

# Chapter 11

## Electron Transfer and Tunneling from Donor to Acceptor in Anharmonic Crystal Lattices

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**Abstract** We model electron transfer from donor to acceptor with a lattice with non-uniform electron on-site energies. The electron motion is described in a tight binding approximation and the lattice site dynamics follows the Morse potential. We focus on the transition time from donor to acceptor which is first determined analytically for a rigid lattice and then numerically from computer simulations of the full system at low temperature. For the parameter ranges explored here a very good agreement is found between the analytical and the numerical transition times. Furthermore, this nonlinear model can account both for the order of magnitude and for the variation with distance of the transition times from donor to acceptor that are measured experimentally, even in the case of long range transitions, i.e., when the distances are well beyond 20 Å. While for short distances and weakly bound electrons the transfer is of the non-tunneling type, for larger distances and/or strongly bound electrons the transfer is tunneling-like, with the transition time varying exponentially.

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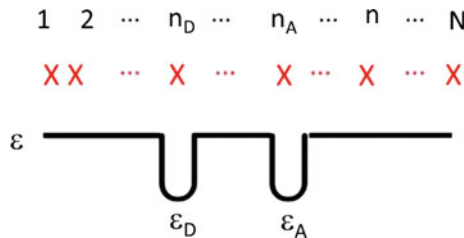
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## 11.1 Introduction

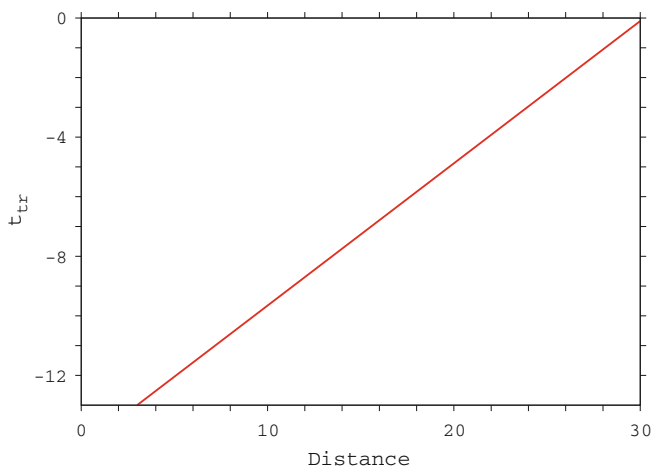
We are interested in the effect of *anharmonic* lattice dynamics on long range electron transfer (ET), that is, ET over distances that are typically larger than  $20 \text{ \AA}$ . What we have in mind are applications to ET in biomolecules like azurin [27, 28] and other proteins and to ET in natural or synthetic DNA [25, 26].

We also aim to describe electron transport in quasi 1d crystals [3–6, 13, 16–18, 24, 27–30, 33, 34, 36, 37, 40–43, 45, 49, 50, 53–56, 59–61, 67, 68, 70, 71] with a particular emphasis to the interference of electron states with *anharmonic* excitations in high  $T_c$  superconducting materials [23, 44, 48, 52]. While many studies of ET in biomolecules are based on the Landau-Zener treatment (see e.g. [28]), we resort to a microscopic formalism, based on the Schrödinger equation. However, in order to find a fruitful approach to such highly complicated problems we need to make drastic approximations. In previous publications [8, 9, 21, 22, 31, 32, 62–66] we investigated some consequences of *anharmonic* lattice excitations on ET. In particular, it was shown that electron trapping by solitons and a new form of ET and electric conduction mediated by solitons, which we designate by solectron can take place in *anharmonic* 1d lattices [1, 10–12, 47, 51, 58, 69]. The solectron state is a modification of the polaron concept since, in this case, a *pre-existing nonlinear* lattice distortion (the soliton) captures a free electron, which then travels along the lattice, carried by the soliton. Thus, the speed of the bound electron state, i.e. the speed of the solectron, is strongly dependent on the speed of the soliton, which is determined by the lattice characteristics only. The previous studies showed that solitons, in homogeneous lattices, lead to electron transfer times that are too large when compared with experimental data. In this chapter, we extend the previous studies and report results for the *inhomogeneous* system obtained by including an electron donor and an electron acceptor explicitly in the lattice. The donor and acceptor are represented by the different electron on-site energies of the corresponding sites, as shown in Fig. 11.1.

Thus, contrary to other studies in which the on-site electronic energies were uniform along the lattice electronic energies are different at the sites where the electron



**Fig. 11.1** Illustration of the donor-acceptor model investigated here. X is a site in a lattice with N sites and D and A mark the sites of the electron donor and acceptor. The on-site electron energies are equal for all sites (and set to zero), except for the donor and electron sites, where their values are  $\varepsilon_D$  and  $\varepsilon_A$ , respectively



**Fig. 11.2** Transition times, in seconds, (in  $\log_{10}$  scale) versus distance (in Å), measured in the protein azurin. The parameters for the line in this figure are taken from [28]

donor and acceptor are located. Also, the variable we are mostly interested in is the transition time from donor to acceptor (or, inversely, the electron transfer rate) and our ultimate aim is to reproduce the order of magnitude, as well as the dependence on distance, of the electron transition times that are measured experimentally [27, 28]. Furthermore, we wish to develop a formalism that can treat short distances between donor and acceptor, i.e. distances  $\leq 20$  Å, but also distances well beyond 20 Å, which are referred to as long range electronic transfer between donor and acceptor. Figure 11.2 summarizes the experimental values of the transfer times that we aim to explain.

In order to deal with phenomena such as electron tunneling (in and out of the donor and acceptor) it is important to treat the electron as a quantum particle. To that end, and as was done in the previous work, the electron motion in the lattice is considered within the tight binding approximation (TBA) [2, 38, 60, 61]. On the other hand, the motion of the lattice sites is treated classically, with the nonlinearity of the lattice interactions being modelled by the Morse potential [46]. The Morse potential (akin to the Lennard-Jones potential), allows for phonon- and soliton- longitudinal vibrations, with the compressions being governed by the repulsive part of the potential. Finally, the interactions between the electron and lattice are modelled by a Su-Schrieffer-Heeger (SSH)-type Hamiltonian [29], in which the electron transfer term from site to site is dependent on the distance between the lattice sites. The Morse potential together with the quantum electron Hamiltonian just described, constitute a *mixed* classical-quantum evolution problem [15]. We apply this Hamiltonian to transitions between *local* electronic states, such as tunneling processes, under the influence of a nonlinear coupling to a cold *anharmonic* lattice. The main aim is to determine how the transition time for the electron to go from the donor to the acceptor is influenced by the dynamics of the *anharmonic* lattice.

