Regular Article

Double path integral method for obtaining the mobility of the one-dimensional charge transport in molecular chain

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Abstract. We report on a theoretical investigation concerning the polaronic effect on the transport properties of a charge carrier in a one-dimensional molecular chain. Our technique is based on the Feynman's path integral approach. Analytical expressions for the frequency-dependent mobility and effective mass of the carrier are obtained as functions of electron-phonon coupling. The result exhibits the crossover from a nearly free particle to a heavily trapped particle. We find that the mobility depends on temperature and decreases exponentially with increasing temperature at low temperature. It exhibits large polaronic-like behaviour in the case of weak electron-phonon coupling. These results agree with the phase transition (A.S. Mishchenko *et al.*, Phys. Rev. Lett. **114**, 146401 (2015)) of transport phenomena related to polaron motion in the molecular chain.

1 Introduction

Studying the nature of the charge transport mechanism in a DNA molecule may gain more basic knowledge about the signalling and repairing process of damaged DNA that are related to the mutation of the DNA resulting in cancer. The mechanism of charge transport through DNA could also be used to protect from damage, caused by oxidizing chemicals [1,2], of genomes in some organisms. Moreover, DNA could be possibly used as a tool to develop numerous tiny devices such as DNA biosensors, templates for assembling nanocircuits and electric DNA sequencings, which are expected to be different from those existing traditional electronic devices [3–7]. There have been many experimental results which indicate that DNA could be a conductor. The first confirmation was from Eley and Spivey [8] initiating that DNA exhibits conductor property. Consequently, scientists have been attracted to investigate the electronic properties of DNA which could be a conductor because of the formation of a π-bond across the different A-T and C-G base-pairs[1]. The π-stacking interaction is a key function for the electrical properties of other organic molecules. Fink *et al.* [10,11] have shown the result of the *I-V* characteristic of DNA suggesting that DNA is a conductor. Later, Porath *et al.* [3] also created an experiment to show that DNA could be treated as a large-band-gap semiconductor. However, the charge transfer mechanism in the DNA chain is not yet well understood and remains very controversial[2]. At temperatures above 1 K, DNA may behave as conductors, semiconductors, or insulators, while below this temperature DNA may exhibit the properties of a proximity-induced superconductor [3,10,15–17]. Interestingly in [17], the electric conductivity of λ-DNA using DNA covalently bonded to Au electrodes was investigated. They found that λ-DNA is an excellent insulator on the micron scale at room temperature. Many theoretical models proposing to study the electrical properties of DNA were based on incoher-

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[1] In many experiments, it is possible to synthesis poly(dC)-poly(dG) and poly(dA)-poly(dT) DNA molecules containing identical base-pairs for studying static conductivity of the DNA molecules [9].

[2] Literature on DNA conductivity can be found in [12–14].

ent phonon-assisted hopping [18,19], classical diffusion under the conditions of temperature-driven fluctuations [20], variable range hopping between localised states [21], transport via coherent tunnelling [8] and polaron and soliton mechanisms [9,22–26]. The quantum model of charge mobility has been studied by Lakhno [27, 28]. The Kubo theory was needed to approximate the model yielding that the mobility increases with a temperature decrease. Another approach is to use Feynman path integrals[3] which was used to study the ground-state energy and the effective mass of the electron in DNA by Natda [39].

In the present paper, we will concentrate on the theoretical description of the mobility of the charge moving along *a model of the one-dimensional molecular chain*. We use the path integral as a key technique to study the problem. The Hamiltonian of the system can be written in the analogue form with the Holstien's Hamiltonian. We will show both analytical and numerical results of the study and we will try to give evidences: Could the one-dimensional molecular chain be a conductor and what are the conditions and factors effecting to its conductivity? The structure of the paper is organised as follows. In sect. 2, we will discuss the model of the one-dimensional molecular chain. The path integral method is used to eliminated the coordinates of the oscillators leading to the effective action of the system. In sect. 3, the steady-state condition at finite temperatures of the charge in the chain under the presence of the external electric field is studied. In sect. 4, the impedance function is computed from the equation of motion by relaxing the steady-state condition. Furthermore, the mobility at low temperatures of the charge is studied by varying the coupling constants and number of oscillators. The effective mass at zero temperature of the charge interacting with the chain is also calculated. In sect. 5, the physical concept of the analytical analysis and numerical results in the previous sections will be presented. In sect. 6, the summary of results and some open problems along with possible future developments will be mentioned.

2 The model of charge transport in the one-dimensional chain

In the literature, one of the famous models to study the motion of charge transport through the molecular chain is the Holstien polaron [40] which describes the small polarons formed by electron and localised phonons. In the present work, we model the one-dimensional molecular chain analogous to the DNA structure, see fig. 1.[4] An electron is now moving along the molecular chain and there is

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[3] The Feynman path integrals were successfully used to study the dynamics of the electron in the polar crystal [29–38].

[4] DNA is composed of two major long polymers which are made from repeating units called nucleotides. For all living things, DNA is in the shape of a double helix which is bonded together with backbones made from alternating phosphate and sugar residues, *i.e.*, A-T and C-G pairs.
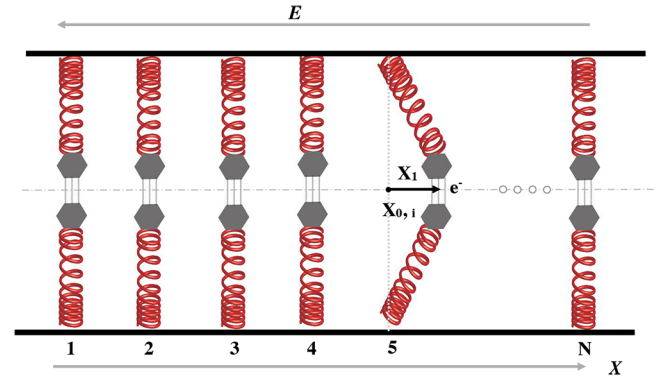

