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Thermo Electronic Properties of DNA Molecule as a Single Electron Transistor(SET)

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Abstract :

In this paper, a DNA molecule is modeled as a basis for studying the properties of a single electron transistor (SET). Solid binding model (SET) characterization and stationary-state equation are adopted to elucidate the electron transport properties through this model. In this work, a good pattern is presented for the calculation of curves (IV) for a single electron transistor and theoretical calculations for the drain current as a function of the source bank voltage and study the effect of heat and gate voltages on it. All calculations of this model are based on the transmittance spectrum. The results of the transmittance spectrum were calculated at equilibrium. The current was evaluated using the Landauers formula. Through the results obtained, it is clear that there is a mutual effect between the gate voltage and the source-drain voltage on the current of the source-drain. Also, there is a clear effect of the temperature of the electrodes on the values of the source-drain in all the studied cases. Through all these calculations of the DNA molecule the results were encouraging and gave the common features of SET. These results are very useful for getting closer and closer to the fabrication of nanoscale electronic parts.

Keyword: Drain current; Source-Drain Voltage ; The tight jointing prototype; Gate Voltage; (SET), DNA.

1. Introduction

Nanotechnology is a modern advanced technology for processing materials at the atomic, molecular, or ultra-molecular level, which is attracting increasing interest from all researchers and specialists in the field of nanotechnology with great support from the government and industries around the world, which gives a great opportunity to study modern advanced nanotechnologies such as carbon nanotubes and DNA at the nanoscale[1]. Transistors are the basic building block of modern electronic devices used to amplify or control electronic signals. Most common transistors have three terminals, two of which carry current from the source to the drain, and the third (gate or base) controls the current through the transport channel [2]. However, gold nanoelectrodes are not stable at room temperature [3]. During the discovery of single electron tunneling and coulomb blockade mechanism, many Researchers predicted that shrinking the dimensions of quantum dots to the nanometer range is quite possible to manufacture applicable sets [4]. A single electron transistor is a three–terminal single electron device which offers low power consumption and high operating speed in addition, as the size reaches nano, quantum mechanical effects come into action, which makes SET work more efficiently [5]. The applications of single electron transistor include switching devices, single electron memory, high-sensitivity electrometer, sensor, and single electron spectroscopy [6]. We present a design based on the permeability spectra to investigate the electronic and thermal properties of the SET. Analytical models in physics [7] and the main equation [8] solve this problem with a thorny manipulation that can calculate the tunnel capacitance and impedance [9]. These designs require impedance and tunnel capacitance as inputs, while the presented design depends on permeability spectrum as input. The permeability spectra provides important insights into the physics of nanoscaleregimes, especially about the density of states of nanoparticles. The pattern is easily altered by changing the contact coupling, the gate coupling and the density of states changes due to the change in the size of the nanoparticles. Relying on the permeability spectra the current is calculated using Landauersformularization.A single–electron transistor is an electronic device that works relying on a strange quantum phenomenon called quantum tunneling, as it exploits it to transport single electrons through a thin slice of insulating material, and the device work, as a switch that transfers between two states, cutting and passing, at the smallest level an available. When the voltage is applied if the change of voltage causes the charge change in the molecule to be less than one electron charge, then no current will pass until the voltage increases to cause a change in the electron charge. Therefore, the electronic current relationship is a nonlinear relationship. In order to improve the operating temperature of single–electron transistors, molecules must be less than 10 nanometers in size.

The SET pattern was designed theoretically, and its electronic properties and thermal effects were investigated. All theoretical calculations were carried out relying on the tight jointing pattern of the stability-status formula. Accordingly, the theoretical results of the drain current and its relationship to the source-drain voltage with the presence or absence of the gate voltage and the study of the heat effects on it, which clearly show the electronic properties of the Single Electron Transistor (SET), this study is useful for the manufacture of a single electron transistor in the nanoscale.

2. Theoretical treatment

In this theoretical treatment, the used pattern is the close link pattern of the stability-status formula, where the bridging regime is used, where the bridge here is the DNA molecule as a single scattering region. And taking into consideration the energy level of each DNA molecule and the coupling interaction between the molecules. The eigenvalues of SET were calculated using the relationship[10]:

$$\mathrm{E_j} = \mathrm{E_Q} - 2V_{mn}\cos\left(\frac{\pi \mathrm{j}}{\mathrm{N}+1}\right) + \sqrt{(V_{mn}\cos\left(\frac{\pi \mathrm{j}}{\mathrm{N}+1}\right))^2 + 2\mathrm{V}_{AT}^2} \qquad (1)$$

Where E_Q is the energy level of the molecule, V_{mn} is the coupling interaction between the nearest adjacent molecules, N stands for the total number of particles within one scattering region and V_{AT} is the Hydrogen bonds

between Adenine and Thymine molecules. Theoretical treatment for SET as a one-dimensional series, all connection between the sites of molecules means that there is a coupling interaction between them, those describe the regime under study (shown in Fig. (1)).

