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Long-range correlation and charge transfer efficiency in substitutional sequences of DNA molecules

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We address the relation between long-range correlations and coherent charge transfer in substitutional DNA sequences using the transfer matrix approach. The substitutional sequences exhibit long-range correlations and show good transmittivity in comparison with uncorrelated random ones. It is found that the charge transfer efficiency varies for different substitutional sequences and many will present electronic delocalization in the system. Further, the resistivity for substitutional sequences may range from decreasing with the length, length independence, or increasing with the length. The conduction mechanisms of various behaviors observed for these sequences are analyzed.

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I. INTRODUCTION

In recent years, the nature of DNA-mediated charge migration has triggered extensive attention among physics, chemistry, and biology communities [1–3], owing to their potential applications in molecular electronic engineering and understanding the damage recognition process and protein binding [4–6]. Nevertheless, the results of direct charge transport measurements of DNA molecules are inconsistent, indicating that they might be insulators [7–9], semiconductors with a voltage gap [10–12], or conductors [13–18]. Even though, many theoretical efforts, mainly in investigating the electronic structure and conductivity of DNA, have been derived via several approaches, including the *ab initio* calculations (Hartree-Fock method, density functional theory) [7,19–27], the transfer matrix method plus a tight-binding model (TBM) [28–35], the Green's function plus a TBM [36–42], and the renormalization approach plus a TBM [33,43,44]. And some consensus on the dominant mechanisms of charge transport in DNA seems to be emerging currently [2,33]. The transport may result from either coherent tunneling (superexchange) [28,35,39,45,46] or incoherent hopping (phonon-assisted processes) [40,41,47], while taking into account different DNA samples and ambient environment.

Nevertheless, the role of sequence in charge transport through DNA remains the subject of controversial debate and should deserve particular concern. The DNA molecules, which are made up from the nucleotides guanine (G), adenine (A), cytosine (C), and thymine (T), determine the sequence of amino acids to form proteins. Thus characteristic sequence-dependent charge transport may provide valuable clues to biological functions of transport. On the other hand, recent outcomes of some communities indicated strong sequence dependence of charge transport [12,48,49] or sequence independence of delocalization in DNA [32]. In the case, the nucleotide correlations were neglected and may play a significant role in charge transfer efficiency. Moreover, the nature of long-range correlations has been recently discussed in aperiodic artificial or genomic DNA sequences [30,50,51] and tends to support electronic delocalization in the one-dimensional Anderson model [52]. However, it would not be sufficient to conclude that any kind of long-range correlations be strong enough to support charge transport through the chains. The two DNA molecules: Fibonacci quasiperiodic sequence and Rudin-Shapiro one, all of which belong to the family of substitutional sequences and have long-range correlations, exhibit different transmission patterns (for a review of the physical properties of the quasiperiodic structures, see Ref. [53,54]). The former shows many robust transmission energies in the spectrum [51], whereas the latter shows weak transmission ability [30] with increasing sequence length. This important difference, however, motivates us to address the relation between long-range correlations and charge transfer efficiency in substitutional DNA sequences. And we find that these DNA sequences present high charge transfer efficiency and different sequences show various transmission patterns. From a statistical analysis over many substitutional sequences, we find the following: (1) These DNA sequences can also be generated from the concatenation rules which reflect the feature of self-similarity. (2) These sequences exhibit long-range correlations and present high charge transfer efficiency. (3) Different sequences show various transmission patterns, and the resistivity ranges from decreasing with the length, length independence, or increasing with the length.

In the present work, we focus on the conductivity and Lyapunov coefficient of single-stranded DNA molecules, of which the conductance has been recently measured [11,55]. In the next section, the theoretical model is presented based on an effective tight-binding Hamiltonian, which is appropriate to describe the single-stranded DNA molecules. Then, the statistical properties of the substitutional sequences are shown in Sec. III, all exhibiting long-range correlations. Section IV deals with the conductivity of the chains, while Sec. V deals with the Lyapunov coefficient. Finally, a summary is made in Sec. VI.

II. MODEL

Several models, such as the simplest one-dimensional model [30,51,56–58], the polaron model [34,59,60], the two-leg ladder model [29,32,35,38], the three chain model [37,61,62], the three-dimensional model [63,64], as well as

TABLE I. List of the substitution rules, the concatenation rules, and the statistical properties of several substitutional sequences.