Fig. 1. A model of the one-dimensional molecular chain can be considered as a double-helix structure of the DNA chain unfolding into a strip. The oscillators, which will be treaded as having the same physical structure, are represented by springs which can move back and forth along the x-direction.

an interaction between the electron and lattices throughout the chain. We choose to describe the motion of the electron with the Hamiltonian, proposed by Natda [39], given by

$$H_e = \frac{p^2}{2m} + \frac{1}{2}\sum_{i=1}^{N}\left[\frac{P_i^2}{M} + M\Omega^2 x_i^2\right]$$
$$+ M\Omega^2\alpha\sum_{i=1}^{N}x_i\delta(x - x_{0,i}). \qquad (1)$$

The first term is the kinetic energy where p and m are the momentum and mass of the charge, respectively. The second term represents the physics of the oscillators where M and Ω are the mass and oscillation frequency and x_i is the displacement along the x-axis of the i-th from its equilibrium $x_{0,i}$. The last term describes the interaction[5], which is modeled by the Dirac delta function, between the electron and the oscillators where α is the coupling constant. The Hamiltonian in eq. (1) is indeed in a different expression from those of Holstein's model, but they equivalently describe the physics of charge transfer in the one-dimensional molecular chain. Moreover, the advantage of the Hamiltonian (1) is that it allows us to analytically solve the problem through the Feynman path integral approach in the same fashion with the Frohlich polaron [29, 31, 35, 39].

To proceed with the problem, we start to write the action of the system in the form

$$S_e = \int_0^T \mathrm{d}t\left(\frac{m\dot{x}^2}{2} + \frac{M}{2}\sum_{i=1}^{N}\left[\frac{\dot{x}_i^2}{M} - \Omega^2 x_i^2\right]\right.$$
$$\left. - M\Omega^2\alpha\sum_{i=1}^{N}x_i\delta(x - x_{0,i})\right), \qquad (2)$$

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[5] We assume that the interaction will take place only on the i-th oscillator, not for other oscillators (undistorted).

and the propagator can be written as

$$I_e = \int_{x(0)}^{x(T)} \mathscr{D}[x(t)] \prod_{i=1}^{N} \int_{x_i(0)}^{x_i(T)} \mathscr{D}[x_i(t)] e^{\frac{i}{\hbar} S_e}. \quad (3)$$

Eliminating the oscillators' coordinates, we obtain the effective propagator

$$I_{\text{eff}} = \int_{x(0)}^{x(T)} \mathscr{D}[x(t)] e^{\frac{i}{\hbar} S_{\text{eff}}}, \quad (4)$$

where the S_{eff} is the effective action given by

$$S_{\text{eff}} = \int_0^T \mathrm{d}t \left(\frac{m\dot{x}^2}{2} + \frac{M\Omega^3\alpha^2}{4} \sum_{i=1}^{N} \int_0^T \mathrm{d}\sigma f_i(t,\sigma) \right.$$
$$\left. \times \frac{\cos(\Omega|t-\sigma| - T/2)}{\sin(\Omega T/2)} \right), \quad (5)$$

where $f_i(t,\sigma) = \delta[x(t) - x_{0,i}]\delta[x(\sigma) - x_{0,i}]$. Using the fact that the delta function can be written in the form

$$\delta(x - \xi) = \sum_{n=1}^{\infty} \varphi_n(x)\varphi_n^*(\xi),$$

where φ_n are arbitrary orthonormal basis sets, then we find that

$$\sum_i \delta[x(t) - x_{0,i}]\delta[x(\sigma) - x_{0,i}] =$$
$$\sum_i \sum_m^{\infty} \sum_n^{\infty} \varphi_m(x(t))\varphi_m^*(x_{0,i})\varphi_n(x_{0,i})\varphi_n^*(x(\sigma)) =$$
$$N \sum_n^{\infty} \varphi_n(x(t))\varphi_n^*(x(\sigma)) = N\delta[x(t) - x(\sigma)]. \quad (6)$$

The effective action becomes

$$S_{\text{eff}} = \int_0^T \mathrm{d}t \left(\frac{m\dot{x}^2}{2} + \eta \int_0^T \mathrm{d}\sigma \int_{-\infty}^{\infty} \mathrm{d}k\, e^{ik(x(t)-x(\sigma))} \right.$$
$$\left. \times \frac{\cos(\Omega|t-\sigma| - T/2)}{\sin(\Omega T/2)} \right), \quad (7)$$

since $\delta[x(t) - x(\sigma)] = \frac{1}{2\pi}\int_{-\infty}^{\infty} \mathrm{d}k\, e^{ik(x(t)-x(\sigma))}$ and we define $\eta \equiv \frac{M\Omega^3\alpha^2 N}{8\pi}$. After eliminating the oscillators' coordinate, the action of the system (7) can be written in terms of the electron coordinate.

3 The steady-state condition

In this section, we consider the system of an electron moving along the molecular chain under the influence of the external constant electric field E_0. The Hamiltonian of the system now is

$$H_e = \frac{p^2}{2m} - E_0 x + \frac{1}{2} \sum_{i=1}^{N} \left[\frac{P_i^2}{M} + M\Omega^2 x_i^2 \right]$$
$$+ M\Omega^2\alpha \sum_{i=1}^{N} x_i\delta(x - x_{0,i}). \quad (8)$$

When the electric field is turned on, the electron will be accelerated. However, the electron will interact with the oscillators while it moves along the molecular chain resulting in a loss of some amount of energy with respect to oscillators. Then if we leave the system on long enough the system will reach the steady state.

