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Bloch oscillations of a soliton in a molecular chain

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Abstract. This paper presents the results of numerical experiments simulating Bloch oscillations of solitons in a deformable molecular chain subject to a constant electric field. By using as an example a homogeneous polynucleotide chain, it is shown that the system under consideration can exhibit complicated dynamical behaviour: when subject to field intensities less than a certain critical value, a soliton exhibits oscillations as a whole, while at field intensities exceeding this threshold, the soliton becomes a breather that oscillates. It is shown that the motion of a charge in a deformable chain is infinite, which in contrast to that in a rigid chain.

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It is well-known that an electron situated in an ideal rigid periodic molecular chain, or in a solid-state superlattice, will exhibit Bloch oscillations in response to a constant electric field [1–5]. In an external, time-periodic field, the motion of a charge along a rigid chain can be both infinite and finite (dynamical localisation) [6–10]. In a deformable crystal chain, the role of the external field is played by oscillations of the lattice nodes, which can be represented as superpositions of plane travelling waves, or phonons. In this case, the motion of an electron along the chain is thought to be infinite, since the electron scatters on phonons and Bloch oscillations do not take place [11].

It is common knowledge that in quasi-one-dimensional molecular chains, the interaction of an electron with lattice oscillations is not weak. Therefore, we cannot safely assume that the electron wave function goes off-phase (in view of scattering of the electron off of phonons), and that Bloch oscillations will fail.

To clear up this point, we consider the case in which a charge, placed in a molecular chain, transfers into a soliton state as a result of interaction with lattice oscillations. This occurs, for example, in homogeneous polynucleotide chains, where the charge's motion is described by a Holstein Hamiltonian in which each site represents a nucleotide pair considered as a harmonic oscillator [12–14]:

$$\hat{H} = \hat{H}_h + \hat{T}_k + \hat{U}_p,$$
$$\hat{H}_h = \nu \sum_{n=1}^{N} (a_n^+ a_{n-1} + a_n^+ a_{n+1}) + \sum_{n=1}^{N} \alpha_n a_n^+ a_n,$$
$$\hat{T}_k = \sum_{n=1}^{N} \frac{\hat{P}_n^2}{2M}, \hat{U}_p = \sum_{n=1}^{N} k\frac{q_n^2}{2}, \quad \alpha_n = \alpha' q_n + n\hbar\omega_B. \quad (1)$$

Here, $\hat{H}_h$ is the Hamiltonian of a charged particle, a_n^+, a_n are the operators for creation and annihilation of the charge on site n, ν is the matrix element for the transition from the n-th site to the $(n \pm 1)$-th site, α_n is the energy of the particle at the n-th site, $\hbar\omega_B = e\mathcal{E}a$ where $\mathcal{E}$ is the intensity of the electric field, e is the electron charge, and a is the distance between neighbouring bases. $\hat{T}_k$ is an operator for the kinetic energy of different sites, while $\hat{U}_p$ gives the potential energy of sites, $\hat{P}_n$ is an impulse operator canonically conjugated to the displacement q_n, M is the effective mass of the site, k is an elastic constant, and α' is the particle-site displacement coupling constant.

We can now consider a semi-classical description of the wave function of the system $|\Psi(t)\rangle$ as an expansion over coherent states:

$$|\Psi(t)\rangle = \sum_{n=1}^{N} b_n(t) a_n^+ \exp\left\{-\frac{i}{\hbar}\sum_j \left[\beta_j(t)\hat{P}_j - \pi_j(t)q_j\right]\right\}|0\rangle, \quad (2)$$

where $|0\rangle$ is the vacuum wave function, and the quantities $\beta_j(t)$ and $\pi_j(t)$ satisfy the relations:

$$\langle\Psi(t)|q_n|\Psi(t)\rangle = \beta_n(t), \quad \langle\Psi(t)|\hat{P}_n|\Psi(t)\rangle = \pi_n(t). \quad (3)$$

Dynamical equations for the quantities $b_n(t)$ and $\beta_n(t)$ resulting from (1–3) have the form:

$$i\hbar\dot{b}_n = \alpha_n b_n + \nu(b_{n-1} + b_{n+1}), \quad (4)$$

$$M\ddot{\beta}_n = -\gamma\dot{\beta}_n - k\beta_n - \alpha'|b_n|^2. \quad (5)$$

The equations in (4) are Schrödinger equations, where b_n is the amplitude of the particle's localisation at the nth site. The equations in (5) are classical motion equations describing the dynamics of nucleotide pairs with respect to

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dissipation, where γ is the friction coefficient. We believe that a semi-classical description, in which the motion of a charge along a chain is described by quantum motion equations (4) and the motion of individual nucleotides is represented by classical motion equations (5), is valid in the case of a large nucleotide mass (≈300 proton masses).

