

## Static and steady State of polarons in DNA system

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### Abstract

This study investigate in details the effect of the phonon vibration on the electrical properties for some short sequences of DNA. The theoretical study is based on the Anderson-Holstein model Hamiltonian for small polaron and on the extended Holstein model Hamiltonian for large polaron. These models provides a convenient description of the charge transport with local and non-local electron –phonon on site interaction. It is extensively, investigated the properties of the stationary state polaron and the stady state polaron. Where, It is showed that the system parameters such us local and non-local electron-phonon interactions, the electron interaction between DNA bases, the DNA base vibration frequency and base on site energy all have pronounced effects on all kinds of polarons states .

**Key words:** local and non-local electron-phonon interactions, Steady State of Polarons, Static of Polarons

## الحالة الثابتة والمستقرة للبولارون في نظام DNA

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### الخلاصة

تم دراسة تأثير اهتزاز الفونون على الخصائص الكهربائية لبعض سلاسل قصيرة من الحمض النووي وبصورة مفصلة. حيث نتجت دراسة نظرية الى نموذج هاميلتونيان أندرسون هول سرتاين للبولارون الصغير وعلى نموذج هاميلتونيان هول سرتاين الموسع للبولارون الكبير. وتوفر هذه النماذج وصفا ملائما لنقل الشحنة بوجود التفاعل الموضعي غير الموضعي للالكترون والفونون وتم التحقق على نطاق واسع في خصائص الحالة الثابتة والمستقرة للبولارون. حيث تبين لنا أن معاملات النظام مثل تفاعلات الإلكترون والفونون المتموضعة وغير المتموضعة، وتفاعل الإلكترون بين قواعد الحمض النووي، وترددات الاهتزاز لقاعدة الحمض النووي وطاقة القاعدة لها تأثيرات مهمة على جميع أنواع حالات البولارون.

**الكلمات المفتاحية:** التفاعل الموضعي وغير الموضعي للإلكترون والفونون، الحالة الثابتة للبولارون، الحالة المستقرة للبولارون.

## Introduction

We study the electron-phonon coupling effects on the electron transfer through vibrating DNA molecules we choice two models, the first model describes the interaction of charges with local vibration (small polaron) and second model describes the interaction of charges with local and non-local vibration (large polaron). Our concern in this paper is to investigate the effects of the system parameters on the static as well as dynamic states of the polaron in DNA system.

Our concern in this paper is to investigate a Hamiltonian model describing the DNA coupling under the presence of dynamic structural fluctuations. Such local and non-local vibrations, are known to strongly influence charge transfer in DNA molecules [1, 2, 3, 4]. For simplicity, we consider a system bases sites where electronic degree of freedom is coupled to an effective local vibrational degree of freedom. Let us assume that initially the charge is entirely localized on the  $j^{\text{th}}$  base site (source base) with energy  $E_{B_j}$ , then, the tunneling of the charge takes place from this base (source base) to the other bases sites with the same energy.

### (1) Theoretical treatment for small polaron model

We choice dimensional dependent Holsten Hamiltonian which contain harmonic dispersion of optical phonons that contain N basis of DNA molecules, identifying every base pair with one electronic site. This is motivated by the fact that the molecular orbitals (HOMOs) of the charge carriers (holes) are located mainly on the purine bases, G or A [5,6]. In the small-polaron theory, which has been developed to describe strong electron vibration coupling is that every DNA base can vibrate (quasi) independently from its neighbors, i.e. every site is connected to an independent oscillator. Thus, the Hamiltonian is read as[6],

$$\begin{aligned} \hat{H} = & \sum_i E_{B_i} C_{B_i}^+(t) C_{B_i}(t) + \sum_i \hbar \omega_i (B_i^+(t) B_i(t) + 1/2) \\ & + \sum_i \lambda_i C_{B_i}^+(t) C_{B_i}(t) (B_i(t) + B_i^+(t)) \\ & + \sum_i [t_{ii+1} C_{B_i}^+(t) C_{B_{i+1}}(t) + t_{ii-1} C_{B_i}^+(t) C_{B_{i-1}}(t) + c.c.] \end{aligned} \quad (1)$$

Where,  $C_{B_i}^+(t)$ ; ( $C_{B_i}(t)$ ) denotes the creation (annihilation) operator, with  $E_i$  represents the  $i^{\text{th}}$  energy level position, with the index  $i$  denote the base number. The vibronic degrees of freedom are described by the boson operators  $B_i^+$  and  $B_i$  for the vibron with frequency  $\omega_i$ . The  $t_{ij}$  is represent the coupling interaction constant between the bases number  $i$  and  $j$ , with  $t_{ij} = t_{ji}$ . The parameter  $\lambda_i$  is

the electron-phonon coupling which represent the interaction between the electronic charge and the vibrated of the base in  $i^{th}$  site.

Equation of motion for  $C_{Bi}(t)$  can be obtained by using [7],

$$\dot{C}_{Bi}(t) = -\frac{d\hat{H}(t)}{dC_{Bi}(t)} \quad \dots(2)$$

$$\dot{C}_{B1}(t) = -\frac{i}{\hbar} \left\{ [E_{B1} + \lambda_1(B_1(t) + B_1^+(t))]C_{B1}(t) + t_{12}C_{B2}(t) \right\} \quad \dots(3a)$$

$$\dot{C}_{BN}(t) = -\frac{i}{\hbar} \left\{ [E_{BN} + \lambda_N(B_N(t) + B_N^+(t))]C_{BN}(t) + t_{N,N-1}C_{Bn-1}(t) \right\} \quad (3b)$$

$$\dot{C}_{Bi}(t) = -\frac{i}{\hbar} \left\{ [E_{Bi} + \lambda_i(B_i(t) + B_i^+(t))]C_{Bi}(t) + t_{i,i-1}C_{Bi-1}(t) + t_{ii+1}C_{bi+1}(t) \right\} \quad 1 < i < N \quad (3c)$$

$$\dot{B}_i(t) = -\frac{i}{\hbar} \left\{ \hbar\omega_i B_i(t) + \lambda_i C_{Bi}^+(t) C_{Bi}(t) \right\} \quad \dots (3d)$$

## (2) Stationary state of small polaron

The stationary state solution technique allow us to discuss the static state polaron for our model, then we used the following stationary state technique,

$$0 = \left\{ [E_{B1} + \lambda_1(B_1 + B_1^+)]C_{B1} + t_{12}C_{B2} \right\} \quad \dots(4a)$$

$$0 = \left\{ [E_{BN} + \lambda_N(B_N + B_N^+)]C_{BN} + t_{N,N-1}C_{Bn-1} \right\} \quad \dots(4b)$$

$$0 = \left\{ [E_{Bi} + \lambda_i(B_i + B_i^+)]C_{Bi} + t_{i,i-1}C_{Bi-1} + t_{ii+1}C_{bi+1} \right\} \quad 1 < i < N \quad (4c)$$

$$0 = \left\{ \hbar\omega_i B_i + \lambda_i C_{Bi}^+ C_{Bi} \right\} \quad \dots (4d)$$

$$B_i = -\frac{\lambda_i}{\hbar\omega_i} n_i \quad \dots (5)$$

In order to solve the system of linear equations which described by eqs.(4), we construct the following matrix-form equation after defining,

$$A_i = E_{Bi} + \lambda_i(B_i + B_i^+); \quad G = t; \quad t = t_{ij} \quad \dots (6)$$

$$\begin{array}{cccccccccc|c|c|c|c|c|c|c|c|c|c}
 A_1 & G & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & C_{B1} & & & & & & & & & & 0 \\
 G & A_2 & G & 0 & 0 & 0 & 0 & 0 & 0 & 0 & C_{B2} & & & & & & & & & & 0 \\
 0 & G & 0 \\
 0 & 0 & & & & & G & & & & & & & & & & & & & & & 0 \\
 0 & 0 & & & G & A_{j-1} & & & & & & & & & & & & & & & & -GC_{Bj} \\
 0 & 0 & & & & & & A_{j+1} & G & & & & & & & & & & & & & -GC_{Bj} \\
 0 & 0 & & & & & & G & & & & & & & & & & & & & & 0 \\
 0 & 0 & & & & & & & & G & & & & & & & & & & & & 0 \\
 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & G & A_{N-1} & G & & & & & & & & & & 0 \\
 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & G & A_N & C_{BN} & & & & & & & & & 0
 \end{array} \dots(7)$$

Assume, initially the base number  $j$  is the donor base i.e.  $C_{Bj} = 1$ . Then, solving the above set of equations (eqs.(7)) to obtain the values of  $C_{Bi \neq j}$ . However, we can determined the charge on the

source base  $j$  by,  $C_{Bj}^2 = 1 - \sum_{i \neq j} C_{Bi}^2$

The displacement or the stretching length is related to,

$$X_i = (B_i + B_i^+) = -2 \frac{\lambda_i^2}{\hbar \omega_i} C_{Bi}^2$$

In the following, we suppose the charge initially is localized on the 5<sup>th</sup> base site (we call it donor base).

