Polaron dynamics in double-stranded DNA under electric fields

Elena Díaz, R. P. A. Lima and F. Domínguez-Adame

Quantum Nanosystems Group-GISC

Departamento de Física de Materiales

Universidad Complutense de Madrid

elenadg@fis.ucm.es

Outline

1. DNA and its physical interest
2. Peyrard-Bishop-Holstein model

   2.1 Origin of the model

   2.2 Polaronic effects in DNA

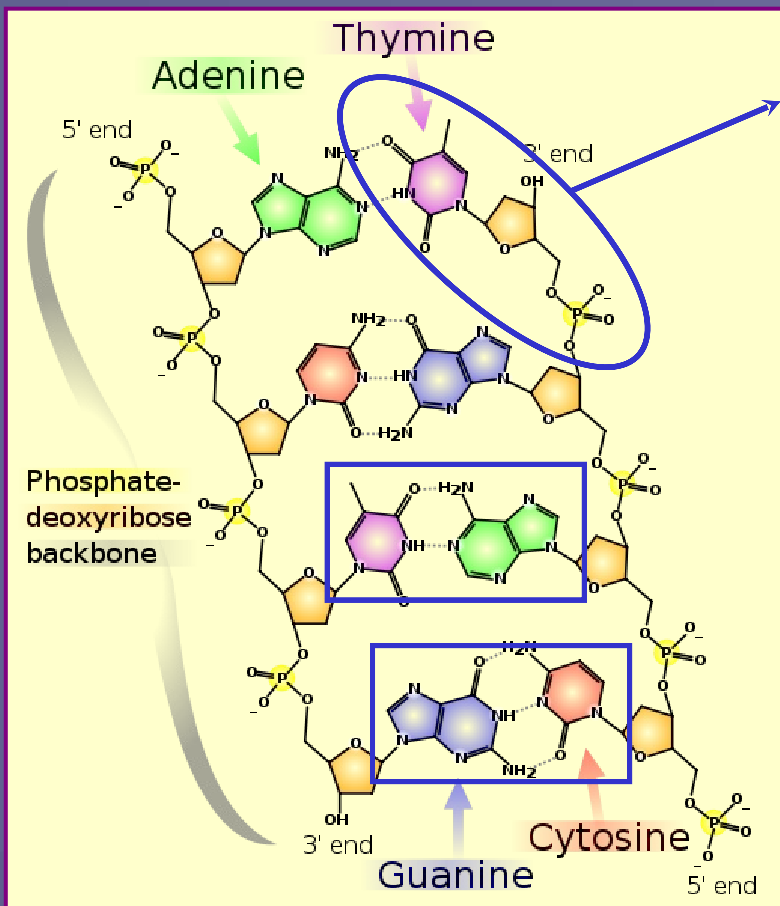
3. Bloch Oscillations

   3.1 Definition and experimental evidence

   3.2 Bloch-like oscillations in DNA

4. Conclusions

What is DNA?