Sequence	Substitution rule	Concatenation rule	τ	$R(10^4)$
GGCSCC	$S_r(\mathrm{G})=\mathrm{GGC}$, $S_r(\mathrm{C})=\mathrm{CC}$	$S_{n+1}=S_nS_n(2^{n-1}\mathrm{C})$	2	478
Copper mean	$S_r(\mathrm{G})=\mathrm{GCC}$, $S_r(\mathrm{C})=\mathrm{G}$	$S_{n+1}=S_nS_{n-1}S_{n-1}$	2	13.9
GGCSGG	$S_r(\mathrm{G})=\mathrm{GGC}$, $S_r(\mathrm{C})=\mathrm{GG}$	$S_{n+1}=S_nS_nS_{n-1}S_{n-1}$	$1+\sqrt{3}$	5.02
Fibonacci	$S_r(\mathrm{G})=\mathrm{GC}$, $S_r(\mathrm{C})=\mathrm{G}$	$S_{n+1}=S_nS_{n-1}$	$\frac{1+\sqrt{5}}{2}$	2.74
Bronze mean	$S_r(\mathrm{G})=\mathrm{GGGC}$, $S_r(\mathrm{C})=\mathrm{G}$	$S_{n+1}=S_nS_nS_nS_{n-1}$	$\frac{3+\sqrt{13}}{2}$	2.54
GCGSGGC	$S_r(\mathrm{G})=\mathrm{GCG}$, $S_r(\mathrm{C})=\mathrm{GGC}$	$S_{n+1}=S_n(S_{n-1}S_n-S_{n-1})S_n$	3	2.83
GGCSCCG	$S_r(\mathrm{G})=\mathrm{GGC}$, $S_r(\mathrm{C})=\mathrm{CCG}$	$S_{n+1}=S_nS_n\tilde{S}_n$	3	15.4
Rudin-Shapiro	$S_r(\mathrm{G})=\mathrm{GC}$, $S_r(\mathrm{A})=\mathrm{TC}$, $S_r(\mathrm{C})=\mathrm{GA}$, $S_r(\mathrm{T})=\mathrm{TA}$	$S_{n+1}=S_nS_{n-1}(ST)_{n-2}(-S_{n-2}+S_{n-1})$	2	134

other models associated with the phonon [40,65,66], have been put forward to simulate the DNA molecules. In this paper, the simplest one-dimensional model is adopted. The Hamiltonian is [30,51,57]

$$\mathcal{H}=\sum_n \varepsilon_n c_n^\dagger c_n-\sum_n t_d(c_n^\dagger c_{n+1}+c_{n+1}^\dagger c_n), \tag{1}$$

where $c_n^\dagger$ (c_n) is the creation (annihilation) operator for a hole at nth site. The on-site energies ε_n are evaluated by ionization potentials of respective bases and are taken as $\varepsilon_G=7.75$ eV, $\varepsilon_A=8.24$ eV, $\varepsilon_C=8.87$ eV, $\varepsilon_T=9.14$ eV [19], while the electronic coupling (hopping term) t_d, simulating the π-π stacking between successive nucleotides, is properly chosen as $t_d=1$ eV [51]. The DNA chains are assumed to be connected in between two semi-infinite electrodes with adjusted on-site energies $\varepsilon_m=\varepsilon_G=7.75$ eV and hopping integral $t_m=t_d=1$ eV. Such choices for modeling the external leads render us to be capable of scanning the transmission spectrum within the interval $[\varepsilon_m-2t_m,\varepsilon_m+2t_m]$, since the dispersion relation of the hole in electrodes is $\varepsilon_m+2t_m\cos(ka)=E$ [67], with the stacking distance $a=3.38$ Å. Notice that *ab initio* calculations have reported t_d ranging from 0.01 to 0.4 eV [21,58,68], but the choice $t_d/t_m=1$ reduces backscattering effects at the contact interface [28] and thus allow for a better understanding of DNA's intrinsic conduction. Finally, each site represents a nucleotide of the sequences for $n\in[1,N]$, whereas sites denote the semi-infinite electrodes for $n\in[-\infty,0]\cup[N+1,+\infty]$.

In what follows, we will discuss the charge transport properties using the above TBM for such single-stranded DNA molecules. We are aware that in order to model specific transport properties of DNA, it would be important to consider not only their double-stranded character, but also intrinsic and extrinsic complications, including structural fluctuations, sugar-phosphate backbone, Coulomb interactions, frequency, contacts, counterions, and water. However, we believe that the relative role of long-range correlations in the nucleotide sequence can be ascertained in great detail by the simplest one-dimensional model, with correlated diagonal disorder.