In the next section the general Hamiltonian for the system, the particular scaling we use to obtain a-dimensionless variables and the derivation of the equations of motion are explained in details. For a more clear presentation of this subject, in Sects. 11.3 and 11.4 we deal with simplified versions of the original Hamiltonian, namely, with the cases of an electron donor and acceptor in a rigid lattice, with periodic boundary conditions (Sect. 11.3), and with fixed boundary conditions (Sect. 11.4), which allow for the derivation of analytical expressions for the transition times between donors and acceptors. In Sect. 11.5 we compare the analytical results for the rigid lattice with the numerical results obtained in computer simulations for the full system, i.e., when the lattice can also move, and in Sect. 11.6 we make a preliminary investigation of the influence of a stronger electron-lattice interaction on the electron transition times. We find that this microscopic model of ET can explain the exponential variation of the transition times with distance that is portrayed in Fig. 11.2 and that, for certain values of the parameters, the rigid lattice provides a sufficiently accurate approximation to the full system. In Sect. 11.7 we discuss the results obtained within the context of long distance ET.

## 11.2 Hamiltonian and Equations of Motion of the Electron-Lattice Dynamics

The model Hamiltonian for charge transport that we consider here consists of the following two terms

$$H = H_{el} + H_{lattice}, \quad (11.1)$$

where  $H_{el}$  provides a quantum mechanical description of ET along the 1d lattice and  $H_{lattice}$  represents the classical dynamics of longitudinal vibrations of the units, viz. the deformations of the corresponding bonds between them. In the TBA we have

$$H_{el} = - \sum_n \left[ \varepsilon_n c_n^* c_n + V_{nn-1} (c_n^* c_{n-1} + c_n c_{n-1}^*) \right]. \quad (11.2)$$

The index  $n$  denotes the site of the  $n$ th unit on the lattice and  $|c_n|^2$  determines the probability to find the electron (charge) residing at such site.  $\varepsilon_n$  is the electron on-site energy at site  $n$ . In absence of donor and acceptor  $\varepsilon_n$  is equal for all sites (and set to zero). On the other hand, donor and acceptor sites are identified by finite values of the on-site energies which represent their electronic energies with respect to energy of the bridge sites. The quantities  $V_{nn-1}$  are the transfer matrix elements whose values are determined by an overlap integral. They account for the nearest-neighbor hopping of the electron along the chain. The interaction between the quantum electron dynamics and the classical vibrational degrees of freedom yields modifications of the electron parameters  $V_{nn-1}$  due to the displacements of

the units from their equilibrium positions. To be specific, following Slater [57] and other authors who have shown that this distance dependence should be exponential [35] we set

$$V_{nn-1} = V_0 \exp[-\alpha (q_n - q_{n-1})]. \quad (11.3)$$

The quantity  $\alpha$  regulates how strongly  $V_{nn-1}$  is influenced by the relative distance,  $r_n = q_n - q_{n-1}$ , between neighbouring lattice sites. The coordinates  $q_n$  quantify the displacements of the sites from their equilibrium positions along the lattice axis. On the other hand, the actual charge occupation has its (local) impact on the longitudinal distortion of the chain (polaron-like effect) [7, 60, 61]. Note that here the exponential form of the electron-lattice interaction accounts for both small and large displacements of the lattice sites thus going beyond the range of linear interaction considered in most earlier studies.

For the lattice part of the Hamiltonian (11.1) we set

$$H_{lattice} = \sum_n \left\{ \frac{p_n^2}{2M} + D (1 - \exp[-B (q_n - q_{n-1})])^2 \right\}. \quad (11.4)$$

$D$  is the break-up energy of a bond,  $B$  is the stiffness of the Morse potential, and  $M$  denotes the mass of a lattice unit (all units are taken with equal mass). The Morse potential exhibits an exponential-repulsive part preventing the cross-over of neighboring lattice particles (molecules) for large displacements. Needless to say, with a Taylor expansion of the exponential function one recovers in lowest order the harmonic limit, and taking into account higher-order terms one recovers the anharmonic potentials, like the cubic power or go to the quartic power, of standard use in condensed matter physics [2, 10, 38].

For universality in our arguments it is convenient to suitably re-scale quantities. Thus, time is scaled as:  $\tilde{t} = \Omega_{Morse} t$ , with  $\Omega_{Morse} = \sqrt{2D B^2/M}$  being the frequency of the harmonic oscillations that take place around the minimum of the Morse potential, and the energy of the system is measured in units of two times the depth of the Morse potential, i.e.  $H \rightarrow H/(2D)$ . Note that  $D \approx 0.1$  eV for physically interesting cases. The dimensionless representation of the remaining variables and parameters of the system follows from the relations:

$$\tilde{q}_n = B q_n, \quad \tilde{p}_n = \frac{p_n}{\sqrt{2MD}}, \quad \tilde{V} = \frac{V_0}{2D} \quad (11.5)$$

$$\tilde{\alpha} = \frac{\alpha}{B} \quad \tilde{\varepsilon}_n = \frac{\varepsilon}{\hbar \Omega_{Morse}}. \quad (11.6)$$

In what follows we drop the tildes. The equations of motion derived from the Hamiltonian (11.1), with (11.2) and (11.4), read as

$$i \frac{dc_n}{dt} = \varepsilon_n c_n - \tau \left\{ \exp[-\alpha(q_{n+1} - q_n)] c_{n+1} + \exp[-\alpha(q_n - q_{n-1})] c_{n-1} \right\} \quad (11.7)$$

$$\begin{aligned} \frac{d^2 q_n}{dt^2} = & \left[ 1 - \exp\{-(q_{n+1} - q_n)\} \right] \exp[-(q_{n+1} - q_n)] \\ & - \left[ 1 - \exp\{-(q_n - q_{n-1})\} \right] \exp[-(q_n - q_{n-1})] \\ & + \alpha V \left\{ (c_{n+1}^* c_n + c_{n+1} c_n^*) \exp[-\alpha(q_{n+1} - q_n)] \right. \\ & \left. - (c_n^* c_{n-1} + c_n c_{n-1}^*) \exp[-\alpha(q_n - q_{n-1})] \right\}. \end{aligned} \quad (11.8)$$

The *adiabaticity* parameter  $\tau = V/(\hbar \Omega_{Morse})$ , appearing in the r.h.s. of (11.8) is the ratio of the two time scales involved, i.e., between the (fast) *electronic* and the (slow) *acoustic* phonon processes. For illustration in our computer simulations we use (unless stated otherwise) the following values:  $\tau = 10$ ,  $V = 0.1$ , and  $\alpha = 1.75$  which are relevant for ET in biomolecules [18, 27, 28, 32, 55, 63]. We also consider the behaviour at low temperature and to mimic thermal agitation (11.8) are augmented with Langevin terms (delta correlated Gaussian noise forces and damping, obeying Einstein's relation between the noise strength and temperature), representing an appropriate heat bath [19, 20, 39].

