

# B850 Ring from Photosynthetic Complex LH2 – Influence of Static Disorder

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**Abstract:** Photosynthesis starts with the absorption of a solar photon by one of the light-harvesting (LH) pigment-protein complexes and transferring excitation energy to the reaction center where charge separation is initiated. The geometric structure of some LH complexes is known in great detail, e.g. for LH2 complex of purple bacteria. Properties of such complex are strongly influenced by its interactions with environment. These interactions could be modeled by static and dynamic disorder. Four uncorrelated Gaussian types of fluctuations (in transfer integrals, in radial positions of molecules on the ring, in angular positions of molecules on the ring and in directions of dipole moments of molecules) are taken into account. The influence of these types of static disorder on Hamiltonian of B850 ring from LH2 complex is investigated in present paper. Results obtained for different types of static disorder are discussed and compared.

**Key-Words:** LH2 complex, B850 ring, static disorder, Hamiltonian, transfer integrals

## 1 Introduction

Photosynthesis is the process by which green plants and certain other organisms (bacteria, blue-green algae) transform light energy into chemical energy. During this process light energy is captured and used to convert water, carbon dioxide, and minerals into oxygen and energy-rich organic compounds. In chemical terms, photosynthesis is a light-energized oxidation–reduction process. Oxidation refers to the removal of electrons from a molecule; reduction refers to the gain of electrons by a molecule. These reactions occur in two stages: the light stage, consisting of photochemical (i.e., light-capturing) reactions; and the dark stage, comprising chemical reactions controlled by enzymes. During the first stage, the energy of light is absorbed and used to drive a series of electron transfers, resulting in the synthesis of ATP and the electron-donor reduced nicotinic adenine dinucleotide phosphate (NADPH). During the dark stage, the ATP and NADPH formed in the light-capturing reactions are used to reduce carbon dioxide to organic carbon compounds [1].

Our interest is mainly focused on first (light) stage of photosynthesis in purple bacteria. Solar photons are absorbed by a complex system of membrane-associated pigment-proteins (light-harvesting (LH) antenna) and the electronic excited state is efficiently

transferred to a reaction center, where the light energy is converted into a chemical energy [2]. The antenna systems of photosynthetic units from purple bacteria are formed by ring units LH1, LH2, LH3, and LH4. The geometric structure is known in great detail from X-ray crystallography. The general organization of above mentioned light-harvesting complexes is the same: identical subunits are repeated cyclically in such a way that a ring-shaped structure is formed. However the symmetries of these rings are different.

Crystal structure of LH2 complex contained in purple bacterium *Rhodospseudomonas acidophila* was first described in high resolution by McDermott et al. [3], then further e.g. by Papiz et al. [4]. The bacteriochlorophyll (BChl) molecules are organized in two concentric rings. One ring (B800 ring) features a group of nine well-separated BChl molecules with absorption band at about 800 nm. The second ring (B850 ring) consists of eighteen closely packed BChl molecules (B850) absorbing around 850 nm. Dipole moments in LH2 ring have tangential arrangement. The whole LH2 complex is nonameric, it consists of nine identical subunits. LH2 complexes from other purple bacteria have analogous ring structure.

Some bacteria contain also other types of complexes such as the B800-820 LH3 complex (*Rhodospseudomonas acidophila* strain 7050) or LH4

complex (*Rhodospseudomonas palustris*). LH3 complex like LH2 one is usually nonameric but LH4 one is octameric (it consists of eight identical subunits). The other difference between LH2 complex and LH4 one is the presence of two additional BChl rings in LH4 complex [5]. Dipole moments in main B- $\alpha$ /B- $\beta$  ring from LH4 complex are oriented radially. In addition, mutual interactions of the nearest neighbour BChls in this LH4 ring are approximately two times smaller in comparison with B850 ring from LH2 complex and they have opposite sign.

The intermolecular distances under 1 nm determine strong exciton couplings between corresponding pigments. That is why an extended Frenkel exciton states model could be used in theoretical approach. In spite of extensive investigation, the role of the protein moiety in governing the dynamics of the excited states has not been totally clear yet. At room temperature the solvent and protein environment fluctuates with characteristic time scales ranging from femtoseconds to nanoseconds. The simplest approach is to substitute fast fluctuations by dynamic disorder and slow fluctuations by static disorder.