III. STATISTICAL PROPERTIES OF SUBSTITUTIONAL SEQUENCES

All the substitutional sequences are constructed by starting from a G nucleotide as a seed and following a certain substitution rule. For instance, a sequence of the rule G →GGC [$S_r(\mathrm{G})=\mathrm{GGC}$] and C→CC [$S_r(\mathrm{C})=\mathrm{CC}$], namely GGCSCC (SQ1), can be generated successively G, GGC, GGCGGCCC, GGCGGCCCGGCGGCCCCCCC,…, for sequences $S_1,S_2,S_3,S_4,\ldots$, respectively. Such sequences can also be obtained from the equivalent method, i.e., the concatenation rule $S_{n+1}=S_nS_n(2^{n-1}\mathrm{C})$, starting with $S_1=\mathrm{G}$, such that the feature of self-similarity is revealed on a broad length scale range. The scale factor τ, measuring the inflation speed of the chain and related to the ratio τ_{GC} (number of G)/(number of C) for an infinite sequence, is then given in the asymptotic limit [54]

$$\tau=\lim_{n\to\infty}\frac{N_{S_n}}{N_{S_{n-1}}}, \tag{2}$$

where N_{S_n} is the total number of nucleotides of S_n. These properties are summarized in Table I for several typical substitutional sequences. Obviously, the larger τ is, the faster the sequence inflates. And $\tau_{\mathrm{GC}}=\tau$ if τ is the irrational, whereas τ_{GC} varies for different sequences if τ is the integer, e.g., $\tau_{\mathrm{GC}}=2$ for GCGSGGC (SQ3) and $\tau_{\mathrm{GC}}=1$ for GGCSCCG (SQ4). Meanwhile, it can be conjectured that the sequences of copper mean (CM), GGCSGG (SQ2), Fibonacci, and bronze mean may perfectly exhibit self-similarity according to the well-organized concatenation rules, while others may exhibit complicated features associated with self-similarity, where $(S_{n-1}S_n-S_{n-1})$ means S_{n-1} should be discarded from the end of $S_{n-1}S_n$ and S_{n-2} from the beginning of S_{n-1} for $(-S_{n-2}+S_{n-1})$, $\tilde{S}_n$ is the complementary chain of S_n, and $(ST)_{n-2}$ is the similar Rudin-Shapiro (RS) sequence but with a T nucleotide as a seed.

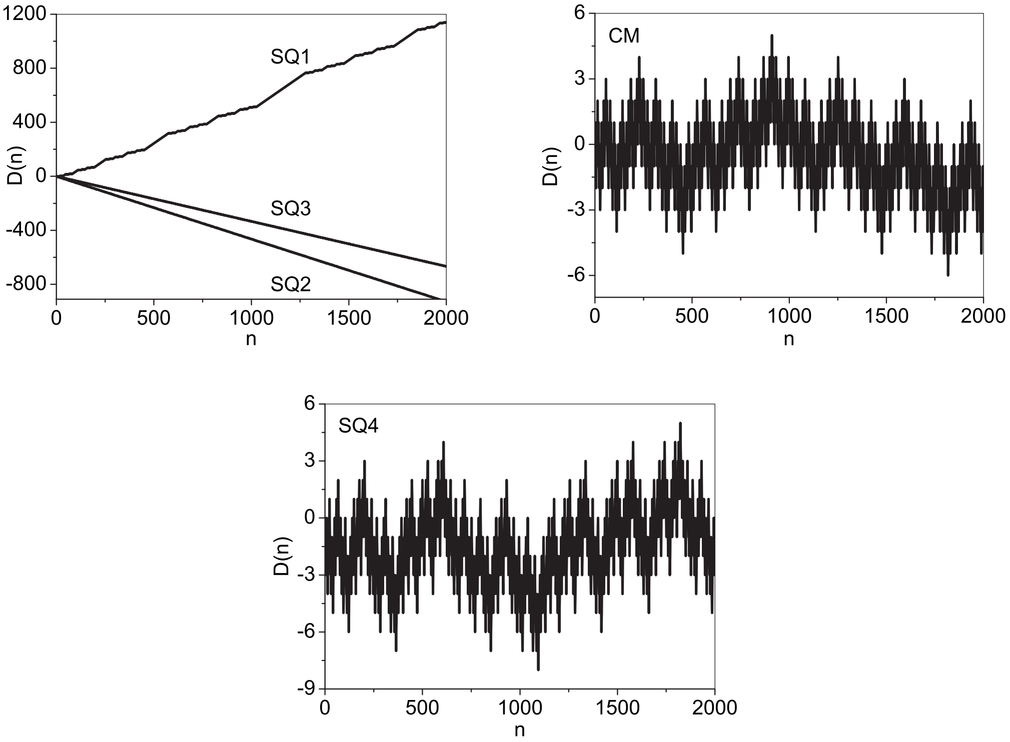

FIG. 1. Random DNA walks generated from the first nucleotide of the chain for SQ1, SQ2, SQ3, CM, and SQ4 sequences. The profiles of SQ1, CM, and SQ4 sequences may somewhat reflect the self-similar character.