### 11.3 Free Electron Dynamics with One Bound State in a Lattice with Periodic Boundary Conditions

Let us first consider the electron dynamics in the case of no coupling to the lattice dynamics ( $\alpha = 0$ ) and equal on-site energies (no donors or acceptors,  $\varepsilon_D = \varepsilon_A = 0$ ). In this regime, which is valid when the oscillations of lattice sites are negligibly small (rigid lattice), the electrons hop from site to site, according to the quantum-mechanical TBA dynamics. Then the Schrödinger equation corresponding to (11.2) reduces to:

$$i \frac{dc_n}{dt} = \tau (c_{n+1} + c_{n-1}). \quad (11.9)$$

The eigen energies  $E_j$  and the eigenfunctions with periodic boundary conditions read [14]:

$$E_j = 2\tau \cos \left[ \frac{2\pi(j-1)}{N} \right] \quad (11.10)$$

$$c_{jn} = \sqrt{\frac{1}{N}} \exp \left[ \frac{2\pi i j n}{N} \right] \quad (11.11)$$

where  $N$  is the number of sites,  $j = 1, \dots, N$  and  $c_{jn}$  is for the probability amplitude for an electron to be in the  $n$ th-site in the  $j$ th eigenstate. Using the eigenstates above as a basis set, the general wavefunction for an electron in a uniform lattice can be written as follows:

$$|\psi(t)\rangle = \sum_{j=1,N} d_j \exp\left(-\frac{i}{\hbar} E_j t\right) |\psi_j\rangle \quad (11.12)$$

where  $|\psi_j\rangle = \sum_{n=1,N} c_{jn}|n\rangle$  is the eigenfunction for the state with energy  $E_j$ ,  $|n\rangle$  is the state in which there is an electron in site  $n$  and  $d_j$  is the probability amplitude for the occupation of eigenstate  $j$ . Substituting expression (11.11) in (11.12) and setting  $t = 0$  we get:

$$|\psi(t=0)\rangle = \frac{1}{\sqrt{N}} \sum_{n,j=1,N} d_j \exp\left(\frac{2\pi i j n}{N}\right) |n\rangle \quad (11.13)$$

For an electron to be initially in site  $r$ , we must have:

$$\langle r|\psi(t=0)\rangle = \frac{1}{\sqrt{N}} \sum_{j=1,N} d_j \exp\left(\frac{2\pi i j r}{N}\right) = \delta_{nr} \quad (11.14)$$

which is valid if the complex coefficients  $d_j$  obey the following equality:

$$d_j = \frac{1}{\sqrt{N}} \exp\left(-\frac{2\pi i j r}{N}\right) \quad (11.15)$$

Thus, the wavefunction for an electron that starts at site  $r$ , taken to be the donor site, is:

$$|\psi(t)\rangle = \frac{1}{N} \sum_{j,n=1,N} \exp\left(-\frac{i}{\hbar} E_j t\right) \exp\left[\frac{2\pi i j (n-r)}{N}\right] |n\rangle \quad (11.16)$$

and the probability amplitude that the electron, after a time interval  $t$ , is at site  $m$ , taken to be the acceptor site, is:

$$\langle m|\psi(t)\rangle = \frac{1}{N} \sum_{j=1,N} \exp\left(-\frac{i}{\hbar} E_j t\right) \exp\left[\frac{2\pi i j (m-r)}{N}\right] \quad (11.17)$$

where  $E_j$  is given by (11.10). We note that the wavefunction (11.16) is a periodic function and so all electronic processes in a homogeneous lattice with periodic boundary conditions are periodic.

In order to study ET from a donor to an acceptor we need an inhomogeneous lattice, i.e. the on-site energies of the electron cannot be equal for all sites. Let us

start by the smallest inhomogeneous lattice possible, i.e. when  $N = 2$ , with a donor with energy  $\varepsilon_D = \varepsilon_1 = \varepsilon$  in site 1 and an acceptor with energy  $\varepsilon_A = \varepsilon_2 = 0$  in site 2. This leads to a simple system which, in the site representation,  $|n\rangle$ , used above, is characterized by the energy matrix:

$$\begin{bmatrix} \varepsilon & -1 \\ -1 & 0 \end{bmatrix}$$

where we have considered the energies in units of  $\tau$ . We are interested in describing the transfer of one electron from the donor in site 1 to the acceptor in site 2.

As before, we calculate the eigen energies of the system:

$$E_1 = \frac{\varepsilon - \sqrt{\varepsilon^2 + 4}}{2} \quad (11.18)$$

$$E_2 = \frac{\varepsilon + \sqrt{\varepsilon^2 + 4}}{2} \quad (11.19)$$

and the corresponding normalized eigenvectors:

$$|\varphi_1\rangle = \begin{bmatrix} \varphi_{11} \\ \varphi_{12} \end{bmatrix} = \begin{bmatrix} \frac{1}{\sqrt{E_2^2 + 1}} \\ \frac{E_2}{\sqrt{E_2^2 + 1}} \end{bmatrix} \quad (11.20)$$

$$|\varphi_2\rangle = \begin{bmatrix} \varphi_{21} \\ \varphi_{22} \end{bmatrix} = \begin{bmatrix} -\frac{1}{\sqrt{E_1^2 + 1}} \\ \frac{|E_1|}{\sqrt{E_1^2 + 1}} \end{bmatrix} \quad (11.21)$$

from which we can determine a general expression for the wave function as a superposition of the two eigenstates (see (11.12)); then we calculate the coefficients  $d_1$  and  $d_2$  so that the probability for the electron to be at the donor in site 1 initially is unity (i.e.,  $p_D(t = 0) = p_1(t = 0) = 1$ ); once we have these new coefficients  $d_1$  and  $d_2$ , we can determine the probability,  $p_A = p_2$ , that the electron is at the acceptor in site 2 at time  $t$ , given that it started at the donor. The result is:

$$p_2(\varepsilon, t) = \frac{2}{\varepsilon^2 + 4} \left[ 1 - \cos\left(\sqrt{\varepsilon^2 + 4} t\right) \right]. \quad (11.22)$$

As expected, this probability is periodic, but notice that it does not necessarily oscillate between 0 and 1! Indeed, the probability,  $p_2$ , for the electron to be at the acceptor when it starts at the donor only reaches its maximum value of unity when  $\varepsilon = 0$ , i.e. when the electronic energies of the donor and acceptor are equal (something that in solid state physics is known as the resonance condition). When the electron energies of the donor and acceptor are different,  $p_2 < 1$  at all times and its maximum value,  $\frac{4}{\varepsilon^2 + 4}$ , decreases as the energy difference between donor and acceptor,  $\varepsilon$ , increases



(in absolute value). *Unless otherwise is stated we define the transition time for an electron to go from donor to acceptor as the smallest time in which this maximum probability is reached.* Equation (11.22) shows that for arbitrary  $\varepsilon$  the transition time for an electron to go from the donor to the acceptor is given by:

$$t_{tr} = \frac{\pi}{\sqrt{\varepsilon^2 + 4}} = \frac{\pi}{E_2 - E_1}. \quad (11.23)$$

Thus, we conclude that, for a two-site system, the first passage time is inversely proportional to the difference between the two lowest eigenvalues, or, in other words, that the difference between the two lowest eigenvalues is proportional to the rate of the first transition from the donor to the acceptor. In the next section, we will see that although this expression, well known from the quantum theory of atoms and molecules, is exactly valid for a two-site system, it is also approximately true for larger lattices.

