Computational Materials Science 137 (2017) 1–5

Contents lists available at ScienceDirect

Computational Materials Science

journal homepage: www.elsevier.com/locate/commatsci

Bloch oscillations in two-dimensional crystals: Inverse problem

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ARTICLE INFO

Article history:
Received 20 February 2017
Received in revised form 25 April 2017
Accepted 26 April 2017

Keywords:
Bloch oscillations
Artificial neural networks
Square lattice

ABSTRACT

Within an artificial neural network (ANN) approach, we classify *simulated signals* corresponding to the semi-classical description of Bloch oscillations on a two-dimensional square lattice. After the ANN is properly trained, we consider the inverse problem of Bloch oscillations (BO) in which a new signal is classified according to the lattice spacing and external electric field strength oriented along a particular direction of the lattice with an accuracy of 96%. This approach can be improved depending on the time spent in training the network and the computational power available. This work is one of the first efforts for analyzing the BO with ANN in two-dimensional crystals.

1. Introduction

Flat two-dimensional crystals are unstable against thermal fluctuations according to the Mermin-Wigner theorem [1]. Therefore, the early study of these crystals was considered just for academic convenience. More recently, it has been known, nevertheless, that some interesting phenomena occur effectively in two-dimensions, like quantum Hall effect [2,3] and high-T_c superconductivity in cuprates [4]. Soon after the first isolation of graphene flakes [5,6], a new era of materials science emerged [7] with a huge variety of two-dimensional (2D) systems discovered in the recent past [8]. The 2D materials are nowadays a cornerstone of solid state physics and materials science because of their potential technological applicability and their impact in fundamental research. Many of these 2D crystals have the crystal structure of the square lattice, which due to its high symmetry, allows the study of a number of interesting phenomena, like Bloch oscillations (BO) [9]. It is well known that BO are not observed directly on crystals because of intraband tunneling and ultrafast electron scattering; BO are directly observed in high purity superlattices under different experimental setups [10–19]. The equations of motion of BO are also relevant for a number of optical systems [20,21]. For that purpose, in a previous work [22], some of us posed the inverse problem of BO for the linear chain within an artificial neural network (ANN) approach [23,24]. The idea is to use simulated signals for BO in a semiclassical approximation to train the ANN and then classify a new signal according to the lattice spacing and electric field strength with high accuracy. In this paper we extend these ideas to the 2D square lattice.

We develop a framework in which the ANN is trained using the simulated signals corresponding to the semiclassical description of BO for a 2D square lattice considering only the nearest neighbor influence. We then predict the strength of electric field along a particular direction of the lattice and the lattice spacing that produce such trajectories. We achieve up to 96% of accuracy in our classification scheme, which can be improved depending on the computational time and computer power available.

For the presentation of ideas, we have organized the remaining of this paper as follows: In Section 2 we give a description of the BO phenomenology in the semiclassical approach. In Section 3, we describe how the signals were generated and the ANN configuration. In Section 4 the results for all the analyzed cases are discussed and finally, in Section 5, the conclusions are presented.

2. Bloch oscillation: semiclassical approach

We start our discussion from the tight-binding Hamiltonian of a monoatomic 2D square lattice of spacing a. Considering the nearest neighbors approximation, we have

$$\begin{aligned} H\psi_{n,m}(\mathbf{k}) &= -t\psi_{n+1,m}(\mathbf{k}) - t\psi_{n-1,m}(\mathbf{k}) \\ &\quad - t\psi_{n,m+1}(\mathbf{k}) - t\psi_{n,m-1}(\mathbf{k}) + \epsilon_0\psi_{n,m}(\mathbf{k}) \\ &\equiv \mathcal{E}^{(n,m)}(\mathbf{k})\psi_{n,m}(\mathbf{k}), \end{aligned} \tag{1}$$

where t is the hopping parameter and $\mathbf{k} = k_1\hat{e}_x + k_2\hat{e}_y$ is the crystal-momentum of electrons in 2D. From Bloch theorem, it is straightforward to find that the energy-momentum dispersion relation is:

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http://dx.doi.org/10.1016/j.commatsci.2017.04.030
0927-0256/

$$\mathcal{E}^{(n,m)}(k_1,k_2)=\epsilon_0-\epsilon^{(n,m)}(k_1,k_2), \tag{2}$$

where

$$\epsilon^{(n,m)}(k_1,k_2)=w(1-\cos(k_1a)-\cos(k_2a)), \tag{3}$$

ϵ_0 is the on-site energy and $w=2t$. Next, we recall the semiclassical equations of motion for an electron moving in an external electric field $\mathbf{E}$ oriented parallel to one direction of the square lattice,

$$\frac{d\mathbf{k}}{dt}=-e\mathbf{E}, \tag{4}$$

$$\frac{d\mathbf{r}}{dt}=\frac{1}{\hbar}\frac{\partial}{\partial\mathbf{k}}\epsilon^{(n,m)}(k_1,k_2). \tag{5}$$

We can straightforwardly integrate the equations of motion and obtain the velocities and trajectories for a given external field strength. Considering the lattice oriented along the $x-y$ plane and a uniform electric field $\mathbf{E}=E_1\hat{e}_x+E_2\hat{e}_y$, we integrate Eq. (4) assuming the initial condition $k_j(0)=0$ with $j=1,2$. Thus

$$k_j(t)=-\frac{eE_j}{\hbar}t. \tag{6}$$

Rewriting Eq. (5), the electron velocity is given by:

$$\begin{aligned} v_j^{(n,m)}(k_j(t)) &= \frac{wa}{\hbar}\sin(k_j(t)a),\\ &= -\frac{wa}{\hbar}\sin\left(\frac{eE_ja}{\hbar}t\right), \end{aligned} \tag{7}$$

and the electric current is simply $j_i=-ev_i$. Integrating Eqs. (7) we get the profile of BO obtaining the position of the electrons as function of time:

$$\begin{aligned} x_j^{(n,m)}(t) &= \frac{w}{eE_j}\cos\left(\frac{eE_j}{\hbar}at\right),\\ &= \frac{w}{eE_j}\cos(\omega_{E_j}t), \end{aligned} \tag{8}$$

with $\omega_{E_j}=eE_ja/\hbar$. Eqs. (8) describe the trajectories which are in fairly good agreement with the experimental observations of BO. In the next Section we describe how the oscillations described by Eq. (7) are simulated and how ANN processes them in order to give an accurate result.

