Resonant and nonresonant transfers of Frenkel excitons in double helical DNA-like regular structures*

I.J. Lalov

Faculty of Physics, Sofia University "St. Kl. Ohridski", 1164 Sofia, Bulgaria

Abstract. Frenkel excitons (FEs) as collectivized electronic excitations are studied using the models of two-strands regular structures with B-DNA geometry. As basic excitations we consider the excitations of the pairs of complementary bases, not the excitations of separate bases, because of the following reasons: 1. Permanent pairing of complementary bases A-T and C-G; 2. Small inter-bases distances. The following cases are treated:

A. Resonant transfer of FEs between equal pairs of complementary bases, e.g. A-T. The models of homopolymers are supposed to contain the equal pair at each step of double helix and one strand contains one base (A-A-A- ...) or alternatively ordered bases (A-T-A-T-…).

B. Non resonant transfer of FEs between different pairs AT↔CG. Two models are studied: a) two-step order sequence with bases in one strand A-C-A-C…; b) four-step order sequence in one strand A-C-T-G-A-C-…

The studied FEs originate from electronic excitations of the pair with transition electric dipole moment perpendicular to the helical axis (for π-π* transitions) or parallel to the axis (for n-π* transitions). The corresponding Hamiltonians for each case allow to calculate the tensors of dielectric permittivity and of gyration, by using Green functions method (at temperature T=0). The calculations give formulas for excitonic spectra and the manifestation of FEs in linear absorption and in Circular Dichroism spectra

1. Introduction

In this paper we study the spectra and manifestation of transferable electronic excitations (Frenkel excitons – FEs) in regular double helix of DNA type with symmetry point group (∞). DNA is the biggest molecule and the sequences of pairs of complementary bases carry genetic information and information for production of proteins. It is also very stable independently of sequences of pairs AT and CG and on orientation of the pairs (AT or TA) at given location [1,2].

Our models treat regular double helical structures of B-form of DNA with perfect order of the pairs and of orientation of the bases. These models do not describe FEs in native DNA. But the transfers of electronic excitations in DNA are studied, as a first step, namely in regular structures (see e.g. [3]). In this way we understand the mechanism of transfer and corresponding excitonic spectra. Regular structures demand equivalent coupling of excitations with both nearest neighbors, mutatis mutandis.

As basic electronic excitations we introduce excitations of the pairs AT or CG, not of their complementary bases. Our approach differs the approaches of many other studies of FEs in DNA, see Ref. [4,5,3,6] in which as initial are used the excitations of the four bases (A, T, C, G). We prefer to study FEs transferred in stacking coupling of the pairs which are structural units of DNA (see [7]). On the other hand, the inter-bases distance in the pair is small and permanent pairing requires the treating of the pair as a hole.

Our description concerns two types of electronic transitions in the pairs: π→π* transitions which are strong and their transition electric dipole moments are parallel to the planes of the pairs and perpendicular to helical axis and n→π* transition with transition moments parallel to the helical axis.

In our calculations we are interested in the excitonic spectra and their demonstrations in linear absorption and in Circular Dichroism (CD). Applying methodics of condensed matter physics

---

*The paper is presented and discussed on BPU12 in Bucharest, Romania – 8-12.07.2025.

[8-10] we calculate dielectric permittivity *ε(ω,k)* and gyration tensor *ρ(ω,k)* near excitonic resonances. The necessary Green functions are calculated at temperature T=0. It is gyration tensor which describes optical activity (gyration) and correspondingly CD.

The organization of the paper is as follows: Section 2 contains short description of methodics of calculations. In Section 3 we treat two models of resonant transfers of FEs between equal pairs. Other two models in Section 4 allow to study the non-resonant transfers of FEs between different pairs. Section 5 is concluding and summarize some results and recommendations.