## 11.4 Free Electron Dynamics in a Lattice with Fixed Boundary Conditions

In this section we consider a 1d lattice of  $N$  sites with fixed b.c. In the absence of donor and acceptor, i.e., when the on-site energies are equal for all  $N$  sites, we find the following eigenvalues and eigenstates [14]:

$$E_j = 2 \tau \cos \left( \frac{\pi j}{N+1} \right), \quad (11.24)$$

$$c_{jn} = \sqrt{\frac{2}{N+1}} \sin \left( \frac{\pi j n}{N+1} \right), \quad (11.25)$$

where  $j = 1, \dots, N$ . Following the same reasoning as in Sect. 11.3 we find that the probability amplitude for an electron to be in site  $m$  after a time  $t$  when it starts from site  $r$  is:

$$\begin{aligned} \langle m | \psi(t) \rangle &= \frac{2}{N+1} \sum_{j=1, N} \exp \left( -\frac{i}{\hbar} E_j t \right) \\ &\quad \sin \left( \frac{\pi j r}{N+1} \right) \sin \left( \frac{\pi j m}{N+1} \right). \end{aligned} \quad (11.26)$$

Also in this case the eigenfunctions are periodic functions and, consequently, in the absence of thermal baths, the probability for an electron to be in site  $m$  when it was initially in site  $r$  is periodic.

Let us now consider the second smallest lattice with a donor and acceptor, namely, when  $N = 3$  and in which the energy of the donor is equal to that of the acceptor ( $\varepsilon_D = \varepsilon_A = \varepsilon$ ), with both of them being different from the electron energies in the bridging site, which is set to zero. With fixed b.c. and also in the site basis  $|n\rangle$ , the corresponding energy matrix is the following:

$$\begin{bmatrix} \varepsilon & -1 & 0 \\ -1 & 0 & -1 \\ 0 & -1 & \varepsilon \end{bmatrix} \quad (11.27)$$

where again the energies are given in units of  $\tau$ . The eigenvalues for this matrix are:

$$E_1 = \frac{\varepsilon - \sqrt{\varepsilon^2 + 8}}{2} \quad (11.28)$$

$$E_2 = \varepsilon \quad (11.29)$$

$$E_3 = \frac{\varepsilon + \sqrt{\varepsilon^2 + 8}}{2} \quad (11.30)$$

and the corresponding normalized eigenvectors are:

$$|\varphi_1\rangle = \begin{bmatrix} \varphi_{11} \\ \varphi_{12} \\ \varphi_{13} \end{bmatrix} = \begin{bmatrix} -\sqrt{\frac{1}{E_3\sqrt{\varepsilon^2+8}}} \\ -\sqrt{\frac{E_3}{\sqrt{\varepsilon^2+8}}} \\ -\sqrt{\frac{1}{E_3\sqrt{\varepsilon^2+8}}} \end{bmatrix} \quad (11.31)$$

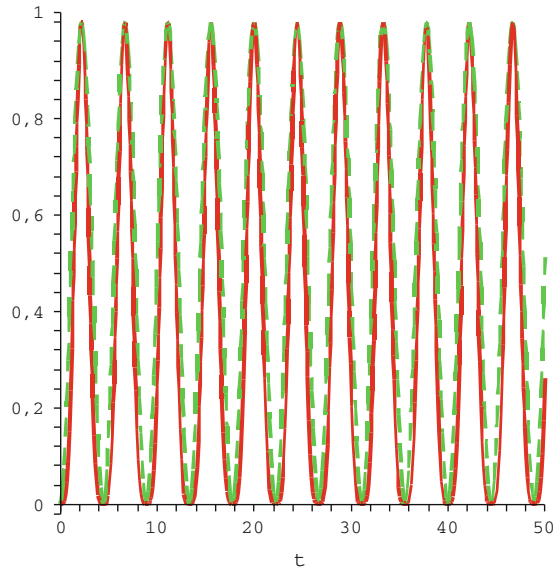
$$|\varphi_2\rangle = \begin{bmatrix} \varphi_{21} \\ \varphi_{22} \\ \varphi_{23} \end{bmatrix} = \begin{bmatrix} -\frac{\sqrt{2}}{2} \\ 0 \\ \frac{\sqrt{2}}{2} \end{bmatrix} \quad (11.32)$$

$$|\varphi_3\rangle = \begin{bmatrix} \varphi_{31} \\ \varphi_{32} \\ \varphi_{33} \end{bmatrix} = \begin{bmatrix} -\sqrt{\frac{1}{E_1\sqrt{\varepsilon^2+8}}} \\ \sqrt{\frac{E_1}{\sqrt{\varepsilon^2+8}}} \\ -\sqrt{\frac{1}{E_1\sqrt{\varepsilon^2+8}}} \end{bmatrix} \quad (11.33)$$

Using the same reasoning as before we can find the probability,  $p_A = p_3$ , as a function of  $\varepsilon$  and time, for an electron to be at the acceptor (in site 3), given that it started at the donor (in site 1). The result is:

$$\begin{aligned} p_3(\varepsilon, t) &= \frac{\varepsilon^2 + 6}{2(\varepsilon^2 + 8)} - \frac{E_3}{2\sqrt{\varepsilon^2 + 8}} \cos(E_1 t) \\ &+ \frac{1}{\varepsilon^2 + 8} \cos(\sqrt{\varepsilon^2 + 8} t) + \frac{E_1}{2\sqrt{\varepsilon^2 + 8}} \cos(E_3 t) \end{aligned} \quad (11.34)$$

**Fig. 11.3** Analytical results for transition processes between a donor and an acceptor separated by one lattice site in a 1d-TBA-lattice with fixed boundary conditions ( $T = 0$ ,  $\alpha = 0$ ). We show the time evolution for the probability of an electron to be at the acceptor (site 3), given that it is at the donor (site 1) to start with, calculated with (11.35) for  $\varepsilon = 0$  (red curve) and with the simplified equation  $1/2 [1 - \cos(\sqrt{2}t)]$  (green curve)



This probability oscillates, as expected, but the oscillations now involve the interference of three different frequencies, which makes it less straightforward to define a transition time. But, as we will see, it is still possible to define this value on average, with the same expression as before (11.23). To show that, let us consider different values of  $\varepsilon$ . For  $\varepsilon = 0$ , (11.34) becomes:

$$p_3(\varepsilon = 0, t) = 3/8 - 1/2 \cos(\sqrt{2}t) + 1/8 \cos(2\sqrt{2}t) \tag{11.35}$$

