

DNA-based tunable THz oscillator

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Abstract

The intrinsic double helix conformation of the DNA strands is known to be the key ingredient of control of the electric current through the DNA by the perpendicular (gate) electric field. We show theoretically that Bloch oscillations in the DNA are also strongly affected by such lateral field; the oscillation frequency splits into a manifold of several generally non-commensurate frequencies leading to a complicated pattern of the charge motion. The frequency of the oscillations falls in the THz domain, providing for a possibility to design a nano-scale source of THz radiation.

Key words: Nano-electronic devices, field effect devices, DNA

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1 Introduction

The helical symmetry of the DNA is almost always neglected when modeling the charge transport through the DNA-based devices: a DNA is usually considered as a flat ladder-like sequence (periodic or stochastic) of base pairs [1,2,3,4,5]. Very recently the intrinsic helix conformation of the DNA strands was put forward as the key ingredient allowing for control of the electric current through the molecule by the electric field perpendicular to the DNA axis [6]. In the presence of such a field the helical conformation leads to an additional periodic modulation of the base pair energies, which affects strongly the charge transport through the DNA. On this basis, prototypes of the single-DNA-based field effect transistor and the Esaki diode analogue have been proposed [6].

In this contribution, we aim to further exploit the symmetry of the DNA molecules and demonstrate, by means of numerical simulations, that (i) - a single dry periodic DNA molecule (such as the ploy(G)-poly(C)) subjected to a collinear uniform electric field can exhibit Bloch oscillations [8] and (ii) - because of the helical conformation, the oscillations become more complex in the presence of the perpendicular (gating) electric field. The frequency of these oscillations falls in the THz domain, the region which is in the focus of an intense research nowadays (see Ref. [7] for a recent overview). The above-mentioned property provides therefore for a possibility to design a DNA-based tunable THz oscillator.

2 Model

Bloch [9] and Zener [10] argued on the theoretical grounds that an electron, moving in an ideal periodic potential and subjected to a uniform electric field F , is confined within a finite region because of the Bragg reflection. Due to the confinement, it undergoes a periodic motion which is characterized by the angular frequency $\omega_B = eFa/\hbar$ and a spatial extension $L_B = W/(eF)$, where $-e$ is the electron charge, F is the applied electric field, a is the lattice constant, and W stands for the band width (see also Ref. [11]).

For simplicity, we consider here a single-stranded uniform poly(G) helix for which we assume the conformation parameters of the double-stranded DNA (dsDNA) in its B form, in particular, the full-twist period of 10 base molecules. For a periodic dsDNA, such as the poly(G)-poly(C), the picture of Bloch oscillations is more complicated as compared to the considered case, however, the physics is very similar. We use the *minimum* tight-binding model, extending it to include a uniform electric field \mathbf{E} that is tilted by the angle θ with respect to the axis of the helix. The field has therefore both the collinear component, $F = E \cos \theta$, and the lateral (gating) one, $E \sin \theta$. The Hamiltonian of our model in site representation reads:

$$H = \sum_{n=1}^N \left| \varepsilon_n |n\rangle \langle n| + J \sum_{n=1}^{N-1} |n+1\rangle \langle n| + h.c. \right. \quad (1)$$

Here, $|n\rangle$ is the state vector of the n -th base molecule and the corresponding energy ε_n is given by

$$\varepsilon_n = \varepsilon_n^{(0)} - U_{\parallel} n - U_{\perp} \cos \left(\frac{2\pi n}{10} + \varphi_0 \right) \quad (2)$$

where $\varepsilon_n^{(0)}$ is the site energy of the n -th base molecule at zero field. We assume all molecules to be the same, so we set the unperturbed energies $\varepsilon_n^{(0)}$ to zero from now on. The term $U_{\parallel} n$ describes the linear potential along the helix axes; the potential drop across a base molecule in the stacking direction is $U_{\parallel} = eaE \cos \theta$, where a is the nearest-neighbor distance along the helix axis, $U_{\perp} = eEr \sin \theta$ is the potential drop across the helix in the perpendicular direction, $r \approx 1$ nm being the helix radius. The phase φ_0 which determines the azimuth of the strand with respect to the field, is set to zero. The term J in Eq. (1) describes the transfer interaction between the nearest-neighbor bases; it is chosen to be positive which implies that the considered charge is a hole [12].

The parallel component of the electric field, $E \cos \theta$, yields the potential ramp along the stacking direction, which sets the frequency of the Bloch oscillations, as in the traditional case. However, Eq. (2) shows that the helix in the lateral field acquires the additional periodic modulation of the potential. This modulation leads to the modification of the electronic structure of the system: the bare energy band splits into several different minibands, which is crucial for the charge transport properties [6]. Each such miniband has its own Bloch frequency, resulting in a more complex overall picture of Bloch oscillations as we show below. The amplitude of the periodic

modulation is controlled by the magnitude of the perpendicular component of the electric field, $E \sin \theta$, providing for a mechanism to alter the fundamental properties of the system.

