Nonlinear charge transport in DNA mediated by twist modes

F. Palmero, C. Katerji,
J.F.R. Archilla, D. Hennig
and F.R. Romero

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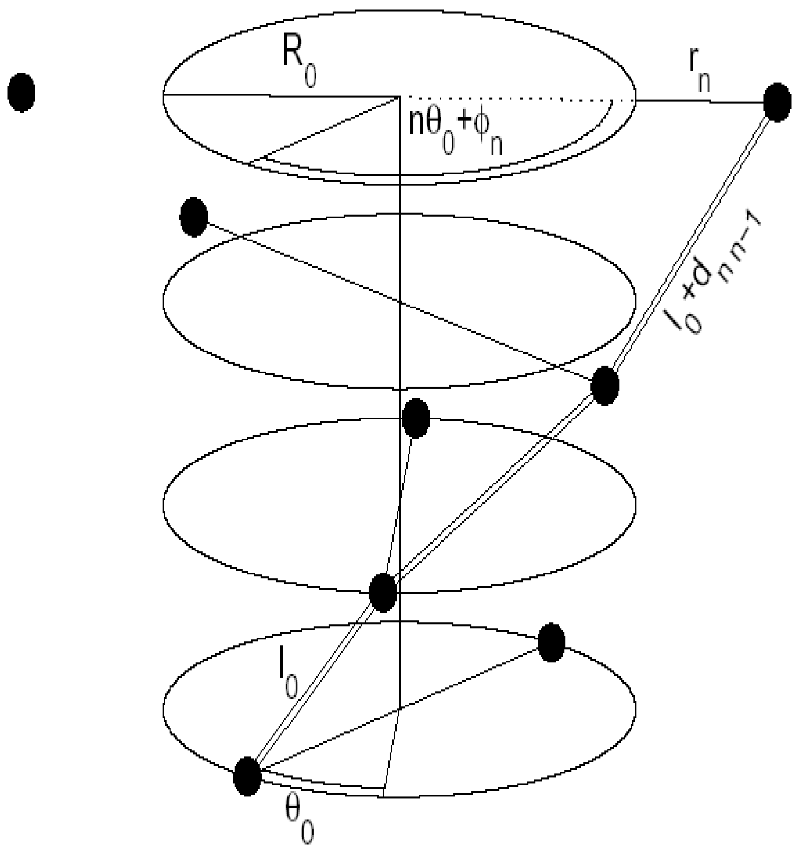
Charge transport in DNA

- Important role for biological functions. Biosynthesis and DNA repair after radiation damage.
- Technological interest. Possibility of building electronic devices based on biomaterials.

The model

- Modification of the *twist-opening* model.
- Bond potential treated as harmonic ones.
- Three dimensional, semi-classical, tight-binding model.



Hamiltonian

- Lattice oscillators treated classically

$$H_{rad} = \sum_n \left[\frac{1}{2M} (p_n^r)^2 + \frac{M\Omega_r^2}{2} r_n^2 \right],$$

$$H_{twist} = \sum_n \left[\frac{1}{2J} (p_n^\phi)^2 + \frac{J\Omega_\phi^2}{2} (\phi_n - \phi_{n-1})^2 \right]$$

- Charge described by a tight-binding system

$$\widehat{H}_{el} = \sum_n E_n |n\rangle\langle n| - V_{n-1,n} |n-1\rangle\langle n| - V_{n+1,n} |n+1\rangle\langle n|$$

$$E_n = E_n^0 + k r_n \qquad V_{n,n-1} = V_0 (1 - \alpha d_{n,n-1})$$

$$d_{n,n-1} = [a^2 + (R_0 + r_n)^2 + (R_0 + r_{n-1})^2 - 2(R_0 + r_n)(R_0 + r_{n-1}) \cos(\theta_0 + \theta_{n,n-1})]^{1/2} - l_0$$