2. Methods

Let operators $T_{in}(T_{in}^{+})$ are operators of annihilation (creation) of electronic excitations with number *i* in the step *n* of B-ladder of regular DNA. The transition electric dipole moment is

$$\vec{R}^{(i)}(n) =< 0|T_{in}\sum_m (\overrightarrow{er_m})\,|0 > \tag{1}$$

in which $|0>$ is the ground state of the pair and sum *m* concerns all electric charges and their positions in the pair *n*. In our calculations we need also the matrix elements of the tensor $Q_{\alpha,\beta}^{(n)}$ which is the sum of electric quadrupole plus magnetic dipole transition moments. They can be expressed in the same way as $\vec{R}^{(i)}$, notably:

$$D_{\alpha\beta}^{i}(n) =< 0|T_{in}Q_{\alpha\beta}^{n}|0 > \tag{2}$$

The helical symmetry lead to the following relations (in the simplest model with equal and equally positioned steps, see Section 3, model A).

$$R_\alpha^{(i)}(n) = \sum \alpha_{\alpha\beta}^{(n)} R_\beta^{(i)}(0)\ ;\ D_{\alpha,\beta}^{(i)}(n) = \sum_{\gamma,\delta} \alpha_{\alpha,\gamma}^{(n)} \alpha_{\beta,\delta}^{(n)} D_{\gamma,\delta}^{(i)} \tag{3}$$

in which $\vec{R}^{(i)}(0)$ and $D^{(i)}$ are corresponding quantities for the step n=0, and $\alpha_{\alpha\beta}^{(n)}$ are expressed in the following matrix (supposing the helical axis directed along axis $\hat{z}$ and arbitrary axis (x,y)⊥z):

$$\left\|\alpha_{\alpha\beta}^{(n)}\right\| = \left\|\begin{matrix}\cos(n\varphi) & -\sin(n\varphi) & 0\\ \sin(n\varphi) & \cos(n\varphi) & 0\\ 0 & 0 & 1\end{matrix}\right\| \tag{4}$$

In more complicated models of Sections 3,4 the similar formulas (1) – (4) are valid but the arguments (nφ) in formula (4) are replaced, depending on the model (for model B the argument is n(π+φ).

Using matrix elements (1) – (2) we can calculate the tensor $\varepsilon_{\alpha\beta}(\omega,\vec{k})$ which connects vector *D* of electric displacement and vector $E(\omega,\vec{k})$ of electric field of electromagnetic wave (see [4-7]):

$$\Delta\varepsilon_{\alpha\beta}(\omega,k) = -A\sum_{\substack{n,m\\ i,j=1,2\\ \gamma=(x,y,z)}} \Big[R_\alpha^{(i)}(n)R_\beta^{(j)}(m) + ik_\gamma\Big(R_\beta^{(i)}(m)D_{\alpha\gamma}^{(j)}(n) - \\ -R_\alpha^{(j)}(n)D_{\beta\gamma}^{(i)}(m)\Big)\Big].e^{-i\vec{k}(\vec{n}-\vec{m})} < 0|T_{in}(t)T_{jm}^{+}(0)| > \tag{5}$$

in which A~N/*v*, where N is number of the steps in helix and *v* is volume of one step. The last multiple is Fourier-component of the following retarded Green function ($\theta(t)$ is step function):

$$G_{ij}(n,m) = -i\theta(t) < 0|T_{in}(t)T_{jm}^{+}(0)|0 > \tag{6}$$

Green functions (6) are calculated using well known methodics [8,10] and averaging in calculations is at temperature T=0 because of big excitation energy of FE, E_{FE}»k_BT (k_B – Boltzman constant). Green functions depend on Hamiltonian of the system.

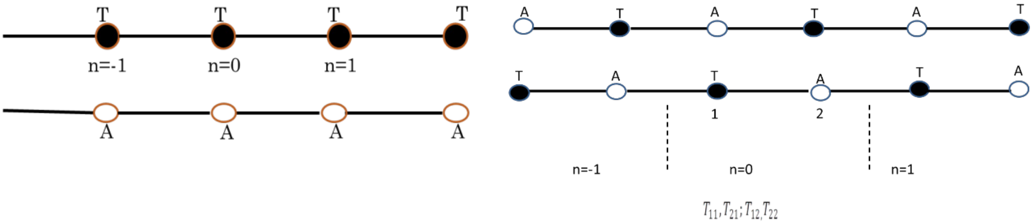
Tensor $\rho_{\alpha\beta}(\omega,k)$ of gyration describes optical activity and CD. It is connected with dielectric permittivity $\varepsilon_{\alpha\beta}(\omega,k)$ with relations [9,11]:

$$\varepsilon_{\alpha\beta}(\omega,k) = \varepsilon^{(1)}_{\alpha\beta}(\omega) + i\sum_{\gamma,\delta} k_\gamma e_{\alpha\beta\delta}\rho_{\delta\gamma} + O(k^2) \tag{7}$$

in which functions $\varepsilon^{(1)}_{\alpha\beta}(\omega)$ describe linear absorption in UV-spectra, $e_{\alpha\beta\delta}$ is Levi-Civita unit tensor and $O(k^2)$ depends on higher powers of wave vector k.

3. Resonant transfers of FEs in homopolymers

In this Section we consider two models of homopolymers with the same pair (e.g. AT) at each step of double helix. Thus transfers of FEs between neighbor steps are resonant.



Model A: complementary homopolymers

Model B: self – complementary co-polymers

FIGURE 1. Schemes of two models of homopolymers. Corresponding contacting bases A or T are denoted on two strands of double helix.

The schemes of two models are shown on Fig. 1. A more simple model A is described with formula (4). The realistic case of nondegenerate excitations of the pair is treated. For π→π* transitions the transition dipole moment is perpendicular to the helical axis $\hat{z}$. The case of collinear transition dipole moments of two different excitations is exotic. But in regular structures the transfers in both directions along helical axis must be equivalent and this is impossible at non collinear transition moments. That is why stacking coupling makes possible inter-step transfers of the same excitation only. For n→π* transitions with parallel to the axis $\hat{z}$ transition moments, (equal for all steps for a given excitation) the transfers with the change of excitations are possible. The Hamiltonians are as follows:

(π→π*) $$\hat{H}_{xy} = \sum_{k,i}[E_i + 2V_i\cos(ka)]T^{+}_{ik}T_{ik} \tag{8a}$$

(n→π*) $$\hat{H}_z = \sum_{k,i=3,4}\{[E_i + 2V_i\cos(ka)]T^{+}_{ik}T_{ik} + V\,[T^{+}_{3k}T_{4k}(1+e^{ika}) + h.c]\} \tag{8b}$$

(a – inter-step distance along helical axis $\hat{z}$).

In Hamiltonian $\hat{H}_z$ three transfers parameters V_3, V_4, V modulate excitonic spectra which at k=0 (these spectra enter tensors ε and ρ) for z-excitations):

$$E_{FE}(k=0) = \frac{1}{2}[E_3 + E_4 + 2(V_3+V_4)] \pm \sqrt{\left[\frac{E_3 - E_4 + 2(V_3 - V_4)}{2}\right]^2 + 4V^2} \tag{9}$$

Using formulas of Section 2, one obtains:

$$\Delta\varepsilon_{xx} = \Delta\varepsilon_{yy} = -\frac{A}{2}\sum_i R^{(i)2}(0)G_i\left(q=\frac{\varphi}{a}\right) \tag{10a}$$

$$\Delta\varepsilon_{xy} = -\Delta\varepsilon_{yx} = ik\left(\frac{A}{2}\right)\sum_i R^{(i)^2}\frac{\partial G_i}{\partial q}\Big|_{q=\frac{\varphi}{a}} \tag{10b}$$

$$G_i(q) = \frac{1}{\hbar\omega - E_i - 2V_i\cos(qa)} \tag{10c}$$

$$\varepsilon_{zz} = -\frac{A}{2\Delta_z(k=0)}\left[R_z^{(3)2}(\hbar\omega - E_4 - 2V_4) + R_z^{(4)2}(\hbar\omega - E_3 - 2V_3) + 4VR_z^{(3)}R_z^{(4)}\right] \tag{10d}$$

$$\Delta_z(k=0) = (\hbar\omega - E_3 - 2V_3)(\hbar\omega - E_4 - 2V_4) - 4V^2 \tag{10e}$$

As usual, excitonic spectra with q=φ/a are manifested in the plane of the pairs, whereas FEs with q =0 are active for polarization along helical axis $\hat{z}$. The component ε_{xy} expresses so called excitonic contribution to gyrotropy [12] and in CD spectra it gives sigmoidal curves with zero at excitonic maximum of linear absorption.