To further compare other statistical properties of the above-mentioned DNA sequences, the rescaled range method which has been considered as a useful measure of nucleotide correlations in DNA molecules [30,51] is employed. This statistical analysis is based on a DNA walk defined by a rule. Here the purine-pyrimidine (RY) rule is considered [51,69], i.e., the walker steps down $[u(j)=-1]$ if a purine (G, A) occurs at the jth position or steps up $[u(j)=+1]$ if a pyrimidine (C, T) occurs at the jth position. After n steps, the net displacement is

$$D(n) = \sum_{j=1}^{n} u(j), \tag{3}$$

and the standard deviation of the walks averaged over the sequence is

$$\sigma^2(n) = 1 - \frac{1}{n^2} D^2(n). \tag{4}$$

The random DNA walks for SQ1, SQ2, SQ3, CM, and SQ4 sequences are shown in Fig. 1. Note that $D(n)$ is shifted to the negative (positive) value for SQ2 and SQ3 sequences (SQ1 sequence), since they (it) contain(s) a large number of purines (pyrimidines). The larger the number is, the stronger the shift is. And the oscillations observed for CM and SQ4 sequences imply $\tau_{\mathrm{GC}}=1$.

Following Hurst's analysis, the rescaled variables are defined as

$$X(k,n) = D(k) - \frac{k}{n} D(n), \tag{5}$$

and the range $S(n)$ for a DNA walk of lengths n is then given by

$$S(n) = \max_{1 \leqslant k \leqslant n} [X(k,n)] - \min_{1 \leqslant k \leqslant n} [X(k,n)]. \tag{6}$$

Thus the rescaled range function $R(n)$ is written as

$$R(n) = \frac{S(n)}{\sigma(n)} \propto n^H, \tag{7}$$

where $R(n)$ and the Hurst exponent H measure the nucleotide correlations, because the rescaled range function for uncorrelated random walk reads $R(n)=\sqrt{\pi n/2}-1$ with $H=0.5$. Therefore, the parameters $R(10^4)$ listed in Table I indicate long-range correlations in substitutional DNA sequences. For some sequences (CM, SQ4, and RS), a single Hurst exponent H can fully characterize them; while for others, the exponent will vary for different segments of the chain [51]. Figure 2 plots $R(n)$ for the six DNA sequences associated with the uncorrelated random one. On the one hand, $R(n)$ for SQ1 sequence illustrates a scale dependent Hurst exponent, which oscillates between a persistent behavior $(0.5<H<1)$ and an antipersistent behavior $(0<H<0.5)$. This point is further illustrated by the difference of $R(n)$ for RS sequence between this work and Ref. [30]. On the other hand, it clearly appears that the substitutional DNA sequences exhibit long-range correlations and will present good transmission ability as compared with the uncorrelated one. And RS sequence will

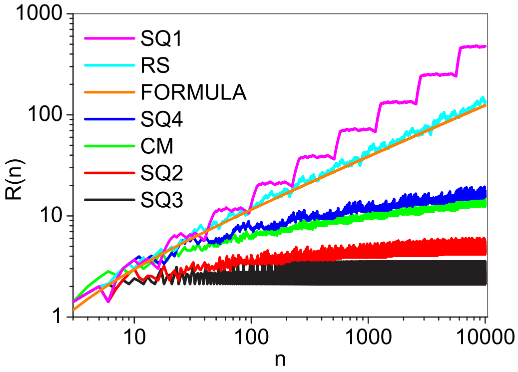

FIG. 2. (Color online) $R(n)$ versus n for the six substitutional DNA sequences. The orange smooth line corresponds to $R(n)=\sqrt{\pi n/2}-1$. The profiles of SQ1 (steplike appearance), CM, SQ4, and RS sequences may also reflect the self-similar character.

show relatively weak transmittivity as its long-range correlations is not strong enough ($H=0.51$). To have some details, we now turn to evaluate charge transfer properties in these sequences.

