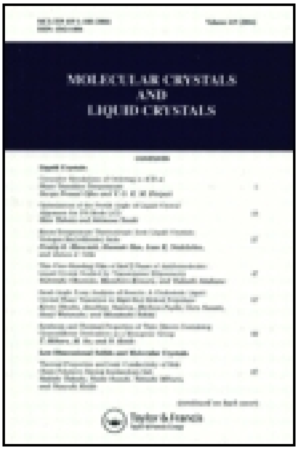

Molecular Crystals and Liquid Crystals

# A Simple Model for Charge Transport in Discotic Liquid Crystals

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# A SIMPLE MODEL FOR CHARGE TRANSPORT IN DISCOTIC LIQUID CRYSTALS

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*In this paper we have examined and revised the treatment of charge transfer phenomena along the columns in discotic liquid crystals. Dynamics of molecules forming the columns is described by a simple harmonic elastic model. Different regimes depending on the ratio of a characteristic molecular oscillation amplitude and an electronic localization length, are examined.*

*Keywords*: discotics; hopping; conductivity

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## 1. INTRODUCTION

This paper is dedicated to Prof. S.Chandrasekhar, who is not only a great and fascinating scientist, but also a source of inspiration on many aspects of liquid crystals. His discovery of discotic liquid crystals has created a new and fruitful (from both the fundamental science and applications points of view) branch of liquid crystalline science. In spite of its 25 year long history the study of discotic liquid crystals is still in an accelerating stage. Chandrasekhar continues to work and we look forward for further insights and discoveries from these endeavours. This investigation is also motivated by one recent Chandrasekhar publication "Discotic liquid crystals as quasi-one-dimensional electrical conductors". In order for the later discussions to be smooth we give here a brief summary of the results of that paper [1].

- The phase diagram of the investigated discotic liquid crystal, includes, a low temperature highly ordered hexagonal columnar phase *H* with discs

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stacked regularly within each column (thus strictly speaking the *H* structure is a 3D crystalline one). At higher temperatures it is transformed into $\mathrm{Col_h}$ phase, the hexagonal columnar phase with a disordered stack of discs, and finally - into the isotropic liquid;

- The addition of the dopant hardly changes the conductivity in the isotropic phase relative to the undoped sample. On the contrary, the conductivity in the columnar phase (along the columns) increases by nearly seven orders of magnitude from the value in the doped isotropic phase;
- The conductivity in the mesophase does not depend on the frequency in the doped state, and on the other hand the conductivity does show an increase with frequency in the isotropic phase in the doped state. In the undoped state the frequency dependence is observed in the mesophase.

The enlisted results clearly manifest that charge transport mechanisms along the columns in the undoped state (and also in the isotropic phase of the doped state), and in the columnar phases *H* and $\mathrm{Col_h}$ in the doped state are drastically different. Moreover, in the liquid crystalline phases, owing to specific molecular dynamic motions within the columns, charge transport in discotic liquid crystals might be different considerably from that in solid state materials.

The very fact of the observation of so strong (seven orders of magnitude (!)) variation of the conductivity with doping is a direct indication of the prevailing role of hopping processes along the discotic columns. Indeed the physical argument leading to a strong (exponential) dependence of the conductivity on the doping (impurity concentration $\mathrm{N_D}$) may be rationalized as follows. The hopping probability to jump between two impurity sites, is determined by the corresponding states wave functions overlapping. We are interested in scales larger than say the Bohr radius $a$ of the charge bounded to the individual impurity site. At such a scale the overlapping depends exponentially on the distance. When $\mathrm{N_D}$ decreases, the average length (the charge must jump to provide the hopping conductivity) increases $\propto \mathrm{N_D}^{-1/3}$, and therefore the hopping probability decreases exponentially $\propto \exp(-\mathrm{N_D}^{-1/3}/a)$.

We believe that in the isotropic state of the doped sample or in any state of the undoped one, the conductivity is determined mainly by the carriers from ionized shallow impurities, always existing in such organic materials (see e.g. [2], and let us emphasize that we are talking about say natural impurities in the undoped samples). In the temperature region $\mathrm{E_i} \leq \mathrm{T} \ll \mathrm{E_g}$ (where $\mathrm{E_i}$ is the characteristic energy scale for the impurity levels, $\mathrm{E_g}$ is the forbidden energy gap for the undoped material), almost all these impurities are ionized, and their concentration in the conduction band only weakly depend on the temperature (there is an increasing contribution superimposed to decrease due to some reduction of the mobility, since the electron phonon scattering slightly increases). The scenario will be discussed in the next section 2.