For this model, there are two important functions depends on the number of bases, namely the charge on the bases  $C_{Bi}^2$ , the quantity related to the displacement or the stretching length  $X_i$ . And, one needs to study the effect of the following system parameters, the electron-vibration coupling constant  $\lambda_i = \lambda_o$ , the electron transfer integral  $t_{ij} = t$  and the frequency of vibration  $\omega_i = \omega_o$ .

Fig.(1a,b) shows the vibration coupling constant  $\lambda_o$  effects the charge distribution  $C_{Bi}^2$  and the stretching length  $X_i$  as a function of bases number.

It is obvious that a narrower and higher polaron will form when the value of  $\lambda_o$  increases, i.e., increasing the localization of charge in their site. When the value of  $\lambda_o$  is nearly 1.0 eV, a polaron will extend only a few base pairs, even locate at one base pair for large values of  $\lambda_o$ . Contrasting to the effect of a vibration coupling constant, the increasing values of a transfer integral and vibration frequency can make polaron more extended as depicted in fig.(2a,b) and fig.(3a,b). The value of the charge transfer integral  $t$  depends on the configuration of the DNA geometry and the solvent

environment [8]. Experiments shows  $t$  might be smaller far from 0.01 eV [8,9], while the scope of 0.05–0.3 eV is estimated theoretically [10,11].

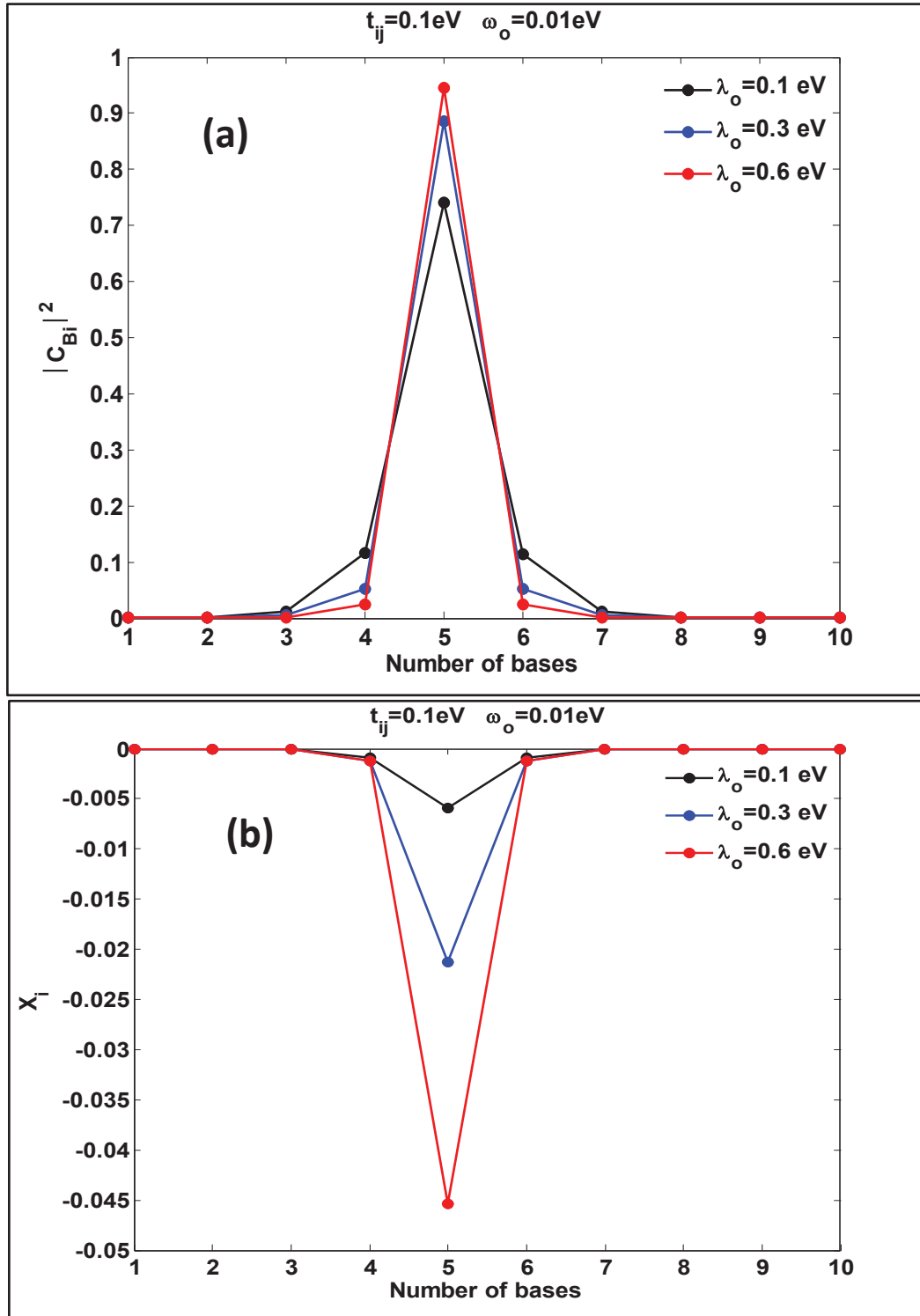


Fig.(1): The influence of the vibration coupling constant  $\lambda_o$  on (a) the charge distribution  $C_{Bi}^2$  and on (b) the stretching length  $X_i^-$ .

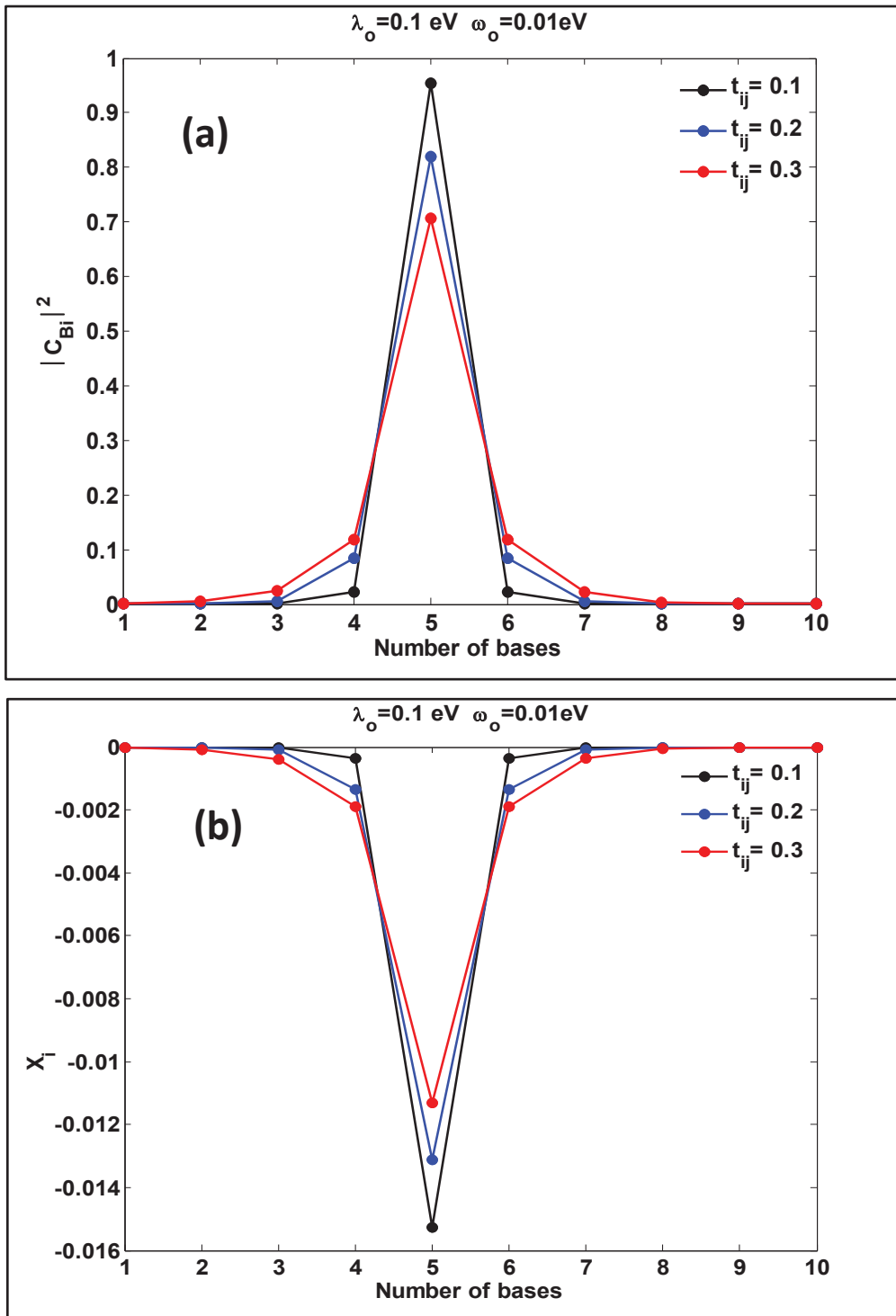


Fig.(2): The effect of increasing the values of transfer integral  $t_{ij}$  on (a) the charge distribution  $C_{Bi}^2$  and on (b) the stretchinglength  $X_i$ .