In the case of a rigid chain, when $\alpha' = 0$ is the solution of the system (4), (5) will be [15,16]:

$$b_n(t) = \sum_{m=-\infty}^{\infty} b_m(0)(-i)^{n-m} e^{-i(n+m)\omega_B t/2} J_{n-m}\left(\xi(t)\right),$$
$$\xi(t) = \frac{4\nu}{\hbar\omega_B} \sin\left(\frac{\omega_B t}{2}\right), \tag{6}$$

where $J_n(x)$ is a Bessel function of the first kind. Solution (6) corresponds to Bloch oscillations of a particle in a chain subject to an electric field, for which the particle's centre of mass

$$X(t) = \sum_{n=1}^{N} |b_n(t)|^2 na \tag{7}$$

exhibits periodic oscillations with a frequency ω_B:

$$X(t) = X(0) + \frac{2a\nu}{\hbar\omega_B} |S_0| \left(\cos\theta_0 - \cos(\omega_B t + \theta_0)\right),$$
$$S_0 = \sum_{m=-\infty}^{\infty} b_m^*(0) b_{m-1}(0) = |S_0|\, e^{i\theta_0}, \tag{8}$$
$$X(0) = a \sum_{m=-\infty}^{\infty} m |b_m(0)|^2,$$

where a is the distance between neighbouring nucleotides, which is equal to 3.4 Å for DNA.

For $\alpha' \neq 0$ in the absence of an electric field, a stationary solution of equations (4) and (5) corresponds to a localised state of soliton type. To study the evolution of a soliton state in an electric field, we will use an initial charge density distribution such that:

$$|b_n(0)| = \frac{\sqrt{2}}{4} \cosh^{-1}\left(\frac{\kappa(n-n_0)}{4\eta}\right), \tag{9}$$
$$n_0 = \frac{N}{2} + 1, \quad \eta = \frac{\nu\tau}{\hbar}, \quad \kappa = \frac{\tau\alpha'^2}{k\hbar}.$$

Initial values of x^0 and y^0 ($b_n = x_n + iy_n$) for $\nu > 0$ have the form:

$$x_n^0 = |b_n(0)|(-1)^n \Big/ \sqrt{2}\,, \;\; y_n^0 = |b_n(0)|(-1)^{n+1} \Big/ \sqrt{2}\,, \tag{10}$$

which correspond to the ground state of a particle in the absence of an electric field [13,14].

Figure 1 shows the results of solving equations (4) and (5) for some values of the parameter κ, which is responsible for the intensity of the charge's interaction with the lattice oscillations when the electric field intensity $E = \mathcal{E}ea\tau/\hbar = 0.1$, $\widetilde{\omega} = \omega\tau = 0.01$, and $\eta = 1.276$. Here, the values of the parameters ω and η are the same as those in

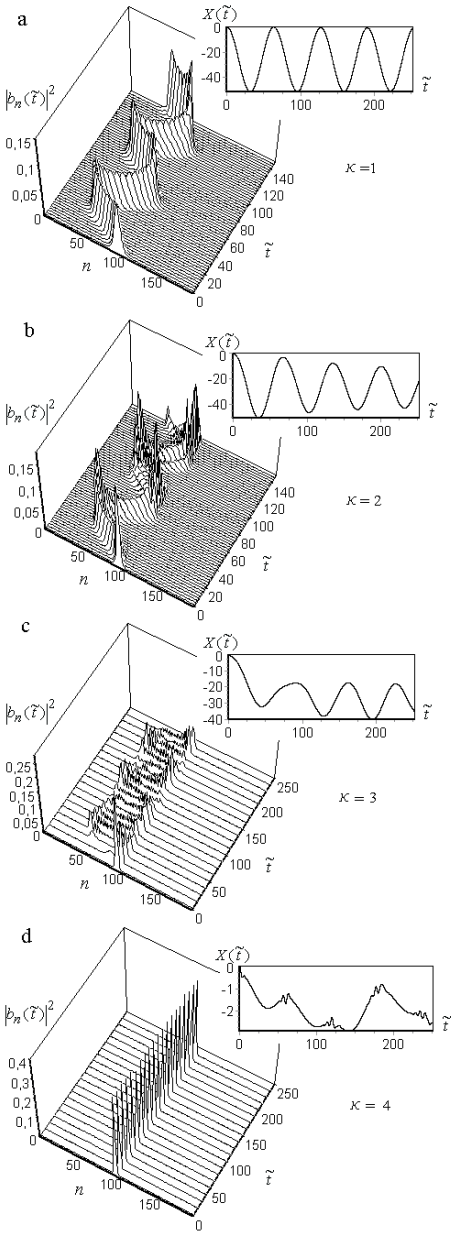

Fig. 1.

reference [12], and $\tau = 10^{-14}$ s. In dimensional units, these parameter values correspond to $\mathcal{E} = 1.94 \times 10^5$ V/cm, $\omega = \sqrt{k/M} = 10^{12}$ s^{-1}, and $\nu = 0.084$ eV. The parameter for electron-phonon strength is $\kappa = 4$, which in dimensional units corresponds to $\alpha' = 0.13$ eV/Å, and is the same as in reference [12]. This value is close to that used by other authors (for example, in [18] α' was found to be $\alpha' \approx 0.23$ eV/Å).