IV. TRANSMISSIVITY AND CONDUCTIVITY

Within the framework of the transfer matrix method, the transmission coefficient $T_N(E)$ is expressed as [28,51]

$$T_N(E)=\left(4-\frac{(E-\varepsilon_m)^2}{t_m^2}\right)\Bigg/\left(2+\sum_{i,j=1,2}\mathcal{P}_{ij}^2+\frac{(E-\varepsilon_m)}{t_m}\right.$$
$$\left.\times(\mathcal{P}_{11}-\mathcal{P}_{22})(\mathcal{P}_{12}-\mathcal{P}_{21})-\frac{(E-\varepsilon_m)^2}{t_m^2}(\mathcal{P}_{12}\mathcal{P}_{21}+1)\right), \tag{8}$$

with $\mathcal{P}=M_N M_{N-1}\cdots M_1$, and $M_n=\begin{pmatrix}(E-\varepsilon_n)/t_d & -1\\ 1 & 0\end{pmatrix}$. For a given energy, $T_N(E)$ measures the level of backscattering events in the charge transport through the chain. In our situation, as any A, T, C base behaves as a potential barrier, the hole (electron) transport will experience sequence-dependent backscattering effects, which dramatically reduce coherent tunneling with increasing length in random DNA sequences [51]. However, the long-range correlations in aperiodic DNA chains tend to induce coherent charge transport. Consequently, there will be a competition between backscattering effects and long-range correlations in substitutional DNA sequences.

Figures 3 and 4 present the comparison of $T_N(E)$ among the substitutional sequences. General trends of Fig. 3 are that the energy spectra show many energies with high transmission even resonances [$T_N(E)=1$]. As the sequence length increases, more states will present good transmittivity (Fig. 3, top frames), due to strong long-range correlations and the increasing number of energy levels [70], although the number of the potential barriers is much larger in SQ1 sequence ($\tau_{\mathrm{GC}}=0$). From a statistical analysis over many substitutional sequences, a great number of them exhibit this property, in-

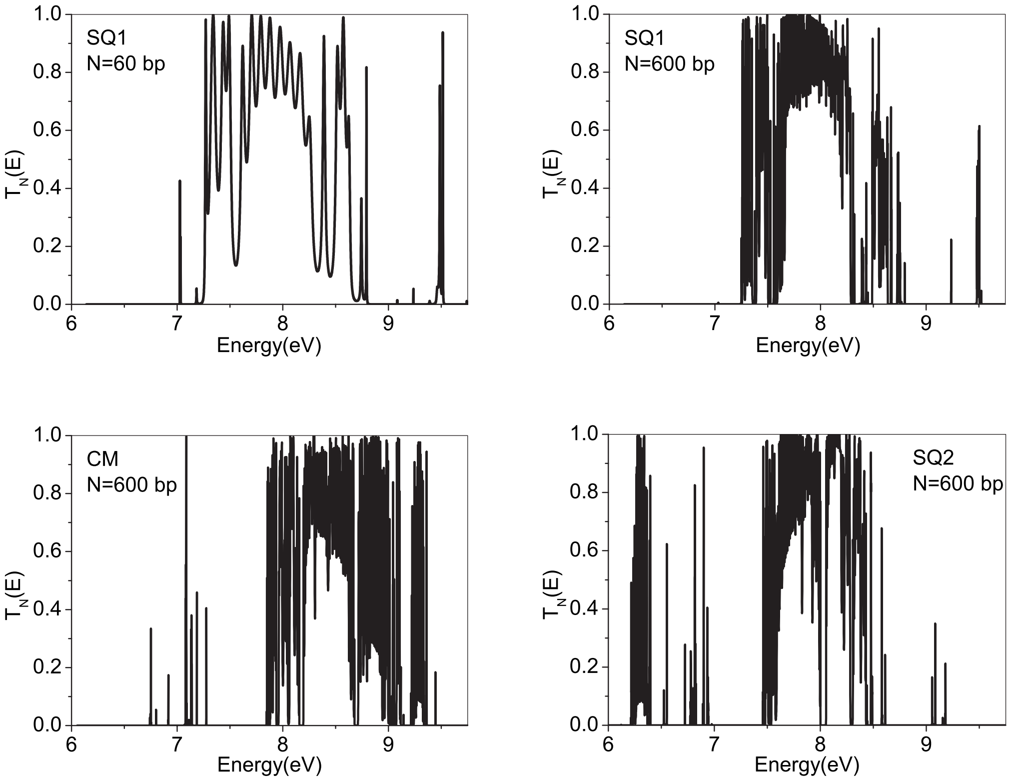

FIG. 3. Transmission coefficient for SQ1 (top frames), CM (bottom left frame), and SQ2 sequences (bottom right frame).