Dynamical equations

$$
\begin{aligned}
\mathrm{i}\,\tau\dot{c}_n &= (E_n + k\,r_n)\,c_n \\
&\quad - (1-\alpha\,d_{n+1,n})\,c_{n+1} - (1-\alpha\,d_{n\,n-1})\,c_{n-1}, \\
\ddot{r}_n &= -r_n - k\,|c_n|^2 \\
&\quad - \alpha\left[\frac{\partial d_n}{\partial r_n}(c_n^* c_{n-1} + c_n c_{n-1}^*) + \frac{\partial d_{n+1}}{\partial r_n}(c_{n+1}^* c_n + c_{n+1} c_n^*)\right], \\
\ddot{\phi}_n &= -\Omega^2\,(2\phi_n - \phi_{n-1} - \phi_{n+1}) \\
&\quad - \alpha\,V\left[\frac{\partial d_n}{\partial \phi_n}(c_n^* c_{n-1} + c_n c_{n-1}^*) + \frac{\partial d_{n+1}}{\partial \phi_n}(c_{n+1}^* c_n + c_{n+1} c_n^*)\right]
\end{aligned}
$$

- Scaled parameters

$\tau = 0.053$, $\Omega^2 = 0.013$, $V = 2.5\times 10^{-4}$

$R_0 = 63.1$, $l_0 = 44.5$ No reliable data k=1, α adjustable

Stationary polaron-like states

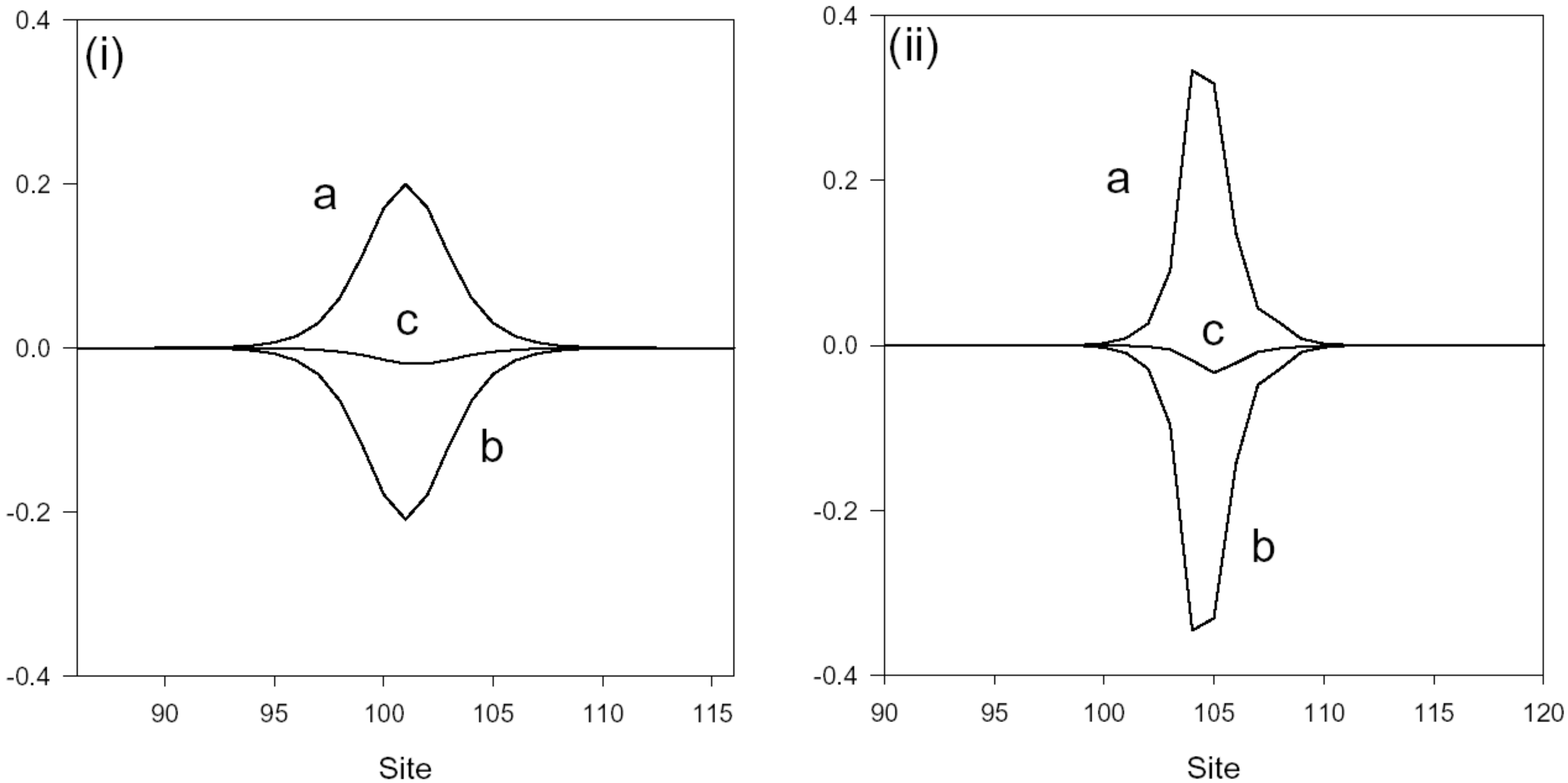
- τ small.
- Born-Oppenheimer approximation.
- Stationary solutions must be attractors of the map:

$$
\begin{aligned}
r_n' &= -k\,|c_n|^2 \\
&\quad - \alpha \left[\frac{\partial d_{n,n-1}}{\partial r_n}(c_n^* c_{n-1} + c_n c_{n-1}^*) + \frac{\partial d_{n+1,n}}{\partial r_n}(c_{n+1}^* c_n + c_{n+1} c_n^*) \right], \\
\phi_n' &= \frac{1}{2}(\phi_{n+1} + \phi_{n-1}) \\
&\quad - \frac{\alpha V}{2\Omega^2} \left[\frac{\partial d_{n,n-1}}{\partial \phi_n}(c_n^* c_{n-1} + c_n c_{n-1}^*) + \frac{\partial d_{n+1,n}}{\partial \phi_n}(c_{n+1}^* c_n + c_{n+1} c_n^*) \right], \\
c_n' &= \frac{[(E_n + k\,r_n')\,c_n - (1 - \alpha\,d_{n+1,n}')\,c_{n+1} - (1 - \alpha\,d_{n\,n-1}')\,c_{n-1}]}{\|(E_n + k\,r_n')\,c_n - (1 - \alpha\,d_{n+1,n}')\,c_{n+1} - (1 - \alpha\,d_{n\,n-1}')\,c_{n-1}\|}, \\
d' &= d(r', \phi')
\end{aligned}
$$

