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Kinetic Analysis of Hole Migration Through DNA

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The mechanism of hole migration through donor-DNA-acceptor systems is studied using a kinetic model, in which the time evolution of the hole population at guanine sites is expressed in terms of the hopping rates between neighboring guanine-cytosine (GC) base pairs. The hole hopping rates are empirically determined and effectively include all important factors of the hole migration process. We present quantitative and qualitative descriptions of hole migration along DNA by analyzing such quantities as survival probabilities, mean residence times, and mean first passage times for a number of different donor-DNA-acceptor systems. The sequence dependence and distance-dependence of the hole-migration mechanism are examined in depth for both short and long donor-DNA-acceptor systems. Some important consequences obtained from our analysis are as follows: (i) The path that a hole takes in going through cross-linked adenine-thymine (AT) base pairs is 1.5 times longer than the typical base-stacking distance; thus, the hole transfer rate decreases about twice as fast for each cross-linked AT base pair as for a directly linked one. (ii) If the GC and AT base pairs are properly arranged the hole migration time can be changed, while keeping the transfer rate the same. (iii) A formula is derived for estimating the maximal length of regular DNA bridges for use in hole-migration experiments.

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I. INTRODUCTION

The phenomena of charge migration through DNA have received a lot of attention during the last decade due to their large number of applications. Today, there is no doubt that long-distance charge transport through DNA occurs, and some progress [1–4] has been made in understanding the underlying aspects of processes of charge migration in DNA. Recent theoretical [3,4] studies suggest that there are two distinct mechanisms for charge migration processes along DNA. The first mechanism is single-step charge transfer mediated by superexchange interactions between nucleobases. This mechanism is characterized by a strong exponential distance-dependence of the charge transfer rate which is expressed as

$$k_{\rm CT} = k_0 e^{-\beta R_{\rm DA}} \ , \qquad (1)$$

where k_0 is a pre-exponential factor, β is a falloff parameter, and $R_{\rm DA}$ is the distance between the donor and the acceptor. The value of β is experimentally found to be about $0.6 - 1.6$ Å^{-1} [5–8]. The other mechanism for charge migration through DNA is multistep hopping transport. Contrary to the superexchange-mediated single-step tunneling, multistep charge transport weakly depends on the distance between the donor and the acceptor. In real experimental data, the effects of both mechanisms coexist, and the prevalence of one is determined by the energetic configuration of the DNA sequences. For off-resonance coupling, the single-step tunneling mechanism prevails while for resonance coupling results in the multistep hopping mechanism prevails [3].

Most of the recent experiments for studying charge transport in DNA have been performed by oxidating a DNA strand in solution, and their results characterize hole migration through DNA. The energetic control of the hole migration mechanism is mainly determined by the oxidation potentials of the nucleobases. Among the four DNA bases, guanine (G) is most easily oxidized, providing the lowest hole state. The second lowest hole state is found at adenine (A) whose oxidation potential is about 0.5 eV [9] above that of guanine. Accordingly, the hole transfer from a GC base pair to an AT base pair takes place via off-resonance coupling between G and A which discourages the hopping mechanism, whereas a hole hops between GC base pairs via resonance coupling between G's.

In theoretical studies of the hole migration mechanism [10–12], the donor-DNA-acceptor system is usually modeled as one-dimensional coupled harmonic oscillators on which a hole hops. The methods vary in how to implement irreversible processes such as hole trapping by the acceptor. Although these methods manage to de-

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scribe important features of the processes of hole migration through DNA, ambiguity in determining the values of key parameters, such as the hole-oscillator coupling constant and the oscillation period, severely limits theirs applicability. Besides, a simplified description of the motion of a hole in DNA excludes some quantitatively important effects inevitably occurring in real experiments (*e.g.*, the trapping of holes by water), which basically prohibits a quantitative analysis. Another theoretical approach to the hole migration problem in DNA is a kinetic treatment of the process of hole migration [13–15]. In this approach, the time evolution of hole populations on GC base pairs is expressed in terms of hopping rates between neighboring guanines. Recently, Berlin *et al.* [14] suggested a plausible way of determining the G-G hopping rates by making use of the transfer rates for AT base pair bridges and achieved good agreement with experimental data.