Static disorder effect on the anisotropy of fluorescence for LH2 complexes was studied by Kumble and Hochstrasser [6] and Nagarajan et al. [7, 8]. We extended these investigations by consideration of dynamic disorder. We studied this effect for simple model systems [9–11] and then for models of B850 ring (from LH2) [12, 13]. Various types of uncorrelated static disorder (in local excitation energies, in transfer integrals, etc.) and correlated one (e.g., elliptical deformation) were used in the past [14–16] and also different arrangements of optical dipole moments were compared [17–20]. Recently we have focused on the modelling of absorption and steady state fluorescence spectra of LH2 and LH4 complexes within the nearest neighbour approximation model [21–25]. We have also extended our model to full Hamiltonian model and published the results for different types of static disorder [26–33].

Main goal of the present paper is the investigation of four types of static disorder (Gaussian fluctuations in transfer integrals, in radial positions of molecules on the ring, in angular positions of molecules on the ring and in directions of dipole moments of molecules) and comparison of their influence on Hamiltonian of B850 ring from LH2 complex. The rest of the paper is structured as follows. Section 2 introduces the ring model with different types of static disorder, used units and parameters could be found in Section 3, results are presented and discussed in Section 4 and some conclusions are drawn in Section 5.

## 2 Model

We consider only one exciton on molecular ring which can model B850 ring from LH2 complex. The Hamiltonian of an exciton on this ring reads

$$H = H_{\text{ex}}^0 + H_{\text{ph}} + H_{\text{ex-ph}} + H_{\text{s}}. \quad (1)$$

### 2.1 Ideal ring

First term in Eq. (1),

$$H_{\text{ex}}^0 = \sum_{m=1}^N E_m^0 a_m^\dagger a_m + \sum_{m,n=1(m \neq n)}^N J_{mn}^0 a_m^\dagger a_n, \quad (2)$$

corresponds to an exciton, e.g. the system without any disorder. The operator  $a_m^\dagger$  ( $a_m$ ) creates (annihilates) an exciton at site  $m$ ,  $E_m^0$  is the local excitation energy of  $m$ -th molecule and  $J_{mn}^0$  (for  $m \neq n$ ) is the so-called transfer integral between sites  $m$  and  $n$ . Local excitation energies  $E_m^0$  are the same for all bacteriochlorophylls on unperturbed ring, i.e.

$$E_m^0 = E_0, \quad m = 1, \dots, N.$$

Inside one ring the pure exciton Hamiltonian  $H_{\text{ex}}^0$  can be diagonalized using the wave vector representation with corresponding delocalized Bloch states  $\alpha$  and energies  $E_\alpha$ . Using Fourier transformed excitonic operators  $a_\alpha$ , the Hamiltonian in  $\alpha$ -representation reads

$$H_{\text{ex}}^0 = \sum_{\alpha=1}^N E_\alpha a_\alpha^\dagger a_\alpha. \quad (3)$$

The interaction strengths between the nearest neighbour bacteriochlorophylls inside one subunit and between subunits are almost the same in B850 ring from LH2 complex (see Figure 1 (B) in [5]). That is why such ring can be modeled as homogeneous case. If we consider the nearest neighbour approximation model (only the nearest neighbour transfer matrix elements are nonzero), we have

$$J_{mn}^0 = J_0(\delta_{m,n+1} + \delta_{m,n-1}). \quad (4)$$

In that case the form of operators  $a_\alpha$  is

$$a_\alpha = \sum_{n=1}^N a_n e^{i\alpha n}, \quad \alpha = \frac{2\pi}{N}l, \quad l = 0, \dots, \pm \frac{N}{2}, \quad (5)$$

where  $N = 18$  and the simplest exciton Hamiltonian for B850 ring from LH2 complex in  $\alpha$ -representation is given by Eq. (3) with

$$E_\alpha = E_0 - 2J_0 \cos \alpha. \quad (6)$$

In dipole-dipole approximation, transfer integrals  $J_{mn}$  can be written as

$$J_{mn} = \frac{\vec{d}_m \cdot \vec{d}_n}{|\vec{r}_{mn}|^3} - 3 \frac{(\vec{d}_m \cdot \vec{r}_{mn})(\vec{d}_n \cdot \vec{r}_{mn})}{|\vec{r}_{mn}|^5} = |\vec{d}_m||\vec{d}_n| \frac{\cos \varphi_{mn} - 3 \cos \varphi_m \cos \varphi_n}{|\vec{r}_{mn}|^3}. \quad (7)$$