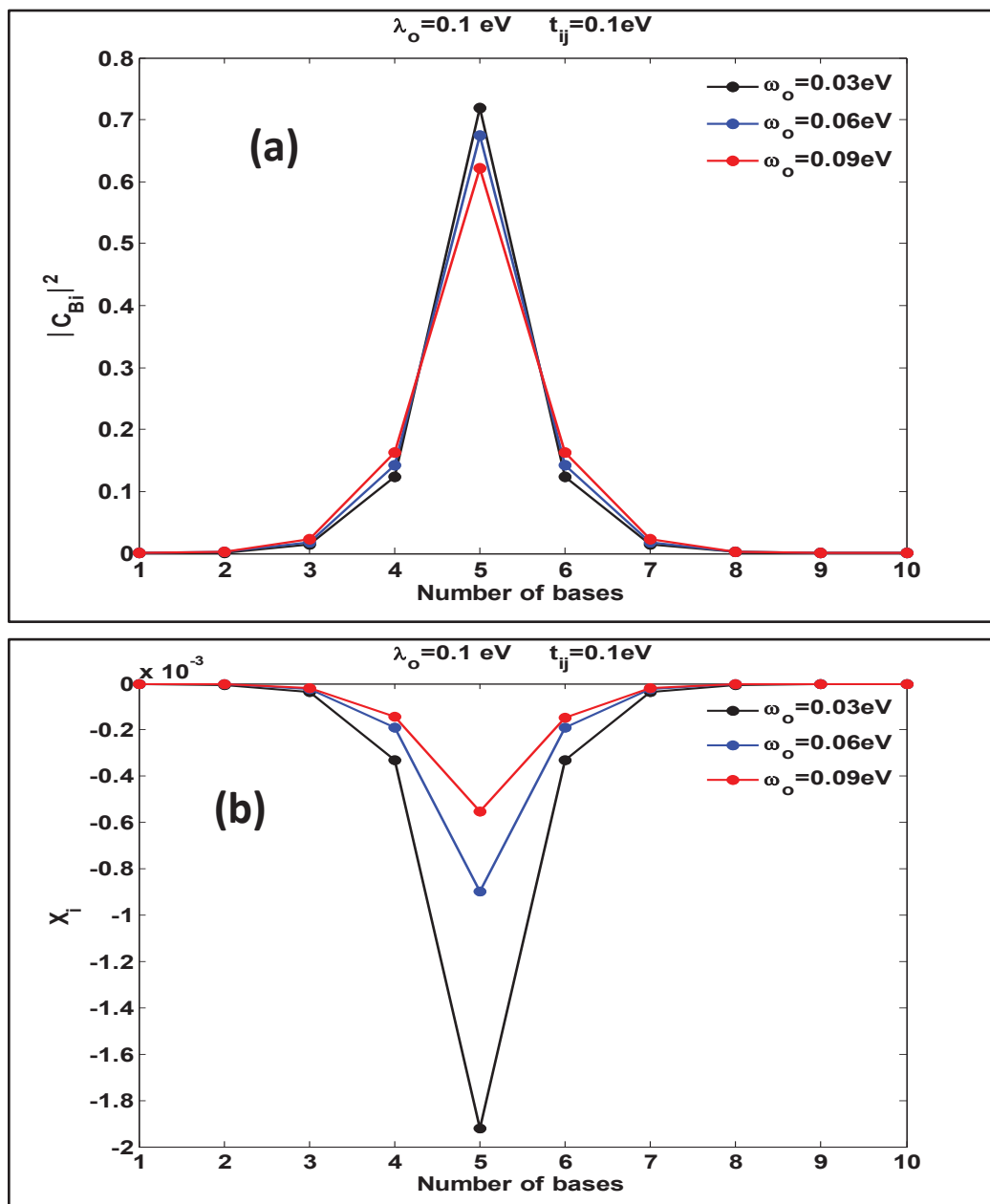


Fig.(3): The effect of increasing the values of vibration frequency  $\omega_o$  on (a) the charge distribution

$C_{Bi}^2$  and on (b) the stretching length  $X_i$ .

From the result of figs.(1,2,3),we note that

- 1- On increasing the electron-phonon coupling  $\lambda_o$  it led to:
  - a- Localization of the charge on the base (charge increases on the 5<sup>th</sup> base (donor base) and decreases on the others).
  - b- Consequently, the value of the stretching length of the corresponding base is increased (due to the increasing of the Coulomb force).



- 2- When increasing the hopping integral  $t$  between the bases led to:
  - a- Largely charge decreasing on the base (5<sup>th</sup>base) due to increasing the hopping of the charge to other bases.
  - b- Consequently, the value of the stretching length decreases for the corresponding base (5<sup>th</sup>base) and it is increases for other bases.
- 3- When increasing the vibration frequency  $\omega_o$  led to the charge decreasing on the base (5<sup>th</sup>base) and increases on the other bases. Consequently, the value of the stretching length of the corresponding 5<sup>th</sup> base is also decreased, while it is increases for the others.

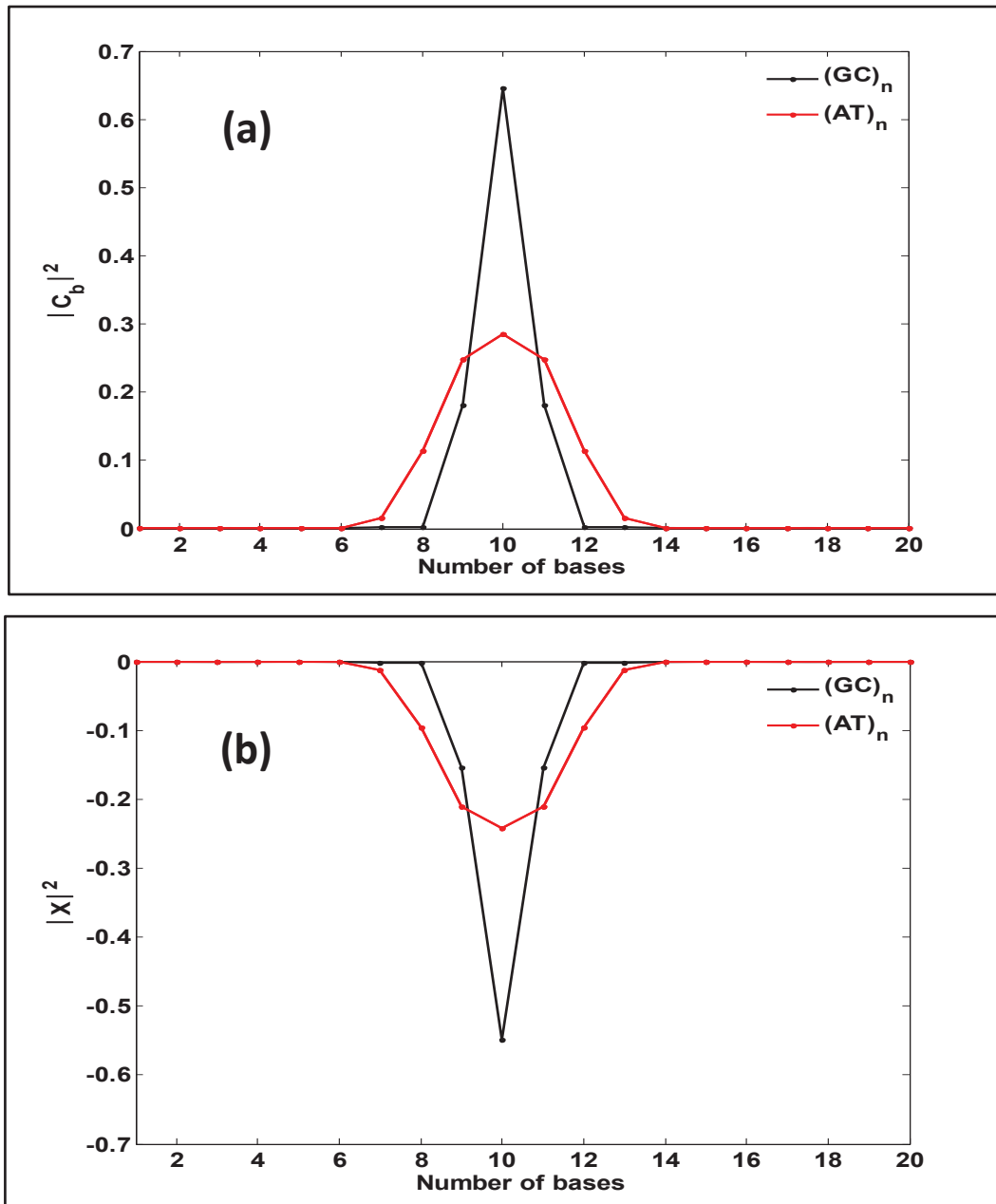
The polaron play an important role in the process of charge migration through duplex DNA stack. We investigate properties of hole polarons in DNA molecules containing identical base pairs, either poly(G)-poly(C) or poly(A)-poly(T). The transfer integral and electron-phonon coupling parameters, according to the theoretical calculations have different values for different base pair dimers.