In this work, we adopt a kinetic approach. Following the procedure suggested by Berlin *et al.* [14], We determine the hopping rates between adjacent GC base pairs by using recent experimental results [6, 16] for superexchange-mediated single-step tunneling cases, which enables us to treat the hole migration process in DNA without losing any significant factor. We investigate various aspects of hole migration in a number of donor-DNA-acceptor systems and carry out both qualitative and quantitative analyses of the underlying mechanism. The kinetic model and the computational methods which we employ are presented in Sec. II. In Sec. III. , the results are analyzed and fully discussed. Finally, conclusions are drawn in Sec. IV.

II. MODEL AND COMPUTATIONAL DETAILS

In hole transfer between two GC base pairs separated by small number of AT base pairs, AT base pairs have been experimentlly shown not to be not oxidized and holes to be exclusively detected on GC base pairs, especially on guanines. [4,8,16] This experimental observation indicates that guanines practically act as hole carriers whereas AT base pairs serve as barriers, mediating the resonant interactions between GC base pairs via superexchange couplings. The kinetic scheme that we use for analyzing hole transport is based on this observation

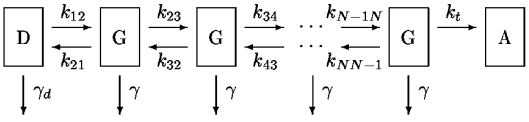

Fig. 1. Schematic representation of the kinetic model for hole hopping in a donor-DNA-acceptor system. D, G, and A denote the donor, the GC sites of a bridge, and the acceptor, respectively.

and is described in Fig. 1. A hole is initially injected into the donor (site 1) and subsequently hops back and forth between nearest neighbor GC base pairs until it arrives at the acceptor where the hole is irreversibly trapped. The guanine radical cation G^+ undergoes an irreversible reaction with water, which also affects the efficiency of hole transport. In our model, we assume that the rate constant for the reaction of G^+ with water is independent of sites.

The hole population (or probability) $P_i(t)$ on site i $(i = 1, \ldots, N)$ at time t can then be calculated from

$$\begin{aligned}\frac{dP_i(t)}{dt} &= -\gamma_d P_i(t)\delta_{i,0} - \gamma P_i(t)(1-\delta_{i,0}) \\ &\quad + \sum_{j=1}^{N} \left[k_{ji}P_j(t) - k_{ij}P_i(t)\right]\delta_{j,i\pm1} \\ &\quad - k_t P_i(t)\delta_{i,N} \ , \end{aligned} \tag{2}$$

where γ_d and γ are the rates of reactions of G^+ with water (*i.e.*, hole trapping by water) at the donor and the GC sites, and k_{ij} and k_t are the hopping rates from site i to j and from the last GC site (site N) to the acceptor, respectively. The first two terms on the right-hand side of Equation. (2) describe the hole trapping reaction by water, the third term represents the hopping process on the bridge, and the fourth term represents the irreversible process of hole trapping by the acceptor. Since a hole is initially generated on the donor, Equation. (2) should be solved with the condition

$$P_i(t=0) = \left\{ \begin{array}{ll} 1 & \text{for } i = 1 \\ 0 & \text{for } i = 2, \ldots, N \end{array} \right\} \tag{3}$$

It is often useful to express the set of coupled differential Equations given by Equation. (2) in a matrix form as

$$\frac{d\hat{P}(t)}{dt} = \hat{W}\hat{P}(t) \ , \tag{4}$$

where

$$\hat{P}(t) = (P_1(t) \ \cdots \ P_N(t))^T$$

and $\hat{\mathrm{W}} =$

$$\begin{pmatrix} -\gamma - k_{12} & k_{21} & 0 & \cdots & 0 \\ k_{12} & -\gamma - k_{21} - k_{23} & k_{32} & \cdots & 0 \\ 0 & k_{23} & -\gamma - k_{32} - k_{34} & \cdots & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & -\gamma - k_{NN-1} - k_t \end{pmatrix} .$$