We have recently shown (for a 1D model with time dependent random hopping [3,4]), that one can successfully attack the similar problem of charge transfer through DNA base pairs stack between donor and acceptor molecules. The model enables us on equal footing to investigate both diffusion of electrons and their tunneling between different sites. We detail key results necessary for our investigation in section 3. Section 4 is devoted to a simple treatment of 1D molecular dynamics which enables us to study possible hopping amplitudes statistics. Depending on the ratio of a characteristic molecular oscillation amplitude and electronic localization length different regimes are examined. We end with some brief conclusions in Section 5.

## 2. ISOTROPIC PHASE AND UNDOPED SAMPLES

As was mentioned above, we believe that ionization into the conduction band of the shallow intrinsic impurities, provides the carriers, and this scenario explains some decrease of the conductivity when the temperature decreases. On further temperature decrease most of these carriers should recombine with the oppositely charged impurity sites, and therefore the conductivity band becomes empty. In this temperature region (i.e. $\mathrm{T} \leq \mathrm{E_i}$) the conductivity is provided by a hop from an occupied impurity site to a vacant site, separated by a distance $z$. The law describing this kind of hopping conductivity was found long ago by Mott (see e.g. [5]). Since we are interested in only 1D hopping along the columns the probability $P$ for such a hop is

$$\mathrm{P} \simeq \exp\left(-2\alpha z - \frac{W}{T}\right), \tag{1}$$

where $\alpha^{-1}$ is the electron localization length, and $W$ is the energy difference between the two sites.

According to Mott's so-called variable range hopping argument, there is a certain competition between the two terms in the exponent (Eq. (1)), and an electron may optimize its hopping distance $z$ to achieve the largest hopping rate (therefore, the largest conductivity). If we assume that the site energy has a uniform distribution between $-\Delta$ and $+\Delta$, the average energy spacing for sites separated by a distance $z$, would be $a\Delta/z$ (where $a$ is the average intermolecular distance along the columns).

Thus

$$P \simeq \exp\left(-2\alpha z - \frac{a\Delta}{zT}\right). \tag{2}$$

The optimum hopping distance $z_0$ is determined by maximizing this expression,

$$\mathrm{z}_0 = \sqrt{\frac{8a\alpha\Delta}{T}},$$

and the hopping conductivity is

$$\sigma \simeq \exp\left(-\sqrt{\frac{8\alpha a\Delta}{T}}\right), \tag{3}$$

and it gives more slow than the standard activation law temperature dependence, which becomes even more slow if one takes into account that localization length $\alpha^{-1}$can increase with the temperature increase.

As it concerns a.c., i.e. frequency dependent conductivity, for qualitative analysis of Chandrasekhar data [1] it is convenient to use the following scaling arguments [6] which can be applied to any 1D system with static and dynamic disordering. The starting point of the approach is the wave packet time spreading

$$\Delta z^2(E,t) = \left\langle (\hat{z}(t) - \hat{z}(0))^2 \right\rangle_E, \tag{4}$$

where $\hat{z}(t)$ is the Heisenberg representation for the electronic position along the column operator, and quantum mechanical averaging performed at a given electronic energy $E$. In turn this quantity (Eq. (4)) can be related to the velocity self-correlation function $C(E, t)$

$$C(E,t) = \langle \hat{v}_z(t)\hat{v}_z(0) + \hat{v}_z(0)\hat{v}_z(t)\rangle_E, \tag{5}$$

and comparing (Eqs. (4, 5)) we get

$$\frac{d^2}{dt^2}\Delta z^2(E,t) = C(E,t). \tag{6}$$

Therefore for small time interval we have (from Eq. (6)) so-called ballistic propagation

$$\Delta z^2(E,t) \simeq C(E,0)t^2. \tag{7}$$

whereas for the larger times due to disordering, the propagation is no more ballistic, e.g. it could be diffusive

$$\Delta z^2(E,t) = D(E)t, \tag{8}$$

where $D$ is the energy dependent diffusion coefficient. In a more general case of the dynamic and static disordering we are dealing within the discotic liquid crystals, one can assume a general scaling behavior for the wave packet spreading

