Bloch oscillations of a soliton in a molecular chain

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

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It is well known that an electron occurring in an ideal rigid periodic molecular chain or in a solid state superlattice exhibits Bloch oscillations in response to a constant electric field \([11]-[15]\). In an external time-periodic field, motion of a charge along a rigid chain can be both infinite and finite (dynamical localization) \([6]-[10]\). In a deformable crystal chain the role of an external field is played by oscillations of the lattice nodes which can be presented as superposition 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 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 on phonons) and Bloch oscillations fail.

To clear up this point we consider the case when a charge placed in a molecular chain transits to a soliton state as a result of interaction with lattice oscillations. This occurs, for example, in homogeneous polynucleotide chains where the charge motion is described by Holstein Hamiltonian in which each site presents a nucleotide pair considered as a harmonical oscillator \([12]-[14]\):

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

Here \(\hat{H}_h\) is a Hamiltonian of a charged particle, \(a_n^\dagger, a_n\) - are operators of creation and annihilation of the charge on site \(n\), \(\nu\) - is the matrix element of the transition from the \(n\) - th site to the \(n \pm 1\) - site, \(\alpha_n\) - 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, \(a\) - is the distance between neighboring bases. \(\hat{T}_k\) is an operator of the kinetic energy of sites, \(\hat{U}_p\) is the potential energy of sites. \(\hat{P}_n\) is an impulse operator canonically conjugated to the displacement \(q_n\), \(\hat{M}\) is the effective mass of the site, \(k\) - is an elastic constant, \(\alpha'\) - is the particle-site displacement coupling constant.

We can pass on to semi classical description of the wave function of the system \(|\Psi(t)\rangle\) as an expansion over coherent states:

\[
|\Psi(t)\rangle = \sum_{n=1}^{N} b_n(t) a_n^\dagger \exp \left\{ -i \sum_{j=1}^{N} \left[ \beta_j(t) \hat{P}_j - \beta_j(t) q_j \right] \right\} |0\rangle,
\]

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

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

Dynamical equations for the quantities \(b_n(t)\) and \(\beta_n(t)\) resulting from \([11]-[14]\) have the form :

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

\[
M \ddot{\beta}_n = -\gamma \dot{\beta}_n - k \beta_n - \alpha' |b_n|^2.
\]

Equations \([11]-[14]\) are Schrödinger equations where \(b_n\) is the amplitude of the particle localization at the \(n\) - th site. Equations \([15]\) are classical motion equations describing dynamics of nucleotide pairs with regard for dissipation,
The length of the homogeneous nucleotide chain is

\[ \kappa \text{ parameter } = t \]

Fig. 1. Oscillatory motions of a soliton for some values of

- \( \omega' = \gamma/M = 6 \cdot 10^{11} \text{ sec}^{-1} \)
- \( \gamma = 0.01 \)
- \( \eta = 1.276 \)

where \( \gamma \) is friction coefficient. We believe that a semiclas-
sical description in which motion of a charge along a chain
is described by quantum motion equations \[4\] and motion
of individual nucleotides is presented by classical motion
equations \[5\] is valid in view of a large nucleotide mass
(\( \approx 300 \) proton mass).

In the case of a rigid chain, when \( \alpha' = 0 \) the solution
of the system \(4, 5\) will be \[13, 16\]:

\[ b_n(t) = \sum_{m=-\infty}^{\infty} b_m(0)(-i)^{n-m} e^{-i(n+m)\omega t/2} J_{n-m}(\xi(t)), \]

\[ \xi(t) = \frac{4\nu}{h\omega_B} \sin \left(\frac{\omega_B t}{2}\right), \]

\[ J_n(x) \] is Bessel function of the first kind. Solution \(6\)
corresponds to Bloch oscillations of a particle in the chain
affected by an electric field for which the particle’s centre
mass:

\[ X(t) = \sum_{n=1}^{N} |b_n(t)|^2 n a, \]

demonstrates periodic oscillations at the frequency of \(\omega_B\):

\[ X(t) = X(0) + \frac{2\alpha}{h\omega_B} |S_0| \left(\cos \theta_0 - \cos(\omega_B t + \theta_0)\right), \]

\[ S_0 = \sum_{m=-\infty}^{\infty} b_m^*(0)b_{m-1}(0) = |S_0| e^{i\theta_0}, \]

\[ X(0) = a \sum_{m=-\infty}^{\infty} m |b_m(0)|^2, \]

where \( a \) is the distance between neighboring nucleotides,
which for DNA is equal to 3.4\( \AA \).

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

\[ |b_n(0)| = \frac{\sqrt{2}}{4} \cosh^{-1} \left(\frac{\kappa(n - n_0)}{4\eta}\right), \]

\[ n_0 = \frac{N}{2} + 1, \quad \eta = \frac{\nu \tau}{h}, \quad \kappa = \frac{\tau \alpha'^2}{k h}. \]

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

\[ x^0_n = |b_n(0)|(-1)^n \sqrt{2}, \quad y^0_n = |b_n(0)|(-1)^{n+1} \sqrt{2}, \]

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

Fig.1 shows the results of the solution of equations
\[4, 5\] for some values of parameter \( \kappa \), responsible for
the intensity of the charge interaction with lattice oscil-
lations at the electric field intensity \( E = \bar{E} e \alpha t/h = 0.1 \)
(\( \bar{\omega} = \omega \tau = 0.01 \)), \( \eta = 1.276 \). Here the values of parameters
\( \omega \) and \( \eta \) are the same as in work \[12\], and \( \tau = 10^{-14} \text{sec} \). In dimensional units these parameter values correspond.
analogy between the influence of a periodic external electric field on a particle and oscillations of phonons. Quite nontrivial is the finding that under this influence, in the case of a strong particle-phonons interaction, i.e. when a soliton is formed, Bloch oscillations of the particle persist in the electric field as oscillations of a soliton as a whole or a breather, depending on the system parameters.

In conclusion it may be said that this picture of the 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 Bloch oscillations. In this case motion of the charge over the chain will be infinite along the lines of the field and have an ordinary band character.

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