Here  $\vec{d}_m$  and  $\vec{d}_n$  are local dipole moments of  $m$ -th and  $n$ -th molecule respectively,  $\vec{r}_{mn}$  is the vector connecting  $m$ -th and  $n$ -th molecule and  $\varphi_m$  ( $\varphi_n$ ) is the angle between  $\vec{d}_m$  ( $\vec{d}_n$ ) and  $\vec{r}_{mn}$ . The angle between  $m$ -th and  $n$ -th vector of local dipole moment ( $\vec{d}_m$ ,  $\vec{d}_n$ ) is referred to as  $\varphi_{mn}$ . Geometric arrangement of the ring has to correspond with the interaction strengths between the nearest neighbour bacteriochlorophylls. That is why distances  $r_{m,m+1}$  of neighbouring molecules in B850 ring from the LH2 complex have to be the same (without any disorder) and angles  $\beta_{m,m+1}$  have to be the same too ( $\beta_{m,m+1} = 2\pi/18$ , see Figure 1).

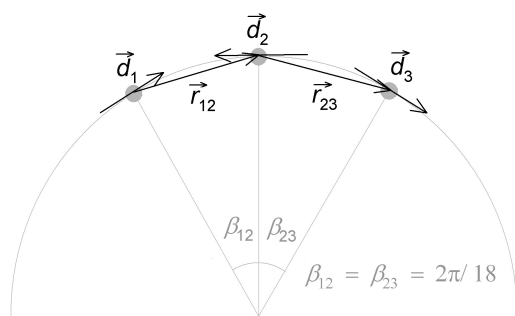


Figure 1: Geometric arrangement of ideal B850 ring from LH2 complex (without any fluctuations)

## 2.2 Dynamic disorder

The second term in Eq. (1),

$$H_{\text{ph}} = \sum_q \hbar \omega_q b_q^\dagger b_q, \quad (8)$$

represents phonon bath in harmonic approximation. Phonon creation and annihilation operators are denoted by  $b_q^\dagger$  and  $b_q$ , respectively.

The third term,

$$H_{\text{ex-ph}} = \frac{1}{\sqrt{N}} \sum_m \sum_q G_q^m \hbar \omega_q a_m^\dagger a_m (b_q^\dagger + b_q), \quad (9)$$

describes exciton-phonon interaction which is assumed to be site-diagonal and linear in bath coordinates (the term  $G_q^m$  denotes the exciton-phonon coupling constant).

## 2.3 Static disorder

Last term in Eq. (1),  $H_s$ , corresponds to static disorder. Different types of static disorder can be taken into account. Fluctuations in local excitation energies of bacteriochlorophylls  $\delta \varepsilon_m$ ,

$$E_m = E_0 + \delta \varepsilon_m, \quad (10)$$

represent one of the most commonly used types of static disorder.

Consideration of fluctuations in transfer integrals  $\delta J_{mn}$  ( $m \neq n$ ),

$$J_{mn} = J_{nm} = J_{mn}^0 + \delta J_{mn}, \quad (11)$$

is another way how the static disorder can be modeled.  $\delta J_{mn}$  can be treated as uncorrelated Gaussian fluctuations (with the standard deviation  $\Delta_J$ ) or they can be connected with deviation in geometric arrangement of the ring. In following, from various types of geometric deviations we deal with three ones:

- a) uncorrelated fluctuations of radial positions of molecules  $\delta r_m$  on the ring (Gaussian distribution and standard deviation  $\Delta_r$ ),

$$r_m = r_0 + \delta r_m, \quad (12)$$

where  $r_0$  is the radius of the ring without any disorder (see Figure 2);

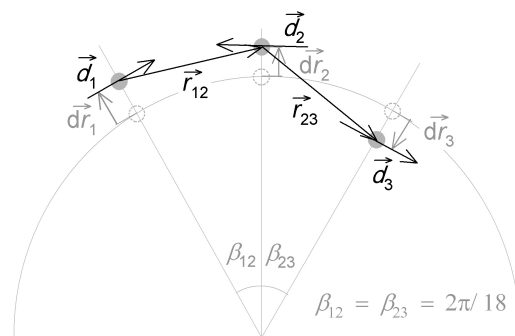


Figure 2: B850 ring from LH2 complex – fluctuations in radial positions of bacteriochlorophylls  $\delta r_m$