The solution of Equation. (4) can be written as

$$\hat{P}(t) = e^{\hat{W}t}\hat{e}_1 \ , \tag{5}$$

where $\hat{e}_i = (0 \ \cdots 0 \ 1 \ 0 \cdots 0)^T$ is a column matrix whose ith component is 1 and whose other components are 0. Note that in obtaining Equation. (5), we used the initial condition of Equation. (3). From Equation. (5), the hole population $P_i(t)$ is obtained as

$$P_i(t) = \hat{e}_i^T \hat{P}(t) = \hat{e}_i^T e^{\hat{W}t}\hat{e}_1 \ . \tag{6}$$

The rate of hole transport through a DNA bridge can be investigated by examining the survival probability, which is defined as

$$\Phi(t) = \sum_{i=1}^{N} P_i(t) \ . \tag{7}$$

$\Phi(t)$ is the probability of finding a hole on the DNA at time t and describes the detailed time evolution of hole hopping on the DNA chain. Another useful quantity is the mean residence time (MRT) [17, 18], which is the average time that a hole spends at a given site before leaving a DNA chain. The MRT for the ith guanine site is

$$\tau_i = \int_0^\infty P_i(t)dt \ , \tag{8}$$

and by substituting Equation. (6) into Equation. (8), we obtain the useful relation

$$\begin{aligned} \tau_i &= \int_0^\infty \hat{e}_i^T e^{\hat{W}t}\hat{e}_1 dt = -\hat{e}_i^T \hat{W}^{-1}\hat{e}_1 \\ &= -\hat{W}_{i1}^{-1} \ , \end{aligned} \tag{9}$$

which reveals that the MRTs are directly related to the first column of the inverse of $\hat{W}$. The mean first passage time (MFPT) is also a useful measure for quantifying the efficiency of hole migration and is given by

$$\tau_{\rm MF} = \sum_{i=1}^{N} \tau_i \ . \tag{10}$$

It represents the average time that a hole takes to travel from the donor to the acceptor.

III. RESULTS AND DISCUSSION

The systems that we consider consist of a guanine radical cation G^+ as the hole donor and a G-triad as the acceptor which are connected to each other by a bridge of AT and GC base pairs. The DNA bridges to which the kinetic analysis has been applied are listed in Table 1. Sequences I to VII were studied in recent experiments [6, 16], and the experimental results for them are also presented. The experimental data are given in terms of the reaction yields of G^+ with water at the GC sites, and among them, the most important quantities are those at

Table 1. Sequences and hole transport characteristics of DNA bridges.

	Bridges	ϕ		$\tau_{\rm MF}$ (γ^{-1})
		Experimental	Calculated	
I	T A	30 ± 6 [6]		0.003
II	TT AA	8.9 ± 1.8 [16]		0.10
III	TA AT	3.2 ± 0.6 [6]		0.24
IV	TTA AAT	0.44 ± 0.2 [6]		0.69
V	TATA ATAT	0.03 ± 0.015 [6]		0.97
VI	TGTA ACAT	3.4 ± 0.7 [6]	2.81	0.40
VII	TACA ATGT	3.8 ± 0.8 [6]	2.81	0.28
VIII	TTGTT AACAA		4.21	0.26
IX	TTGTTGTT AACAACAA		2.57	0.42
X	TTGTTGTTGTT AACAACAACAA		1.71	0.57

the donor and the acceptor which are in our notation expressed as

$$Y_{\rm D} = \int_0^\infty \gamma P_1(t)dt = \gamma\tau_1 \ , \tag{11}$$

$$Y_{\rm A} = \int_0^\infty k_t P_N(t)dt = k_t\tau_N \ , \tag{12}$$

where $Y_{\rm D}$ and $Y_{\rm A}$ are the water reaction yields at the donor and the acceptor, respectively, and in Equation. (11) $\gamma_d = \gamma$ was used. Especially, their ratio, the so-called the damage ratio

$$\phi = \frac{Y_{\rm A}}{Y_{\rm D}} = \frac{k_t}{\gamma}\frac{\tau_N}{\tau_1} \tag{13}$$

provides information on the hole transfer rate [6]. It is important to note that in the case of $N = 1$, ϕ becomes the hopping rate relative to the water reaction rate:

$$\phi = \frac{k_t}{\gamma} \ . \tag{14}$$

Since the values of ϕ for superexchange-mediated single-step tunnelings to a GC base pair and to a GC base triad are found to be very close [13,14], the experimental values of ϕ for sequences I to V can be used as the hopping rates between GC base pairs separated by corresponding AT