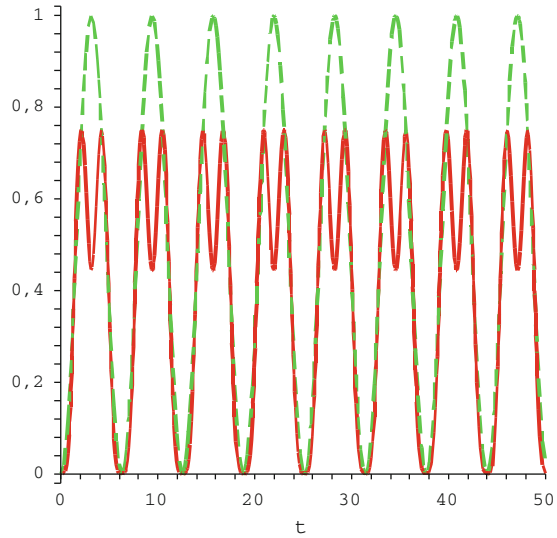
Figure 11.3 shows that, for  $\varepsilon = 0$ , the oscillations have a period that is related essentially with the lowest frequency, that is, that is related to the energy difference between the two lowest states,  $t_{tr} \approx \frac{\pi}{E_2 - E_1} = \frac{\pi}{\sqrt{2}}$ .

If we now consider  $\varepsilon = -1$ , the probability for the electron to be in site 3 becomes:

$$p_3(\varepsilon = -1, t) = \frac{7}{18} - 1/3 \cos(t) + 1/9 \cos(3t) - 1/6 \cos(2t). \tag{11.36}$$

Figure 11.4 shows that the interference between the three frequencies results in that, for  $\varepsilon = -1$ , the probability for the electron to be in the second well never reaches a value of unity as happened for the two-site system. On the other hand, the residence time for the electron in the second well is effectively increased because of the interference. Also in this case, the lowest frequency provides an *average* estimate for the transition time which is related to the energy difference between the two lowest energy states.

**Fig. 11.4** Analytical results for transition processes between a donor and an acceptor separated by one lattice site in a 1d-TBA-lattice with fixed boundary conditions ( $T = 0$ ,  $\alpha = 0$ ). We show the time evolution for the probability of an electron to be at the acceptor (site 3), given that it is at the donor (site 1) to start with, calculated with (11.36) for  $\varepsilon = -1$  (red curve) and with the simplified equation  $1/2 [1 - \cos(t)]$  (green curve)

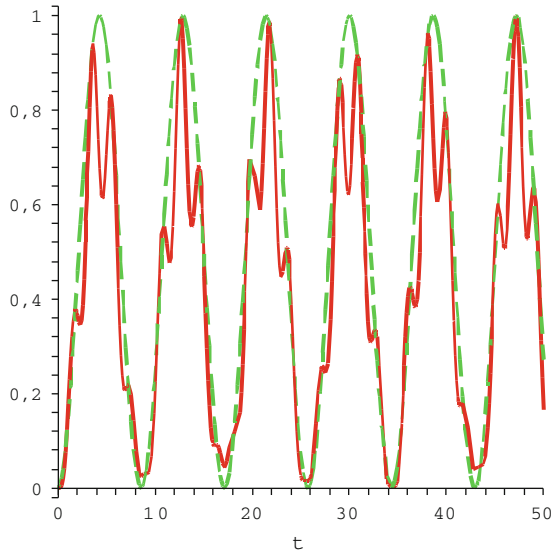


For  $\varepsilon = -2$ , the probability for the electron to be in site 3 becomes:

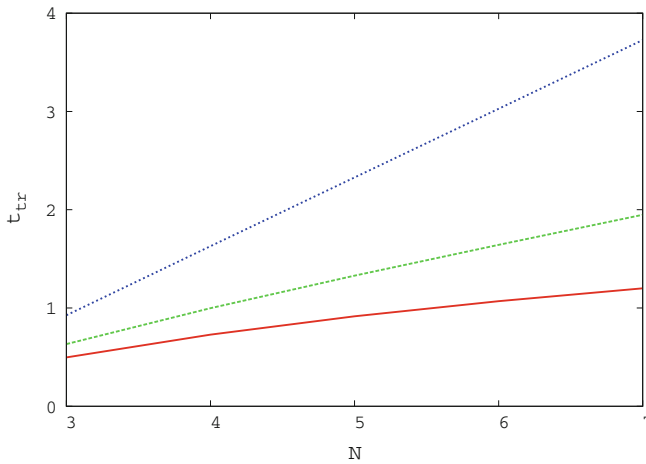
$$p_3(\varepsilon = -2, t) = \frac{5}{12} + \frac{1}{12} \cos(2\sqrt{3}t) + \frac{\sqrt{3}-3}{12} \cos[(\sqrt{3}+1)t] - \frac{\sqrt{3}+3}{12} \cos[(\sqrt{3}-1)t] \quad (11.37)$$

and the time evolution is displayed in Fig. 11.5. It appears that, for  $\varepsilon = -2$ , although the interference between the three frequencies leads to a variety of oscillatory patterns, the overall transition time is still related to the energy difference between the two lowest energy states, as given by (11.23). Thus we conclude that, although the expression (11.23) widely used for the first passage time is only strictly valid for a lattice with two sites, it does provide a good approximation in a lattice with three sites in which the donor is at site 1 and the acceptor is at site 3. Notice that also in this case the interference between the three frequencies results in that, for certain values of  $\varepsilon$ , the probability for the electron to be at the donor may never reach unity, as happened for the two-site system. However, the time to reach a maximum probability can still be related to the energy difference between the two lowest energy states.

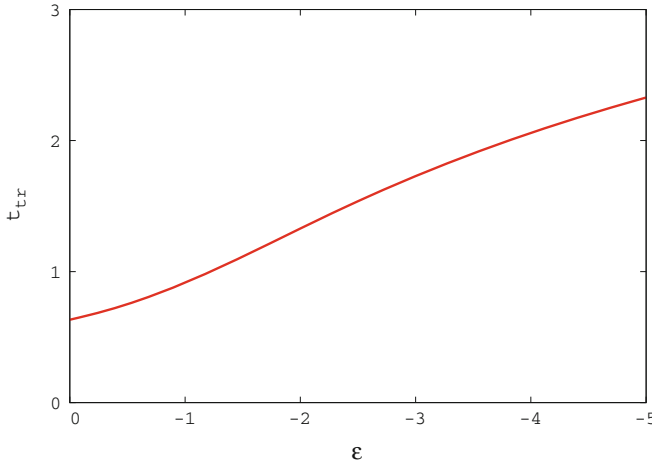
Since the analytical expressions for lattices with more than three sites are not illuminating, we will use (11.23) to determine numerically the dependence of the transition time for an electron to go from the donor to the acceptor, as a function of the electronic energy of the donor (assumed equal to that of the acceptor) and of the distance between the donor and acceptor. In Fig. 11.6 a donor and acceptor with electronic energies  $\varepsilon = -5, -2, -1$  (blue, green and red, respectively) and separated by  $N - 2$  sites have been considered and the two lowest eigenvalues have been determined numerically. Given the average separation between sites in azurin [63]  $N = 5$  in the figure is close to 20 Å. This figure shows that for the larger elec-