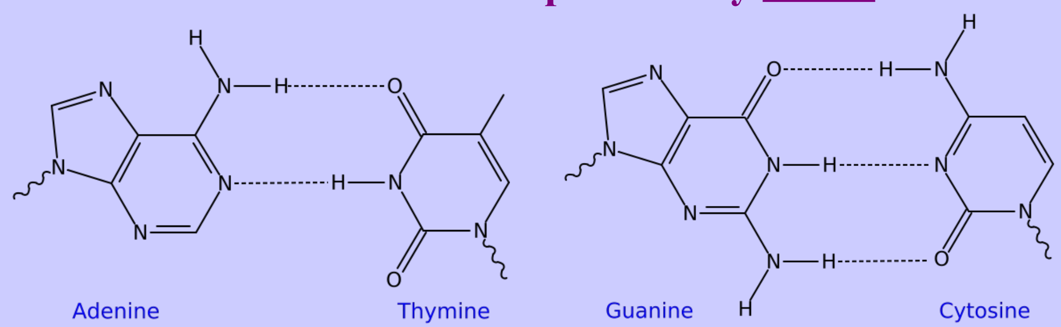


Nucleotide = Base + Sugar + Phosphate

Base → A, T, G, C

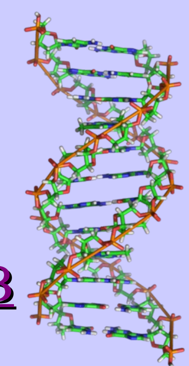
Sugar + Phosphate → Backbone

Watson-Crick Pair = 2 Complementary Bases + H-Bonds



Several possible conformations

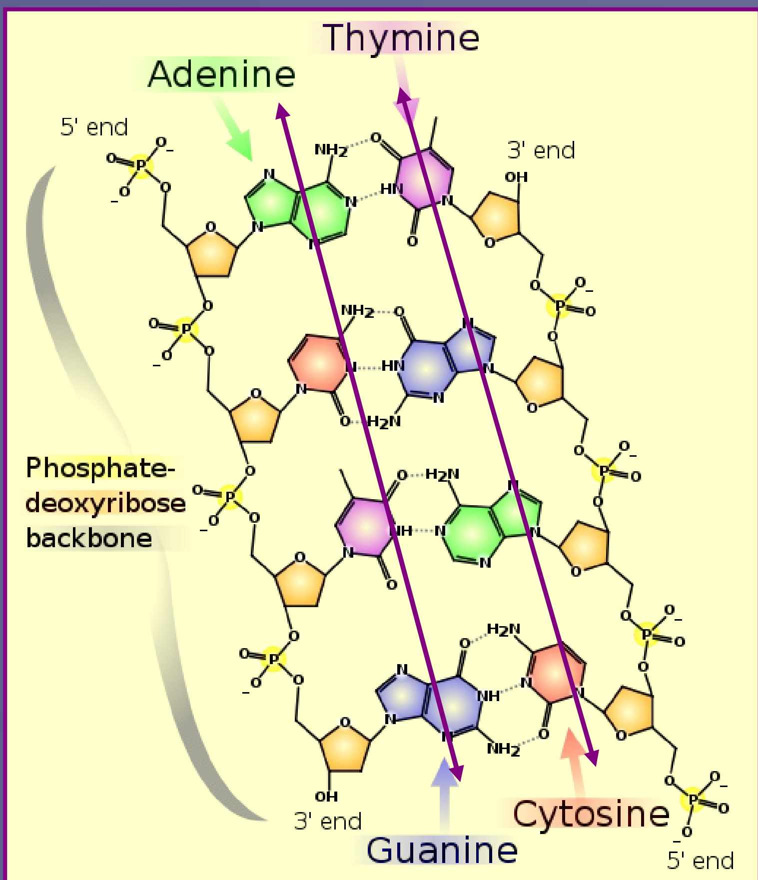
Most Common: type B



Physical interest

Nitrogenous bases = Purine/Pyrimidine Rings

Aromatic Rings:
i.e. Benzene

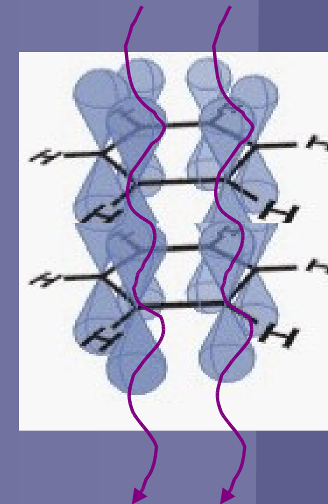


Saturday, February 7th

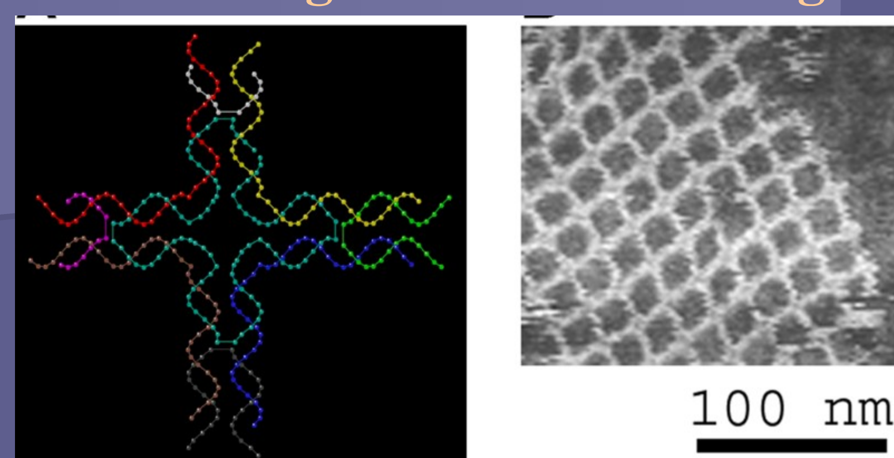
Session 9 Plenary contribution (Sala de Grados)

9:30-10:30 Francisco Domínguez-Adame (UCM-Madrid)

Challenges of the electronic transport across single DNA molecule

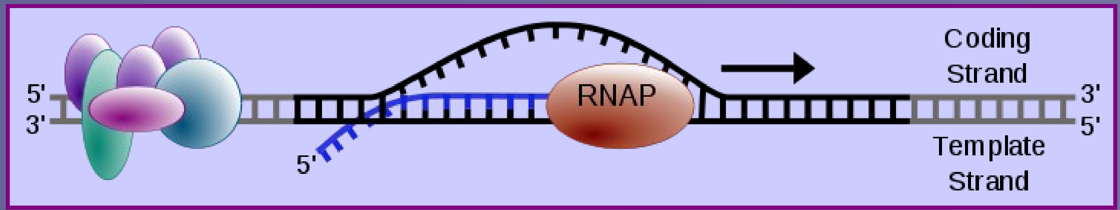


Self-assembling **Molecular Recognition**



Origin of Peyrard-Bishop Model

Description of thermal denaturation: first step of the transcription process



VOLUME 62, NUMBER 23 PHYSICAL REVIEW LETTERS 5 JUNE 1989

Statistical Mechanics of a Nonlinear Model for DNA Denaturation

M. Peyrard
Laboratoire d'Optique du Réseau Cristallin, Faculté des Sciences, 6, Boulevard Gabriel, 21100 Dijon, France and Center for Nonlinear Studies, Los Alamos National Laboratory, Los Alamos, New Mexico 87545