Now we turn to model B, see Fig. 1. The unit cell of self-complementary co-polymers contains two equal pairs with opposite orientation. For π→π* transitions the following model Hamiltonian can be used:

$$\widehat{H}_{(xy)} = \sum_{k,i}\left\{[E_i + 2V_i\cos(2ka)][T_{i1}^{+}T_{i1} + T_{i2}^{+}T_{i2}] + F_i\left[T_{i1}^{+}T_{i2}\left(1 + e^{2ika}\right) + h.c\right]\right\} \qquad (11)$$

in which second index of operators denotes the number of step in unit cell, and F_i is transfer parameter of FEs between two neighbor steps. In excitonic spectra so called Davydov splitting is observed [4,6], notably:

$$W_i(k) = E_i + 2V_i\cos(2ak) \pm 2F_i cos(ka) \qquad (12)$$

But in linear absorption and in CD spectra only the level with sign "-" is active. One obtains:

$$\Delta\varepsilon_{xx} = \Delta\varepsilon_{yy} = -\frac{A}{2}\sum_i R^{(i)2}\frac{\partial G_i(q)}{\partial q}_{|q=\frac{\varphi}{a}} \;;\; G_i(q) = \frac{1}{\hbar\omega - E_i - 2V_i\cos(2aq) + 2F_i cos(qa)} \qquad (13)$$

The excitonic contribution $\varepsilon_{xy} = -\varepsilon_{yx}$ can be expressed with formula (10b) with Green functions (13) and multiplied by 2. Using formulas of Section 2 we obtain the following components of gyration tensor for model A:

$$\rho_{xx} = \rho_{yy} = \left(\frac{A}{2}\right)\sum_i\left[R_y^{(i)}D_{zx}^{(i)} - R_x^{(i)}D_{zy}^{(i)}\right]G_i\left(\frac{\varphi}{a}\right) \qquad (14a)$$

$$\rho_{zz} = A\sum_{i=1,2}\left[R_x^{(i)}D_{yz}^{(i)} - R_y^{(i)}D_{xz}^{(i)}\right]G_i\left(\frac{\varphi}{a}\right) \qquad (14b)$$

The component $\rho_{xy} = -\rho_{yx}$ does not enter the formula for "effective" gyration tensor for light beam which includes angle θ with helical axis $\hat{z}$, namely:

$$\rho^{(\theta)} = \rho_{xx}sin^2\theta + \rho_{zz}cos^2\theta \qquad (15)$$

For n→π* transitions the transition dipole moments of excitation I of the pair 1 and 2, being parallel to helical axis, have opposite directions in model B. That is why the only active superposition can be expressed with the operators:

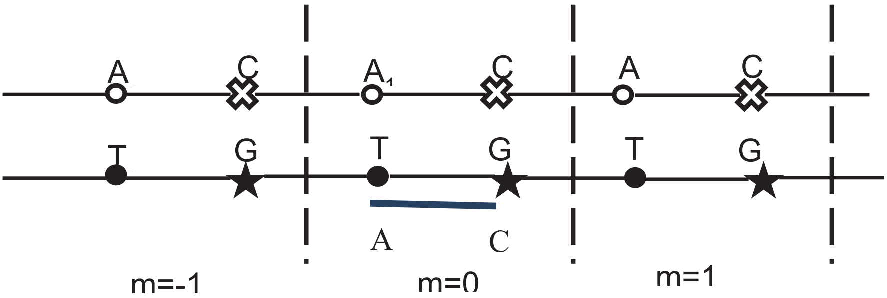
$$Z_{in} = \frac{1}{\sqrt{2}}(S_{i1}(n) - S_{i2}(n)), i = 3,4 \qquad (16)$$

Model Hamiltonian and components ε_{zz} can be represented using formulas (8b) and (10d) for operators (16) at k=0.