**Fig. 11.5** Analytical results for transition processes between a donor and an acceptor separated by one lattice site in a 1d-TBA-lattice with fixed boundary conditions ( $T = 0, \alpha = 0$ ). We show the time evolution for the probability of an electron to be at the acceptor (site 3), given that it is at the donor (site 1) to start with, calculated with (11.38) for  $\epsilon = -2$  (red curve) and with the simplified equation  $1/2 [1 - \cos((\sqrt{3} - 1) t)]$  (green curve)



**Fig. 11.6** Transition time (in  $\log_{10}$  scale and in units of  $\Omega_{Morse}^{-1}$ ) versus the number of lattice sites  $N$  for an electron to go from a donor to an acceptor in 1d-TBA-lattice ( $3 \leq N \leq 7$ ), with the donor and acceptor at the ends ( $T = 0, \alpha = 0$ ). The electronic energies of the donor and acceptor are  $\epsilon = -5$  (upper dotted line, blue),  $\epsilon = -2$  (center dashed line, green) and  $\epsilon = -1$  (lower solid line, red), in units of  $\tau$



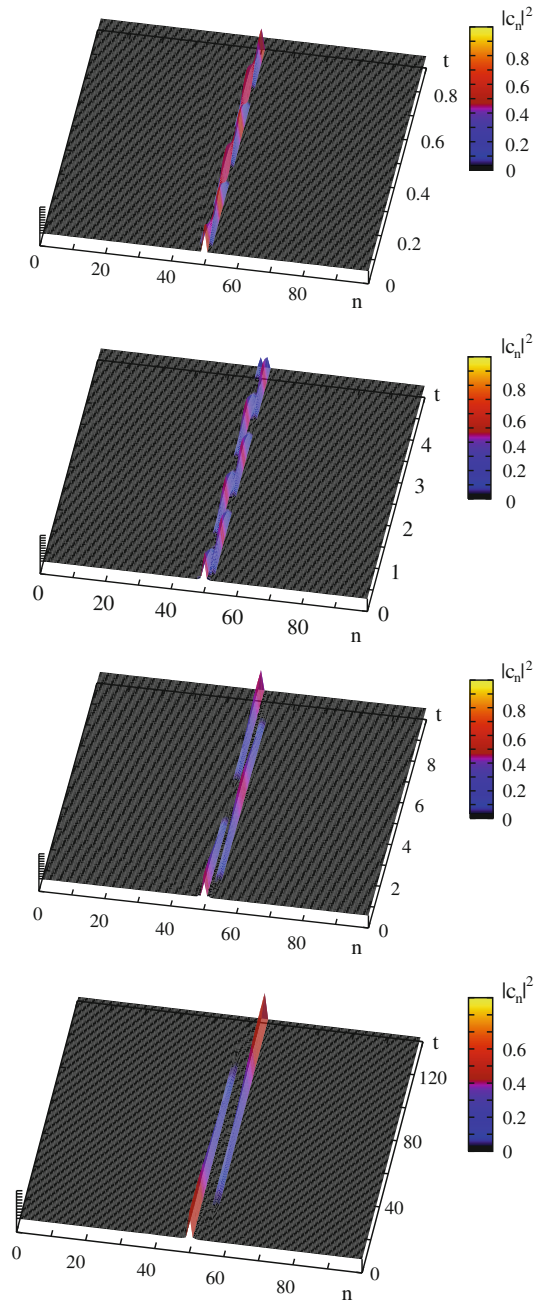
**Fig. 11.7** Transition time (in  $\log_{10}$  scale and in units of  $\Omega_{Morse}^{-1}$ ) versus  $\epsilon$  (in units of  $\tau$ ) for an electron to go from a donor and to an acceptor separated by a 3 site bridge. ( $N = 5$ ,  $T = 0$ ,  $\alpha = 0$ ).  $\epsilon$  is the energy of the electron at the donor and at the acceptor

tronic energies (in absolute terms), the transition time from donor to acceptor varies exponentially with the distance which is usually identified with the *tunneling* regime. On the other hand, when the electronic energies of donor and acceptor are comparable to the hopping term  $\tau$ , the transition time does not vary exponentially with the distance, that is, *non-tunneling* quantum interference processes become important. This is particularly visible the shorter the bridge between donor and acceptor is, as shown in Fig. 11.7. Indeed, this figure shows the transition time as function of donor and acceptor energies, for a lattice with seven sites (a 5 site bridge between the donor and acceptor). While in the *tunneling* regime the dependence of the transition time is *exponential* in the electronic energy  $\epsilon$ , for this small number of bridge sites this is not the case for the smaller values of the on-site electronic energies (in absolute terms). On the other hand, for the larger values of  $\epsilon$  the transition times do scale exponentially with the on-site energies of donor and acceptor which suggests that, for these values, the electronic transfer is in the tunneling regime.

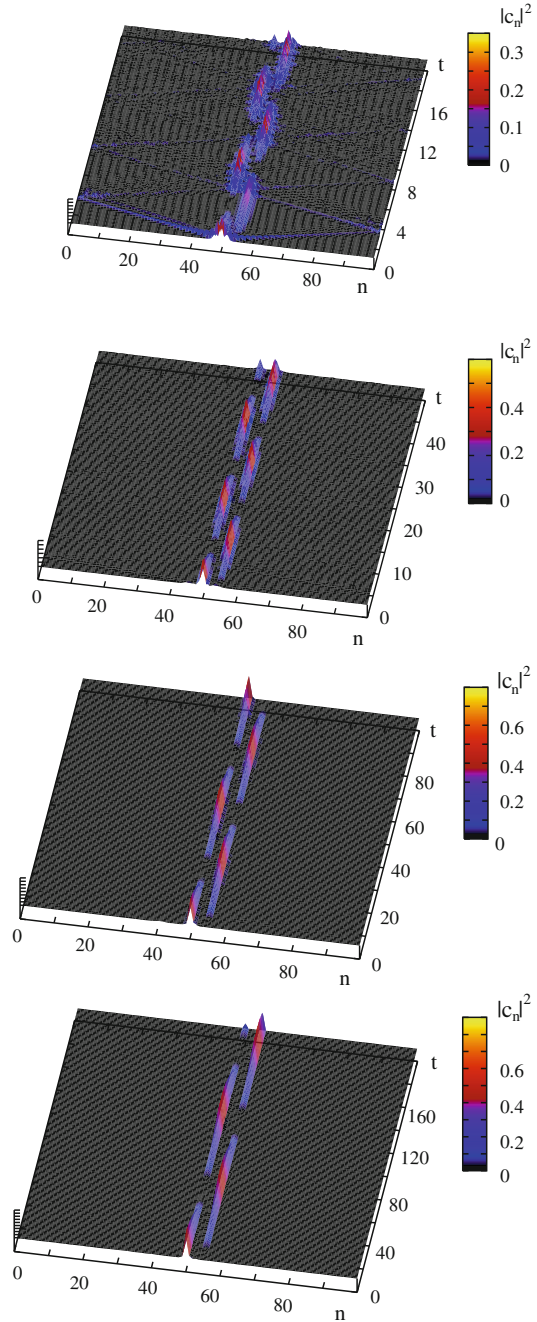
## 11.5 Computer Simulations of ET from Donor to Acceptor in a Lattice at Low Temperature

