Electronic Conduction in Base Pairs of DNA Mediated by Phonons

P. M. Fonseca Alfonso a, R. R. Rey-Gonzalez b

aGrupo de Óptica e Información Cuántica, Departamento de Física, Universidad Nacional de Colombia - Bogotá
bGrupo de Física de Materiales, Universidad Pedagógica y Tecnológica de Colombia - Tunja

Recibido 22 de Oct. 2007; Aceptado 6 de Mar. 2009; Publicado en línea 30 de Abr. 2009

Resumen
El ADN es un alambre molecular o un alambre cuántico natural. Uno de los mecanismos propuestos para la conducción electrónica corresponde al tunelamiento entre pares de bases de ADN que forman un escalón. Como la probabilidad de tunelamiento electrónico directo puede ser despreciable en primera aproximación, tenemos en cuenta un tunelamiento electrónico asistido por phonones, considerando sólo un modo vibracional debido a variaciones en la distancia entre los pares de bases. La probabilidad de tunelamiento en ciertos tiempos es uno en condiciones muy rigurosas tanto sobre el valor de los parámetros como en el estado inicial de los phonones.

Palabras Clave: ADN, conducción electrónica, phonones.

Abstract
DNA is a molecular wire or one natural quantum wire. One of the proposed mechanisms of the electronic conduction corresponds to tunneling between base pairs that constitute one step. Since the direct electronic tunneling probability can be neglected in the leading order, we take into account electronic tunneling assisted by phonons, considering only the vibrational mode due to the distance variation between base pairs. The tunneling probability at certain times is one under very stringent conditions over the value of the parameters and the initial phonon states.

Keywords: DNA, electronic conduction, phonons.

©2008. Revista Colombiana de Física. Todos los derechos reservados.

1. Introducción

The deoxyribonucleic acid or DNA is one of the most interesting and mysterious biological molecules. It possesses a very important biological function that consists in the aptitude to preserve and transfer genetic information.

On the other hand, as a result of the continuous and rapid progress of the Nanotechnology, the need to miniaturize electronic devices is becoming increasingly palpable. The study of the electronic conduction in long molecules like DNA is interesting not only from point of view of basic science but also due to the potential technological applications. DNA constitutes an excellent candidate to use in Nanotechnology, because it has two important properties that are extremely valuable in the development of nanodevices: recognition and self assembling. The recognition is the property of the molecule to keep the information and to respond according to the interaction with other biomolecules; for example, the proteins. The self assembling is the capacity to assemble itself spontaneously, based on its chemical
and structural properties. These properties could handle the construction of individual components of circuits due to their ability to keep the information, to select the correct component and to organize molecules in different still more complex configurations, increasing therefore the efficiency of devices of reduced size. Moore’s law, which predicted an exponential increase of the number of transistors contained in a chip, has been roughly obeyed since its formulation in 1964. Moore’s law is expected to be finally broken that by the end of this decade or the next one, as a consequence of the current limits in the technologies of miniaturization. The use of molecules with diameters of the order of a few nanometers, as an essential part of the electronic circuits, might help in keeping the exponential increase of the number of transistors packed in a chip.

Despite the intensive research of the electronic properties of DNA, its “true” nature remains elusive. In fact, the scientific reports indicate very different behaviors in different still more complex configurations, increasing therefore the efficiency of devices of reduced size. Moore’s law is expected to be finally broken that by the end of this decade or the next one, as a consequence of the current limits in the technologies of miniaturization. The use of molecules with diameters of the order of a few nanometers, as an essential part of the electronic circuits, might help in keeping the exponential increase of the number of transistors packed in a chip.

Despite the intensive research of the electronic properties of DNA, its “true” nature remains elusive. In fact, the scientific reports indicate very different behaviors in different still more complex configurations, increasing therefore the efficiency of devices of reduced size. Moore’s law is expected to be finally broken that by the end of this decade or the next one, as a consequence of the current limits in the technologies of miniaturization. The use of molecules with diameters of the order of a few nanometers, as an essential part of the electronic circuits, might help in keeping the exponential increase of the number of transistors packed in a chip.

2. Physical and theoretical model

We consider a bases pair and one electronic state per base. In addition we suppose that the distance between the bases is not constant, but it can change. If the oscillations around the classic equilibrium point are small, the phononic mode can be treated in the harmonic approximation. Since we moreover assume localized electronic states with an almost vanishing overlap, the Hamiltonian that describes the system, in the independent electron approximation, can be written as follows

\[ \hat{H} = \epsilon_1 \hat{c}_1^\dagger \hat{c}_1 + \epsilon_2 \hat{c}_2^\dagger \hat{c}_2 + \hbar \omega \hat{a}^\dagger \hat{a} + \hbar \lambda (\hat{a}^\dagger + \hat{a}) (\hat{c}_1^\dagger \hat{c}_2 + \hat{c}_2^\dagger \hat{c}_1), \]

(1)

where \( \epsilon_i, i = 1, 2 \) are the eigenenergies of the electrons in the \( i \)-th electronic state, \( \hbar \omega \) is the phonon energy and \( \lambda \) is the electron - phonon coupling constant. The operators of annihilation \( \hat{c}_i \) and creation \( \hat{c}_i^\dagger \) of the electrons in the states \( |i\rangle = 1, 2 \), satisfy the usual anticommutation relations \( \{ \hat{c}_i, \hat{c}_j^\dagger \} = \delta_{i,j} \). The symbols \( \hat{a} \) and \( \hat{a}^\dagger \) represent the operators of annihilation and creation of phonons, which satisfy the usual commutation relations \( [\hat{a}_i, \hat{a}_j^\dagger] = 1 \).