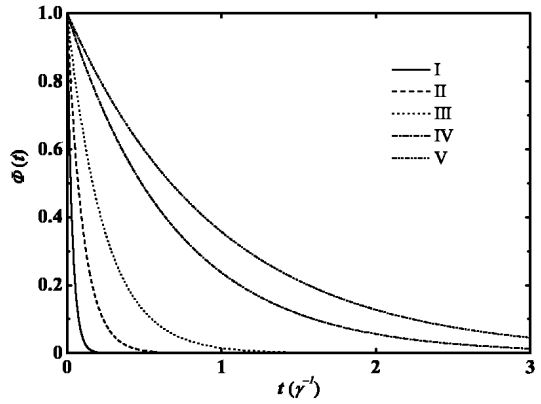

Fig. 2. Survival probabilities for sequences I, II, III, IV and V.

barriers in the sequences VI to X Thus, Equation. (2) can be rewrittn as

$$\frac{dP_i(t')}{dt'} = -P_i(t') + \sum_{j=1}^{N}\left[\frac{k_{ji}}{\gamma}P_j(t') - \frac{k_{ij}}{\gamma}P_i(t')\right]\delta_{j,i\,\pm\,1} - \frac{k_t}{\gamma}P_i(t')\delta_{i,N}, \quad (15)$$

where $t' = \gamma t$. In our calculations, we assume $k_{ij} = k_{ji}$, as there is no directional bias in hole hopping along the DNA bridges.

The values of $\tau_{\rm MF}$ and ϕ calculated using Equations. (10) and (13) are given in Table 1. The main factors determining the characteristics of hole migration in donor-DNA-acceptor systems are the numbers and the orders of AT and GC base pairs in the DNA bridges, and the donor-acceptor distance. In what follows, we examine their effects separately, as their roles are quite distinct.

1. Effects of AT Base pairs on Hole Migration

Figure 2 shows the survival probabilities for sequences I to V. As the number of AT base pairs in the bridge increases, the efficiency of hole migration dramatically decreases, resulting in a large increase of $\tau_{\rm MF}$. As discussed in Sec, I. the mechanism of hole transfer for sequences I to V is single-step tunneling mediated by superexchange couplings between AT base pairs and the transfer rate is given by Equation. (1) with $\beta = 0.6 - 0.7$ Å^{-1} [6,8]. As ϕ is proportional to $k_{\rm CT}$, the distance dependence of ϕ is

$$\phi \propto e^{-\beta R_{\rm DA}} \ , \quad (16)$$

indicating that ϕ decreases with the addition of an AT base pair by a factor of

$$\delta_\phi \equiv e^{-\beta r_o} \simeq 0.11 \pm 0.02 \ , \quad (17)$$

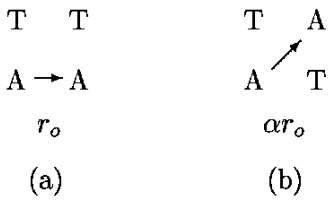

Fig. 3. Effective paths and lengths of AT base pair bridges for hole transport are schematically represented. (a) is for sequence II, and (b) is for sequence III, where $\alpha \simeq 1.5$.

where $r_o = 3.4$ Å is the base stacking distance.

Though useful for the qualitative description of the superexchange-mediated single-step tunneling, Equations. (16) and (17) provide only a rough explanation of the experimental data and predict the same values for sequences of the same size. The experimental results, however, indicate that in addition to the distance between the donor and the acceptor, the relative location of adjacent adenines has a considerable effect on hole transfer. For example, although the lengths of sequences II and III are the same, the MFPT of sequence III is more than twice as large as that of sequence II. To explain the dependence of hole migration on the specific sequences of AT base pairs, we need to take into account the path that a hole actually takes through the AT base pairs. Since adenine has a lower oxidation potential than thymine, a hole passes through adenines when it migrates along stacked AT base pairs. Thus, as Fig. 3 shows, the effective length of a two cross-linked AT base-pair bridge (Fig. 3(b)) is longer than that of directly linked one (Fig. 3(a)) by a factor of