It can be seen from Figure 1a that in the presence of an electric field, a soliton executes periodic motion, returning to the point where the soliton's centre of mass was initially located. This oscillatory motion corresponds to Bloch oscillations with a period of $T = 2\pi/\omega_B$. The total amplitude of the oscillations L is close to that determined from the solution of the linear problem (6), and is written

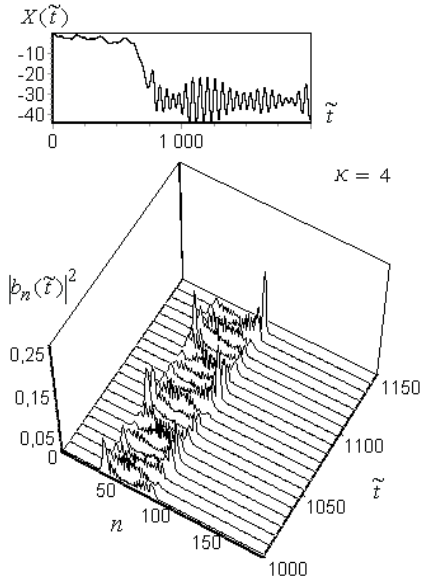

Fig. 2. Transformation of a soliton into a breather for $\kappa = 4$ (Fig. 1d at large times).

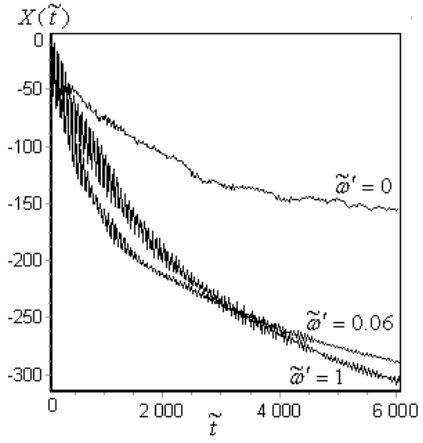

Fig. 3. The function $X(\widetilde{t})$ for various values of $\widetilde{\omega}'$.

as $\Delta W a/E$, where $\Delta W = 4\eta$ stands for the width of the conductivity band, and is equal to $\Delta W \tau/\hbar$ in dimensional form. For the parameter values presented above, $L \approx 51a$ (with a characteristic size for the soliton of $\approx 10a$).

Figures 1b–1d show the evolution of the dynamical behaviour of a soliton at the initial stages of motion, as the parameter κ increases. After a period of time, Bloch oscillations are restored (the restored Bloch oscillations are not given in Figs. 1b–1d).

In the case of the strong electric fields represented in Figure 1, a soliton executing Bloch oscillations in time turns into a breather, oscillating at the Bloch frequency (Fig. 2). At rather large values of κ, a breather can arise from the initial soliton state immediately, i.e. by-passing the phase of the Bloch oscillations as a whole.

Without going into the details of the nonstationary regimes of the particle's motion in the cases under consideration, we will restrict ourselves to a purely qualitative description of the picture. It has been observed that the case of a deformable chain ($\alpha' \neq 0$) differs qualitatively from the limiting case of a rigid chain ($\alpha' = 0$), in that at finite α', the quantity $X(t)$ given by (7) grows infinitely as $t \to \infty$ (Fig. 3). This result could have been predicted from the aforementioned analogy between the influence of a periodic external electric field on a particle and the oscillation of phonons. Quite nontrivial, however, is the finding that under this influence, in the case of strong particle-phonons interactions (i.e. when a soliton is formed), Bloch oscillations of the particle persist in the electric field as oscillations of the soliton as a whole or as a breather, depending on the system's parameters.

In conclusion, it may be said that this picture of charge motion in a deformable molecular chain in a constant electric field at zero temperature $T = 0$ seems to be rather general: a positive charge introduced in the chain will move along the field executing Bloch oscillations. At finite temperatures, a soliton or breather state will break, thus leading to failure of the Bloch oscillations. In this case, the motion of the charge over the chain will be infinite along the lines of the field and will possess an ordinary band character.

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