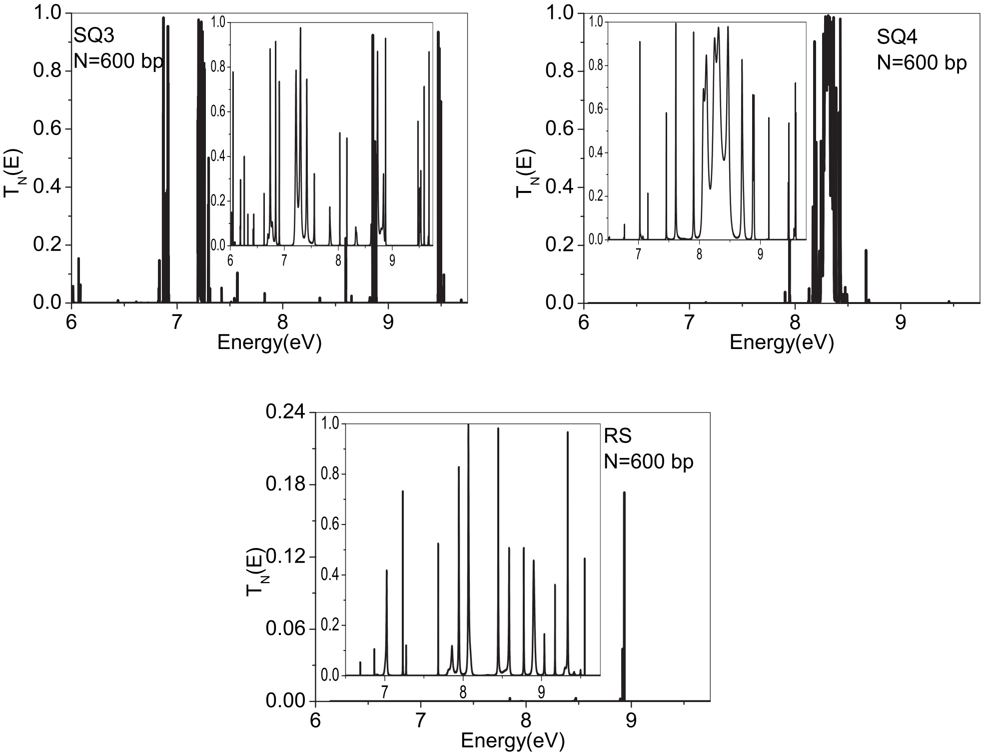

FIG. 4. Transmission coefficient for SQ3 (top left frame), SQ4 (top right frame), RS sequences (bottom frame) with $N=600$ bp (main frames) and with $N=60$ bp (insets).

dicating that the long-range correlations in these DNA chains are strong enough to induce electronic delocalization [32,52] and hence they will have a big conductivity. While for other substitutional sequences, only a few states will present good transmission ability (Fig. 4, top frames) because of the stronger fluctuations in diagonal energetics (Fig. 2, SQ4 to CM, SQ3 to SQ2). These states are also robust enough to persist against backscattering effects with increasing length, and will intersperse or assemble along the energy spectrum. Nevertheless, the transmissivity of RS sequence remarkably decreases with increasing length, due to the weak long-range correlations and stronger fluctuations in diagonal energetics (Fig. 2, RS).

To get a clear picture of the competition and the length dependent transport properties in substitutional sequences, the mean transmission coefficient is calculated by assuming a linear drop across the DNA chains (i.e., $\mu_{L,R}=\mu\pm e\mathcal{V}/2$, with μ the Fermi level and $\mathcal{V}\to 0$) [67], and the equation is

$$\bar{T}(N) = \int_{5.75}^{9.75} T_N(E)\left[\cosh\left(\frac{E-\mu}{k_BT}\right)+1\right]^{-1} dE \Bigg/ \int_{5.75}^{9.75}\left[\cosh\left(\frac{E-\mu}{k_BT}\right)+1\right]^{-1} dE, \tag{9}$$

with $k_BT=26$ meV. The intrinsic resistivity of the DNA molecules is then estimated by [28,34]

$$\rho = \frac{h}{2e^2}\frac{1-\bar{T}(N)}{\bar{T}(N)}\frac{S_{\mathrm{DNA}}}{L_{\mathrm{DNA}}}, \tag{10}$$

with $h/2e^2=12.9\ \mathrm{k}\Omega$ the quantum resistance, $S_{\mathrm{DNA}}=3\times 10^{-14}\ \mathrm{cm}^2$ the effective cross section, and $L_{\mathrm{DNA}}=Na$ the length.

Figure 5 plots the dependence of the resistivity on the length for SQ2, SQ4, RS, and poly(G) sequences. Notice that poly(G) has the biggest conductivity and the resistivity is about the order of $10^{-4}\ \Omega\,\mathrm{cm}$, whereas the resistivity of poly(GC) is about the order of $10^{-3}\ \Omega\,\mathrm{cm}$ [Fig. 5, inset, poly(GC)] which accords with the theoretical calculation in

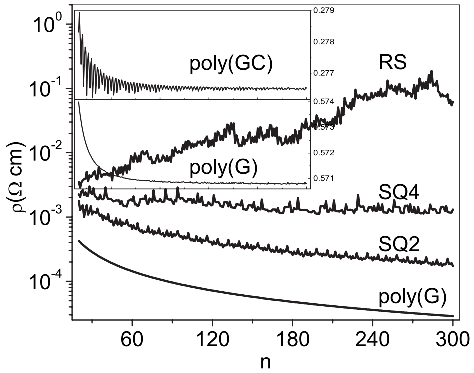

FIG. 5. Typical results of the resistivity for substitutional DNA sequences (main frame). And that for poly(G) is shown for comparison. Inset: $\bar{T}(n)$ versus n for poly(G) and poly(GC) from $n=20$ to 300 bp.