$$\Delta z^2(t) = At^{2\beta}, \tag{9}$$

where the exponent $\beta = 1$ describes a ballistic propagation, and $\beta = 1/2$ - diffusive one. The time dependent diffusion coefficient is also related to the Kubo a.c. conductivity. Introducing a characteristic relaxation time $\tau$ (at $t > \tau$ the electronic wave function looses its phase memory) we end up with

$$\sigma(\omega)\alpha \int_0^\infty dt \exp\left[\left(i\omega - \frac{1}{\tau}\right)\right] \frac{d^2\Delta z^2}{dt^2} \alpha\, A\left(\frac{\tau}{1 - i\omega\tau}\right)^{2\beta-1}. \tag{10}$$

It follows from (Eq. 10) that at $\beta > 1/2$, the real part of the a.c. conductivity increases with $\omega$, and it conforms to the data presented in [1] and with our conjecture (based on the temperature dependence) that in the undoped samples (and in the isotropic phase in the doped samples) the conductivity is governed mainly by the ionized from shallow impurities carriers activated into the conductivity band.

This expression (Eq. (10)) is a quite general one, and based only on quantum mechanical treatment of non-interacting charge carriers. Therefore to have frequency independent a.c. conductivity (as it was observed in [1] for the doped samples in the discotic $H$ and $Col_h$ phases, one must admit that for this case $\beta = 1/2$, i.e. there is pure diffusional broadening of the wave packet. As we will show in the next section molecular vibrations assisted hopping along the columns can provide this diffusional process.

## 3. 1D HOPPING MODEL FOR THE DOPED SAMPLES

The experimental data [1] clearly indicate that in the doped samples in the ordered discotic liquid crystalline phase, the conductivity has nothing to do with thermal activated more or less free carriers. Since the transversal (with respect to the columns) conductivity is negligible, we can restrict ourselves to one column which we treat as 1D linear chain of stacked molecules - discs.

The model we will work with takes into account the most minimal amount of physical ingredients needed to describe charge transport phenomena in discotic liquid crystals. The charge is carried through the columns of the discotic liquid crystal by excited electrons (or holes) which can jump between the molecules. We assume that efficient charge transfer between neighboring molecular pairs takes place for relatively rare events, i.e. the picture which (as we believe) reflects basic features of the electron transport in discotic liquid crystals, assumes as the key point that for the static equilibrium configuration of a column charge hopping is expected to be negligibly small since there is no significant electronic overlapping between adjacent molecules. Nevertheless, sometimes, due to thermal fluctuations, exclusively favourable for hopping configurations of the molecules occur, when an efficient hopping is possible. If the separation between the molecules is larger than the amplitude of their thermal vibrations, then probability of such events (which can be called "contacts" or "collisions" ) is small. Duration of the contact can be estimated as the characteristic oscillation time $\omega_b^{-1}$.

The above reasoning leads to an 1D hopping Hamiltonian for electrons

$$H = \hbar \sum_i \left( \xi_i a_i^+ a_{i+1} + \xi_i^* a_{i+1}^+ a_i \right) \tag{11}$$

Here $a_i$ and $a_i^+$ are electronic annihilation and creation operators at the site (i.e. molecular coordinate along the column) $i$, and $\xi_i$ are the hopping amplitudes, which are functions of the time $t$. The equations for the Heisenberg operators $a_i$ are

$$\partial_t a_i = -i\xi_i a_{i+1} - i\xi_{i-1}^* a_{i-1} \tag{12}$$

The hopping matrix element $\xi_i$ can be decomposed into a constant part $\langle \xi_i \rangle$, that describes the coherent charge carrier motion in a completely rigid lattice, and a fluctuating part. We assume the inequality $\langle \xi_i \rangle^2 \ll \langle \xi_i^2 \rangle$, that allows us to neglect $\langle \xi_i \rangle$.