In order to get the steady-state condition, we will apply the method, called Double path integral [30,32,35,38], that was used to study the motion of the electron in the polar crystal. Let ρ be the density matrix of the system and the expectation value of any operator $\mathbf{Q}$ at time t is given by

$$\langle \mathbf{Q}(t) \rangle = \mathsf{Tr}\left(\mathbf{Q}\rho(t) \right). \quad (9)$$

We now assume that the system is in thermal equilibrium initially, $\rho(t = 0) = \exp(-\beta H_e)$ where $\beta = 1/k_B\mathsf{T}$, T and k_B are the temperature and Boltzmann constant, respectively. To obtain the density matrix at any time t, we need to solve the time evolution equation

$$i\hbar \frac{\partial\rho}{\partial t} = [H_e, \rho], \quad (10)$$

and therefore we have[6]

$$\rho(t) = e^{-\frac{i}{\hbar}\int_0^T H(s)\mathrm{d}s}\rho(0)e^{+\frac{i}{\hbar}\int_0^T H'(s)\mathrm{d}s}. \quad (11)$$

As we mentioned earlier at the beginning the molecular chain is in thermal equilibrium, then we may write $\rho(0) = \exp(-\beta \sum_k a_k^\dagger a_k)$, where $a_k^\dagger$ and a_k are creation and annihilation operators of the oscillators.

Next, we will compute the expectation value of the electron displacement at time T as

$$\langle x(T) \rangle = \frac{\partial}{i\partial\gamma}\mathsf{Tr}\rho(T)\big|_{\gamma=0}, \quad (12)$$

where we now put $E_0 \to E_0 + \gamma\delta(t - T)$ and $E_0' \to E_0'$. The problem of integrating $\mathsf{Tr}\rho(T)$ over chain oscillators' coordinate can be performed in the same fashion as we mentioned in sect. 2. For convenience, we transform the electron coordinate to a frame of reference drifting [30,32,35] with the expectation value of the electron velocity v: $x(t) = y(t) + vt$. Then $\mathsf{Tr}\rho(T)$ can be written in the form

$$\mathsf{Tr}\rho(T) = \int \mathscr{D}[y(t)] \int \mathscr{D}[y'(t)] e^{i\Psi_e}, \quad (13)$$

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[6] An unprimed operator acts to the left and is ordered right to left with increasing time, and the primed operator acts to the right and is ordered left to right with increasing time.

where

$$\Psi_e = \Phi_e + \Phi'_e + \Phi_{in}, \tag{14a}$$

$$\Phi_e = \int_0^T \left(\frac{m}{2}\dot{y}^2(t) + (E_0 + \gamma\delta(t-T))y(t) \right), \tag{14b}$$

$$\Phi'_e = \int_0^T \left(\frac{m}{2}\dot{y}'^2(t) + E'_0 y'(t) \right), \tag{14c}$$

$$\Phi_{in} = i\eta \int_{-\infty}^{\infty} \mathrm{d}k \int_0^T \mathrm{d}t \int_0^T \mathrm{d}\sigma \, (S_\Omega(t-\sigma)$$
$$\times e^{-ik(y'(t)-y'(\sigma))} + S_\Omega^*(t-\sigma)e^{ik(y(t)-y(\sigma))}$$
$$- S_\Omega(t-\sigma)e^{ik(y'(t)-y(\sigma))}$$
$$- S_\Omega^*(t-\sigma)e^{ik(y(t)-y'(\sigma))} \Big), \tag{14d}$$

$$S_\Omega(u) = \left(\frac{e^{i\Omega u}}{1-e^{-\beta\Omega}} + \frac{e^{-i\Omega u}}{e^{\beta\Omega}-1} \right) e^{-ikvt}. \tag{14e}$$

Here comes the crucial point. The path integral of (13) can not be performed exactly, so we need to introduce a trail action given by

$$\Psi_{tr} = \Phi_e + \Phi'_e + \Phi_{tr}, \tag{15}$$

where

$$\Phi_{tr} = i \int_{-\infty}^{\infty} \mathrm{d}k \int_0^T \mathrm{d}t \int_0^T \mathrm{d}\sigma (G(t-\sigma)(y'(t)-y'(\sigma))^2$$
$$+ G^*(t-\sigma)(y(t)-y(\sigma))^2$$
$$- G(t-\sigma)(y'(t)-y(\sigma))^2$$
$$- G^*(t-\sigma)(y(t)-y'(\sigma))^2), \tag{16a}$$

$$G(u) = \sum_{j=1}^N \int_{-\infty}^{\infty} \mathrm{d}\Omega'_j G(\Omega'_j)e^{-i\Omega'_j u}. \tag{16b}$$

The function $G(\Omega'_j)$ is the distribution function[7] [30, 35] with frequencies $\Omega'_j = \sqrt{\frac{K_j}{M'}}$ of the j-th fictitious particle. We now expand (13) in the form

$$\int \mathscr{D}[y(t)] \int \mathscr{D}[y'(t)]e^{i\Psi_e}$$
$$= \int \mathscr{D}[y(t)] \int \mathscr{D}[y'(t)]e^{i\Psi_{tr}}e^{i(\Psi_e-\Psi_{tr})},$$
$$= \int \mathscr{D}[y(t)] \int \mathscr{D}[y'(t)]e^{i\Psi_{tr}}(1 + i(\Psi_e - \Psi_{tr}) + \ldots). \tag{17}$$

Using (17), we can write

$$\langle y(T)\rangle_e = \langle y(T)\rangle_{tr} + {}_e\langle y(T)\rangle_{tr} - {}_{tr}\langle y(T)\rangle_{tr} + \ldots, \tag{18}$$

where

$${}_j\langle y(T)\rangle_k = \frac{\partial}{i\partial\gamma} \int \mathscr{D}[y(t)] \int \mathscr{D}[y'(t)]i\Psi_j e^{i\Psi_k} |_{\gamma=0}, \tag{19a}$$

$$\langle y(T)\rangle_k = \frac{\partial}{i\partial\gamma} \int \mathscr{D}[y(t)] \int \mathscr{D}[y'(t)]e^{i\Psi_k} |_{\gamma=0}. \tag{19b}$$

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[7] In refs. [29,30,32,35,39], they considered only one fictitious particle. The reason why we consider N' fictitious particles is to make the trial action more realistic and also to improve the variational result [41,42].