$$\alpha = 1 - \frac{1}{\beta r_o}\ln\left(\phi_{\rm III}/\phi_{\rm II}\right) \simeq 1.5 \ , \quad (18)$$

where $\phi_{\rm II}$ and $\phi_{\rm III}$ are the values of ϕ for sequences II and III, respectively. From the values of ϕ for sequences I and II, the rate-decrease factor for each directly linked AT base pair is estimated to be

$$\delta_{\phi,\rm direct} \simeq 0.2 \ , \quad (19)$$

and by using Equations. (16), (18), and (19), we can calculate the value for each cross-linked AT base pair: Equations. (19) and (20) well account for the results for sequences II to V

$$\delta_{\phi,\rm cross} = \delta^{\alpha}_{\phi,\rm direct} \simeq 0.09 \ . \quad (20)$$

the experimental errors. It is interesting to note that the value of δ_ϕ is midway between the values of $\delta_{\phi,\rm cross}$ and $\delta_{\phi,\rm direct}$. This is reasonable because the value of β is obtained by fitting the experimental results for general sequences of AT base pair bridges, and thus $\delta_{\phi,\rm cross}$ and $\delta_{\phi,\rm direct}$ correspond to the extreme cases. Equations. (19) and (20) apply to any AT base pair sequence and provide useful information on their hopping rates as long as the AT base pair bridges are short enough to ensure that the G-hopping mechanism is valid [8].

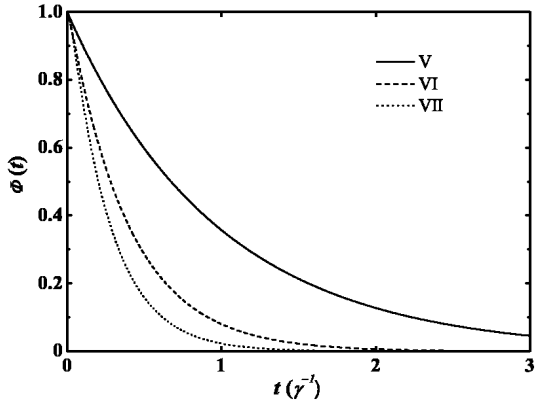

Fig. 4. Survival probabilities for sequences V, VI, and VII.

2. Effects of GC Base Pairs on Hole Migration

One of the most important observations on hole migration through DNA is that the characteristics of hole migration greatly depend on the number of GC base pairs present in the bridge. Comparing the results for sequences V, VI, and VII in Table 1, we observe that the efficiency of hole migration significantly improves when one of the AT base pairs of sequence V is replaced by a GC base pair (see Fig. 4). Especially, hole migration through sequence VII occurs almost as fast as it does through sequence III which is half as long. Obviously, this is a consequence of successive hoppings between GC base pairs. Since the hopping rates between GC base pairs depend on the specific sequences of AT barriers between them, in sequence VII a hole hops from the donor to the GC site at the same rate as in sequence III, and in its subsequent motion, the rate of the hole being trapped by the acceptor is about ten times larger than the rate of the hole hopping back to the donor. The overall efficiency of hole migration for sequence VII, therefore, becomes very close to that for sequence III.

It is worth investigating the reason the values of $\tau_{\rm MF}$ for sequences VI and VII are noticeably different despite their having the same transfer rate. In Fig. 5, the hole populations on the GC sites for sequences VI and VII are compared. $P_2(t)$ is larger for sequence VI than it is for sequence VII for all time while $P_1(t)$ for sequence VI is lower than that for sequence VII only at early times. This can be explained as follows: The rate of hole hopping from the donor (site 1) to the GC site of the bridge (site 2) is much larger for sequence VI than it is for sequence VII. On the other hand, the rate of a hole being trapped by the acceptor is much lower for sequence VI than it is for sequence VII. Note that the arrangements of AT barriers in sequences VI and VII are exactly opposite. As a result, a hole is likely to stay on bridge VI far longer than on bridge VII, which is clearly indicated by the MRTs (see Table 2). This retardation of hole hopping in bridge VI slows down the decay rate of $P_1(t)$ and decreases the efficiency of hole migration, leading to an increase in the MFPT.