Stationary states

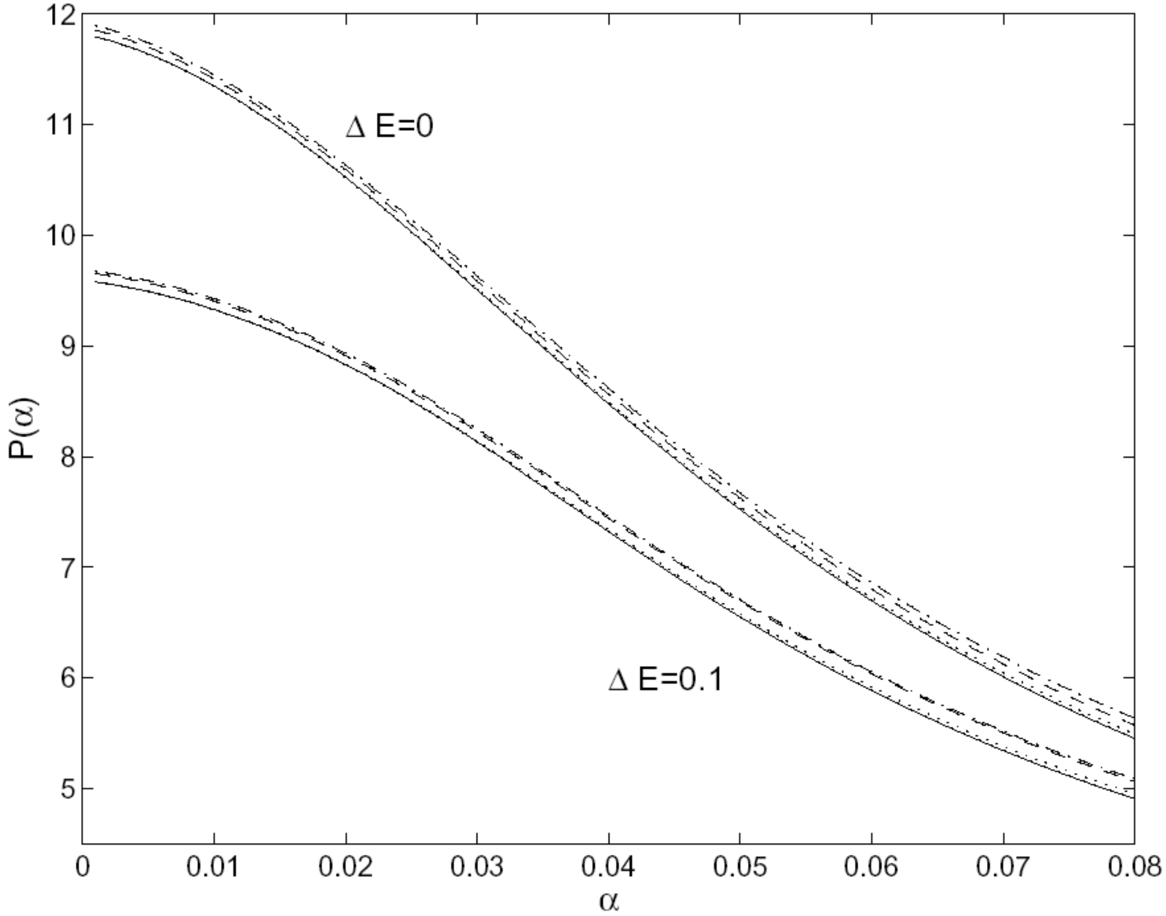
⌘Ordered case $E^0_n = E_0$

⌘Disordered case $E^0_n \in [-\Delta E_0, \Delta E_0]$



a) Electronic amplitude; b)Radial displacements, c) Angular twist

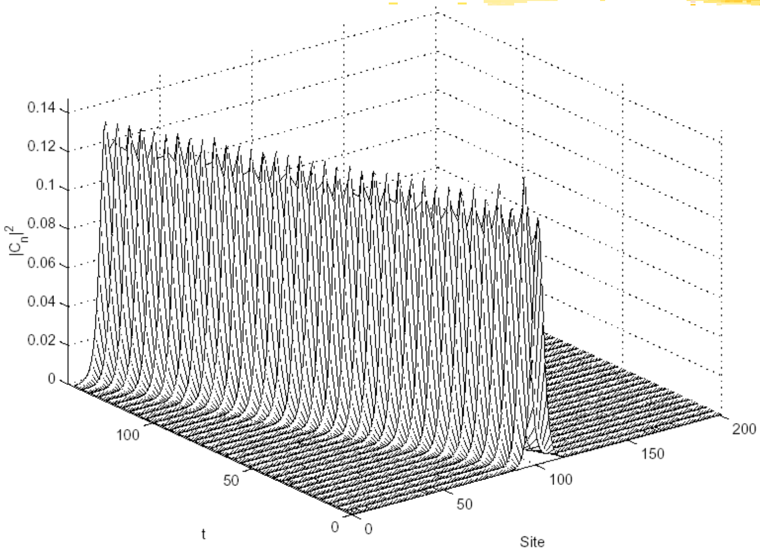
Participation number

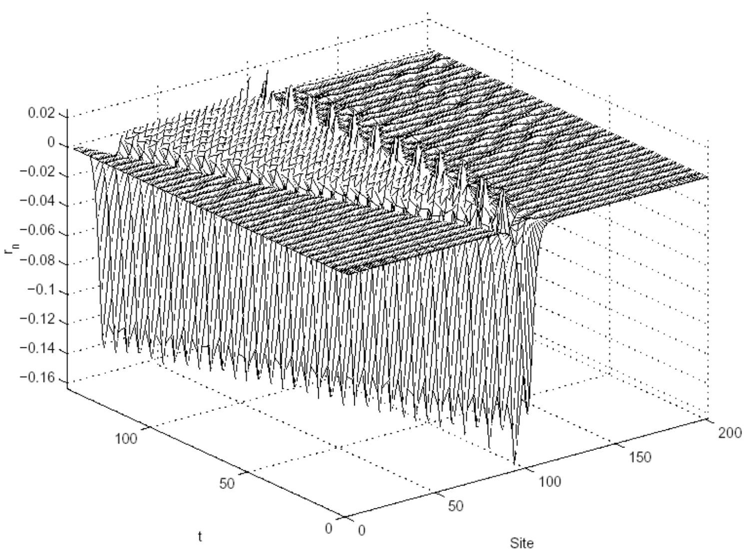


Charge transport in the absence of disorder

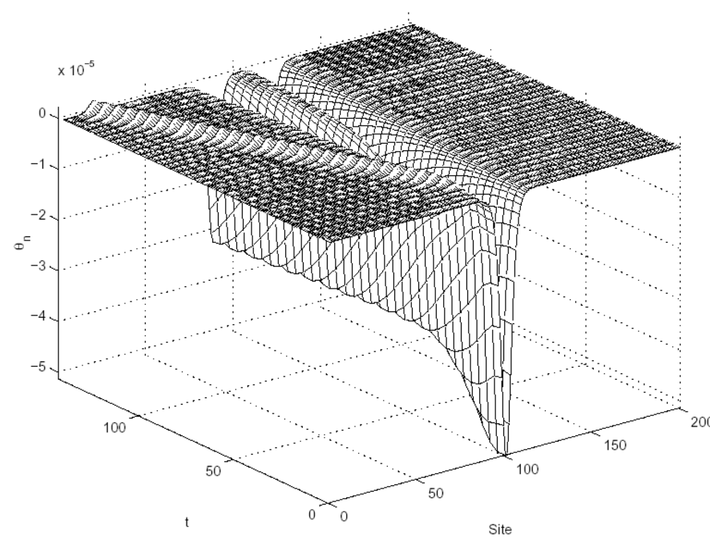