In this section we consider a long lattice ring with  $N = 100$  sites on which the donor and the acceptor are separated by a distance of  $\Delta n$  sites. Furthermore, we include explicitly the interaction of the electron with the motions of the lattice sites, by solving numerically equations (11.7) and (11.8), augmented with the appropriate Langevin terms to account for heating, as explained at the end of Sect. 11.2. Figures 11.8 and 11.9 show the electron transitions as a function of the distance  $\Delta n$  between donor and acceptor (Fig. 11.8) and as a function of the electronic energy of the donor (assumed

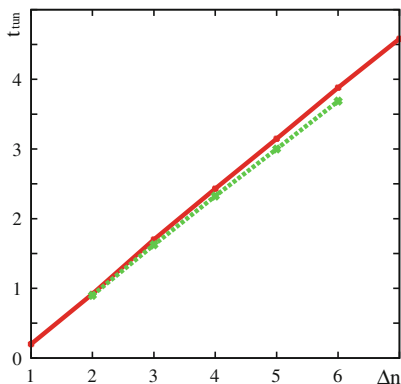
**Fig. 11.8** Computer simulations of electronic transition processes in a 1d-TBA-lattice with periodic boundary conditions, for different distances  $\Delta n$  between donor and acceptor.  $\Delta n = 1, 2, 3$  and  $5$ , from *top* to *bottom*, respectively. For all trajectories:  $\varepsilon = -5$  (in units of  $\tau$ ), ( $N = 100$ ),  $T = 0.002D$ ,  $\alpha = 0.1$ ,  $V = 0.1$  and  $\tau = 10$



**Fig. 11.9** Computer simulations of electronic transition processes in a 1d-TBA-lattice with periodic boundary conditions, for different donor and acceptor energies  $\varepsilon$ .  $\varepsilon = -1, -2, -3$  and  $-4$  (in units of  $\tau$ ), from *top to bottom*, respectively. For all trajectories:  $\Delta n = 5$ , ( $N = 100$ ),  $T = 0.002D$ ,  $\alpha = 0.1$ ,  $V = 0.1$ , and  $\tau = 10$







**Fig. 11.10** Transition time between two wells as a function of the distance between donor and acceptor,  $\Delta n$  ( $N = 100$ ). Comparison between analytical calculations for a lattice with fixed ends (red solid line above) and computer simulations (green dotted line below). The depth of the wells is  $\varepsilon = -5$  (in units of  $\tau$ ). Temperature,  $T = 0.002D$ . Parameter values:  $\alpha = 0.1$ ,  $V = 0.1$  and  $\tau = 10$

to be equal to that of the acceptor) (Fig. 11.9). In all cases displayed the electron moves between donor and acceptor in an oscillatory manner, as predicted by the analytical results obtained in previous sections (cf. 11.22 and 11.34). Moreover, this agreement between the numerical results for the full system and the analytical results for a rigid lattice (cf. 11.23) is not merely qualitative, as demonstrated in Fig. 11.10. Indeed, in Fig. 11.10, a comparison of the *transition* time as a function of the distance between acceptor and donor,  $\Delta n$ , is made between the analytical and the numerical results, namely, the solid line (red, above) corresponds to the analytical transition times, while the dashed line (green, below) corresponds to the numerical transition times obtained from trajectories such as those displayed in Fig. 11.8. Figure 11.10 shows that, for very low temperatures, and weak electron-lattice interactions, the transition times are approximately the same as for a rigid lattice and, for the values of the parameters used, both lead to the exponential dependence on distance that characterizes tunneling.

Finally, we should note that Figs. 11.8 and 11.9 also provide an insight into the localization of the electron states. From inspection of the scales for  $|c_n|^2$ , at the top right end corner of each plot in Fig. 11.9, we find that the electron states at the donor and acceptor become more localized as the binding energy of the electron to the donor (and acceptor) increases. A careful inspection of the top three plots of Fig. 11.8 and of the top two plots of Fig. 11.9 reveals that, on top of the oscillatory motion from donor to acceptor, some radiation leaks into the lattice and is observed to go around the ring a few times, before it disperses, when either the distance between donor and acceptor is very short or their on-site energies are approximately equal to the electron coupling term  $\tau$ .

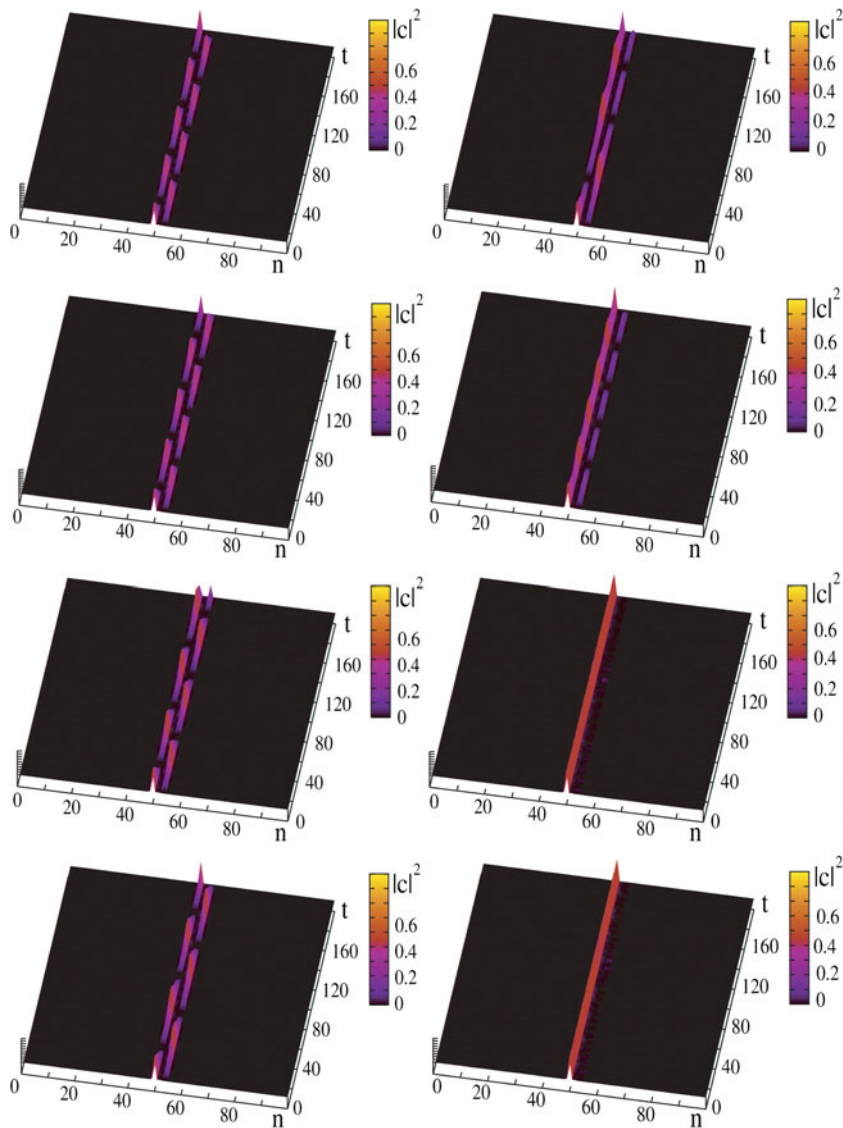
## 11.6 Dependence of Transition Time on $\alpha$