Fig(4) show the Properties of hole polarons in poly(G)-poly(C) and poly(A)-poly(T) DNA molecules, where we see that the polaron in poly(A)-poly(T) has a larger width than polaron in poly(G)-poly(C) DNA molecule, and the hole state in poly(A)-poly(T) is more delocalized than that in the other DNA duplex this results can be interpreted because the transfer integral between GC base pairs is larger than that between AT base pairs in magnitude as calculated with *ab initio* approach[12].

The polaron in the consecutive AT DNA stack is approximately 8 sites wide, while the width of polaron in the other DNA chain is only approximately 4 sites i.e, it is more localize. At the central site of the polaron region, both charge population and relative displacement reach their maximum (absolute value for the relative displacement)[12].

Table (1) the parameters of poly (G)-poly(C) and of poly (A)-poly (T) all in eV units[12].

Types of DNA chain	$E_{B_i}$	$\lambda_o$	$t$	$\omega_o$
$(GC)_n$	-0.35	0.365	0.188	0.016
$(AT)_n$	-0.85	0.164	0.081	0.011



Fig(4): The charge distribution and the stretching length of polaron in poly(G)-poly(C) (a) and in poly(A)-poly(T) DNA (b) molecules with parameters listed in table(2-1).

For the polaron in poly(G)-poly(C), the maximum of charge density is about 0.64, and the greatest reduction of separation distance is about  $-0.55 \text{ \AA}$ . For the polaron in poly(A)-poly(T), the maximum of charge density is about 0.29, and the minimum  $X$  is only  $-0.26 \text{ \AA}$ .

### (3) Steady state of small polaron

To evaluate the energy of small polaron we apply the steady state solution to our system equations. The following steady state technique will be applied,

$$C_X(t) = C_X e^{-iEt/\hbar}$$

Then, we have a similar set of equations as eqs.(4):

$$0 = \{ [E_{B1} - E + \lambda_1(B_1 + B_1^+)]C_{B1} + t_{12}C_{B2} \} \quad \dots(8a)$$

$$0 = \{ [E_{BN} - E + \lambda_N(B_N + B_N^+)]C_{BN} + t_{N,N-1}C_{Bn-1} \} \quad (8b)$$

$$0 = \{ [E_{Bi} - E + \lambda_i(B_i + B_i^+)]C_{Bi} + t_{i,i-1}C_{Bi-1} + t_{ii+1}C_{bi+1} \} \quad 1 < i < N \quad (8c)$$

$$0 = \{ \hbar\omega_i B_i + \lambda_i C_{Bi}^+ C_{Bi} \} \dots (8d)$$

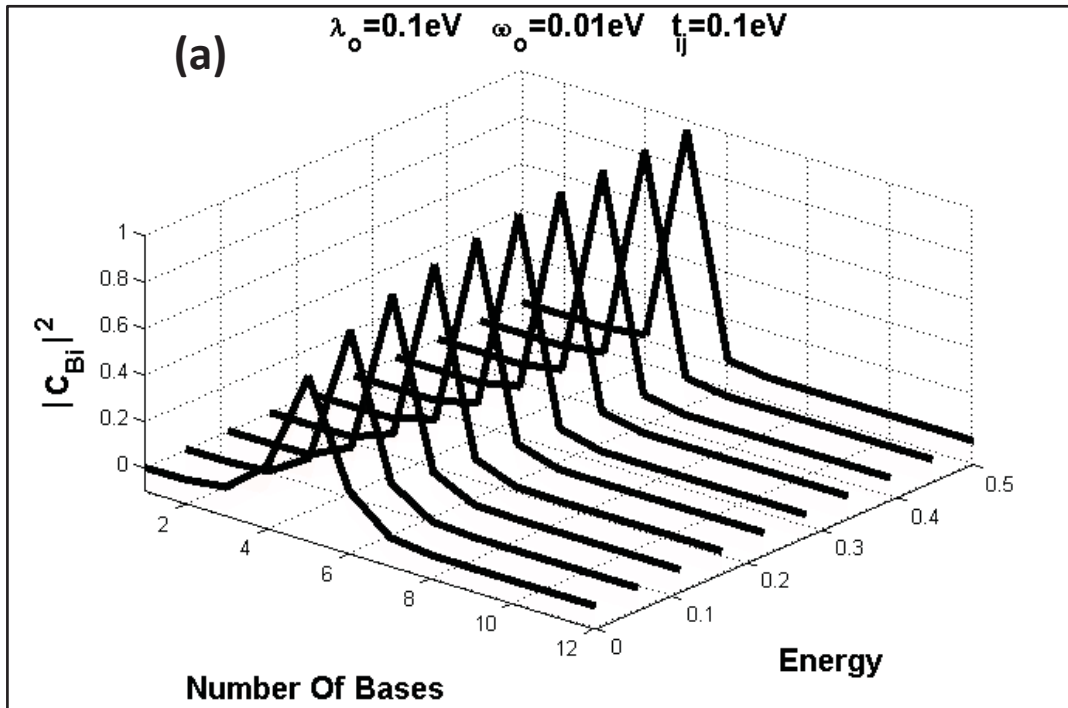
The system of the above linear equations (eqs.(8)) can be put in the following matrix-form equation,

it has same shape as eq.(7) with, ( $t = t_{ij}$ ), and,

$$A_i = E_{Bi} - \lambda_i X_i - E, \quad G = t \quad \dots(9)$$

We note that, increasing the polaron energy led to:

- 1- The polaron become higher, narrower and more localized.
- 2- The central base charge and its stretching length are increases.
- 3-



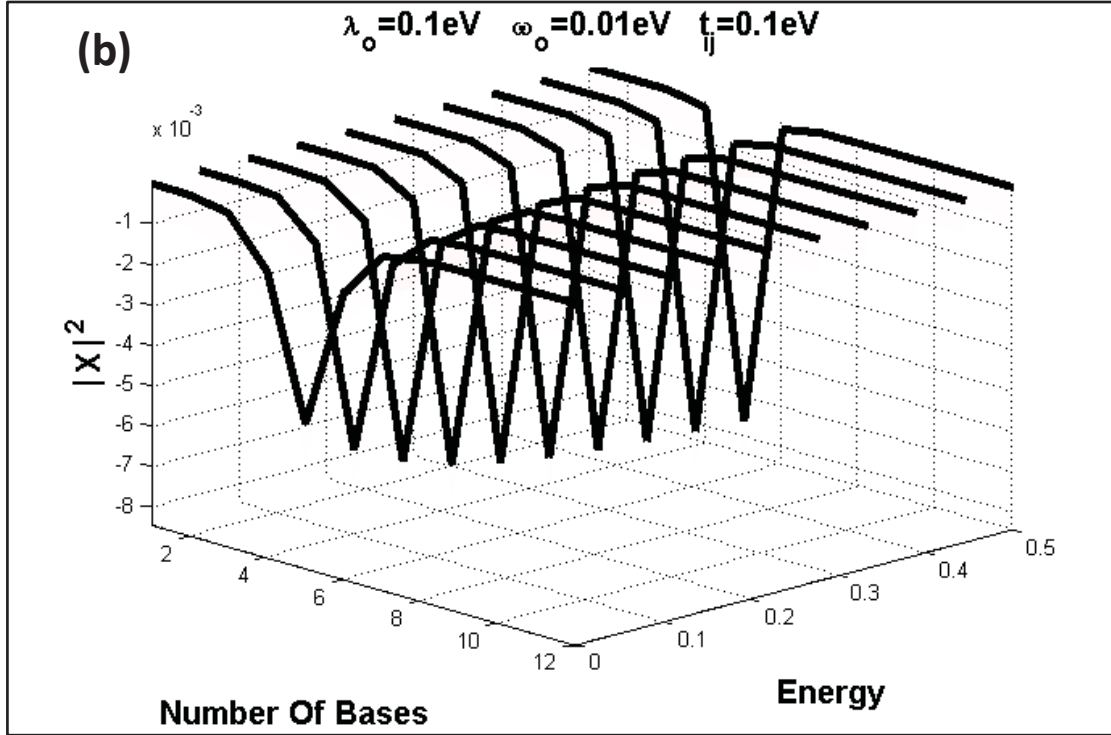


Fig.(5):The steady state of a small polaron (a) The charge distributions on the bases and (b) The corresponding stretching length all as a functions to polaron energy E.