The velocity of the electron can also be expanded in the form

$$v_e = v_{tr} + {}_e v_{tr} - {}_{tr} v_{tr} + \ldots, \tag{20}$$

We are interested in calculating the expectation value of the velocity at $T \to \infty$ at which the steady state is reached. Then we have

$${}_j v_k = \lim_{T\to\infty} \frac{\mathrm{d}}{\mathrm{d}T} {}_j\langle y(T)\rangle_k, \tag{21a}$$

$$v_k = \lim_{T\to\infty} \frac{\mathrm{d}}{\mathrm{d}T} \langle y(T)\rangle_k. \tag{21b}$$

From the relation (20), we may find

$$\frac{1}{v_e} = \frac{1}{v_{tr}} - \frac{{}_e v_{tr} - {}_{tr} v_{tr}}{v_{tr}^2}, \tag{22}$$

which is nothing more than the first-order expansion of the reciprocal of $v_e \simeq v_{tr} + {}_e v_{tr} - {}_{tr} v_{tr}$. The reason why we choose such an expansion for this type of problem is given in refs. [30,32,35]. Moreover, assuming $v_{tr} = -{}_{tr} v_{tr}$ which reduces (22) to

$$\frac{1}{v_e} = -\frac{{}_e v_{tr}}{v_{tr}^2}. \tag{23}$$

From (19b), we find that

$$\langle y(T)\rangle_e = -iE_0 \int_0^T \mathrm{d}t \, (L(t) - L^*(t)), \tag{24}$$

where

$$L(t) - L^*(t) = \int_{-\infty}^{\infty} \frac{\mathrm{d}\nu}{2\pi i} \left(\frac{1}{Z_\nu} - \frac{1}{Z_\nu^\dagger} \right) e^{-i\nu t}, \tag{25a}$$

$$Z_\nu = -\nu^2 - 4\nu \sum_{j=1}^{N'} \int_{-\infty}^{\infty} \frac{\mathrm{d}\Omega'_j}{\Omega'_j} \frac{G(\Omega'_j)}{\Omega'^2_j - \nu^2}. \tag{25b}$$

The first order of velocity in the expansion is

$$v_{tr} = -i2E_0 \, \mathrm{Im} \, L(T). \tag{26}$$

The next velocity in the expansion ${}_e v_{tr}$ can be computed by considering the term $\iint \Psi_e e^{\Psi_{tr}}$

$$\int \mathscr{D}[y(t)] \int \mathscr{D}[y'(t)]i\Psi_e e^{i\Psi_{tr}} =$$
$$-\eta \int_{-\infty}^{\infty} \mathrm{d}k \int_{-\infty}^{\infty} \mathrm{d}\theta \int_{-\infty}^{\theta} \mathrm{d}\zeta \left(S_\Omega(\theta-\zeta) \iint (1) \right.,$$
$$+ S_\Omega^*(\theta-\zeta) \iint (2) - S_\Omega(\theta-\zeta)$$
$$\iint (3) - S_\Omega^*(\theta-\zeta) \iint (4) \bigg). \tag{27}$$

We introduce the shorthand notations where the force terms $\iint[E_0, E_0']$ in $\iint \Psi_e e^{\Psi_{tr}}$ will be inserted as follows:

$$\iint(1) = \iint[E_0 + \gamma\delta(t-T), E_0' \\ +k(\delta(t-\theta) - \delta(t-\zeta))], \quad (28a)$$

$$\iint(2) = \iint[E_0 + \gamma\delta(t-T) \\ +k(\delta(t-\theta) - \delta(t-\zeta)), E_0'], \quad (28b)$$

$$\iint(3) = \iint[E_0 + \gamma\delta(t-T) + k\delta(t-\theta), E_0' \\ +k\delta(t-\zeta)], \quad (28c)$$

$$\iint(4) = \iint[E_0 + \gamma\delta(t-T) + k\delta(t-\zeta), E_0' \\ +k\delta(t-\theta)]. \quad (28d)$$

After performing tedious computation, we put $_e v_{tr}$ into (23) together with another assumption that $v_e \simeq v_{tr} \equiv v$ yielding the steady-state equation

$$E_0 = \eta \int_{-\infty}^{\infty} \mathrm{d}\zeta \int_{-\infty}^{\infty} \mathrm{d}k \frac{k\cos[\Omega\zeta]}{\sinh[\Omega\beta/2]} e^{-ikv(\zeta+i\beta/2)} e^{-k^2\Delta_\beta(\zeta)}, \quad (29)$$

where

$$\Delta_\beta(u) = \frac{1}{2} \sum_{j=1}^{2N'+1} \frac{\prod_{l=1}^{N'}(z_j^2 - \Omega_l^{2\prime})}{z_j \prod_{m\neq j}(z_j - z_m)} \\ \times \frac{\cosh[z_j\beta/2] - \cos[z_j u]}{\sinh[z_j\beta/2]}, \quad (30)$$

and z_j are the roots of the polynomial

$$\nu^2 \prod_{j=1}^{N'}(\nu^2 - \Omega_j^{\prime 2}) - \nu^2 \sum_{j=1}^{N'} \Omega_j^{\prime 2} = 0. \quad (31)$$

Equation (29) represents the equation of motion in the steady-state condition, which holds at any temperatures, for the charge moving along the molecular chain according to the model (1). The charge gains energy from the electric field and gives the energy to the oscillators via the interaction. Note that we compute only the first-order velocity in the expansion (20) corresponding to the fact that the interaction between the electron and oscillators is weak. The expansion in (18) can be pushed further in order to cover the higher range of the interaction.