A. R. Bishop
Theoretical Division and Center for Nonlinear Studies, Los Alamos National Laboratory, Los Alamos, New Mexico 87545
(Received 19 December 1988)

Transfer integral method → **No continuum aproximation is needed**

Transfer integral method → **Large amplitude fluctuations** → **Collective nonlinear excitation-motion of bases**

Peyrard-Bishop Formalism

A single freedom degree is considered for every base pair: y_n → H-bonds stretching

Inhomogeneties due to the base sequence and asymmetries of the two strands are neglected

$$H = \sum_n \left[\tfrac{1}{2} m \dot{y}_n^2 + V(y_n) + W(y_n, y_{n-1}) \right] .$$

Morse Potential for H-bonds

$$V(y_n) = D(e^{-a y_n} - 1)^2$$

H-bonds+repulsion between phosphates+surrounding solvent

Nonlinear Stacking Interaction → Cooperativity

First Aproximation

$$W(y_n, y_{n-1}) = \frac{1}{2} k (y_n - y_{n-1})^2$$

→

Better description: anharmonic potential

$$W(y_n, y_{n-1}) = \frac{k}{2} (1 + \rho e^{-\alpha(y_n + y_{n-1})})(y_n - y_{n-1})^2$$

RAPID COMMUNICATIONS

PHYSICAL REVIEW E VOLUME 47, NUMBER 1 JANUARY 1993

Entropy-driven DNA denaturation

Thierry Dauxois* and Michel Peyrard*
Physique Non Linéaire: Ondes et Structures Cohérentes, Faculté des Sciences, 6 Boulevard Gabriel, 21000 Dijon, France and Center for Nonlinear Studies and Theoretical Division, Los Alamos National Laboratory, Los Alamos, New Mexico 87545
A. R. Bishop
Center for Nonlinear Studies and Theoretical Division, Los Alamos National Laboratory, Los Alamos, New Mexico 87545

(Received 27 May 1992)

Peyrard-Bishop-Holstein (PBH) Formalism

Extra charge in a deformable molecule

distortion to get the minimum energy conformation → **POLARON**

$$H = H_{lat} + H_{ch} + H_{int}$$

Peyrard-Bishop Model

$$H_{lat} = \sum_n \left[\frac{1}{2} m \dot{y}_n^2 + V(y_n) + W(y_n, y_{n-1}) \right],$$

Tight-binding Hamiltonian

$$H_{ch} = -V \sum_n \left(c_n^\dagger c_{n+1} + c_n^\dagger c_{n-1} \right).$$

Charge-lattice interaction

Holstein type coupling

$$H_{int} = \chi \sum_n y_n c_n^\dagger c_n$$

On-site energy correction

PHYSICAL REVIEW E, VOLUME 65, 061905

Effects of intrinsic base-pair fluctuations on charge transport in DNA

S. Komineas,[1,2] G. Kalosakas,[1] and A. R. Bishop[1]
[1]*Theoretical Division and Center for Nonlinear Studies, Los Alamos National Laboratory, Los Alamos, New Mexico 87545*
[2]*Physikalisches Institut, Universität Bayreuth, D-95440 Bayreuth, Germany*
(Received 27 February 2002; published 17 June 2002)

PBH model. Semiclassical aproximation

Bases **Charge**

$m_b \gg m_c$

$t_{ph} = 1/\omega_{ph}$ $\omega_{ph} \sim$ THz $\quad\downarrow\quad$ $t_e = \hbar/V$ $V \sim 0.1$eV

$t_{ph} \sim$ps $\gg$ $t_e \sim$fs

Classical-mechanics for the lattice distorsion dynamics

$$m\frac{d^2y_n}{dt^2} = -V_M'(y_n) - W'(y_n, y_{n-1}) - W'(y_{n+1}, y_n) - \chi|\psi_n|^2,$$