#### (4)Theoretical treatment for large polaron model

We considered a DNA sequence with N base pairs, the first and last of which are coupled to semi-infinite metal electrodes. We further allow for a coupling to (in general multiple) vibrational modes, that can be excited by local and non-local coupling to the charge carriers on the DNA. When later performing the numerical calculations we will restrict ourselves to a single vibrational mode of the DNA, base pair, e.g., the ‘stretch’ mode [13]. We consider an extended Holstein model of an electron hopping between two sites, but interacting with all surrounding ions of the lattice via a long-range electron-phonon coupling, like in a simple case of a one dimensional ionic chain, vibrating in the direction perpendicular to the chain[6], the Hamiltonian is read as,

$$\begin{aligned}
 \hat{H} = & \sum_i E_{Bi} C_{Bi}^+(t) C_{Bi}(t) + \sum_{\alpha} \hbar \omega_{\alpha} (B_{\alpha}^+(t) B_{\alpha}(t) + 1/2) + \\
 & \sum_{\alpha} \sum_i \lambda_i C_{Bi}^+(t) C_{Bi}(t) (B_{\alpha}(t) + B_{\alpha}^+(t)) + \\
 & \sum_{\alpha} (B_{\alpha}^+(t) + B_{\alpha}(t)) \sum_i [\lambda_{ii+1} C_{Bi}^+(t) C_{Bi+1}(t) + \lambda_{ii-1} C_{Bi}^+(t) C_{Bi-1}(t)] \\
 & + \sum_i [t_{ii+1} C_{Bi}^+(t) C_{Bi+1}(t) + t_{ii-1} C_{Bi}^+(t) C_{Bi-1}(t)]
 \end{aligned} \tag{10}$$

The vibronic degrees of freedom are described by boson operators  $B_\alpha^+$  and  $B_\alpha$  for the vibron mode  $\alpha$  with frequency  $\omega_\alpha$ . where  $\lambda_i$  and  $\lambda_{ij}$  are the strengths for the local and non-local electron-vibron coupling, respectively. We further restrict our self the non-local coupling terms to nearest neighbors,  $\lambda_{ij} = \lambda_1 \delta_{i,j=i\pm 1}$ . Note that, the vibron modes and their coupling to electrons assumed independent of the base pairs involved, an approximation that is reasonable for some modes of interest, including the base pair stretch mode [13].

The equation of motion for  $C_{Bi}(t)$  can be obtained by using eq.(2) to get,

$$\dot{C}_{B1}(t) = -\frac{i}{\hbar} \left\{ \begin{array}{l} [E_{B1} + \lambda_1 \sum_{\alpha} (B_{\alpha}(t) + B_{\alpha}^+(t))] C_{B1}(t) \\ + \lambda_{12} \sum_{\alpha} (B_{\alpha}(t) + B_{\alpha}^+(t)) C_{B2}(t) + t_{12} C_{B2}(t) \end{array} \right\} \dots(11a)$$

$$\dot{C}_{BN}(t) = -\frac{i}{\hbar} \left\{ \begin{array}{l} [E_{BN} + \lambda_N \sum_{\alpha} (B_{\alpha}(t) + B_{\alpha}^+(t))] C_{BN}(t) \\ + \lambda_{NN-1} \sum_{\alpha} (B_{\alpha}(t) + B_{\alpha}^+(t)) C_{BN-1}(t) + t_{NN-1} C_{BN-1}(t) \end{array} \right\} (11b)$$

$$\dot{C}_{Bi}(t) = -\frac{i}{\hbar} \left\{ \begin{array}{l} [E_{Bi} + \lambda_i \sum_{\alpha} (B_{\alpha}(t) + B_{\alpha}^+(t))] C_{Bi}(t) \\ + \sum_{\alpha} (B_{\alpha}(t) + B_{\alpha}^+(t)) [\lambda_{ii+1} C_{Bi+1}(t) \\ + \lambda_{ii-1} C_{Bi-1}(t)] + t_{ii+1} C_{Bi+1}(t) + t_{ii-1} C_{Bi-1}(t) \end{array} \right\} 1 < i < N (11c)$$

$$\dot{B}_{\alpha}(t) = -\frac{i}{\hbar} \left\{ \begin{array}{l} \hbar \omega_{\alpha} B_{\alpha}(t) + \sum_i \lambda_i C_{Bi}^+(t) C_{Bi}(t) \\ + \sum_i [\lambda_{ii+1} C_{Bi}^+(t) C_{Bi+1}(t) + \lambda_{ii-1} C_{Bi}^+(t) C_{Bi-1}(t)] \end{array} \right\} (11d)$$

### (5) The stationary state of a large polaron:

We apply the stationary state solution technique to allow us to discuss the static state for the large polaron model, then equations (eqs.(11)) gives,

$$0 = \left\{ \begin{array}{l} [E_{B1} + \lambda_1 \sum_{\alpha} (B_{\alpha} + B_{\alpha}^+)] C_{B1} + \\ \lambda_{12} \sum_{\alpha} (B_{\alpha} + B_{\alpha}^+) C_{B2} + t_{12} C_{B2} \end{array} \right\} \quad 0 = \left\{ \begin{array}{l} [E_{BN} + \lambda_N \sum_{\alpha} (B_{\alpha} + B_{\alpha}^+)] C_{BN} \\ + \lambda_{NN-1} \sum_{\alpha} (B_{\alpha} + B_{\alpha}^+) C_{BN-1} + t_{NN-1} C_{BN-1} \end{array} \right\} (12a)$$

(12b)

$$0 = \left\{ \begin{array}{l} [E_{Bi} + \lambda_i \sum_{\alpha} (B_{\alpha} + B_{\alpha}^+)] C_{Bi} + \\ \sum_{\alpha} (B_{\alpha} + B_{\alpha}^+) [\lambda_{ii+1} C_{Bi+1} + \lambda_{ii-1} C_{Bi-1}] \\ + t_{ii+1} C_{Bi+1} + t_{ii-1} C_{Bi-1} \end{array} \right\} \text{ for } 1 < i < N \quad (12c)$$

$$0 = \left\{ \begin{array}{l} \hbar \omega_{\alpha} B_{\alpha} + \sum_i \lambda_i n_{Bi} + \\ \sum_i [\lambda_{ii+1} C_{Bi}^+ C_{Bi+1} + \lambda_{ii-1} C_{Bi}^+ C_{Bi-1}] \end{array} \right\} \quad (12d)$$

$$B_{\alpha} = - \left\{ \sum_i \lambda_i n_{Bi} + \sum_i [\lambda_{ii+1} C_{Bi}^+ C_{Bi+1} + \lambda_{ii-1} C_{Bi}^+ C_{Bi-1}] \right\} / \hbar \omega_{\alpha} \quad (12e)$$

Then, we have the same shape of matrix eq.(7), with,

$$A_i = E_{Bi} + \lambda_o \sum_{\alpha} (B_{\alpha} + B_{\alpha}^+) \quad G = t + \lambda_1 \sum_{\alpha} (B_{\alpha} + B_{\alpha}^+) \quad ; \quad t = t_{ij}$$

In fig.(2-9) and for certain value of  $\lambda_1 \neq 0$ , we show the influence of the local vibration coupling constant  $\lambda_i = \lambda_o$  on the charge distribution  $C_{Bi}^2$  and on the stretching length  $X_{\alpha}$ . However, now one can see the nonlocal effect of charge, since it spread on the bases. Increasing  $\lambda_o$  led to more localization of charge on the 5<sup>th</sup> base (donor) and faster decreases of the stretching length till it saturated to a zero value. In fig.(10) and for a certain value of  $\lambda_o$  we show the effect of increasing the nonlocal vibration coupling constant  $\lambda_{ij \neq i} = \lambda_1$  led to more charge increasing on the 5<sup>th</sup> base (donor base) and other bases, also increasing the stretching length.

The result of figs.(9,10,11,12) can be summarized as follow:

Increasing  $\lambda_o$  led to more localization of charge on the 5<sup>th</sup> base (donor base) and faster decreases of the stretching length till it saturated to a zero value.

When increasing the hopping integral  $t$  between the bases led to faster charge decreasing on the 5<sup>th</sup> base (donor base) due to increasing the hopping of the charge to other bases. Consequently, the absolute value of the stretching length decreases faster.

When increasing the vibration frequency  $\omega_o$  led to the charge decreasing on the 5<sup>th</sup> base (donor base) and faster decreases the value of the stretching length of the.