Fig.(1): Schematic diagram ofthe Single Electron Transistor(SET).

using the following time-reliant HamiltonianH_{am} (using Dirac symbols). This Hamiltonian gives all the interactions of the sub-regime, as shown below:

$$H_{am} = E_S|S\rangle\langle S| + E_{Dr}|Dr\rangle\langle Dr| + \sum_{k_{AT}} E_{k_{AT}}|k_{AT}\rangle\langle k_{AT}| + \sum_{k_{AT}}[(V_{Drk_{AT}}|Dr\rangle\langle k_{AT}| + h.c) + (V_{Sk_{AT}}|S\rangle\langle k_{AT}| + h.c)] + \sum_{k_L}(V_{Sk_{L1}}|S\rangle\langle k_{L1}| + h.c) + \sum_{k_R}(V_{Drk_{L2}}|Dr\rangle\langle k_{L2}| + h.c) \qquad (2)$$

Where the different symbols S, Dr, L1, L2, and AT denote the source, drain, wire one, wire two, and (Adenine/Thymine) molecules with a total number of N. The energy level $|i\rangle$ and $\langle i|$ are states of ket and bra, respectively. V_{ij} represents the interaction of the conjugation between the two sub-regime i and j, where the regime wave function can be written as,

$$\psi(t) = C_S(t)|S\rangle + C_{Dr}(t)|Dr\rangle + \sum_{k_{AT}} C_{k_{AT}}(t)|k_{AT}\rangle + \sum_{k_{L1}} C_{k_{L1}}(t)|k_{L1}\rangle + \sum_{k_{L2}} C_{k_{L2}}(t)|k_{L2}\rangle, \qquad (3)$$

where $C_i(t)$represent the coefficients of linear expansion. The equations of motion for $\mathrm{C_j(t)}$can be taken from the time reliant Schrödinger equation,

$$\frac{\partial\psi(t)}{\partial t} = -iH\psi(t). \qquad (4)$$

Then by substituting equations (2) and (3) in (4) we obtain,

$$\frac{\bar{C}_{Dr}(E)}{\bar{C}_S(E)} = \frac{X(E)}{Y(E)}, \qquad (5)$$

where,

$$X(E) = V^{DrAT}\,\Gamma_{AT}(E)V^{ATS}, \qquad (6)$$

$$Y(E) = E - E_{Dr} - \sum\nolimits_{DrL1}(E) - \sum\nolimits_{DrAT}(\mathrm{E}), \qquad (7)$$

here $\sum_{Dri}(E) = -i\Delta_{Dri}(E) + \Lambda_{Dri}(E)$, where $\Delta_{Dri}(E)$ is the broadening function, while $\Lambda_{Dri}(E)$ is the quantum shift, where $i = L1, AT$. Thusthe permeability capacity and the permeability probability are both determined by [11],

$$t_{SD}(E) = \frac{\bar{C}_{Dr}(E)}{\bar{C}_S(E)}, \qquad (8)$$

and ,

$$T_{SD}(E) = |t_{SD}(E)|^2. \qquad (9)$$

The current passing through the scattering region is calculated from the Landauerformularization[12],

$$I = \frac{2e}{h}\int_{-\infty}^{\infty} T(E)[f_{L1}(E) - f_{L2}(E)]dE, \qquad (10)$$

where $f_\alpha(E) = \{1 + \exp[E - \mu_\alpha/k_B Te_\alpha]\}^{-1}$ is Fermi distribution function of electrons in the lead$\alpha = L1, L2$. The chemical potential of the lead α is $\mu_\alpha$with$\mu_{L1} = -V_{DS}/2$ and $\mu_{L2} = +V_{DS}/2$ where V_{DS} is the drain-source voltage. The temperature Te_α of the lead α.