Quantum-mechanics for the carrier wave function dynamics

$$i\hbar\frac{d\Psi_n}{dt} = -V(\Psi_{n+1} + \Psi_{n-1}) + \chi y_n \Psi_n$$

Polaronic effects in DNA PBH model

PHYSICAL REVIEW E **72**, 021912

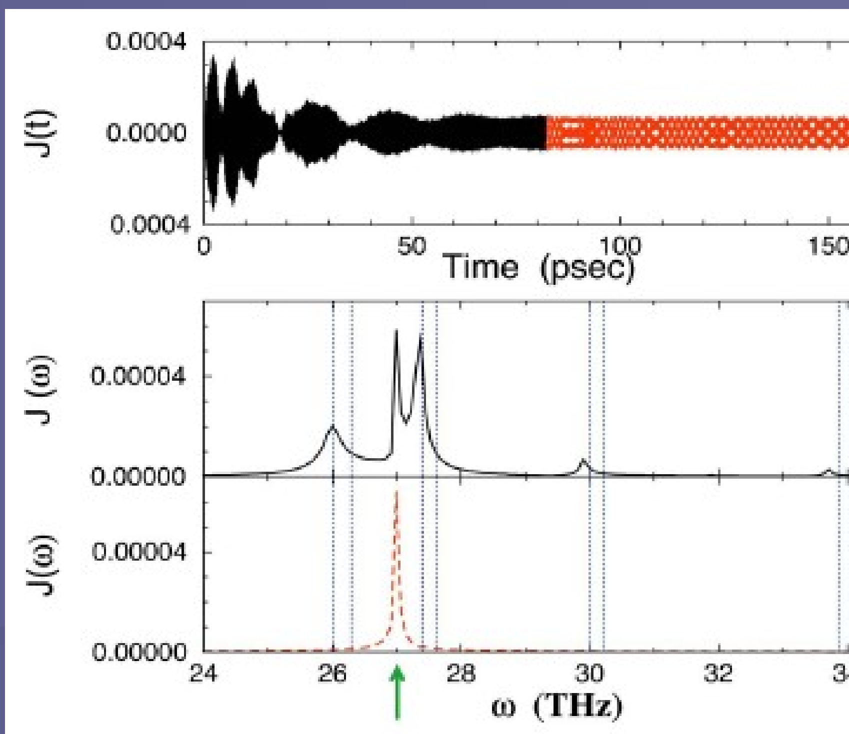
ac conductivity in a DNA charge tr

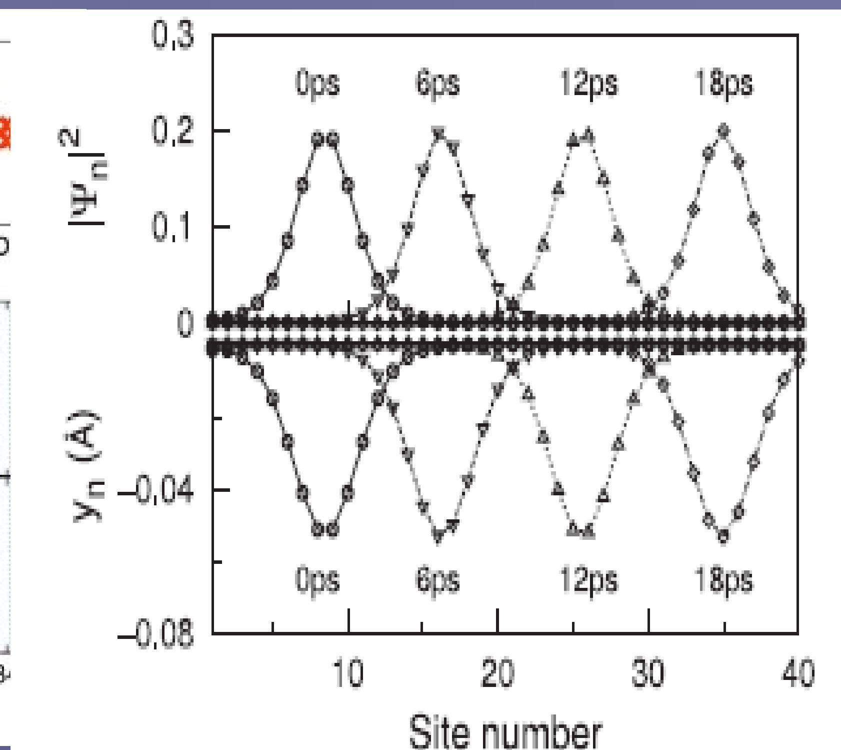
P. Maniadis,[1] G. Kalosakas,[1] K. Ø. Rasmussen

