor the Wannier-Bloch states are normalizable states. Thus the labeling of the vertical axis has only a relative meaning.

2.7 Wannier-Stark Resonances using Complex Scaling

Since the Floquet method of calculating the Wannier-Stark resonances is based on an intuitive (not rigorous) definition of the metastable states, one can doubt if the complex energies found are "true" resonances. To be sure about the results we compare the Floquet data with data obtained by an independent method using complex scaling, which has been proven to be very successful in solving many problems of resonance scattering [15].

Complex Scaling relies on the Balslev-Combes theorem [16], which associates the resonances $\mathcal{E} = E - \mathrm{i}\Gamma/2$ with the square-integrable eigenfunctions of the complex scaled Hamiltonian, $H(x\exp(i\theta))$, provided that $\theta > -E/\Gamma$. It was shown that the theorem also holds in cases where the asymptotic solutions of the Schrödinger equation are not free waves, which is the case for the Stark field [17] (see also the discussion in the review article [4] as well as the analysis of the time-depended case [18]).

The Hamiltonian matrix elements, $\langle\nu|H(x\exp(i\theta)|\nu'\rangle$, $\nu,\nu' = 1, 2, \ldots, N$, are calculated using particle-in-a-box basis functions $|\nu\rangle = L^{-1/2}\sin(\nu\pi x/L)$, where the middle of the box is on one of the local minima of $V(x) + Fx$. $N = 500$ basis functions are used and the box-size L was taken as 10 periods of the potential $V(x)$. In the numerical calculations for the potential $V(x) = \cos x$ (parameters $F = 0.2$, $\hbar = 0.5$) a smooth exterior complex scaling transformation is used, which rotates x to the complex plane by $\theta = 0.3\,\mathrm{rad}$. The resonances are stable with respect to a small variation of the scaling angle θ. The results of the matrix diagonalization of $\langle\nu|H(x\exp(i\theta)|\nu'\rangle$ are presented in Figure 7 by circles.

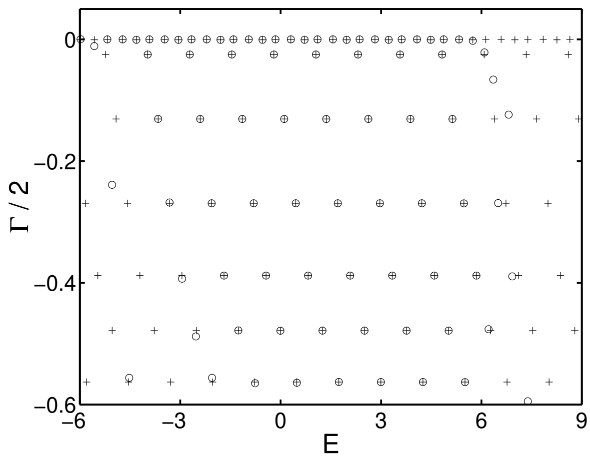

Fig. 7. Complex resonance eigenvalues obtained from the complex scaled Hamiltonian (o) compared with the Wannier-Stark ladder obtained from the present method (+) as described in Section F.

First, we note that due to the finite box size only a segment $\Delta E \approx FL = 4\pi \approx 12.6$ of the Wannier-Stark ladder is spanned by the numerical complex scaling results. As it is seen in Fig. 7, the resonances are arranged along 10 strings, whose real parts are separated approximately by the Wannier-Stark ladder spacing $2\pi F \approx 1.26$. The finite box size and the finite basis set causes numerical differences between the resonances of the different strings. Also shown in Figure 7 are the resonances computed by the novel method proposed in the present paper. The Wannier-Stark ladders $\mathcal{E} + n2\pi F$, $n = 0, \pm 1, \pm 2, \ldots$ of these resonances are in good agreement with the complex scaling results. As expected, the agreement is best for the central strings. The numerical values for the three most stable resonances are $\mathcal{E}_0 = -0.15286770 - i\,3.2363851 \cdot 10^{-09}$, $\mathcal{E}_1 = 0.30482723 - i\,2.3630620 \cdot 10^{-06}$ and $\mathcal{E}_2 = 0.71553772 - i \cdot 6.0492101 \cdot 10^{-04}$ (present method), which are in almost perfect agreement with the complex scaling results $\mathcal{E}_0 = -0.15286771 - i\,3.2363488 \cdot 10^{-09}$, $\mathcal{E}_1 = 0.30482722 - i\,2.3630619 \cdot 10^{-06}$ and $\mathcal{E}_2 = 0.71553771 - i\,6.0492101 \cdot 10^{-04}$ (central string, where the best results are expected). Thus both methods can be considered as reliable. The advantage of the Floquet method is, however, that it essentially reduces the numerical effort.

3 Conclusion

We calculated the positions and widths of the resonances (or metastable states) for a quantum particle in the potential $V(x) = \cos x + Fx$. A generic relation of the metastable states to the particle Bloch states in cosine potential ($F = 0$) was demonstrated. It should be noted, however, that in spite of this generic relation the metastable Wannier states can not be obtained from the Bloch states by any iterative procedure. This fact was proved before by using rather sophisticated arguments. In our approach it just follows from the different structure of the evolution operator for the Wannier and Bloch problems.

We believe that it is useful to compare our approach to find the resonances with the most commonly used approach based on the crystal momentum or Adams representation. In this approach one looks for the solution of the problem in terms of Bloch states, i.e.,

$$\Phi(x) = \sum_l \int_{-1/2}^{1/2} a_l(k)\phi_{l,k}(x)\mathrm{d}k \; . \qquad (33)$$

Since the Hamiltonian (2) is diagonal in the basis of Bloch states, the eigenvalue problem for the Hamiltonian (1) takes the form

$$iF\frac{\partial a_l(k)}{\partial k} + \epsilon_l(k)a_l(k) + F\sum_{l'\neq l} X_{l,l'}(k)a_{l'}(k) = \varepsilon a_l(k) \; , \qquad (34)$$

where a periodic boundary condition on k should be imposed. If we neglect the coupling between the bands (by $X_{l,l'}(k) = 0$), the solution (33) will have the form of the functions (6), which now correspond to the discrete set of levels

$$\varepsilon_{l,m} = 2\pi Fm + \langle\epsilon_l\rangle \; , \quad \langle\epsilon_l\rangle = \int_{-1/2}^{1/2} \epsilon_l(k)\mathrm{d}k \; . \qquad (35)$$

The issue of the approach is that due to the coupling between the bands ($X_{l,l'}(k) \neq 0$) the levels (35) gain a finite width and an effort of the research aims at the calculation of this width (or decay coefficient) as a function of F. This task is rather difficult from both analytical and numerical point of views. Actually the method can provide a solution only for special forms of the periodic potential corresponding to finite number of Bloch bands [5].

In our approach we first find the metastable Wannier-Bloch states and then construct the localized states. If one is only interested in the widths of levels, the latter is unnecessary because the levels widths, as well as their positions, are already defined by diagonalizing the matrix $W^{(k)}(n', n)$ for a *single* arbitrary value of k.

We also would like to stress that we find the resonances for "an infinite crystal". This differs from the larger part of the other numerical studies, where one seeks for the solution of the Schrödinger equation with the Hamiltonian (1) in a finite interval (see [19], for example).

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