Statistics of the hopping coefficients $\langle \xi_i \rangle$ is characterized by the correlation functions

$$\begin{aligned} \langle \xi_i(t_1) \xi_j^*(t_2) \rangle &= \mu_i(t_1 - t_2)\delta_{ij}, \\ \langle \xi_i(t_1) \xi_j(t_2) \rangle &= \zeta_i(t_1 - t_2)\delta_{ij}, \end{aligned} \tag{13}$$

where we assumed that the hopping coefficients for collisions of different molecules are not correlated. The decay time of the functions $\mu_i(t)$ and $\zeta_i(t)$ is determined by the molecular collision time $\tau$. Since the collisions are rare we can disregard higher order irreducible correlation functions of $\xi$. In other words, statistics of the hopping coefficients $\xi_i$ can be treated as Gaussian. Since intensity of the molecular oscillations (leading to the collisions) increases with increasing temperature, the correlation functions (Eq. (13)) are temperature dependent.

Let us consider average occupation numbers

$$F_i(t) = \langle a_i^+(t) a_i(t) \rangle. \tag{14}$$

Here a double averaging is implied. First, we consider time scales larger than $\omega_b^{-1}$, where the hopping amplitudes $\xi_i$ can be treated statistically. Second, we perform quantum averaging, which experimentally corresponds to averaging over a large number of columns. If the characteristic time for variations of $F_i$ is larger than $\tau$ then one derives from Eq. (12) a closed master equation for $F_i$

$$\partial_t F_i = M_i(F_{i+1} - F_i) + M_{i-1}(F_{i-1} - F_i), \tag{15}$$

where $M_i = \int dt \mu_i(t)$. We see, that the (real) factors $M_i$ are probabilities for the electron to jump to neighboring sites.

# 4. PROPAGATING PHONON MODE ASSISTED CHARGE TRANSPORT

In order to provide a more complete account of the charge transfer phenomenom along the columns in discotic liquid crystals described in the previous section, a number of questions remain to be clarified. First we go one step further relating explicitly introduced above hopping amplitudes $\xi_i$ and molecular vibrations.

Lacking sufficient data on the modes, we can at present discuss only the general features of the dynamics. Our aim in this section is to include schematically into the model described in the previous section one propagating weakly damped phonon mode.

## 4.1 Elastic Model for Hopping Amplitudes

Let us introduce displacements $u_j$ of the molecules along the column. It is natural to assume that the hopping amplitudes $\xi_j$ are

$$\xi_j = \eta_j \exp[-\alpha_j(u_{j+1} - u_j)], \tag{16}$$

where we introduced variables $\eta_j, \alpha_j$ to describe characteristic amplitudes of vibrations and charge penetration or localization length. Both quantities are slowly temperature dependent.

The molecular dynamics can be treated in the framework of the elastic energy

$$u = \frac{1}{2}\sum_j K_j(u_{j+1} - u_j)^2, \tag{17}$$

where $K_j$ are corresponding elastic moduli. Then the simultaneous statistics of $u_j$ is very simple: it is Gaussian and is characterized by the pair correlation function

$$\langle (u_{j+1} - u_j)(u_{n+1} - u_n) \rangle = \frac{T}{K_j}\delta_{jn}. \tag{18}$$

Armed with (Eq. (16)) and (Eq. (18)) we are in a position to find some useful relations. Indeed

$$\langle \xi_j \rangle = \eta_j \exp\left[\frac{T\alpha_j^2}{2K_j}\right], \quad \langle \xi_j^2 \rangle = \eta_j^2 \exp\left[\frac{2T\alpha_j^2}{K_j}\right], \tag{19}$$

$$\langle \xi_j \xi_n \rangle = \langle \xi_j \rangle \langle \xi_n \rangle \quad \text{if}\, j \neq n, \tag{20}$$

$$\left\langle \prod_{j=0}^{j=n-1} \xi_j^2 \right\rangle = \exp\left[\sum_{j=0}^{j=n-1} \frac{2T\alpha_j^2}{K_j}\right] \times \prod_{j=0}^{j=n-1} \eta_j^2. \tag{21}$$

We assume that discotic columns can be treated as homogeneous ones and for the case we obtain from Eq. (21)

$$\left\langle \prod_{j=0}^{j=n-1} \xi_j^2 \right\rangle = \eta^{2n} \exp\left[\frac{2T\alpha^2 n}{K}\right]. \tag{22}$$

Therefore we conclude that it is possible to neglect $\langle \xi_j \rangle^2$ in comparison with $\langle \xi_j^2 \rangle$ if

$$T\alpha^2 \gg K. \tag{23}$$

The inequality (Eq. (23)) is a crucial one for the whole scheme.