We solve the Hamiltonian (1) in the Rotating Wave Approximation, RWA. With one electron by base, we observe a set of doublets with an energy splitting much smaller than the energy separation between different doublets. The eigenenergies of the eigenstates of (1) are given by the expression

\[ E_{n \pm} = \frac{\epsilon_1 + \epsilon_2 + (2n - 1) \hbar \omega}{2} \pm \sqrt{\frac{\hbar^2 \lambda^2 n}{2} + \left( \frac{\epsilon_1 - \epsilon_2 - \hbar \omega}{2} \right)^2}, \]

(2)

where \( n = 1, 2, \ldots \) and \( E_0 = \epsilon_1 \). The difference between eigenenergies of the electrons in the absence of interaction, \( \epsilon_1 - \epsilon_2 \), is 0,101 eV and the phonon energy is \( \hbar \omega = 0,1 \text{ eV} \).

The Hamiltonian (1) can also be solved in an exact way by direct numeric diagonalization. The eigenvectors and eigenvalues have been numerically found for typical values of the parameters.

The figure 1(a) shows the exact energy spectra for different electron-phonon coupling constants, \( \lambda \), while figure 1(b) shows the absolute error between numerical and the analytical results for the same values of \( \lambda \).
employed in the former figure. We can see that the error increases as \( \lambda \) approaches \( \hbar \omega \). This shows us that although the Rotating Wave Approximation is a good approximation for values of \( \lambda \ll \hbar \omega \), the limit used in quantum optics, even for values of \( \lambda \) the order of \( \hbar \omega \) the approximation gives surprisingly good values for the lowest energy eigenstates.

The eigenvectors, in the RWA, are given by:

\[
|n, +\rangle = a_n |n-1, 1\rangle - b_n |n, 2\rangle, \\
|n, -\rangle = b_n |n-1, 1\rangle + a_n |n, 2\rangle, 
\]

where

\[
a_n = \frac{\hbar \lambda \sqrt{2n} \sqrt{\hbar^2 \lambda^2 n + \left(\frac{\Delta}{2}\right)^2}}{2 \sqrt{\hbar^2 \lambda^2 n + \left(\frac{\Delta}{2}\right)^2 + \sqrt{\hbar^2 \lambda^2 n + \left(\frac{\Delta}{2}\right)^2}}},
\]

\[
b_n = \frac{\sqrt{\frac{\Delta}{2} + \sqrt{\hbar^2 \lambda^2 n + \left(\frac{\Delta}{2}\right)^2}}}{2 \sqrt{\hbar^2 \lambda^2 n + \left(\frac{\Delta}{2}\right)^2}}.
\]

and \( \Delta = \epsilon_1 - \epsilon_2 - \hbar \omega \).

The time evolution for the analytical states was performed and we find for the probability to have \( n \) phonons at time \( t \):

\[
p(n) = \rho_{nn}(0) \left[ \cos^2 \left(\frac{\Omega_n t}{2}\right) + \left(\frac{\Delta}{\Omega_n}\right)^2 \sin^2 \left(\frac{\Omega_n t}{2}\right) \right] + \rho_{n-1,n-1}(0) \left(\frac{4\lambda^2 n}{\Omega_{n-1}}\right) \sin^2 \left(\frac{\Omega_{n-1} t}{2}\right),
\]

where \( \rho_{nn}(0) = |C_n(0)|^2 \) is the probability of find \( n \) phonons in the initial instant, \( t = 0 \), and \( \Omega_n^2 = (\epsilon_1 - \epsilon_2 - \hbar \omega)^2 + 4 \lambda^2 (n+1) = \Delta^2 + 4 \lambda^2 (n+1) \).

Figure 2 shows the time evolution of level population for different number of phonons, \( n \). Increasing the number phonons the electron population per level oscillates more fast, thus the period diminishes.

3. Conclusiones

In spite of the recent theoretical and experimental efforts, the electronic conduction in the DNA is not understood well enough. It is important to analyze simple models in which possible mechanisms of conduction are found and in which the usual approaches could be successful. In this contribution we have proposed a simple model for the electronic conduction in a step of DNA stairs, made up of two nitrogenic bases. We find that electron conduction assisted by phonons is a possible mechanism by electron transfer through a DNA as molecular wire. We have also found fermion-boson entangles states as a consequence of electron-phonon coupling. These entanglement states can be used for quantum processing, where the phonons might be used as bus qubits.
4. Acknowledgements

This work was partially funded by Fundación para la Promoción de la Investigación y la Tecnología and DIB Universidad Nacional.

Referencias