3. Resultsand Discussion

Starting to give the values of the variables in our calculations. V_{nm} coupling interaction between the nucleons of DNA with each other, $V_{BrS} = -0.5eV$ is coupling interaction between the bridge (DNA) with source,$V_{DrBr} = -0.9eV$ is coupling interaction between the bridge with the drain. The reaction of the source with the left wire is $V_{SL1} = V_{DrL2} = -4.0eV$, where V_{DrL2} is the coupling with the right wire. Fermi energy E_F balanced at zero. The energy levels of the molecules Thymine (T) and Adenine (A) are

4.16 eV and 3.26 eV respectively). The current is measured in units of (2e/h). The results obtained for the single electron transistor pattern can be divided as follows:

3.1. Permeability spectrum:

In Fig.(2), the permeability spectra from the single electron transistor pattern is shown for different values of V$_g$. The lowest unoccupied molecular levels (LUMO) are shown while the highest occupied molecular levels (HOMO) are not shown because they do not contribute to conduction in this case because they are well below the Fermi energy level (E_F= 0). Where we find that the permeability probability as a function of the energy spectra is greatly affected by the change in the gate voltage, as the permeability probability spectra shifts towards the higher energy spectrawhen the value of the gate voltage increases from negative to positive, and we also note that the value of the permeability probability increases with the increase in the value of the gate voltage from values negative towards positive values, where this is due to the fact that the HOMO levels are full of electrons, and the higher gate voltage values, which leads to an increase in the permeability probability, and vice versa, that is, applying a negative gate voltage leads to depletion of electrons in the LUMO levels, which leads to a decrease permeability.The gating effect can be better understood by looking at the distribution of unoccupied orbitals as shown in Fig.(2), the permeability spectra of the single electron transistor are above the Fermi level with gate voltage under the influence of five different gate voltages, +4, +2, 0, -2, -4 volts.Molecular orbitals are greatly affected by the different gate potentials. The molecular orbitals with the highest permeability probability, is ordinarily subject to the influence of gate voltages, i.e. push up with positive voltage and pull down with negative voltage.

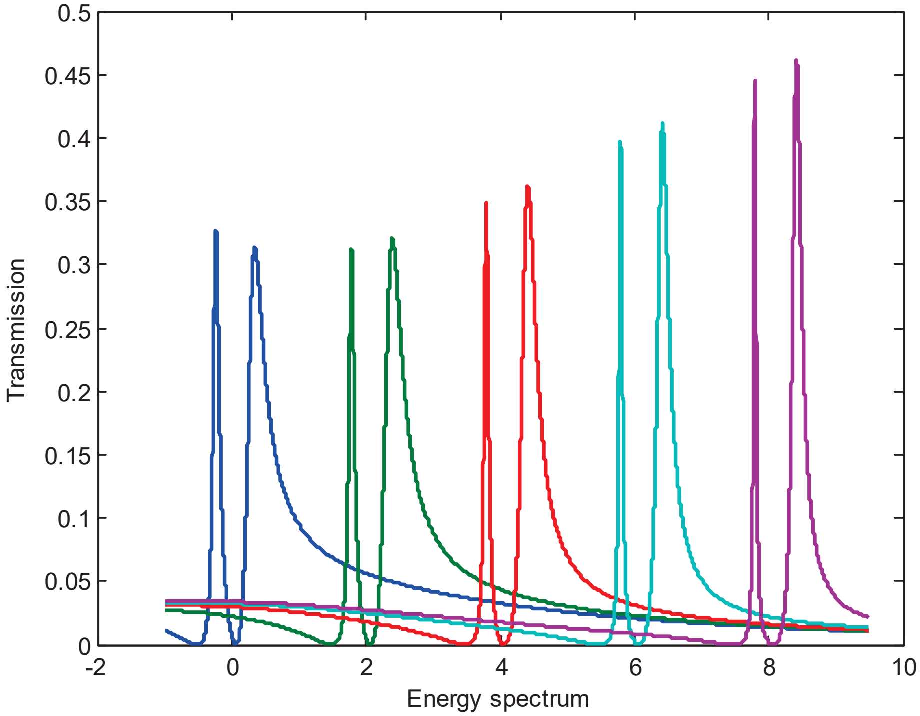

Fig.(2):The transmission as function of energy spectrum at gate voltage(V$_g$=-4eV(dark blue), -2eV(green), 0eV(red), +2eV(bright blue) and +4eV(violet).