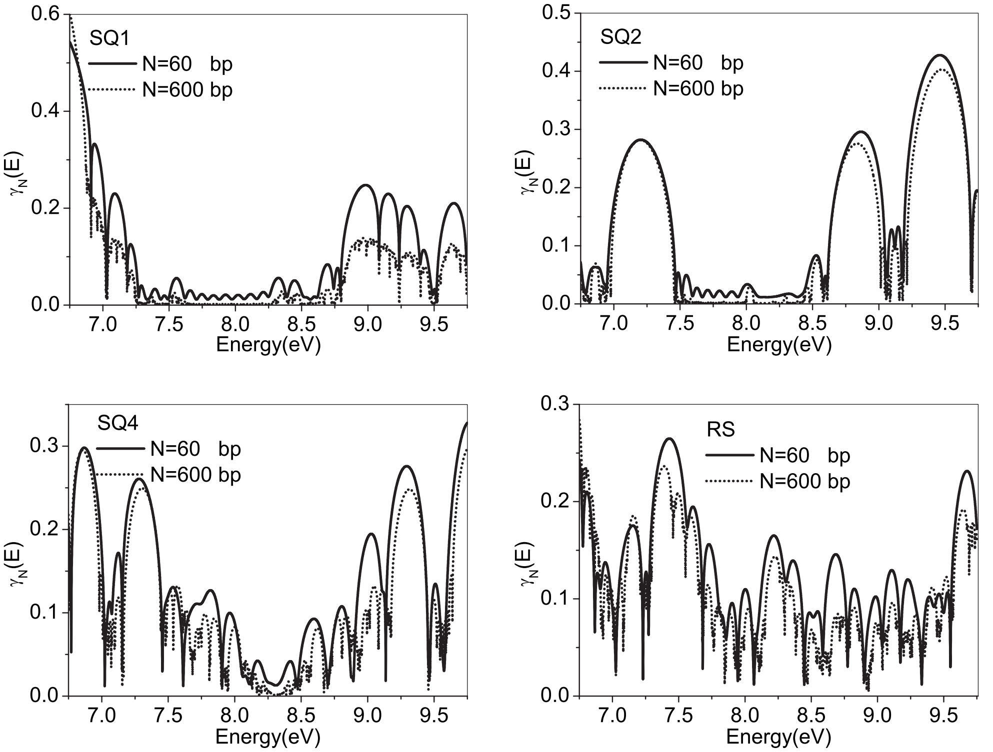

FIG. 6. Energy dependent Lyapunov coefficient $\gamma_N(E)$ for SQ1, SQ2, SQ4, and RS sequences. The Lyapunov spectra of CM and SQ3 sequences are similar to that of SQ2 and SQ4 sequences, respectively.

Ref. [34]. This is due to the periodic arrangement of the nucleotides and the absence of the potential barriers, which result in the smooth resistivity curve and roughly length independent transmission coefficient, although there seems to be a similar crossover [35,71] at $N=130$ bp [Fig. 5, inset, poly(G)]. When the more realistic coupling $t_d=0.15$ eV is adopted [21,37], we find that $\bar{T}=0.02$ for poly(GC) of $N=30$ bp. Accordingly, one deduces $\rho \simeq 0.02\ \Omega\,\text{cm}$ which turns out to be in good agreement with the experimental measurement [16]. Meanwhile, the observed oscillations for poly(G) (Fig. 5, inset) reflect the fact that we have treated the system as a coherent system via ignoring the dephasing effect of the environment and relaxation process of phonons [35,40,47]. These oscillations coexist with the backscattering effects induced fluctuations in all other sequences and the total fluctuations will be more obvious [Fig. 5, inset, poly(GC)]. When it comes to the substitutional sequences, the general trends of these sequences are that ρ is characterized by fluctuations with varying scales for different chains, where the small bumps are related to the occasionally inserted different nucleotides and reflect the backscattering effects as well as the neglecting of incoherences in DNA molecules. Since RS sequence contains A, T, C, and G four nucleotides, the dependence of the resistivity on the length is very intricate and exhibits larger fluctuations. On the other hand, it clearly appears that ρ for the SQ2 sequence decreases with increasing length, ρ for the SQ4 sequence tends toward the length independence, whereas ρ for the RS sequence increases with increasing length. This fact, however, is related to the competition between long-range correlations and backscattering effects in the chains as already discussed above (Figs. 3 and 4). Further, we confirm that the resonant energies can also be found in the transmission spectra and more fluctuations will be observed in the resistivity curves when the smaller coupling is used in these chains.