4 Electrical properties of the molecular chain

In the previous section, the steady-state equation is obtained by observing the expansion of the velocity of the electron moving along the molecular chain. For the present section, we will compute the impedance function of the system from the equation of motion. The electric field is now modified to $E_0 \to E(t) = E_0 e^{i\varpi t}$ where ϖ is the oscillation frequency. From (24), we may write

$$\langle y(T) \rangle_e = -i \int_0^T \mathrm{d}t Y(T-t) E(t). \quad (32)$$

Taking the Fourier transform of (32), we have

$$y_\varpi = Y_\varpi E_\varpi, \quad (33)$$

where Y_ϖ is the Fourier transform of the response function given by

$$Y_\varpi = \int_0^T \mathrm{d}\xi e^{i\varpi\xi} \int_0^T \frac{\mathrm{d}\nu}{2\pi i} \left[\frac{1}{Z_\nu} - \frac{1}{Z_\nu^\dagger} \right] e^{-i\nu\xi} \equiv \frac{1}{Z_\varpi}. \quad (34)$$

The Z_ϖ is the impedance function of the electron moving on the molecular chain. Without imposing the steady-state condition, the equation of motion reads

$$E(T) = \eta \int_{-\infty}^{\infty} \mathrm{d}\zeta \int_{-\infty}^{\infty} \mathrm{d}k \frac{k\cos[\Omega\zeta]}{\sinh[\Omega\beta/2]} \\ \times e^{-ikv(\zeta+i\beta/2)} e^{-k^2\Delta_\beta(\zeta)} + \langle \ddot{y}(T) \rangle_e. \quad (35)$$

Applying (32) to (35), we find that the impedance function can be expressed in the form

$$Z_\varpi = -\varpi^2 + \int_0^{\infty} \mathrm{d}\xi(1 - e^{i\xi\varpi}) \operatorname{Im} S(\xi), \quad (36)$$

where

$$S(\xi) = 2\eta \int_{-\infty}^{\infty} \mathrm{d}k k^2 \left(\frac{e^{i\Omega\xi}}{1 - e^{-\beta\Omega}} + \frac{e^{-i\Omega\xi}}{e^{\beta\Omega} - 1} \right) \\ \times e^{-k^2\Lambda_\beta(\xi)}, \quad (37a)$$

$$\Lambda_\beta(u) = \sum_{j=1}^{2N'+1} \frac{\prod_{l=1}^{N'}(z_j^2 - \Omega_l^{\prime 2})}{z_j \prod_{m\neq j}(z_j - z_m)} \\ \times \frac{\cosh[z_j\beta/2] - \cos[z_j(u - i\beta/2)]}{\sinh[z_j\beta/2]}. \quad (37b)$$

We are now interested for the case of $\varpi < 1$ and $\beta \to \infty$ (zero temperature) and the path of integration along the real axis may be rotated to a path along the positive or negative imaginary axis $\xi \simeq 0$ to $\pm i\infty$ [30]. The impedance becomes

$$Z_\varpi = -\varpi^2 - 2\eta \int_0^{\infty} \mathrm{d}\xi(1 - \cosh[\varpi\xi]) e^{-\Omega\xi} \\ \times \int_{-\infty}^{\infty} \mathrm{d}k k^2 e^{-k^2\Lambda(\xi)}, \quad (38)$$

where

$$\Lambda(u) = \sum_{j=1}^{2N'+1} \frac{\prod_{l=1}^{N'}(z_j^2 - \Omega_l^{\prime 2})}{z_j \prod_{m\neq j}(z_j - z_m)} (1 - e^{-z_j u}). \quad (39)$$

In the case of extremely low frequency ϖ, we may approximate $1 - \cosh[\varpi\xi] \cong -\varpi^2\xi^2/2$. Then the impedance function is simplified to

$$Z_\varpi = -\varpi^2 m^*, \quad (40)$$

where m^* is the effective mass given by

$$m^* = 1 + \frac{\eta\sqrt{\pi}}{2} \int_0^{\infty} \mathrm{d}\xi \xi^2 \frac{e^{-\Omega\xi}}{[\Lambda(\xi)]^{3/2}}. \quad (41)$$
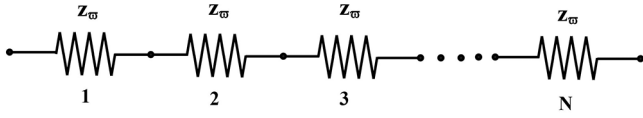
Fig. 2. The chain can be represented as a connected series of impedance functions z_ϖ.

Equation (40) together with (41) suggest that the charge behaves like a free particle with the effective mass m^* when it moves along the molecular chain. According to the model, eq. (38) is the impedance function for the whole molecular chain which consists of N oscillators. If we assume that each oscillator has the same impedance, we find

$$z_\varpi = \frac{Z_\varpi}{N}, \qquad (42)$$

which is the impedance for each oscillator. Then the system can be presented as a connected series of impedance functions shown in fig. 2. In the case that N becomes very large, $N \to \infty$, the impedance function remains finite

$$\lim_{N \to \infty} z_\varpi = -2\eta' \int_0^\infty \mathrm{d}\xi (1 - \cosh[\varpi\xi]) e^{-\Omega\xi}$$
$$\times \int_{-\infty}^\infty \mathrm{d}k k^2 e^{-k^2 \Lambda(\xi)}, \qquad (43)$$

where $\eta' = \frac{M\Omega^3 \alpha^2}{8\pi}$. From the result (42), we see that the conductivity of the chain is directly proportional to the reciprocal of the length of the chain [43].