3. Signals creation and feature processing

For fixed lattice parameters a and t, the trajectories described by Eqs. (7) and (8) are functions of the electric field strength along each spatial direction, which becomes the only free parameter that characterizes a given trajectory in our considerations. We have trained an ANN that associates the electric currents of the electrons with their corresponding electric fields. In other words, the ANN learns through some examples the relationship between the electric current signals in the 2D square lattice and the electric fields that generate those currents. First, let us describe how the training signals were generated then we explain the classification process.

For simplicity and without loss of generality, all signals were created following the next considerations:

- The parameters of Eqs. (7) and (8) were fixed to dimensionless units $e=\hbar=1, w_2=w_2=a=0.5$.
- The signals were generated for a time lapse $\tau=200$.
- We integrate the signals considering the possibility of negative and positive electric fields for both E_1 and E_2 on three different ranges defined by $E_{\min}$ and $E_{\max}$. These cases will be describe more thoroughly later on Section 3.1.

Once the signals were produced, we selected as inputs of the ANN values for each component of the velocity (v_1 and v_2) at one hundred different times defined by $t_i=i\Delta t$, with $\Delta t=\tau/100=2$ and $i=0,1,\ldots,99$. This means that the ANN will analyze a signal V consisting of two hundred values:

$$V=\{v_1(t_1),v_2(t_1),\ldots,v_1(t_n),v_2(t_n)\}. \tag{9}$$

In Fig. 1 we show an example of BO velocities and the corresponding values where the trajectories were evaluated with $E_1=-0.22$ and $E_2=0.14$ generated using Eq. (7).

As the goal is to classify the electric field in 2D, we impose that the feedforward ANN has two outputs $\widetilde{E}_1$ and $\widetilde{E}_2$. Notice the difference between $\tilde{E}_i$ as the predicted value and E_i the physical value. Considering a single hidden layer with 27 neurons, the equation that defines the predicted value given an input signal V is defined by:

$$\widetilde{E}_j=F\left(\sum_{h=1}^{27}\tilde{\sigma}_{hj}F\left(\sum_{i=1}^{200}\sigma_{ih}V_i\right)\right), \tag{10}$$

where $j=1,2$. F is the activation function for the hidden and output layers, in this case the standard sigmoid logistic function were used; σ_{ih} and $\tilde{\sigma}_{hj}$ are the weights between the input and hidden layer and hidden to output layer respectively. The ANN structure is illustrated in the Fig. 2.

3.1. Electric field scenarios

The accuracy of the ANN depends on the frequency of the signals, the electric fields and sampling points. In this Section, we analyze how the performance of the ANN behaves in three different scenarios. Using 625 signals with all the parameters kept fixed except for the electric field that ranges in the scenarios:

(i) Between $[E_{\min}=-0.5, E_{\max}=0.46]$ separated in steps of $\Delta E=0.04$.
(ii) Between $[E_{\min}=-1, E_{\max}=0.92]$ with $\Delta E_j=0.08$.
(iii) Between $[E_{\min}=-0.25, E_{\max}=0.23]$ with $\Delta E_j=0.02$.

Considering that the activation function F used in Eq. (10) is a sigmoid function, the output of the network will be within the range $[0,1]$. The ANN's outputs could be divided in classes that represent the target intervals for E_1 and E_2. This means that the more classes an output has, the more precision is required for a correct classification. For this case, we have decided to divide each output in 5 classes. For clarity, let us develop the case ((i)) where $\Delta E_j=1/25$ and $E_{\min}=-0.5$ and $E_{\max}=0.46$. Therefore for each E_j, every class covers up the range:

$$E_{\min}+5\zeta\Delta E\leqslant E_\zeta<E_{\min}+5(\zeta+1)\Delta E, 0\leqslant\zeta\leqslant 4, \tag{11}$$

where E_ζ index each class for any of signal E_j sections. An schematic representation classes division is presented in Fig. 3. However, because the ANN's output is defined between (0,1), we need to map the electric field class classification into this range. For that, we define the center each one of the five classes $\widehat{E}_\zeta$ in the output neuron as:

$$E_\zeta\equiv\widehat{E}_\zeta=0.1+0.2\zeta. \tag{12}$$

Besides, the center of each class will be used as the target value ($\widehat{E}_\zeta$) in the training phase. For example, if the signal is created with any of the first five values for E_1 ($\zeta=0$) and the last five values of E_2 ($\zeta=4$), then the ANN has correctly classified this signal if:

$$\widehat{E}_0-0.1\leqslant\widetilde{E}_1<\widehat{E}_0+0.1, \tag{13}$$

$$\widehat{E}_4-0.1\leqslant\widetilde{E}_2<\widehat{E}_4+0.1. \tag{14}$$

In the following section we discuss the training procedure used to minimize the error of the predictions.