- b) uncorrelated fluctuations of angular positions of molecules  $\delta \nu_m$  on the ring (Gaussian distribution and standard deviation  $\Delta_\nu$ ),

$$\nu_m = \nu_m^0 + \delta \nu_m, \quad (13)$$

where  $\nu_m^0$  is the angular position of  $m$ -th bacteriochlorophyll on the ring, directions of bacteriochlorophyll dipole moments in new positions are again tangential to the ring (see Figure 3);

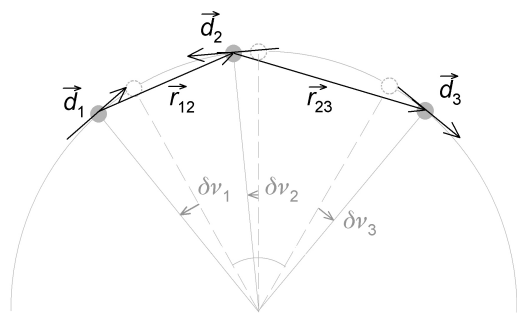


Figure 3: B850 ring from LH2 complex – fluctuations in angular positions of bacteriochlorophylls  $\delta\nu_m$

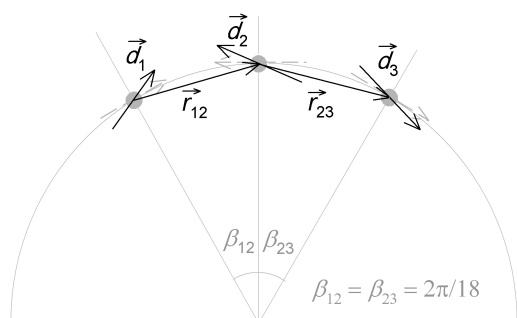


Figure 4: B850 ring from LH2 complex – fluctuations in directions of bacteriochlorophyll dipole moments  $\delta\vartheta_m$

- c) uncorrelated fluctuations of bacteriochlorophyll dipole moment directions  $\delta\vartheta_m$  (Gaussian distribution and standard deviation  $\Delta_\vartheta$ )

$$\vartheta_m = \vartheta_m^0 + \delta\vartheta_m, \quad (14)$$

where  $\vartheta_m^0$  determines dipole moment direction of  $m$ -th bacteriochlorophyll molecule. Positions of bacteriochlorophylls remain the same as in unperturbed ring (see Figure 4).

### 3 Units and Parameters

Dimensionless energies normalized to the transfer integral  $J_{m,m+1} = J_0$  (see Eq. (4)) have been used in our calculations. Estimation of  $J_0$  varies in literature between  $250 \text{ cm}^{-1}$  and  $400 \text{ cm}^{-1}$ .

In our previous investigations [34] we found from comparison with experimental results for B850 ring from the LH2 complex [35] that the possible strength  $\Delta_J$  of the uncorrelated Gaussian static disorder in transfer integrals  $\delta J_{mn}$  is approximately

$\Delta_J \approx 0.3 J_0$ . That is why for this type of static disorder we have taken the strengths

$$\Delta_J \in \langle 0.05 J_0, 0.30 J_0 \rangle. \quad (15)$$

Other above mentioned types of static disorder also manifest themselves through the fluctuations of transfer integrals and therefore we have taken their strengths in connection with strength  $\Delta_J$ :

- a) uncorrelated fluctuations of radial positions of molecules  $\delta r_m$

$$\Delta_r \in \langle 0.03 r_0, 0.18 r_0 \rangle, \quad (16)$$

- b) uncorrelated fluctuations of angular positions of molecules  $\delta\nu_m$

$$\Delta_\nu \in \langle 0.001 \pi, 0.016 \pi \rangle, \quad (17)$$

- c) uncorrelated fluctuations of bacteriochlorophyll dipole moment directions  $\delta\vartheta_m$

$$\Delta_\vartheta \in \langle 0.03 \pi, 0.18 \pi \rangle. \quad (18)$$

## 4 Results and Discussion

Influence of various types of static disorder on Hamiltonian (namely on the nearest neighbour transfer integrals) of B850 ring from LH2 complex is investigated in present paper. Distributions of the nearest neighbour transfer integral  $J_{m,m+1}$  were calculated for above mentioned four types of static disorder. These distributions are graphically presented in two ways – mainly by contour plots and also by line plots. Additionally we calculated expected values  $E(J_{m,m+1})$  and standard deviations  $\sqrt{D(J_{m,m+1})}$  of the distributions. These numerical characteristics are presented in four tables together with corresponding static disorder strengths. Values of  $E(J_{m,m+1})$  and  $E(J_{m,m+1}) \pm \sqrt{D(J_{m,m+1})}$  are also drawn in contour plots.