We now introduce the function

$$\chi_\varpi = \int_0^\infty \mathrm{d}\xi (1 - e^{i\xi\varpi}) \operatorname{Im} S(\xi), \qquad (44)$$

which is the last term of the impedance function (36). For convenience of analytical analysis as mentioned in [30, 32, 35], we may consider

$$\operatorname{Im} \chi_\varpi = \sinh[\varpi\beta/2] \int_0^\infty \mathrm{d}u \cos[\varpi u] \Sigma(u), \qquad (45)$$

where

$$\Sigma(u) = S(u + i\beta/2) = \frac{2\eta}{\sqrt{\pi}} \frac{\cos[u]}{\sinh[\beta/2]}$$
$$\times \frac{1}{[D_\beta(u)]^{3/2}}, \qquad (46a)$$

$$D_\beta(u) = \sum_{j=1}^{2N'+1} \frac{\prod_{l=1}^{N'} (z_j^2 - \Omega_l'^2)}{z_j \prod_{m \neq j} (z_j - z_m)}$$
$$\times \frac{\cosh[z_j \beta/2] - \cos[z_j u]}{\sinh[z_j \beta/2]}. \qquad (46b)$$

The mobility [30, 32, 35] of the charge moving along the molecular chain is defined as

$$\frac{1}{\mu} = \lim_{\varpi \to 0} \frac{\operatorname{Im} \chi_\varpi}{\varpi} = \frac{\beta}{2} \int_0^\infty \Sigma(u) \mathrm{d}u. \qquad (47)$$

We see that the mobility of the charge is a function of the temperature and also the coupling constant α. We also would like to point out that (45) and (47) hold at any temperatures. In the next section, we will show the analytical analysis as well as the numerical results of the effective mass and the charge mobility.

5 Physical concept of the results

In this section, we will focus more on the physical meaning of the results from the previous sections. Before proceeding, we need to reduce the complexity of the trial action (15). Here, we are interested in the case of $N' = 1$. Let υ and Ω' be the variational variables, determined from the minimization of the ground state energy [29,39], given by

$$\Omega' = \sqrt{\frac{K}{M'}}, \quad \upsilon = \sqrt{\frac{K}{\varrho}}, \quad \text{and} \quad \varrho = \frac{m}{m + M'}. \qquad (48)$$

The steady-state condition: With $N' = 1$, eq. (29) becomes

$$E_0 = \eta \int_{-\infty}^\infty \mathrm{d}\varsigma \int_{-\infty}^\infty \mathrm{d}k k \left([1 + n(\Omega)] e^{i(\Omega - kv)\varsigma} \right.$$
$$\left. - n(\Omega) e^{-i(\Omega - kv)\varsigma} \right) e^{-k^2 D_\beta(\varsigma)}, \qquad (49)$$

where

$$n(\Omega) = \frac{1}{e^{\beta\Omega} - 1}, \qquad (50a)$$

$$D_\beta(u) = \frac{1}{2} \frac{\Omega'^2}{\upsilon^2} \left[\left(\frac{\upsilon^2 - \Omega'^2}{\upsilon \Omega'^2} \right) \right.$$
$$\times \frac{\cosh[\upsilon\beta/2] - \cos[\upsilon(u - i\beta/2)]}{\sinh[\upsilon\beta/2]}$$
$$\left. - iu + \frac{u^2}{\beta} \right]. \qquad (50b)$$

We will follow the analysis process of (49) as those in [33, 35]. We start to rewrite (50b) in the following form [33]:

$$D_\beta(u) = \frac{1}{2} \left(\frac{\upsilon^2 - \Omega'^2}{\upsilon^3} \right) \coth[\upsilon\beta/2] - \frac{iu}{2M} + \frac{u^2}{2M\beta}$$
$$- \left(\frac{\upsilon^2 - \Omega'^2}{\upsilon^3} \right) \left([1 + n(\upsilon)] e^{-i\upsilon u} \right.$$
$$\left. + n(\upsilon) e^{i\upsilon u} \right), \qquad (51)$$

where $M = \frac{\Omega'^2}{\upsilon^2}$. We now also introduce the relation [33, 35]

$$e^{-\frac{k^2 u^2}{2M\beta}} = \int \mathrm{d}p f(p) e^{\pm \frac{ipku}{M}}, \quad \text{where} \quad f(p) = \sqrt{\frac{\beta}{2\pi M}} e^{-\frac{\beta p^2}{2M}}. \qquad (52)$$

Inserting (52) and (51) into (49) together with expanding the terms $[1 - n(\upsilon)]$ and $n(\upsilon)$ in the Taylor series, we

$$\text{Im}\,\chi_\varpi = \frac{4\sqrt{2}\eta\beta^{3/2}}{\sqrt{\pi}}\left(\frac{v}{\Omega'}\right)^3 \frac{\sinh[\varpi\beta/2]}{\sinh[\beta/2]} \int_0^\infty \frac{\cos[\varpi u]\cos[u]\mathrm{d}u}{\left[u^2 + \frac{\beta^2}{4} + \beta\left(\frac{v^2-\Omega'^2}{\Omega'^2 v}\right)\coth[\beta v/2] - \beta\left(\frac{v^2-\Omega'^2}{\Omega'^2 v}\right)\frac{\cos[vu]}{\sinh[\beta v/2]}\right]^{3/2}}. \tag{56}$$

obtain

$$E_0 = \eta\sqrt{\frac{\beta}{2\pi}} \sum_{n=0}^{\infty} \sum_{n'=0}^{\infty} \int \mathrm{d}p \int_{-\infty}^{\infty} \mathrm{d}k B(\beta,n,n') k^{2(n+n'-1)}$$

$$\times e^{-\frac{k^2}{2}\left(\frac{v^2-\Omega'^2}{v^3}\right)\coth[v\beta/2]} f(p)k$$

$$\times \left\{ [1 + n(\Omega)] \cdot \delta\left(\Omega - k\left(v + \frac{p}{M}\right) + \frac{k^2}{2M}\right.\right.$$

$$\left. + (n-n')v\right) - n(\Omega) \cdot \delta\left(-\Omega + k\left(v + \frac{p}{M}\right)\right.$$

$$\left.\left. + \frac{k^2}{2M} + (n-n')v\right)\right\}, \tag{53}$$

where

$$B(\beta,n,n') = \frac{\frac{1}{2}\left[\left(\frac{v^2-\Omega'^2}{v^3}\right)[1+n(v)]\right]^n}{n!}$$

$$\times \frac{\frac{1}{2}\left[\left(\frac{v^2-\Omega'^2}{v^3}\right)n(v)\right]^{n'}}{n'!}. \tag{54}$$

The physical meaning of (53) is the following, see also [33, 35]. The term in the second line of (53), with the term $[1 + n(\Omega)]$, represents the process that the electron with momentum $p + Mv$ emits a phonon with energy Ω and momentum k, while the electron state changes from $n' \to n$. The electron momentum is reduced by k and the delta function tells us that energy is conserved, while the $[1 + n(\Omega)]$ shows that a phonon with frequency Ω is emitted. The term in the third line of (53), with the term $n(\Omega)$, describes the opposite situation as follows: the electron with momentum $p + Mv$ absorbs the phonon with frequency Ω.