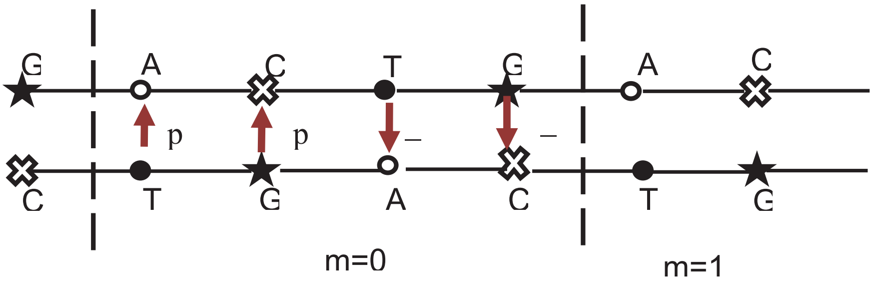
In formula (8b) one obtains E_i-F_i, see (11), and the expression of (10d) is multiplied by 2. A little surprising result, treating model B, is the vanishing of corresponding components of gyration tensor. In calculations of components $\rho_{xx} = \rho_{yy}$ for transitions with transition moments parallel to axis $\hat{z}$, one obtains the difference $d_{xy}^{(i)} = D_{xy}^{(i)} - D_{yx}^{(i)}$. We apply equations (3) – (4) for neighbor step n=1 but with argument n(π+φ) instead of nφ. One obtains the same expressions for $d_{xy}^{(i)}$ of the neighbor steps but their difference is zero for operators (16). Hence corresponding components of tensor ρ are zero. The CD signal is caused by other excitations (not n→π*).

4. Non-resonant transfers of FEs

Non-resonant transfers of FEs are transfers of electronic excitation between different pairs in double helix ladder. Taking into account the functions of DNA molecule they are so important as resonant transfers. We treat again two models of regular structures with different pairs (Fig. 2).



Model C: two – step order



Model D: four – step order

FIGURE 2. Scheme of double helix with different pairs. (AT) and (CG) are complementary bases, m is number of unit cell.

Model C contains two different pairs in unit cell. The pairs $(AT)_0$ and $(AT)_1$ are rotated at angle 2φ along helical axis with the same orientation of bases A and T (also for pair CG). We introduce transition dipole moments $\vec{p}_a(m), \vec{p}_c(m)$ and transition quantities $D_{\alpha\beta}^{(a)}(m), D_{\alpha\beta}^{(c)}$(m) for electronic excitations in the two pairs (AT) and (CG). They can be expressed with the transition parameters of unit m=0 using formulas (3) – (4) with argument 2nφ.

Both vectors $\vec{p}_a(0)$ and $\vec{p}_c(0)$ for π→π* transitions are parallel to the planes of the pairs. But the coupling of the two excitonic modes in regular structures is possible in the case of collinear vectors $\vec{p}_c$ and $\vec{p}_a$ (the last transformed according formulas (3), (4)). Then the following model Hamiltonian can be introduced:

$$\widehat{H}_{(xy)} = \sum_k\{[E_a + 2V^a\cos(2ka)]A_k^+A_k + [(E_c + 2V^c\cos(2ka)]C_k^+C_k + V\,[A_k^+C_k(1 + +e^{-2ika}) + h.c]\,\} \tag{17}$$

in which E_a, E_c are excitation energy of both excitations and V is transfer parameter of FEs between different neighbor pairs. As a result of mixing of the two excitations one obtains the following equation for excitonic levels $E_{1,2}(q)$:

$$\Delta(q) = [E_{1,2}(q) - E_a - 2V^a co\,s(2ka)][(E_{1,2}(q) - E_c - 2V^c\cos(2ka)] - -4V^2cos^2(qa) = 0 \tag{18}$$

with excitonic levels

$$E_{1,2}(k) = \frac{1}{2}[E_a + E_c + 2\cos(2ka)(V^a + V^c)] \pm \sqrt{\left[\frac{E_a - E_c + 2\cos(2ka)(V^a - V^c)}{2}\right]^2 + 4V^2cos^2(ka)} \tag{19}$$