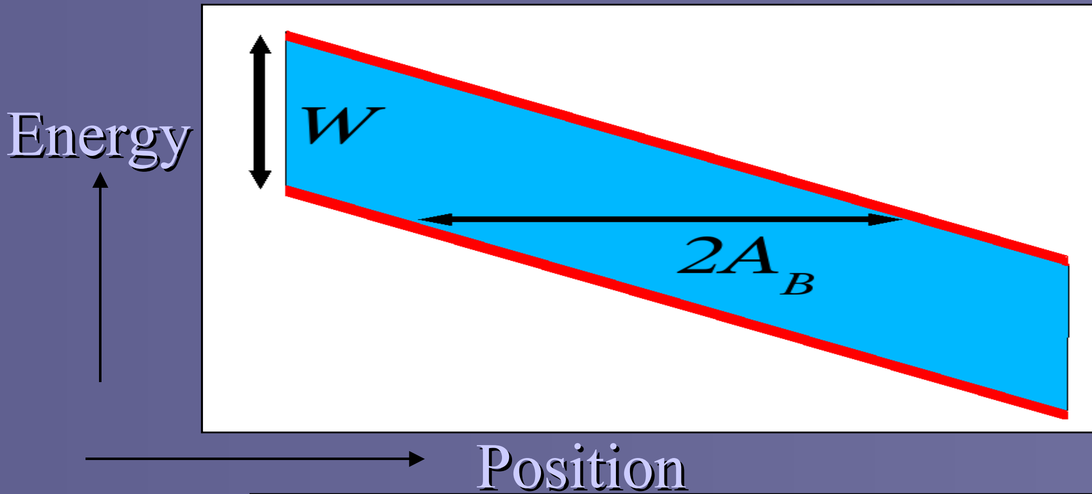
IOP PUBLISHING JOURNAL OF PHYSICS: CONDENSED MATTER
J. Phys.: Condens. Matter **20** (2008) 035207 (5pp) doi:10.1088/0953-8984/20/03/035207

The electric field effect and conduction in the Peyrard–Bishop–Holstein model

Julia A Berashevich, Adam D Bookatz and Tapash Chakraborty







Definition

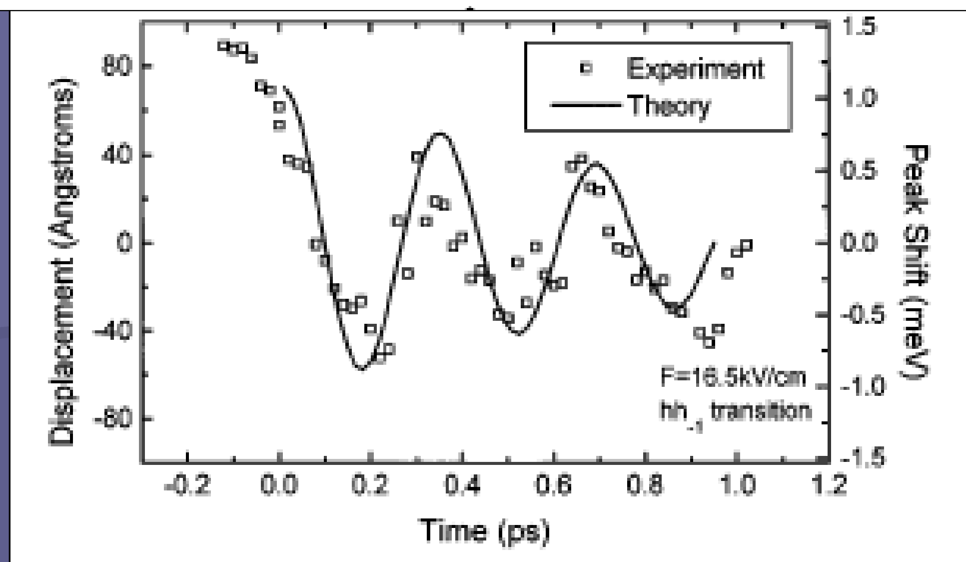
Felix Bloch

$$\omega_B = eUd/\hbar$$

$$L_B = 2A_B = W/eU$$

VOLUME 79, NUMBER 2 PHYSICAL REVIEW LETTERS 14 JULY 1997

Direct Measurement of the Spatial Displacement of Bloch-Oscillating Electrons in Semiconductor Superlattices



Bloch-like oscillations in DNA

Homopolymer DNA: poly(G)-poly(C) poly(A)-poly(T)

$$i\hbar \frac{d\psi_n}{dt} = -Un\psi_n - T(\psi_{n+1} + \psi_{n-1}) + \chi y_n \psi_n,$$

$$m\frac{d^2y_n}{dt^2} = -V'_M(y_n) - W'(y_n, y_{n-1}) - W'(y_n, y_{n+1}) - \chi|\psi_n|^2$$

n=1..(N sites)
a=3.4Å (lattice period)
m=300amu
T =0.1eV
U and χ variables

V_0 =0.04V α=4.45Å

$$V_M(y_n) = V_0(e^{-\alpha y_n} - 1)^2$$

k=0.04 eV/Å^2 β=0.35Å^{-1}

$$W(y_n, y_{n-1}) = \frac{k}{4}(2 + e^{-\beta(y_n + y_{n-1})})(y_n - y_{n-1})^2.$$

(Fitting parameters for experimental melting curves, PRE **47** R44 (93))