V. LYAPUNOV COEFFICIENT

Within the framework, the behavior of the Lyapunov coefficient [72],

$$\gamma_N(E) = \frac{1}{N} \ln(P_{11}^2 + \mathcal{P}_{12}^2 + \mathcal{P}_{21}^2 + P_{22}^2), \qquad (11)$$

comparing the transmission properties of different chains [51], is presented in Fig. 6. Interestingly, the behavior obtained for the Fibonacci sequence is in good agreement with previous theoretical studies [51], suggesting that the underlying structure of $\gamma_N(E)$ given by Eq. (11) can also reflect the self-similarity associated with the partitioning of the spectrum. Note that $\gamma_N(E)$ shown for SQ1, SQ2, SQ4, and RS sequences illustrates these properties but for a different nature. While each of the elliptic bumps found in SQ1 sequence with 60 bp is exactly divided into several parts in the 600 bp sequence due to the additional item (2^{n-1}C) in the concatenation rule (see Table I), the series of them found in the SQ2 sequence with 60 bp is well reproduced in the 600 bp sequence. From an analysis over many substitutional sequences with well-organized concatenation rules, it is found that they perfectly exhibit the self-similarity. Nevertheless, the fragmentation of the spectrum for SQ4 and RS sequences (Fig. 6, bottom frames) considerably reduces the

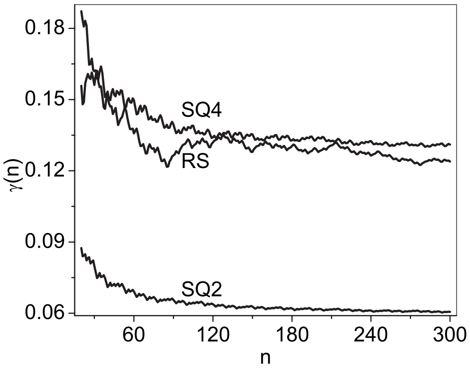

FIG. 7. The averaged Lyapunov coefficient for SQ2, SQ4, and RS sequences.

transmission coefficient of many states with increasing length (Fig. 4), due to the stronger fluctuations in diagonal energetics. The averaged Lyapunov coefficient $\gamma(N) = \langle \gamma_N(E) \rangle$ observed for SQ2, SQ4, and RS sequences will saturate at a different point (Fig. 7). And the fluctuations in the curves reflect the competition between the long-range correlations and the backscattering effects.

VI. CONCLUSIONS

In this paper, the intrinsic conduction properties of single-stranded DNA molecules are investigated by a tight-binding Hamiltonian combining the transfer matrix approach. Since the nucleotide correlations tend to play an important role in charge transfer through the chains, the transmissivity and the Lyapunov coefficient are presented for substitutional DNA sequences, which can be generated by substitutional rules or concatenation rules. From a statistical analysis over many substitutional sequences, it is found that they exhibit long-range correlations and show much higher charge transfer efficiency over longer distances in comparison with the uncorrelated one. Nevertheless, since the competition between long-range correlations and backscattering effects varies for different substitutional sequences, some of them show many energies with high transmission in the spectrum and the resistivity decreases with the length, others show only a few states of good transmittivity and the resistivity tends towards length independence, whereas for RS sequence the transmission coefficient decreases and the resistivity increases with increasing length. The resistivity curves of the substitutional sequences are characterized by fluctuations and reflect the backscattering effects and the neglecting of incoherences in DNA molecules. On the other hand, while the sequences with well-organized concatenation rules are fully characterized by self-similarity, others exhibit self-similarity associated with the fragmentation of the spectrum with increasing length. Therefore, we believe that the charge transfer efficiency can be improved by adjusting the arrangement of nucleotides. In the future, the model will be better constructed by considering the dephasing effect and double-stranded character for the substitutional DNA sequences, since the dephasing effect exists in a real system and the interstrand charge transport is very important [35]. The dephasing effect can result in a weak length dependence for a one-dimensional system [35], that is different from what we have discussed above. We expect that the dephasing effect may help damp the fluctuations of the resistivity curves observed in Fig. 5. And we also expect that a similar experimental study [18] would be undertaken for the short substitutional DNA chains, since the coherent tunneling is proposed to be the predominant conduction mechanism there.

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