Calculations of the components of tensor $\varepsilon(\omega, q)$ give the following results:

$$\varepsilon_{xx}(\omega, \tfrac{\varphi}{a}) = \varepsilon_{yy}(\omega, \tfrac{\varphi}{a}) = -\frac{A}{2\Delta\left(\varphi/a\right)}\,\gamma(\varphi) \tag{20a}$$

$$\gamma(\varphi) = p_a^2(\hbar\omega - E_c - 2V^c\cos(2\varphi)) + p_c^2(\hbar\omega - E_a - 2V^a\cos(2\varphi)) + 4Vp_ap_c cos\varphi \tag{20b}$$

$$\varepsilon_{xy} = -\varepsilon_{yx} = ikA\left\{\frac{\partial\left(1/\Delta(q)\right)}{\partial q}\Big|_{q=\varphi/a}\gamma(\varphi) - \frac{2a}{\Delta\left(\varphi/a\right)}p_ap_cVsin\varphi\right\} \tag{20c}$$

Hamiltonian $\widehat{H}_z$ for n→π* excitations contains the same terms as Hamiltonian $\widehat{H}_{(xy)}$, see (17), but with other values of E_a, E_c, V^a, V^c, V. Consequently, formula for component $\varepsilon_{zz}(\omega,0)$ is analogous of (20a) with new excitonic parameters and (2γ(0)) instead of γ(φ).

Model D of four – step order includes four pairs; the first two different pairs are neighbors of the second row of the same different pairs with opposite orientation of the complementaries bases. We consider only non-resonant transfers between the nearest neighbor steps. For π→π* transitions this type of transfers is possible in regular structures in the case of collinear vectors $\vec{p}_a, \vec{p}_c$ (see model C). Then one obtains the following model Hamiltonian:

$$\widehat{H}_{(xy)} = \sum_k\{E_a(A_{1k}^+A_{1k} + A_{3k}^+A_{3k}) + E_c(C_{2k}^+C_{2k} + C_{4k}^+C_{4k}) + M\left[A_{1k}^+\left(C_{2k} - C_{4k}e^{-i4ka}\right) + \right.$$
$$\left. + A_{3k}^+(C_{4k} - C_{2k}) + h.c\right]\} \tag{21}$$

with one transfer parameter M. For excitonic spectra E_{FE} we obtain a quartic equation

$$(bd)^2 - 4bdM^2 + 4M^4sin^2(2ka) = 0 \tag{22}$$

in which $d = E_{FE} - E_a$, $b = E_{FE} - E_c$. Its roots are as follows:

$$\Delta(q) = [bd - 4M^2cos^2(qa)][bd - 4M^2sin^2(qa)] = 0 \tag{23a}$$

$$E_{FE}^{(1,2)} = \frac{E_a+E_c}{2} \pm \sqrt{\left(\frac{E_a-E_c}{2}\right)^2 + 4M^2cos^2(qa)} \ :\ E_{FE}^{(3,4)} \tag{23b}$$

The pair $E_{FE}^{(3,4)}$ is analogous of $E_{FE}^{(1,2)}$ with $sin^2(qa)$ instead of $cos^2(qa)$. Lengthy calculations of dielectric permittivity give at Hamiltonian (21) curious result, notably

$$\varepsilon_{xx} = \varepsilon_{yy} = \frac{-A}{\mathrm{bd}-4M^2cos^2(qa)}\,\gamma(\varphi);\ \gamma(\varphi) = p_a^2d + p_c^2b - 4p_ap_cMcos\varphi \tag{24}$$

$$\varepsilon_{xy} = -\varepsilon_{yx} = ikA\left\{\frac{\partial}{\partial q}\left(\frac{1}{\Delta(q)}\right)_{q=\frac{\varphi}{a}}\gamma(\varphi)(bd - 4M^2sin^2\varphi) + 8a\frac{Msin\varphi}{\Delta(\frac{\varphi}{a})}[(bd - \right.$$
$$\left. -4M^2cos^2\varphi)p_ap_c - M^2cos\varphi(p_a^2d + p_c^2b)]\right\} \tag{25}$$

The maxima of linear absorption are zeros of the first multiple only in (23a). In CD spectra described with component ε_{xy} the both multiplies in (23a) are active and four peaks would be observed, not two as in linear absorption.