The effective mass: The effective mass (41) can be simplified in the form

$$m^* = 1 + \eta\sqrt{8\pi}v^3$$

$$\times \int_0^\infty \mathrm{d}\xi \frac{\xi^2 e^{-\Omega\xi}}{\left[v\left(1 - \frac{\Omega'^2}{v^2}\right)(1 - e^{-v\xi}) + \Omega'^2\xi\right]^{3/2}}. \tag{55}$$

The numerical results of the effective mass with various coupling constants and the number of oscillators are shown in fig. 3. In the case of the weak coupling, the electron will move freely as the effective mass approximately becomes the mass of the electron: $m^* \to m = 1$. In the case of strong coupling, the electron will behave like a heavy particle as the effective mass increases. The transition between the two regimes is very sharp at the coupling constant about $\alpha \approx 1$. Another effect on the mass of the electron is the number of oscillators N. For large N, the effective mass of the electron will increase drastically. This
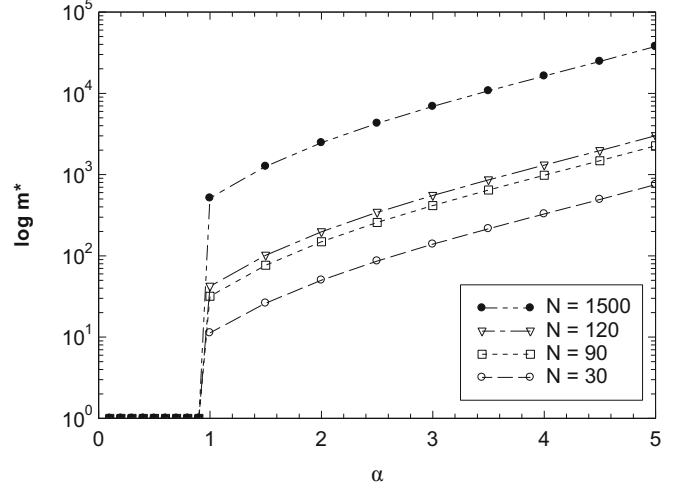

Fig. 3. Coupling interaction dependence of the effective mass for a different number of oscillators. The dashed, dotted, dot-dashed and double-dot-dashed lines show that dependence of the effective mass when the number of oscillators is $N = 30$, 90, 120 and 1500, respectively.

result suggests that the length of the chain has an effect on the charge transfer mechanism as pointed in [43].

The mobility: We consider the function $\text{Im}\,\chi_\varpi$ for the case $N' = 1$

see eq. (56) *above*

We see that the integrand of (56) has the same structure as those (47a) in [30]. If we now consider the system at low temperatures and $\varpi < 1$ we have

$$\text{Im}\,\chi_\varpi = 4\sqrt{2}\eta\left(\frac{v}{\Omega'}\right)^3 \left[\sqrt{1-\varpi}\,e^{-\beta(1-\varpi)}e^{-\left(\frac{v^2-\Omega'^2}{\Omega'^2 v}\right)(1-\varpi)}\right.$$

$$+ \sqrt{1+\varpi}\,e^{-\beta}e^{-\left(\frac{v^2-\Omega'^2}{\Omega'^2 v}\right)(1+\varpi)}$$

$$- \sqrt{1-\varpi}\,e^{-\beta}e^{-\left(\frac{v^2-\Omega'^2}{\Omega'^2 v}\right)(1-\varpi)}$$

$$\left. - \sqrt{1+\varpi}\,e^{-\beta(1+\varpi)}e^{-\left(\frac{v^2-\Omega'^2}{\Omega'^2 v}\right)(1+\varpi)}\right]. \tag{57}$$

The first term describes the process in which the electron absorbs a quantum of energy ϖ from the electric field and emits a phonon with unit energy. The second term shows that the electron absorbs a quantum of energy ϖ and also absorbs a phonon then at the end the electron will carry the momentum $\sqrt{1+\varpi}$. The third term, the electron absorbs a phonon and releases a quantum of energy ϖ to the electric field. The fourth term represents the electron with energy $1 + \varpi$ emitting a phonon as well as a quantum of energy to the electric field. The term $\exp[-\left(\frac{v^2-\Omega'^2}{\Omega'^2 v}\right)(1\pm\varpi)]$ tells the chance that the electron with energy $1 \pm \varpi$ completes the processes. Equation (57)
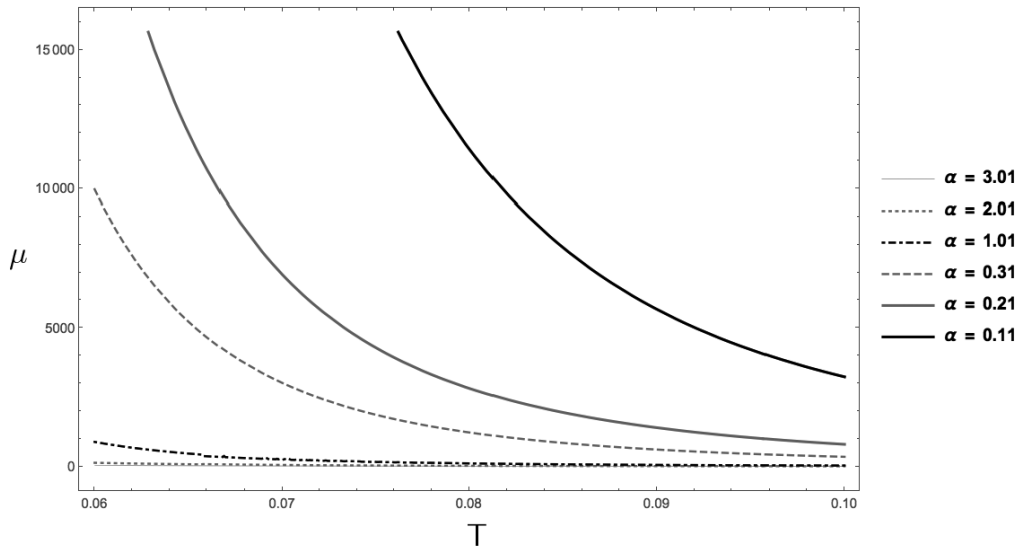
Fig. 4. The mobility *versus* the temperature in one-dimensional molecular chain with various coupling constants.