Uncorrelated Gaussian distributions of  $J_{m,m+1}$  are presented in Figure 5 for comparison to other types of static disorder that are connected with deviations of ring geometry. For this type of fluctuations ( $\delta J_{m,m+1}$ ), of course, the expected value of the distribution of the nearest neighbour transfer integrals  $J_{m,m+1}$  is independent of the strength of static disorder, i.e.  $E(J_{m,m+1}) = J_0$  and the strength of static disorder  $\Delta_J$  equals the standard deviation  $\sqrt{D(J_{m,m+1})}$ .

Figure 6 shows the distributions of  $J_{m,m+1}$  for Gaussian uncorrelated static disorder  $\delta r_m$  in radial positions of molecules on the ring. The distributions of

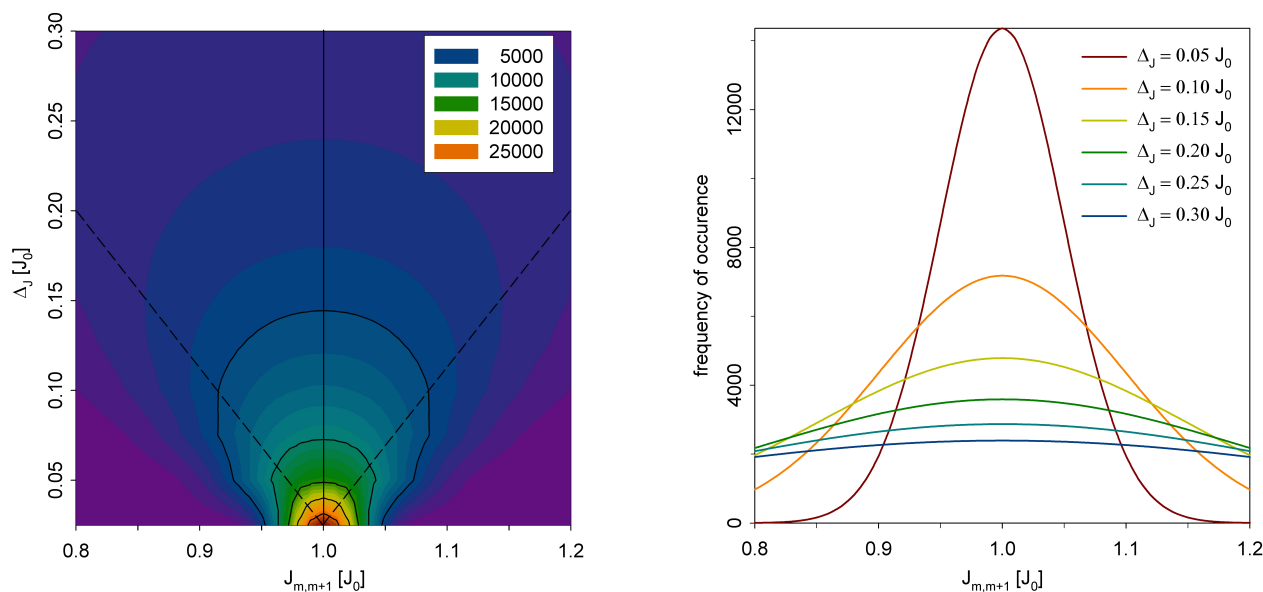


Figure 5: Distributions of the nearest neighbour transfer integrals  $J_{m,m+1}$  for B850 ring from LH2 complex – uncorrelated static disorder in transfer integrals  $\delta J_{mn}$  (six strengths  $\Delta_J = 0.05, 0.10, 0.15, 0.20, 0.25, 0.30 J_0$ )