We further solve the time-dependent Schrödinger equation (the Planck constant $\hbar = 1$)

$$i\dot{\psi}_n = \varepsilon_n \psi_n + J(\psi_{n+1} + \psi_{n-1}) \quad (3)$$

for an electron wave packet ψ_n being initially a narrow Gaussian centered at an arbitrary lattice site n_0 :

$$\psi_n(0) = A \exp \left[-\frac{(n - n_0)^2}{2} \right], \quad (4)$$

where A is the normalization constant. The solution of Eq. (3) can be expressed in terms of the eigenvalues λ_ν and eigenfunctions $\varphi_{\nu n}$ of the Hamiltonian (1) as follows

$$\psi_n(t) = \sum_{\nu=1}^N \sum_{m=1}^N e^{-i\lambda_\nu t} \varphi_{\nu n} \varphi_{\nu m} \psi_m(0), \quad (5)$$

where the eigenfunctions $\varphi_{\nu n}$ are chosen to be real. The quantities we use to characterize the dynamics of the electron wave packet are the mean position of the packet (centroid):

$$x(t) = \sum_{n=1}^N (n - n_0) |\psi_n(t)|^2, \quad (6a)$$

and its Fourier transform:

$$f(\omega) = \frac{1}{2\pi} \int_0^\infty dt e^{i\omega t} x(t). \quad (6b)$$

3 Results and discussions

In all simulations we used the helix of $N = 101$ bases. The hopping integral was chosen to be $J = 0.27$ eV (see, e.g., Ref. [6]). The initial wave packet was placed in the middle of the helix, $n_0 = 51$.

Figure 1 displays results of our calculations of the centroid $x(t)$ for various magnitudes of the gating potential drop U_\perp . At zero gating potential (upper panel), the motion of the centroid represents simple harmonic oscillations with the period $\tau_B = 2\pi/U_\parallel$ and the amplitude $L_B \approx (4J/U_\parallel)a$, where $4J$ is the bandwidth, which is in full correspondence with the standard picture

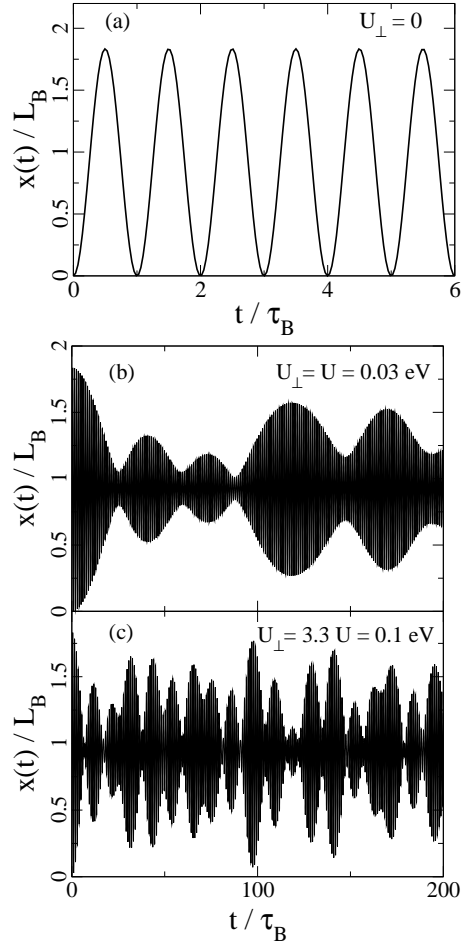


Fig. 1. Bloch oscillations of the centroid $x(t)$, Eq. (6a), calculated for a single-stranded helix of 101 bases at various magnitudes of the gating field. The corresponding gating potentials are indicated in the plots.

of Bloch oscillations in a linear chain. The helical symmetry does not affect the oscillations at $U_{\perp} = 0$.

On turning on the gating field, $U_{\perp} \neq 0$, the motion of the centroid still manifests an oscillatory behavior, however, a more complicated one as compared to simple harmonic oscillations (Fig. 1 middle and lower panels). The Fourier spectra $f(\omega)$ of the centroid plotted in Fig. 2 shed light on the situation. It demonstrates that a nonzero gating field gives rise to a splitting of the Bloch frequency into a multiplet with a frequency spacing dependent on the gating potential U_{\perp} . The resulting signals presented in Fig. 1 (middle and lower panels) are formed because of the superposition of harmonic oscillations with several different and generally non-commensurate frequencies.

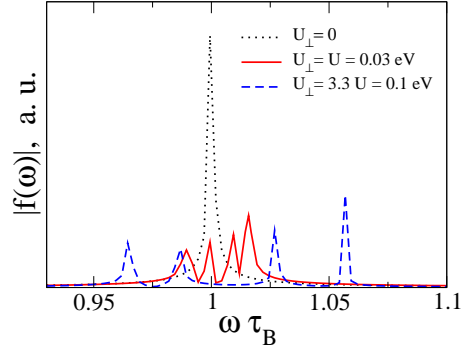


Fig. 2. Spectra of Bloch oscillations of the centroid depicted in Fig. 1.

Finally, for the parameters we use, which are typical for the synthetic dry DNA, the period of oscillations $\tau_B = 2\pi/U_{\parallel} \sim 1$ ps, i.e., it falls in the THz domain.

4 Summary

In summary, we have demonstrated that the intrinsic helix conformation of the DNA strands can have strong impact on its radiation properties. The electric field along the stack direction forces the injected charge to exhibit Bloch oscillations. In a tilted electric field, however, the harmonic Bloch oscillations become a superposition of oscillations with close and generally non-commensurate frequencies which can be tuned by an external electric field. The frequency of the oscillation falls in the THz domain. This finding is important for the self-assembled DNA arrays on gold with the DNA molecules being tilted with respect to the surface [13,14]. Such arrays may provide a nano-scaled source of coherent THz radiation.

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