- Stationary solutions can be moved (under certain condictions).
- Discrete gradient method.
- Three different regimes depending on parameter α
  - Radial movability regime
  - Twist movability regime
  - Mixed regime

Ordered case I. Radial regime

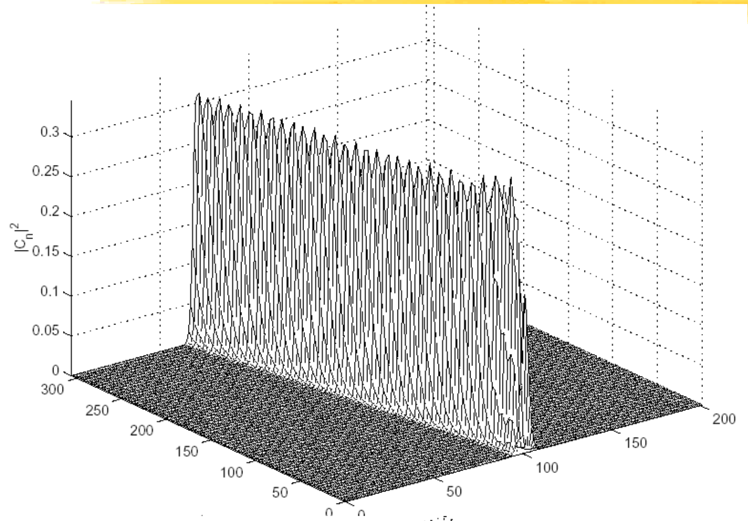


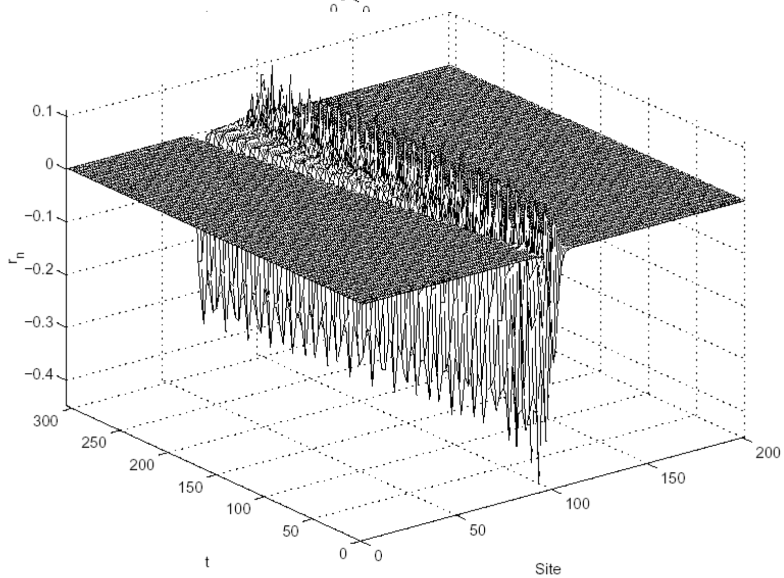


- α small enough (~0.0002).
- Velocity increases with perturbation.