Because the discotic liquid crystal column is a dynamic structure on the charge transport experiment time scale, to examine dynamical characteristics, one should introduce the kinetic energy

$$\frac{1}{2}\sum_j M_j (\partial_t u_j)^2, \tag{24}$$

where $M_j$ is the reduced molecular mass. Putting (Eq. (24)) together with the potential energy (Eq. (17)), one can easily find the dispersion law for this elastic mode. Again assuming that all adjacent molecules are the same (homogeneous case) we get

$$\langle u_j(t) u_n(0) \rangle = \int_0^{2\pi} \frac{\mathrm{d}q}{2\pi} \exp\left[iq(j-n)\right] \frac{T}{M\omega_q^2} \cos(\omega_q t), \tag{25}$$

where

$$\omega_q^2 = \frac{2K}{M}(1 - \cos q), \tag{26}$$

and for the moment we neglected attenuation of the elastic modes. We see that $\omega_b = \sqrt{K/M}/a$. At small $q$ we have $\omega_q = q\sqrt{K/M}$. The integral (Eq. (25)) diverges at small $q$ since the main contribution to $\langle u_j^2 \rangle$ is associated with the most long wavelength mode. It is worth noting also that from Eq. (25) we come to the expression

$$\langle (u_n - u_0)^2 \rangle = \frac{T}{K}\int_0^{2\pi} \frac{\mathrm{d}q}{2\pi}\frac{2-\cos(nq)}{1-\cos q} = \frac{T}{K}n, \tag{27}$$

reproducing actually Eq. (22).

The expression (Eq. (16)) implies that we have to be interested in the correlation function

$$\Phi_{jn}(t) = \langle [u_{j+1}(t) - u_j(t)][u_{n+1}(0) - u_n(0)] \rangle. \tag{28}$$

The function (Eq. (28)) enters, say, the pair correlation function of $\xi_i$:

$$\langle \xi_\mathrm{j}(\mathrm{t})\xi_\mathrm{n}(0) \rangle = \eta^2 \exp\left[\frac{\alpha^2\Phi_{jn}}{2b^2}\right]. \tag{29}$$

Using Eq. (25) one obtains

$$\Phi_{jn}(t) = \frac{T}{K}\int_0^{2\pi}\frac{\mathrm{d}q}{2\pi}\cos(\omega_q t)\exp[iq(j-n)]. \tag{30}$$

Note that the integral (Eq. (30)) converges at small $q$. If $\omega_b t \ll 1$ then it follows from Eq. (30)

$$\Phi_{jn} = \left(\frac{T}{K} - \frac{Tt^2}{M}\right)\delta_{jn} + \frac{Tt^2}{2M}(\delta_{j+1,n} + \delta_{j-1,n}). \tag{31}$$

Coming back now to the expression (Eq. (29)) we conclude that the characteristic correlation time $\tau$ of $\xi$ is

$$\tau\alpha \sim \sqrt{M/T}. \tag{32}$$

We see that at $t \sim \tau$ the non-diagonal correlation functions $\langle \xi_j \xi_n \rangle$ contain the small factor $\exp(-T\alpha^2/2K)$ in comparison with diagonal ones $\langle \xi_j^2 \rangle$. Therefore we can neglect the non-diagonal correlation functions.

To include an attenuation $\gamma(q)$ of the elastic modes one should substitute

$$\cos(\omega_q t) \rightarrow \cos(\omega_q t)\exp(-\gamma|t|)$$

in Eq. (30). The term with $\gamma$ can be neglected provided $\gamma_b\tau \ll 1$, where $\gamma_\mathrm{b}$ is the attenuation at $q \sim 1$.

## 4.2 Columnar Conductivity and Phonon Assisted Hopping and Tunneling

To examine the conductivity in the columnar phase, let us consider the following pure schematic device, when one isolated discotic column is attached to the two metallic electrodes: left (l) and right (r).

After the electron leaves the left electrode, it starts to jump along the column stretched between the left and the right electrodes. During the time the electron is "smeared" approximately uniformly over all sites between the electrodes due to diffusion. Then the relative probability for the electron to get on the right electrodes is determined by the ratio of the probabilities for the electron to jump to the left electrode and to the right one from the neighboring sites. This relative probability appears to be independent of the separation $z$ between the electrodes.