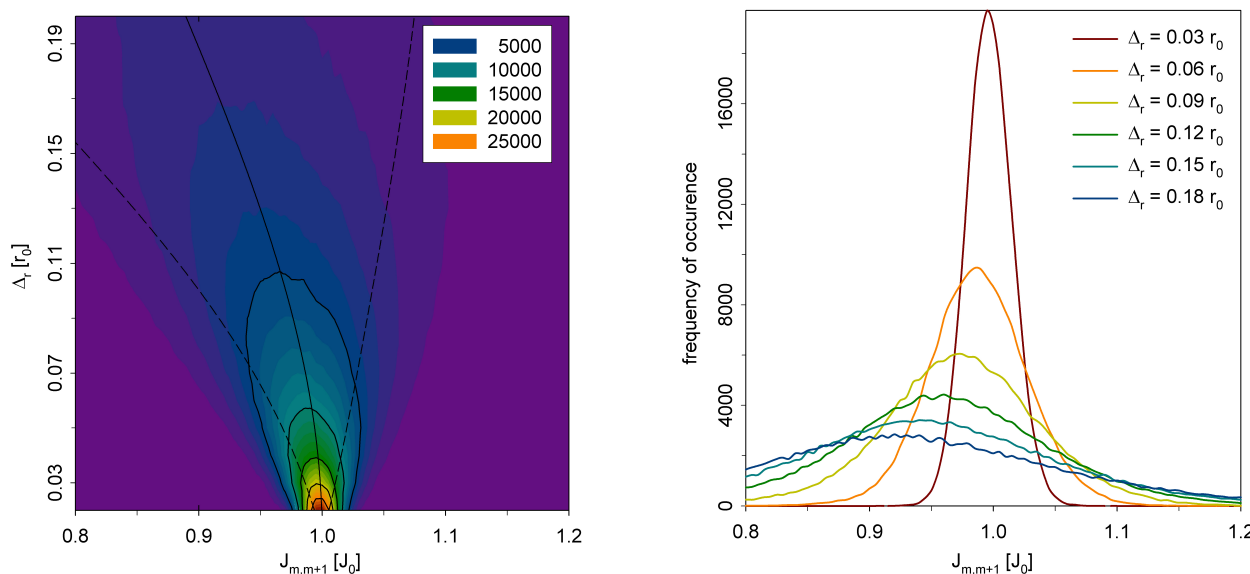


Figure 6: Distributions of the nearest neighbour transfer integrals  $J_{m,m+1}$  for B850 ring from LH2 complex – uncorrelated static disorder in radial positions of molecules  $\delta r_m$  (six strengths  $\Delta_r = 0.03, 0.06, 0.09, 0.12, 0.15, 0.18 r_0$ )

$J_{m,m+1}$  for two other above mentioned types of static disorder can be seen in Figure 7 (Gaussian uncorrelated fluctuations of angular positions of molecules on the ring  $\delta \nu_m$ ) and in Figure 8 (Gaussian uncorrelated fluctuations of molecular dipole moment directions  $\delta \vartheta_m$ ). For these types of static disorder (connected with deviations in ring geometry) expected

value  $E(J_{m,m+1})$  depends on static disorder strength. Dependencies of  $E(J_{m,m+1})$  and  $\sqrt{D(J_{m,m+1})}$  on corresponding static disorder strength are presented in Figure 6 (left column) and Table 1 ( $\Delta_r$ ), Figure 7 (left column) and Table 2 ( $\Delta_\nu$ ) and Figure 8 (left column) and Table 3 ( $\Delta_\vartheta$ ). As concerns expected value