Initial Polaron State. Unbiased System

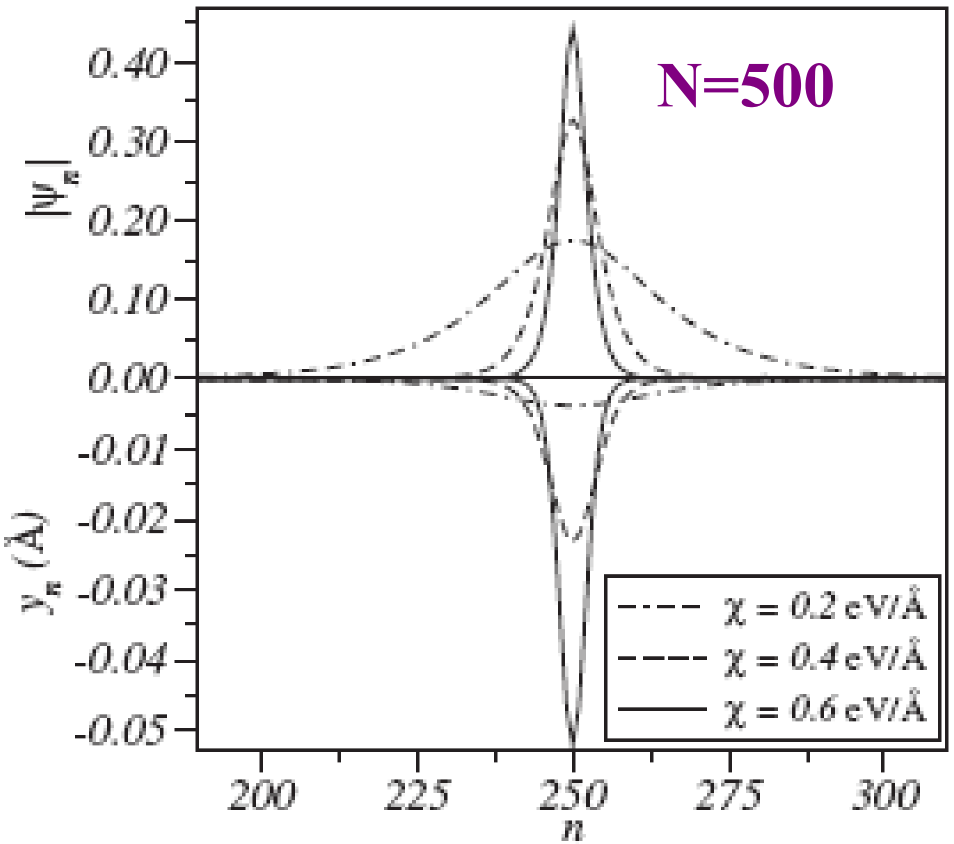
$$m\frac{d^2y_n}{dt^2} = -V'_M(y_n) - W'(y_n,y_{n-1}) - W'(y_n,y_{n+1}) - \chi|\psi_n|^2 - \gamma m\frac{dy_n}{dt}$$

U=0 mV/Å
γ=50 THz

Runge-Kutta method
4th order

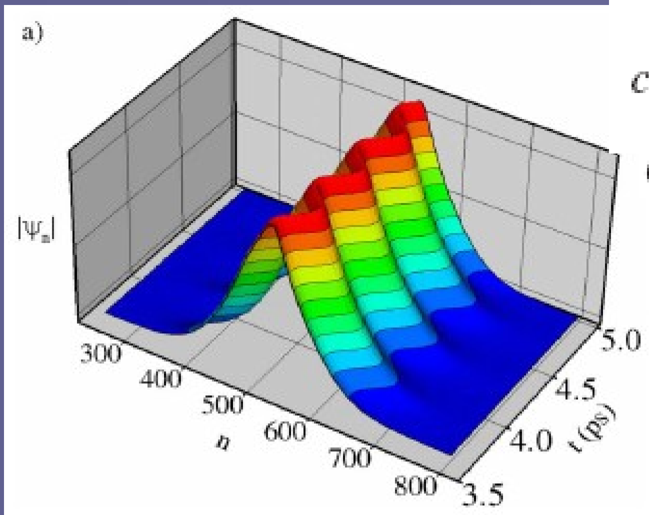
Rigid boundary conditions

Gaussian-like functions
↓
Stationary polaronic ground state



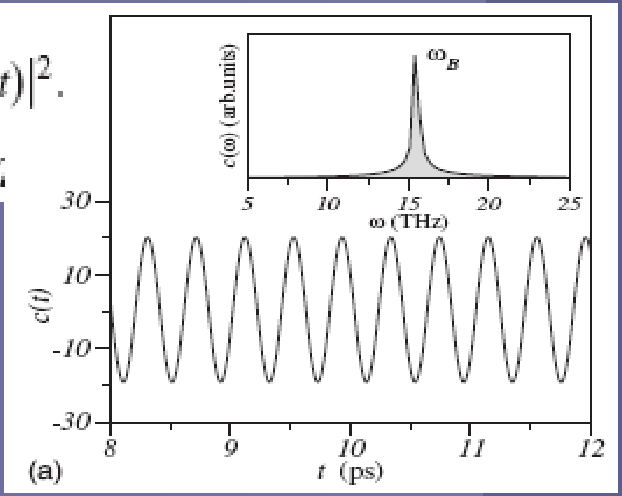
Biased Non-dissipative System. Polaron Dynamics