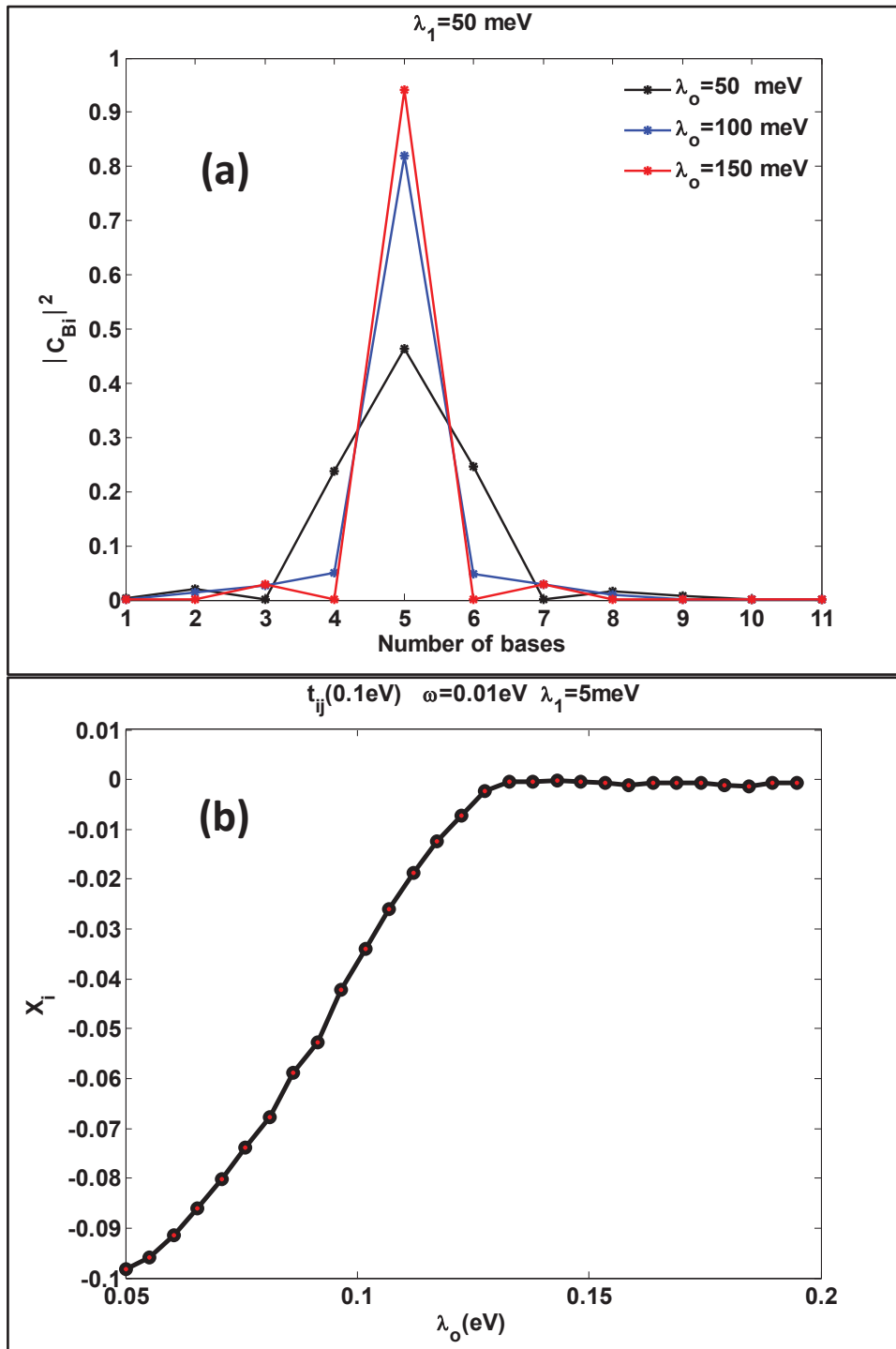


Fig.(6): The influence of the local vibration coupling constant  $\lambda_o$  on (a) the charge distribution on the bases  $C_{Bi}^2$  and (b) the stretching length  $X_\alpha$ .

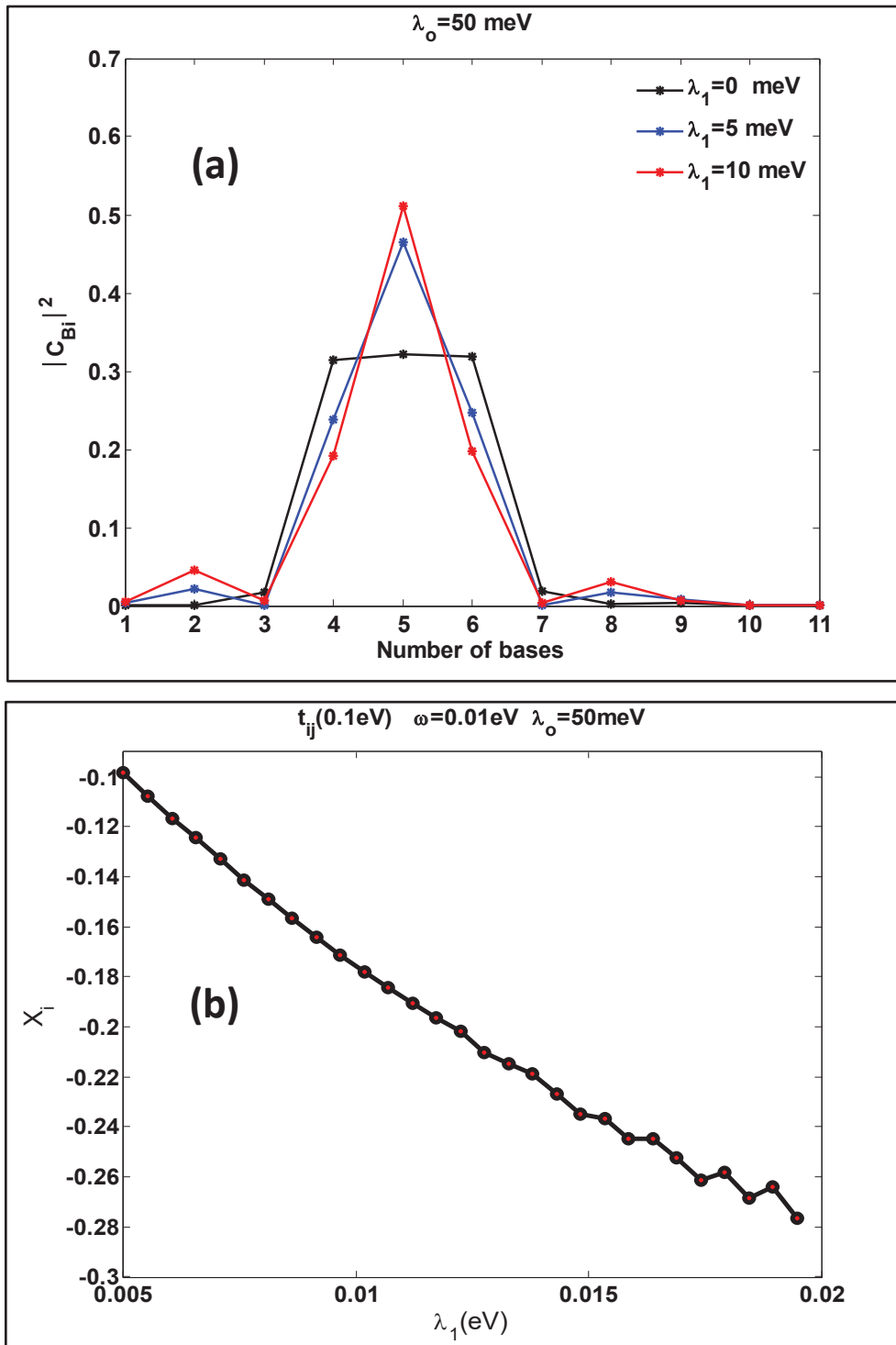


Fig.(7): The influence of the nonlocal vibration coupling constant  $\lambda_0$  on (a) the charge distribution on the bases  $C_{Bi}^2$  and (b) the stretching length  $X_\alpha$ .