$\alpha$  represents the strength of electron lattice interaction (see (11.3)). The higher the  $\alpha$  the stronger this interaction is. Until now we have reported results for  $\alpha \leq 0.1$ . However, the values of this parameter relevant for ET in biomolecules are likely to be higher [18, 27, 28, 32, 55, 63]. Thus, in this section, we investigate the effect on the transition time of increasing values of  $\alpha$ .

Figure 11.11 shows that, initially, the change with  $\alpha$  of the transition time for the electron to go from the donor to acceptor is slow. Indeed, judging from the number of cycles after 180 time units, the transition time only decreases from 4 to 3 when  $\alpha$  increases from 0.1 to 0.9. However, above this value, the effect of increasing  $\alpha$  becomes very marked indeed, first leading to an effective decrease in the probability of finding the electron at the acceptor site (as has been found before for specific values of the on-site energies in small lattices) and finally resulting in an inhibition of the transition altogether when  $\alpha \geq 1.5$ . These results are more clearly seen in Fig. 11.12 in which the dependence of the transition time on the electron-lattice interaction is displayed.

## 11.7 Discussion and Conclusions

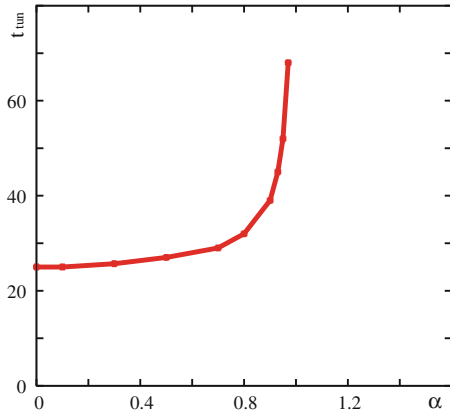
Our ultimate aim is to model the influence of the environment on long range ET, such as that observed in proteins [27, 28] and in synthetic DNA [25, 26]. While Marcus theory [27, 28, 43] can explain ET up to 20 Å, our ultimate aim is to develop a theoretical explanation capable of including ET for larger distances as well, by exploring the hypothesis that solitons in the media between donors and acceptors can constitute carriers for the electron. In this study we have considered a one dimensional lattice in which the electron on-site energies were all equal except at the donor and acceptor sites (see Fig. 11.1). The variable we are interested in is the transition time for the electron to move from the donor to the acceptor. We should note, however, that, our results were obtained in a finite lattice and in a finite size system all the trajectories are necessarily periodic so that the electron keeps moving from donor to acceptor and vice-versa. Therefore, in Sects. 11.3 and 11.4 we have defined the transition time as the first time passage, i.e. the instant in which the probability for the electron to be at the acceptor is maximum for the first time (given that the probability for the electron to be at the donor was 1 initially). We have verified that, to a good approximation, this defined rate of transfer from donor to acceptor in a rigid lattice can be predicted from the energy difference between the two lower energy states of the electron. Furthermore, in Sect. 11.5 we showed that, at low temperature, this rigid lattice rate is very similar to that obtained from the numerical simulations of an electron coupled to a flexible lattice, for an electron-lattice coupling constant  $\alpha = 0.1$ . Indeed, comparison of Figs. 11.2 and 11.10 shows that the nonlinear model



**Fig. 11.11** Computer simulations of electronic transition processes in a 1d-TBA-lattice with periodic boundary conditions, for different values of  $\alpha$ . For all trajectories:  $\varepsilon = -5$  (in units of  $\tau$ ), ( $N = 100$ ),  $T = 0.002D$ ,  $V = 0.1$ ,  $\Delta_n = 5$  and  $\tau = 10$ . From *top to bottom*, respectively,  $\alpha = 0, 0.5, 0.8, 0.9$  (*left column*) and  $\alpha = 0.97, 1, 1.5, 1.75$  (*right column*)

used here (cf. 11.1–11.4) can not only reproduce the exponential distance dependence of the experimentally measured transition times for electron transfer from donors to acceptors but also leads to the right order of magnitude of these transition times. For

**Fig. 11.12** Transition time from donor to acceptor as a function of the electron-lattice interaction,  $\alpha$ , using the data in Fig. 11.11. The depth of the wells is  $\varepsilon = -5$  (in units of  $\tau$ ). Temperature,  $T = 0.002D$ . Parameter values:  $\alpha = 0.1$ ,  $V = 0.1$ ,  $\Delta n = 5$  and  $\tau = 10$ . ( $N = 100$ )



example, it is approximately 3800 time units for  $\Delta n = 7$  when  $\varepsilon_{donor} = \varepsilon_{acceptor} = -5$  (in units of  $\tau$ ) (see Fig. 11.10). In Sect. 11.6 we show that the transition times depends weakly on  $\alpha$  between 0 and 0.9. On the other hand, above 0.9, the probability for an electron to go from the donor to the acceptor decreases markedly and for  $\alpha \geq 1.5$  the transition time becomes virtually infinite.

Regarding the mechanism that underlies the electronic transfer from donor to acceptor, our simulations also demonstrate that, at low temperatures, there is a whole spectrum of possibilities from non-tunneling to tunneling-like donor to acceptor transitions. E.g., in a lattice chain with weakly bound donor and acceptor electrons the electronic transition time is not exponential with distance (see solid bottom curve in Fig. 11.6 and Fig. 11.7). On the other hand, for strongly bound donor (and acceptor) electrons, the electronic transitions from donor to acceptor are of tunneling-type, even when  $\Delta n = 1$ , with the transition time growing very fast, i.e. following an exponential law with  $\Delta n$ . Future work will explore in greater detail the effect of stronger couplings between the electron and the lattice and also of higher temperatures on the electron transfer from donor to acceptor and on the corresponding transition times. It is worth mentioning that other studies with homogeneous lattices [8, 9, 21, 22, 31, 32, 62–66] have already pointed at the potential of this theory to explain faster electron transport as well.

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