contains possible scatterings happening while the electron moves along the chain.

In the case of low temperatures and $\varpi \to 0$, eq. (56) leads to the dc mobility

$$\frac{1}{\mu} = 4\eta\sqrt{\frac{2}{\pi}}\beta^{3/2}\left(\frac{\upsilon}{\Omega'}\right)^3$$
$$\times \int_0^\infty \frac{\cos[u]\mathrm{d}u}{\left[2\left(\frac{\upsilon^2-\Omega'^2}{\Omega'^2}\right)\frac{1-\cos[\upsilon u]}{\upsilon^2}+u^2+\frac{\beta^2}{4}\right]^{3/2}}. \quad (58)$$

The numerical results of the polaron mobility is shown in fig. 4. The mobility will decrease with increasing temperature. The low-temperature behaviour of its mobility is proportional to the temperature in the exponential form [44] which corresponds to the phase diagram of polaron transport [45]. The coupling constant also affects the mobility of the electron as follows. In the case of strong coupling, the electron will have more difficulty moving through a strongly distorted chain. On the other hand, for the case of weak coupling, the electron can move easily through the slightly distorted chain. These results correspond with the result of the effective mass as the electron will gain more mass from the interaction with the chain reflecting to its mobility in the motion.

In this case $\beta^2 \gg (\upsilon^2 - \Omega'^2)$, we have

$$\frac{1}{\mu} = 4\eta\sqrt{\frac{2}{\pi}}\beta^{3/2}\int_0^\infty \frac{\cos[u]\mathrm{d}u}{\left[u^2+\frac{\beta^2}{4}\right]^{3/2}} = 2\eta\sqrt{\frac{2}{\pi}}\beta^{1/2}K_1(\beta),$$
$$(59)$$

where K_1 is the modified Bessel function of second kind and $K_1(\beta) \approx e^\beta/\sqrt{\beta}$, the mobility becomes

$$\mu \propto e^\beta, \quad (60)$$

which agrees with the numerical result in fig. 4. The low-temperature behaviour of the mobility has the characteristic form of an exponential term for the deformable one-dimensional molecular chain. The electron mobility will be influenced strongly by the interaction of the electrons with phonons. In a semiconductor quantum wire, the mobility of an electron interacting with acoustic phonons would follow an exponential behaviour and the energy relaxation of an electron due to emissions of acoustic phonons strongly increased by all the low-temperature acoustic phonon scattering mechanisms, which are exponentially activated in a an electron [46, 47]. The main feature of our results is the identification of the electron transfer in the chain similar to be behaviour of electron scattering in a semiconductor quantum wire. Recent studies of the electrical conductivity of DNA molecules reveal that they may act as semiconductor materials with nanometer scale dimensions [3, 9, 10, 13, 16, 48–57].

6 Summary

We have studied the model of charge transfer in a one-dimensional molecular chain with arbitrary N oscillators employing the Hamiltonian proposed in [39]. The interaction between the charge and the oscillators is represented by the Dirac delta function. The path integral method is used as the key tool to study the physical properties of the system. The main advantage of the path integral is that the oscillators' coordinates can be integrated leading to an effective action. The expectation value of the equation of motion of the electron moving in the chain under the influence of an external electric field can be computed by introducing the trial action. The electron will gain energy from the electric field and will give some to the phonons via the scattering process. In the steady-state condition, the electron is the balance of these two processes. The electron behaves like a heavy particle if the coupling constant and the number of oscillators are large. On the other hand,

the electron moves freely in the weak-coupling region with a small number of oscillators.

The mobility of charge moving along the chain is studied as a major feature. At low temperature the result suggests that our one-dimensional chain can be treated as a semiconductor quantum wire. For the case of extremely low temperatures, the mobility is very high leading to a very high conductivity. This result may be explained by the resonant tunnelling effect. The hopping process [58,59] may be a current candidate to theoretically explain the charge transfer in the one-dimensional molecular chain and agree with many experimental results [60–62]. However, experiments have so many factors as well as conditions to be controlled. This causes a big debate on what a one-dimensional molecular chain conductivity should be as pointed out in [13,14]. Then, we believe that the model in this paper may offer an alternative theoretical description of the charge transfer process.

Finally, we would like to point out that the model can be developed for a more realistic DNA. The results in the present paper can then be improved by taking into account the following points. The first is taking the double-helix structure of DNA into account (quasi-1D). This means that the angular part has to be added into the action but this would lead to complex computation. The second point is to consider the different coupling constants between A-T and C-G pairs. The third point is to consider the anharmonic oscillator of base-pairs in the case of strong coupling. As a last point, the results of path integrals can be corrected by computing the higher terms in the expansion of the velocity equation (20).

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