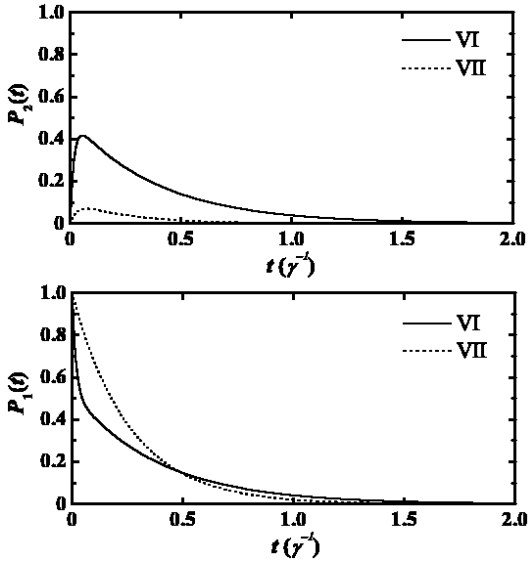

Fig. 5. Hole populations on GC sites in sequences VI and VII. $P_1(t)$ and $P_2(t)$ are for the donor and the GC sites of the bridge, respectively.

Table 2. Mean residence times for the DNA bridges. The time scale is γ^{-1}.

Bridges	1st GC site	2nd GC site	3rd GC site	4th GC site
VI	0.21	0.19		
VII	0.26	0.02		
VIII	0.18	0.08		
IX	0.22	0.14	0.06	
X	0.25	0.17	0.10	0.05

3. Distance Dependence of Multistep Hole Transport

As discussed above, the presence of GC base pairs in the bridges dramatically changes the nature of the distance dependence of hole migration. To study how the multistep hole transport depends on the length of DNA bridges, let us consider a series of GC base pairs separated by the same sequence of AT base pairs, so that

$$k_{12} = k_{23} = \cdots = k_t = k \ . \tag{21}$$

The assumption of homogeneous AT barriers is not necessary for our discussion, but facilitates our analysis. With the condition of Eq. (21), the MRTs given by Equation. (9) can be easily found in closed forms by means of the recursion matrix technique [19], and through Equations. (12) and (13), the analytic expressions for ϕ and

$Y_{\rm A}$ are obtained as

$$\phi = \sqrt{1+\frac{4k}{\gamma}}\frac{1}{(\lambda+\zeta)^N-(\lambda-\zeta)^N} \simeq \sqrt{\frac{k}{\gamma}}\frac{1}{\sinh\left(N\sqrt{\frac{\gamma}{k}}\right)} , \tag{22}$$

$$Y_{\rm A} = \frac{2\zeta}{(\lambda-\zeta)^N(1-\lambda+\zeta)+(\lambda+\zeta)^N(\lambda-1+\zeta)} \simeq \frac{1}{\cosh\left(N\sqrt{\frac{\gamma}{k}}\right)} , \tag{23}$$

where

$$\lambda = 1+\frac{\gamma}{2k} ,$$

$$\zeta = \sqrt{\frac{\gamma^2}{4k^2}+\frac{\gamma}{k}} ,$$

and we have used the fact that γ/k is small. It is seen from Eq. (22) that the characteristics of the multistep hopping mechanism change near $N \simeq N_c \equiv \sqrt{k/\gamma}$; *i.e.*, for $N < N_c$,

$$\phi \simeq \frac{1}{N} , \tag{24}$$

and for $N >> N_c$,

$$\phi \propto e^{-\frac{N}{N_c}} = e^{-\bar{\beta}R_{\rm DA}} , \tag{25}$$

where $\bar{\beta} \equiv (N_c r_{\rm GG})^{-1}$, and $r_{\rm GG}$ is the distance between the nearest GC base pairs. Therefore, for short DNA bridges with $N < N_c$, the rate of hole transport by the multistep hopping mechanism linearly decreases with the length of the bridges. On the other hand, for DNA bridges longer than $N_c r_{\rm GG}$, multistep hopping transport exhibits an exponential decrease with distance, like superexchange-mediated single-step tunneling. The corresponding falloff parameter $\bar{\beta}$ is, however, much smaller than that for superexchange-mediated single-step tunneling. For example, if sequence III is used as the AT barriers of a regular DNA bridge, the critical length is 18.2 Å, and the value of $\bar{\beta}$ is 0.05 Å^{-1}, which is over an order of magnitude smaller than the typical value of β. The survival probabilities for regular bridges with different lengths (sequences VIII, IX, and X) are compared in Fig. 6. Note that the difference in lengths between sequences VIII and X is as large as 20.4 Å. The time dependence of the survival probabilities is clearly seen to be quite insensitive to the donor-acceptor distance. The weak distance-dependence of the multistep hopping mechanism enables a hole to travel long distances.