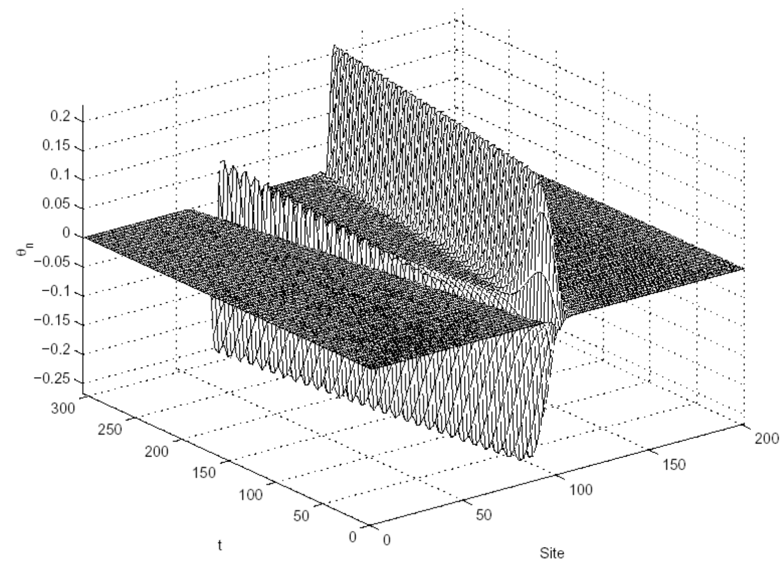


Ordered case II. Twist regime





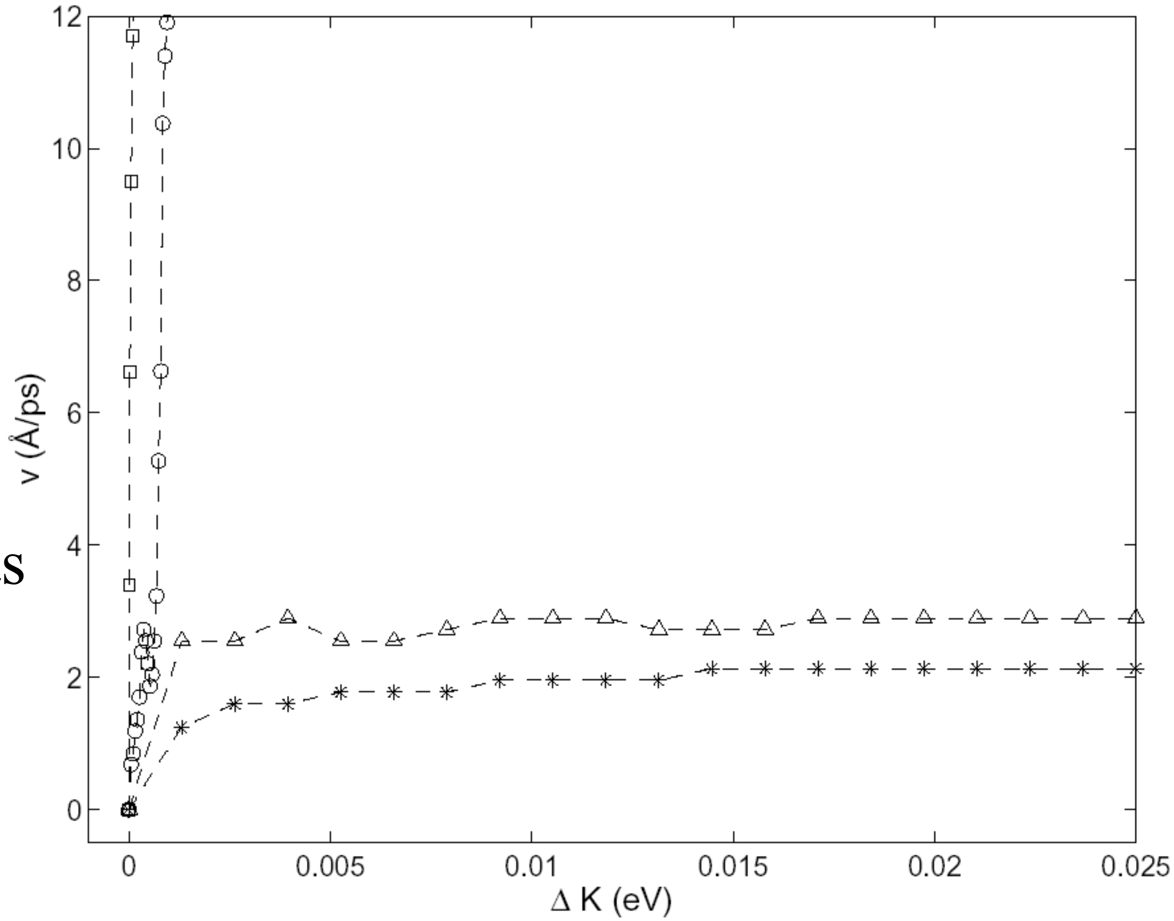
- Larger values of parameter α (~0.05).
- There exist a limit velocity.