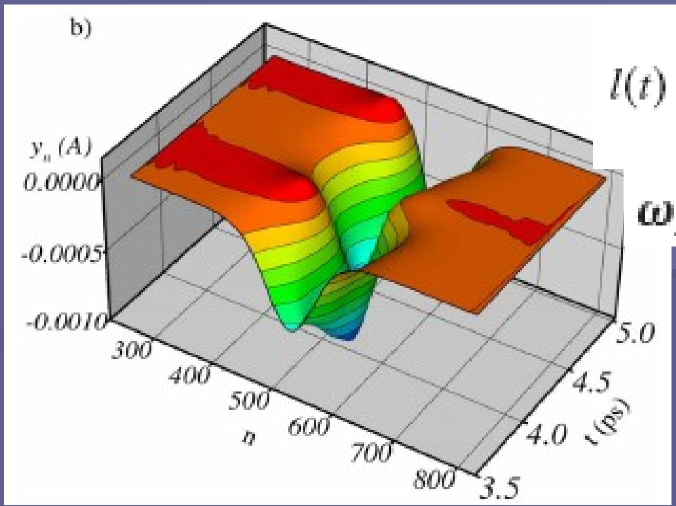
N=1000 F=3mV/Å χ=0.1eV/Å



$$c(t) = x(t) - x(0), \quad x(t) = \sum_{n=1}^{N} n|\psi_n(t)|^2.$$

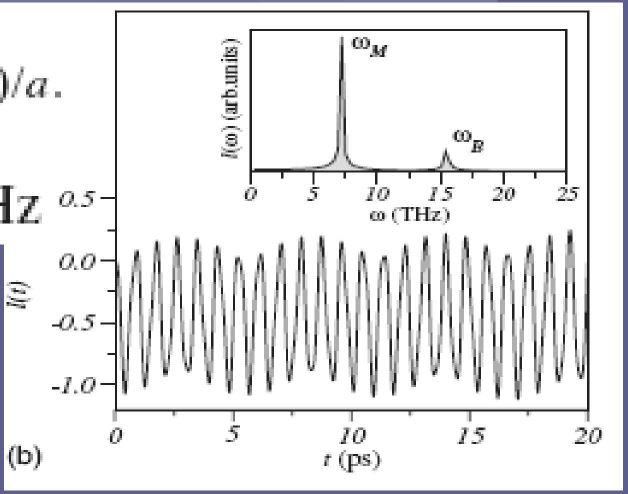
$$\omega_B = eFa/\hbar = 15.502 \text{ TH}$$





$$l(t) = \xi(t) - \xi(0), \quad \xi(t) = \sum_{n=1}^{N} n y_n(t)/a.$$

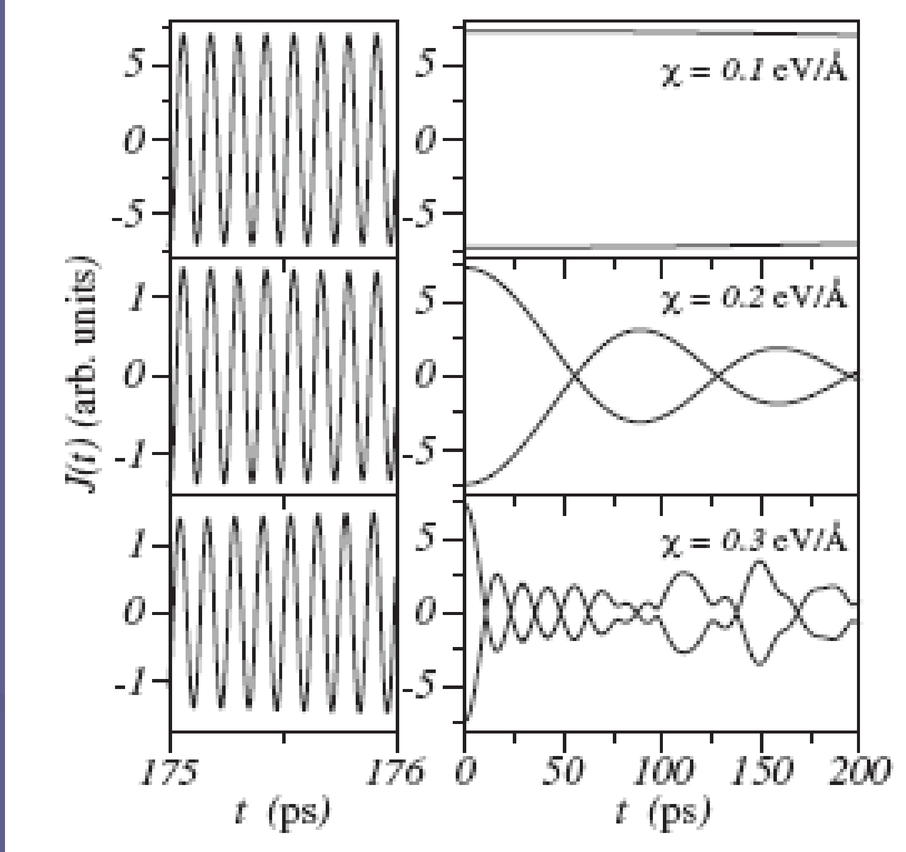
$$\omega_M = \alpha\sqrt{2V_0/m} = 7.138 \text{ THz}$$