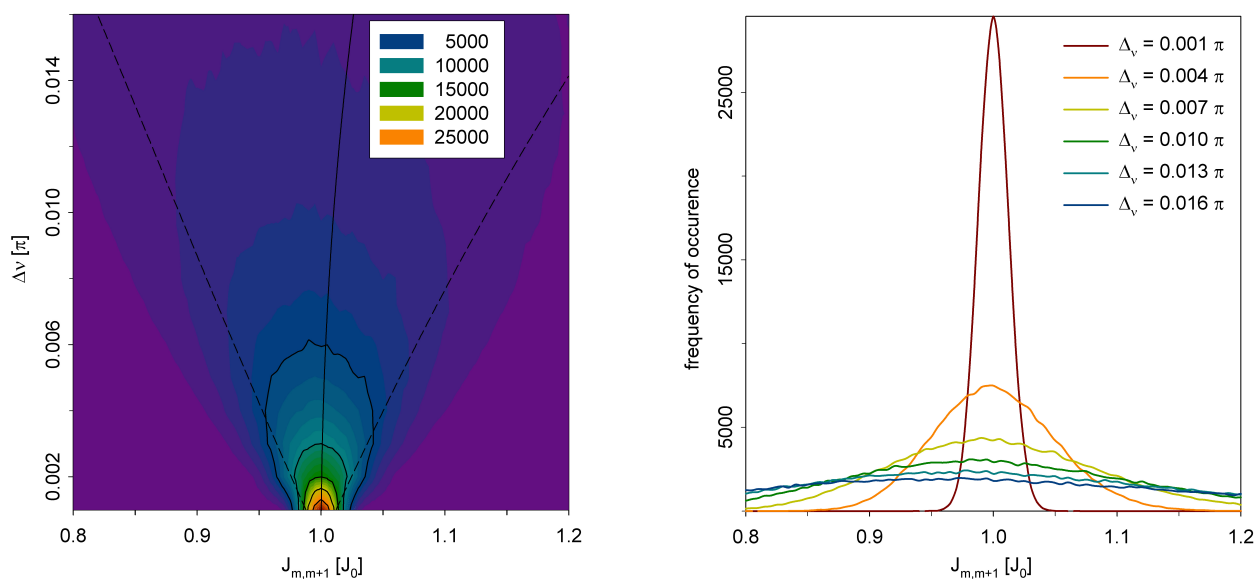


Figure 7: Distributions of the nearest neighbour transfer integrals  $J_{m,m+1}$  for B850 ring from LH2 complex – uncorrelated static disorder in angular positions of molecules  $\delta\nu_m$  (six strengths  $\Delta_\nu = 0.001, 0.004, 0.007, 0.010, 0.013, 0.016 \pi$ )

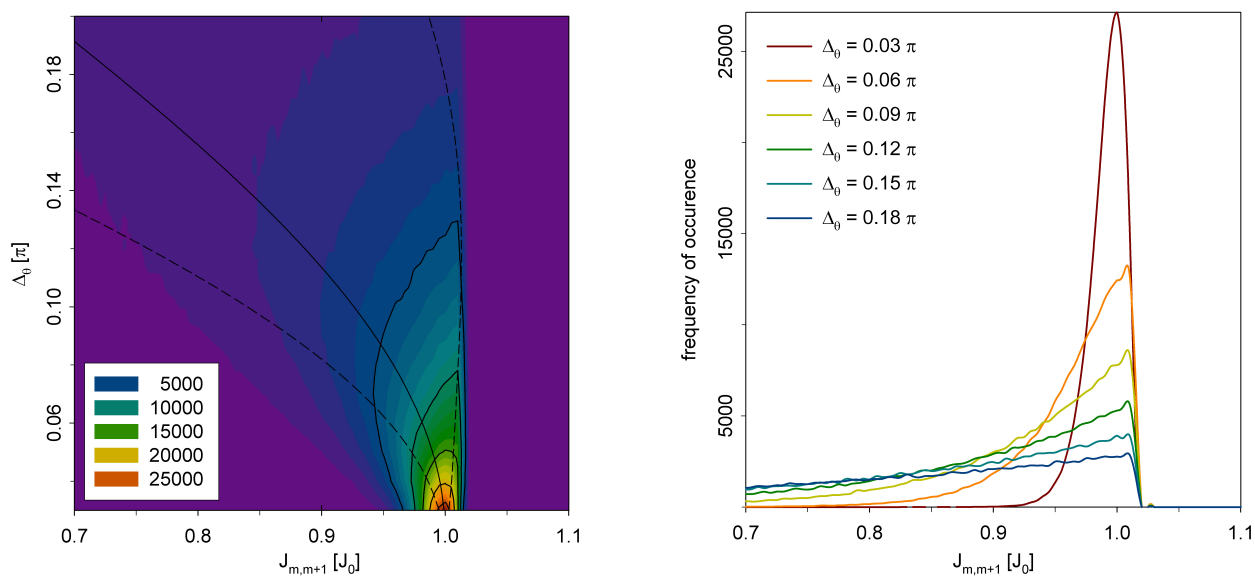


Figure 8: Distributions of the nearest neighbour transfer integrals  $J_{m,m+1}$  for B850 ring from LH2 complex – uncorrelated static disorder in dipole moment directions  $\delta\vartheta_m$  (six strengths  $\Delta_\vartheta = 0.03, 0.06, 0.09, 0.12, 0.15, 0.18 \pi$ )