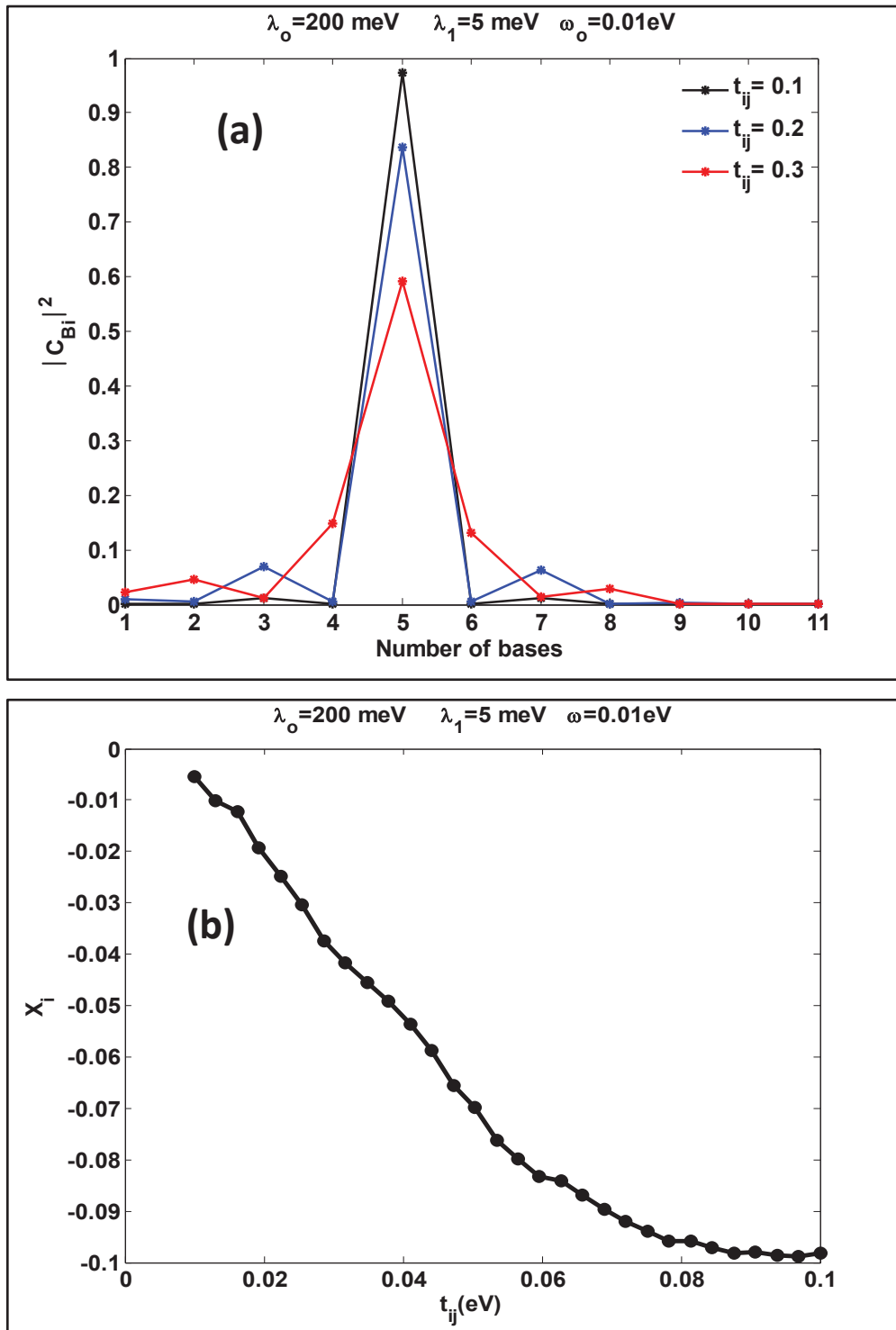


Fig.(8): The effect of increasing the values of a transfer integral  $t$  on (a) the charge distribution on the bases  $C_{Bi}^2$  and (b) the stretching length  $X_{\alpha}$ .

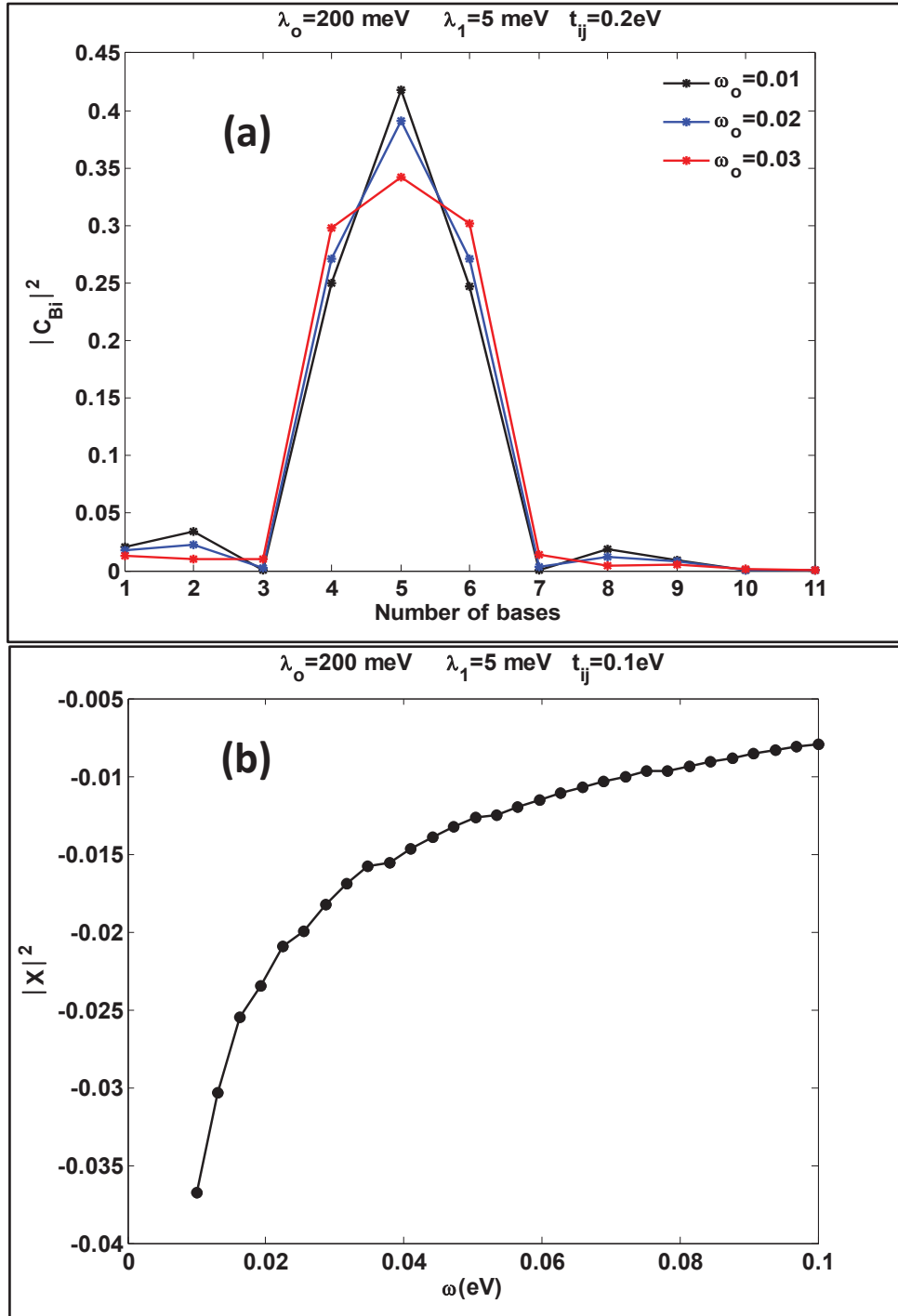


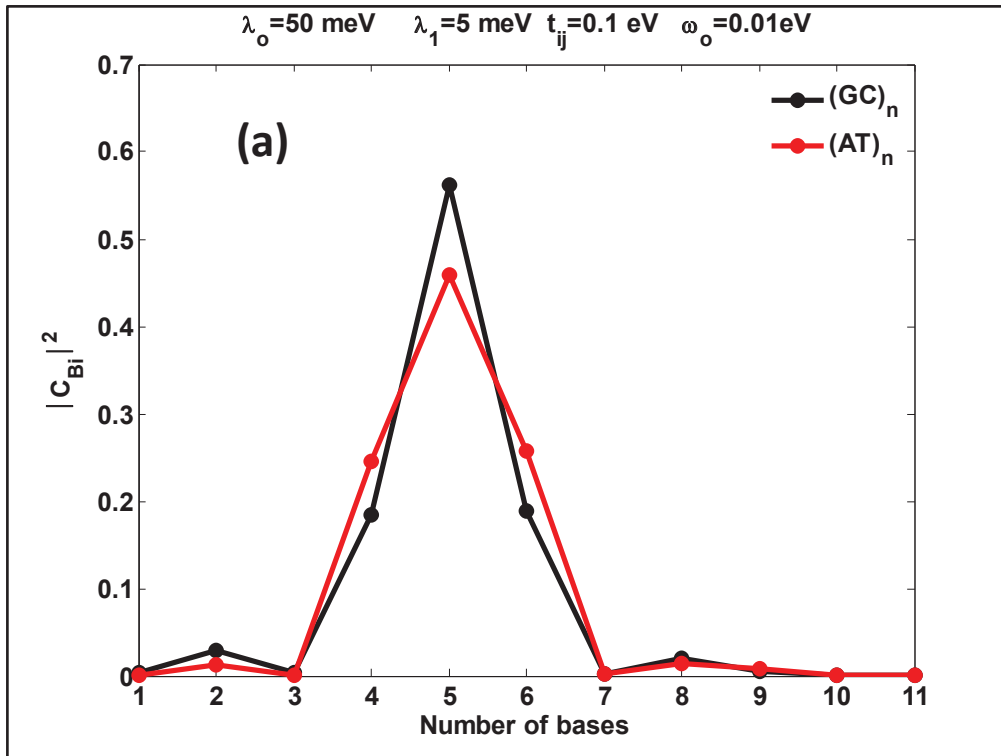
Fig.(9): The effect of increasing the values of vibration frequency  $\omega_o$  on (a) the charge distribution on the bases  $C_{Bi}^2$  and (b) the stretching length  $X_\alpha$ .