In calculations of component ε_{zz} we need Hamiltonian $\widehat{H}_z(k = 0)$ and component $\widehat{P}_z$ of transition dipole moment. Taking into account that z – component, parallel to the helical axis, is equal for all steps of double helix, one obtains:

$$\widehat{P}_z = h_{az}\left(Z_{1,k=0} - Z_{3,k=0}\right) + h_{cz}\left(Z_{2,k=0} - Z_{4,k=0}\right) \tag{26}$$

$$\widehat{H}_z(k = 0) = E_{az}\left(Z_{1,0}^+Z_{1,0} + Z_{3,0}^+Z_{3,0}\right) + E_{cz}\left(Z_{2,0}^+Z_{2,0} + Z_{4,0}^+Z_{4,0}\right) + V_z\left[\left(Z_{1,0}^+ - Z_{3,0}^+\right)\left(Z_{2,0} - \right.\right.$$
$$\left.\left. -Z_{4,0}\right) + h.c\right] \tag{27}$$

$$\varepsilon_{zz} = -\frac{A}{b_1d_1-4V_z^2}[h_{az}^2d_1 + h_{cz}^2b_1 + 4V_zh_{az}h_{cz}] \tag{28}$$

in which $b_1 = \hbar\omega - E_{az}$, $d_1 = \hbar\omega - E_{cz}$,and h_{az}, h_{cz} are parallel to the helical axis transition dipole moments.

5. Conclusions

Our study illustrates the importance of resonant and nonresonant transfers which modulate strongly excitonic spectra of DNA-like structures and as a result change the energy transport. We stress on the permanent pairing of the complementary bases and thus the choice of the excitations of the pairs as initial is natural and preferable (not excitations of separate bases). Nonresonant transfers can be effective in the case of comparable difference of excitation energy in the two pairs and coupling parameters.

In the study we use methodics of treating of FEs in condensed matter structures which is consistent not only because DNA molecule is the biggest one but also because of its helical symmetry and of a common nature of transfer processes in DNA and in other molecular structures. In applications of the excitonic theory one must take into account the existence of several close maxima with big spectral width in spectra of DNA, On the other hand, rotation of the pairs relatively helical axis decreases the coupling between second third and so on neighbors and stacking coupling between first neighbor pairs would prevail. So the feeling of non-very mobile Frenkel excitons in DNA molecule is, perhaps, correct.

Probably the right approach treating DNA – like structures is to consider transfers of FEs in some important units with known sequence of the pairs of complementary bases, and, as next step, transfers between these units.

Acknowledgment

The author thanks N. A. Kojouharova for technical assistance in preparation of presentation and manuscript.

REFERENCES

1. Cantor, Ch. R. and Shimmel, P. R., Biophysical Chemistry, Freeman and Co., San Francisco (1980)
2. Winkler, R. G., Polyelectrolytes and Semiflexible Polymers, in Physics meets biology, Gompper, G. and other (eds), Forchungs zentrum Julich (2004) 82 (1960) 4785
3. Bouvier, B., Gustavson, T., Markovitsi, D. and Milli, P., Chem. Phys. 275 (2002) 75-92 https://doi.org/10.1016/S0301-0104(01)00523-7
4. I. Tinoko Jr., J. Am. Chem. Soc. 82 (1960) 4785
5. I. Tinoko Jr., R. W. Woody and D. F. Bradley, J. Chem. Phys. 38 (1963), 1317
6. Czader A. and Bittner E.R. , J. Chem. Phys.128 (2008), 035101 doi: 10.1063/1.2821384
7. T. Miyata and S. Yomosa, J. Phys. Soc. Jap., 27 (1969) 720
8. Davydov, A. S., Theory of Molecular Excitons, Plenum Press, New York (1971)
9. Agranovich, V. M., Theory of Excitons (in Russian), Nauka, Moscow, 1968
10. Agranovich, V. M., Excitations in Organic Solids, Oxford University Press, New York (2009) https://doi.org/10.1093/acprof:oso/9780199234417.001.0001
11. Lalov, I. J. and Kojouharova, N. A., Chem. Phys. 563 (2022) 111642 https://doi.org/10.1016/j.chemphys.2022.111642
12. Harada, N. and Nakanishi, K., Circular Dichroism Spectroscopy – Excitonic Coupling in Organic Biochemistry, Uni. Sci. Books, Mill Valley, CA (1983)