$E(J_{m,m+1})$ , we can see decrease of it for increasing static disorder strength in case of fluctuations in radial positions of molecules on the ring  $\delta r_m$  (see Figure 6 and Table 1) and fluctuations in molecular dipole moment directions  $\delta\vartheta_m$  (see Figure 7 and Table 2). On the other hand,  $E(J_{m,m+1})$  increases with growing strength of static disorder in angular positions of

molecules on the ring  $\delta\nu_m$  (see Figure 8 and Table 3). In all these three cases dependence of standard deviation on strength of static disorder is nonlinear. The most important change of expected value occurs in case of fluctuations of molecular dipole moment directions  $\delta\vartheta_m$ . In addition, the distribution of  $\delta J_{m,m+1}$  is significantly skewed in this case. In contrast with

$\Delta_r$	expected value $E(J_{m,m+1})$	standard deviation $\sqrt{D(J_{m,m+1})}$
0.03 $r_0$	0.997 $J_0$	0.018 $J_0$
0.06 $r_0$	0.988 $J_0$	0.040 $J_0$
0.09 $r_0$	0.973 $J_0$	0.066 $J_0$
0.12 $r_0$	0.954 $J_0$	0.096 $J_0$
0.15 $r_0$	0.932 $J_0$	0.129 $J_0$
0.18 $r_0$	0.907 $J_0$	0.163 $J_0$

Table 1: Expected values and standard deviations of the nearest neighbour transfer integral  $J_{m,m+1}$  distributions for uncorrelated Gaussian fluctuations  $\delta r_m$  (six strength  $\Delta_r$ )

$\Delta_\nu$	expected value $E(J_{m,m+1})$	standard deviation $\sqrt{D(J_{m,m+1})}$
0.001 $\pi$	1.000 $J_0$	0.012 $J_0$
0.004 $\pi$	1.002 $J_0$	0.049 $J_0$
0.007 $\pi$	1.005 $J_0$	0.086 $J_0$
0.010 $\pi$	1.010 $J_0$	0.124 $J_0$
0.013 $\pi$	1.017 $J_0$	0.164 $J_0$
0.016 $\pi$	1.026 $J_0$	0.206 $J_0$

Table 2: Expected values and standard deviations of the nearest neighbour transfer integral  $J_{m,m+1}$  distributions for uncorrelated Gaussian fluctuations  $\delta \nu_m$  (six strength  $\Delta_\nu$ )

$\Delta_\vartheta$	expected value $E(J_{m,m+1})$	standard deviation $\sqrt{D(J_{m,m+1})}$
0.03 $\pi$	0.991 $J_0$	0.015 $J_0$
0.06 $\pi$	0.965 $J_0$	0.045 $J_0$
0.09 $\pi$	0.923 $J_0$	0.089 $J_0$
0.12 $\pi$	0.868 $J_0$	0.145 $J_0$
0.15 $\pi$	0.801 $J_0$	0.207 $J_0$
0.18 $\pi$	0.727 $J_0$	0.271 $J_0$

Table 3: Expected values and standard deviations of the nearest neighbour transfer integral  $J_{m,m+1}$  distributions for uncorrelated Gaussian fluctuations  $\delta \vartheta_m$  (six strength  $\Delta_\nu$ )

this type of static disorder the changes of  $E(J_{m,m+1})$  are very low for fluctuations in angular positions of molecules  $\delta \nu_m$ .

## 5 Conclusions

Comparison of the results obtained within different types of static disorder can be summarized as follows. Expected value of the nearest neighbour transfer in-

tegral distribution depends on static disorder strength for all presented types of fluctuations connected with ring geometry. The most essential change appears in case of static disorder in dipole moment directions. In this case also the dependence of standard deviation of the distribution on the static disorder strength has the highest nonlinearity. This is connected with the highest skewness of this distribution.

**Acknowledgements:** Support from the Faculty of Science, University of Hradec Králové (project of specific research No. 2106/2016) is acknowledged.

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