As the minimal experimental uncertainty for the measurement of ϕ is about 0.01, a meaningful hole transport measurement should satisfy

$$\phi \geq 0.01 , \tag{26}$$

and from Eqs. (22) and (26), the maximal distance for experimentally measurable hole transport is estimated to be

$$N_{\rm max} = N_c \ln 200 + N_c \ln N_c .$$

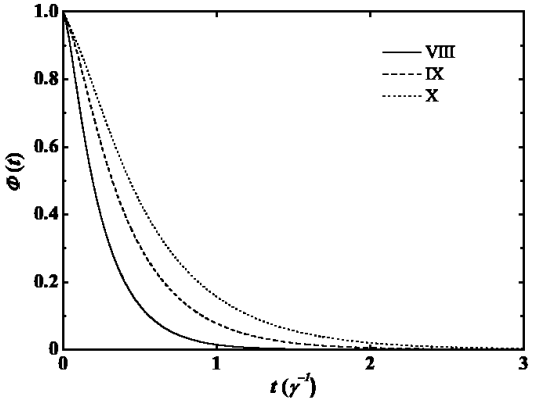

Fig. 6. Survival probabilities for sequences VIII, IX, and X.

As an example, the maximal length of a regular DNA bridge consisting of GC base pairs separated by two directly linked AT base pairs is $r_{\rm GG}N_{\rm max}$ = 194 Å, and the percentage of holes arriving at the acceptor is, from Eq. (23), 0.3 %.

IV. CONCLUSIONS

In this work, we studied the mechanism of hole migration in donor-DNA-acceptor systems by using a kinetic model which describe the time evolution of the system in terms of experimentally measurable quantities, the hopping rates between neighboring guanine sites. Using this model, we calculated hole populations, survival probabilities, mean residence times, and mean first passage times for a number of different DNA bridges and examined the underlying transport mechanism by analyzing them.

In our analysis, the dependence of the efficiency of hole migration on the sequence of DNA bridges was investigated in depth. In addition to its well-known distance dependence, the hole transfer rate was found to significantly depend on the specific arrangement of AT base pairs. The hole transfer rate decrease by the factor of 0.2 for each directly linked AT base pair and by 0.09 for each cross-linked AT base pair. This difference comes from the fact that a hole takes different paths for different linkages of AT base pairs. According to our analysis, a hole travels about 1.5 times farther for a cross-linked AT base pair than it does for a directly linked one. The presence of GC base pairs in DNA bridges was shown to dramatically improve the hole transfer rate, changing the basic mechanism of hole migration, which has already been pointed out by many authors [4,11,12,14]. We discussed how the order of the GC and AT base pairs affected the process of hole migration in DNA and showed that the hole migration time could be controlled by properly ordering GC and AT base pairs without changing the hole transfer rate.

Our analysis confirmed that the long-range hole transport through DNA is due to the multistep hopping mechanism. To draw a clear picture of long-distance transport in DNA we analytically studied the cases of regular DNA bridges, although the qualitative features will apply to irregular DNA bridges as well. Our analysis indicates the existence of a critical length across which the distance dependence of the multistep hopping mechanism changes, which is consistent with other studies [13,14]. For regular DNA bridges, the critical length R_c is given by $r_{\rm GG}\sqrt{k/\gamma}$, and the transfer rate decreases linearly with the donor-acceptor distance for systems with $R_{\rm DA} < R_c$ and shows a weak exponential distance-dependence for systems with $R_{\rm DA} >> R_c$. Using an analytic expression for ϕ, we derived a formula (Eq. (27)) for estimating the maximal length of regular DNA bridges for experimentally measurable hole transport, which will be a useful guide in preparing DNA samples for hole-migration experiments.

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