Ordered case III. Mixed regime

Mixed regime for intermediate values of parameter α.

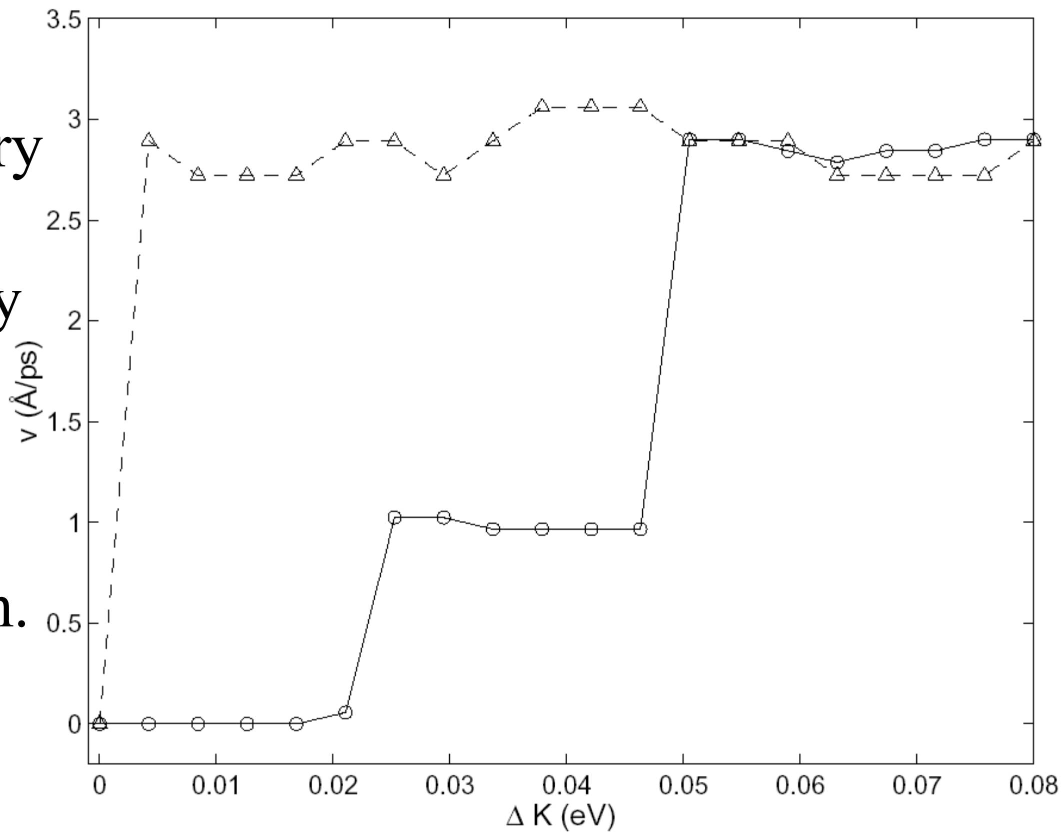
- Radial movability requires less energy.
- Radial movability has higher velocity.



Squares: Radial regime; Circles: Mixed regime, radial activation; Triangles: Mixed regime, angular activation; Starts: Twist regime

Disordered case

•Radial movability regime very sensitive to disorder.
•Twist movability regime very robust to disorder.
•Mixed regime, angular activation leads more robust polarons than radial activation.



Circles: Disordered case; Triangules: Ordered one

Conclusions

- Analysis of the influence of the radial and angular perturbations on the properties of moving polarons in a three-dimensional, semi-classical, tight-binding model for DNA in both the ordered and disorderd case.
- Three regimes in function of the coupling of the transfer integral with the deformations of the hydrogen bonds.
- Properties of the moving polaron different in each regime. Mobility induced by angular activation is more robust with respect to parametric disorder, has lower velocity and the activation energy is higher than in radial movability regime.

Further works

- Analysis of the influence of an impurity in the mouvement of the polaron.
- We consider a different well depth (in radial variables) in a site.
  - Radial activation: Polaron is refected or trapped by the impurity.
  - Twist activation: Polaron cross the impurity.

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