Thus we found that the propagating phonon mode promotes two different mechanisms: diffusion and tunnelling, for the electron to come from the left to the right electrode. The diffusion leads to an independence of the probability on the separation $z$ between the electrodes, while the tunnelling leads to an exponential dependence of the probability on $z$.

It should be noted that to describe charge transfer tunneling phenomena we are going to analyze in this section, we do not really need a quantum transport formalizm, a semiclassical treatment would suffice. We have to deal with dynamic tunnelling which can be effective only when due to fluctuations of $\xi$ there occurs some kind of a "bridge" between the electrodes, and the exponential law is determined in fact by a small probability to create such a bridge, which is realized, when simultaneously many molecular "collisions" occur. We will call this collective mode corresponding to the bridge formation by instanton (general notion used for fairly rare fluctuations related to tails of distribution functions; therefore the probability to have such a fluctuation is very small, however the fluctuation itself can lead to a noticeable effect).

Let the charge population at the left end of the column, attached to the left electrode be $F_0$. At the equilibrium

$$F_0^{eq} = 2f(E_0, u_l), \tag{33}$$

where the factor 2 stems for the spin degeneracy, and

$$f(E, u) = \frac{1}{1 + \exp[(E - \mu)/T]}, \tag{34}$$

is the Fermi distribution function, $E_0$ is the electronic energy in the molecular site $n = 0$, and $\mu_l \equiv E_F$ is the Fermi energy in the left metallic electrode. Similarly if the last right site of the column ($n = N$) is in the equilibrium with the right metallic electrode

$$F_N^{eq} = 2f(E_N, \mu_r), \tag{35}$$

where the notation is self-explanatory.

Under non-equilibrium conditions the actual charge populations $F_0$ and $F_N$ are not the equilibrium ones, and therefore there is a certain current from (or to) the left electrode, and to (or respectively from) the discotic liquid crystal column

$$I_l = \frac{e\Gamma_l}{\hbar}(F_0 - F_0^{eq}), \tag{36}$$

and analogously for the right electrode

$$I_r = \frac{e\Gamma_r}{\hbar}(F_N - F_N^{eq}), \tag{37}$$

where $e$ is the elementary charge, and $\Gamma_{l,r}$ - describe the coupling between the column and the electrodes.

In the stationary conditions we have also hopping or tunneling current between the sites 0 and $N$, and the corresponding current $I_h$ can be found from (Eq. (15)) and reads

$$I_h = \frac{eM}{N}(F_N - F_0). \tag{38}$$

Assuming that the applied voltage $V$ creates the charge population gradient and besides naturally

$$\mu_l = E_F - \frac{eV}{2}; \mu_r = E_F + \frac{eV}{2},$$

one can write down two continuity equations

$$I_l = I_r = I_h. \tag{39}$$

The calculated (from Eq. (39)) $I$ - $V$ characteristic looks like as a smoothed increasing step - like function. It becomes even more smooth if one takes into account level broadening. In any case, the slope of the $I$-$V$ characteristic, i.e. the conductivity $\sigma$ does not depend essentially on the temperature and does not depend at all on the frequency. In fact in the conditions of the experimental data [1] (we tried to simulate somehow by our model) the current flow is the result of a certain imbalance between the contacts. One contact would like to see more electrons than it occupies actually the neighboring site, and keeps pumping them in, while the other would like to see fewer than the actual number at its neighboring site and therefore keeps pulling them out. The net effect is a continuous transfer of electrons from one contact to another and it reveals only very weak temperature dependence due to electronic hopping and tunneling between the attached to the electrodes molecular sites.

## 5. CONCLUSION

In this paper we have examined charge transfer phenomena along the columns in discotic liquid crystals. Dynamics of the disc-like molecules is described by a simple harmonic elastic model. Different regimes depending on the ratio of a characteristic molecular oscillation amplitude and electronic localization length, are examined. The key finding in our study is that a long distance charge transfer can be related to the specific fluctuation formation i.e. with dynamic tunnelling which can be effective only when due to molecular fluctuations there occurs some kind of a "bridge" between the electrodes, and the exponential tunneling law is determined in fact by a small probability of such bridge, which is realized, when simultaneously many molecular "collisions" occur. This collective mode corresponding to the bridge formation can be called by instanton (general notion used for fairly rare fluctuations related to tails of distribution functions; therefore the probability to have such a fluctuation is very small, however the fluctuation itself can lead to a noticeable effect).

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