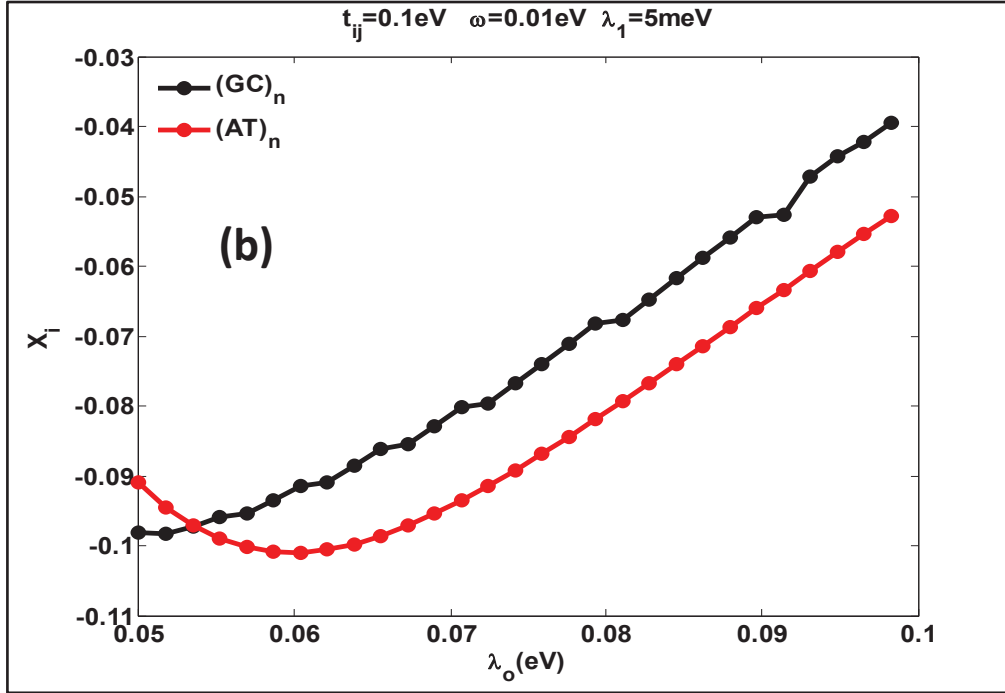
Also, we investigate properties of hole polarons in DNA molecules containing identical base pairs, either poly(G)-poly(C) or poly(A)-poly(T) in the presence of the nonlocal electron-phonon coupling parameters.

Fig(13) show the Properties of hole polarons in poly(G)-poly(C) and poly(A)-poly(T) DNA molecules, where we see that the polaron in poly(A)-poly(T) still has a larger width than polaron in poly(G)-poly(C) DNA molecule, and the hole state in poly(A)-poly(T) is less delocalized than that in the other DNA duplex this results can be interpreted because the larger transfer integral between GC base pairs than that in between AT base pairs.

At the central site of the polaron region, the charge population for GC base pairs is larger than that for AT base pairs and on increasing the local electron-phonon coupling  $\lambda_0$  then the relative displacement decreases for both kind of base pairs but small values for GC base pairs for the range  $\lambda_0 > 0.058$ .

For the polaron in poly(G)-poly(C), the maximum of charge density is about 0.57, and the greatest reduction of separation distance is about  $-0.091 \text{ \AA}$ . For the polaron in poly(A)-poly(T), the maximum of charge density is about 0.48, and the minimum  $X_\alpha$  is only  $-0.098 \text{ \AA}$ .





Fig(10): (a) The charge distribution as function of base number and (b) The stretching length of polaron as a function of  $\lambda_o$  in poly(G)-poly(C) and in poly(A)-poly(T) DNA molecules with  $E_{GC} = -0.35eV$ ,  $E_{AT} = -0.85eV$ .

#### (6) The steady state of a large polaron:

The steady state technique solution of our system equations (eqs.(11), give the following set of equations,

$$0 = \left\{ \begin{array}{l} [E_{B1} - E + \lambda_1 \sum_{\alpha} (B_{\alpha} + B_{\alpha}^+)] C_{B1} + \\ \lambda_{12} \sum_{\alpha} (B_{\alpha} + B_{\alpha}^+) C_{B2} + t_{12} C_{B2} \end{array} \right\} \quad (13a)$$

$$0 = \left\{ \begin{array}{l} [E_{BN} - E + \lambda_N \sum_{\alpha} (B_{\alpha} + B_{\alpha}^+)] C_{BN} \\ + \lambda_{NN-1} \sum_{\alpha} (B_{\alpha} + B_{\alpha}^+) C_{BN-1} + t_{NN-1} C_{BN-1} \end{array} \right\} \quad (13b)$$

$$0 = \left\{ \begin{array}{l} [E_{Bi} - E + \lambda_i \sum_{\alpha} (B_{\alpha} + B_{\alpha}^+)] C_{Bi} + \\ \sum_{\alpha} (B_{\alpha} + B_{\alpha}^+) [\lambda_{ii+1} C_{Bi+1} + \lambda_{ii-1} C_{Bi-1}] \\ + t_{ii+1} C_{Bi+1} + t_{ii-1} C_{Bi-1} \end{array} \right\} \quad \text{for } 1 < i < N \quad (13c)$$

$$0 = \left\{ \begin{array}{l} \hbar\omega_\alpha B_\alpha + \sum_i \lambda_i n_{Bi} + \\ \sum_i [\lambda_{ii+1} C_{Bi}^+ C_{Bi+1} + \lambda_{ii-1} C_{Bi}^+ C_{Bi-1} + c.c.] \end{array} \right\} \quad (13d)$$

$$B_\alpha = - \left\{ \sum_i \lambda_i n_{Bi} + \sum_i [\lambda_{ii+1} C_{Bi}^+ C_{Bi+1} + \lambda_{ii-1} C_{Bi}^+ C_{Bi-1} + c.c.] \right\} / \hbar\omega_\alpha \quad (13e)$$

Here, we have the same shape of matrix eq.(2-7) but with,

$$A_i = E_{Bi} + \lambda_o \sum_\alpha (B_\alpha + B_\alpha^+) - E \quad ; \quad G = t + \lambda_1 \sum_\alpha (B_\alpha + B_\alpha^+) \quad ; \quad t = t_{ij} \dots (14)$$

We note that for  $\lambda_1 \neq 0$ , increasing the polaron energy led to:

- 1- The polaron become not localized, the charge spread to other bases.
- 2- The charge of the central base (the 5<sup>th</sup> base) decreases.

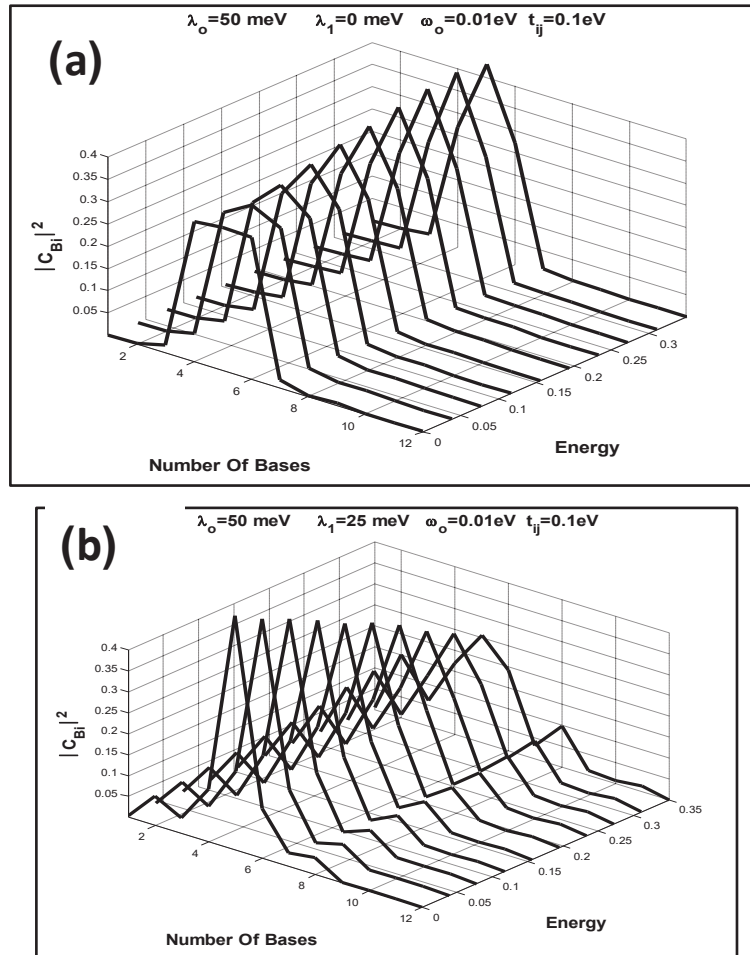


Fig.(11): The steady state of a large polaron with (a)  $\lambda_1 = 0$  and (b)  $\lambda_1 \neq 0$ .

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