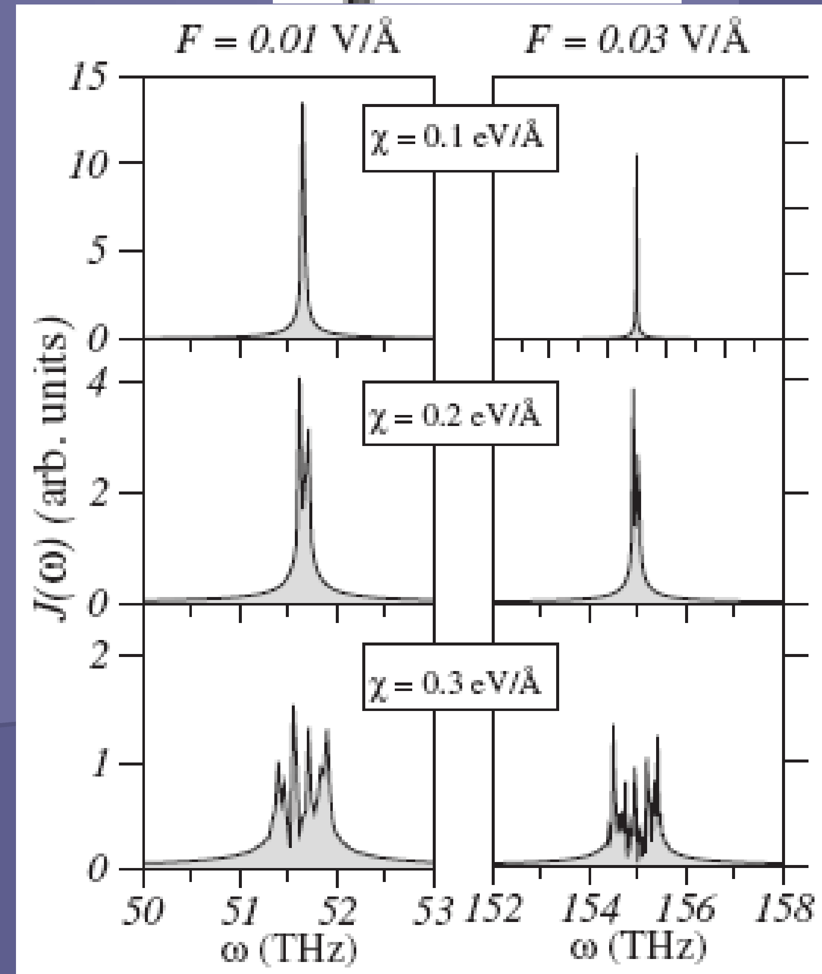


Biased Non-dissipative System. Average Current Density N=1000

$$J(t) = \frac{\hbar e}{m_e N a^2} \sum_{n=1}^{N} \mathrm{Im}[\psi_n^*(\psi_{n+1} - \psi_{n-1})],$$

$$\omega_B = eFa/\hbar$$





Conclusions

- Bloch Oscillations arise even considering charge-lattice coupling in a biased system within the Peyrard-Bishop-Holstein model.

- DNA may be a potential candidate for electronic applications in THz range. i.e. Bloch frequency ~ 15-150THz

- The charge-lattice coupling should be as small as possible to allow BO. Berashevich et al. (J. Phys. Condens. Matter 20 075104 (08))

  χ(poly(A)-poly(T))~0.4eV/Å <χ(poly(G)-poly(C))~1.0eV/Å

  χ decreases by increasing the number of nucleotides

- Our results should be relevant at short times after the initial excitation since the scattering destroys the coherence neccesary to see BO. Lakno and Fialko (Pis`ma Zh. Eksp. Teor. Fiz. 79 575 (04))

  $\tau_{scatt} \sim T^{-2/3}$ $\tau_{scatt} > \tau_{Bloch}$ i.e. F=3.0 meV/Å $T < T_{min} \sim 50K$

Thanks for the attention