3.2.Source-Drain current vs. Source-Drain Voltage:

3.2.1.Gate voltage effects

Transistors are three-terminal electronic devices wherethetransmission between the source and the drain is done by controlling the applied gate voltage (V_g). Electrostatic gates are considered to be orbital energy levels in molecular conductorssimilar to conventional field effect transistors. The experimental constructions of this device have an important goal at the level of nanoelectronics to make electronic devices smaller and smaller and to develop mechanisms for transporting charge at the molecular or atomic level. The tunneling current can be changed by changing the molecular energy levels of individual molecules by changing the gate voltage. The calculated (IV) Source-Drain curves are shown in Figs.((3) to (7)) where the gate bias (V_g) varies from -4 eV to 4 eV and the V_{sd} is tuned from -2 to 2 eV. The most important feature of the Isd-Vsd curves is the change of current by controlling the gate voltage. Gate-controlled molecular conduction is observed for the single electron transistor model. It can be noted here that the value of current in the single electron transistor model increases with increasing V_{sd} bias in the regime bias range from -2 to 2 eV. The effect of gate voltages (V_g) on the I_{sd}–V_{sd} curves is clearly observed in this low-bias regime. It is noted that the current intensity I_{sd} is related to Vsd in a non-linear relationship. that the value of current changes significantly more for the same V_{sd} with different values of gate voltages V_g in both positive and negative bias regimes. Under the influence of negative gate voltage values, charge transfer occurs through the metallic-molecular junction by a non-resonant tunneling process.Each curve in Figs. (3) to (7) shows that there is a region of low conductivity that is due to the source-drain biases, and then the absolute value of the source-drain current increases with the increase in the value of those biases, whether those values are negative or positive. The drop in conductivity at low bias voltages is a direct consequence of insufficient charge energy and is called a Coulomb blockade. The width of the Coulomb block changes relying on the change in gate voltages. Coulomb blockade is what characterizes the behavior of single electron transistors.The source-drain current threshold voltage for the source-drain voltage depends on the gate voltage (Coulomb the siege).When the gate voltage is applied, the operating state is faster. However, the on and off state of the device does not change monotonously with the change of the gate voltage, due to the inconsistency of the transfer coefficient around the theoretical value of the Fermi energy.From Figs.((3) to (7)) it was found that the value of (I_{sd}) current changes whenever the gate voltage values change in the negative direction so that the current value reaches the highest possible when the gate value reaches (-4) eV.

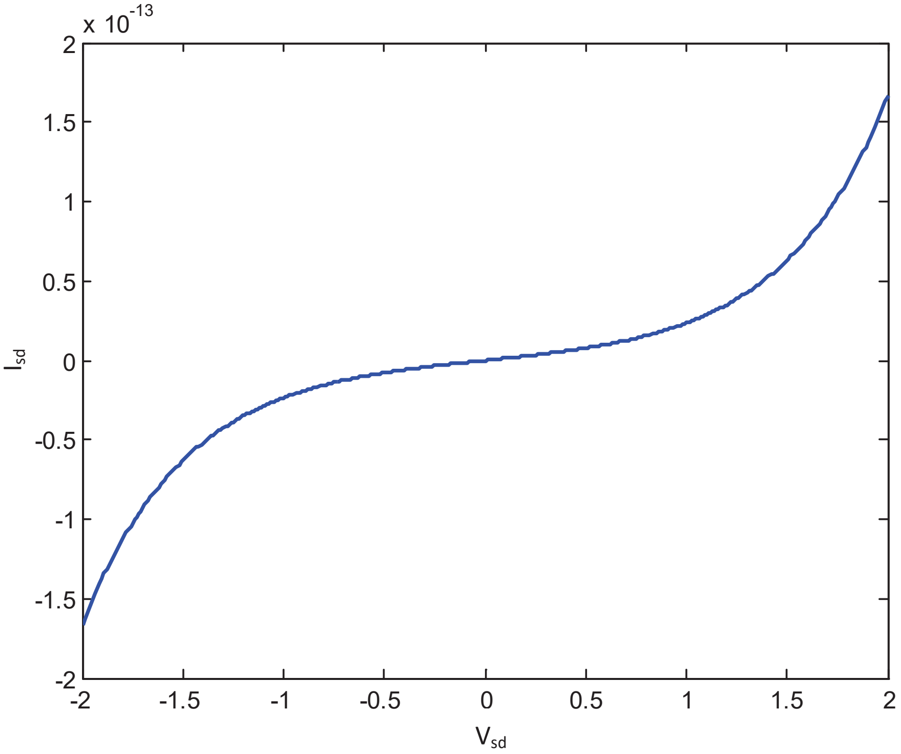

Fig.(3) The current source-drain as functions of the source-drain voltage of DNA molecule as single electron transistor with gate voltage($V_g = +4\ eV$) at temperature(300K).

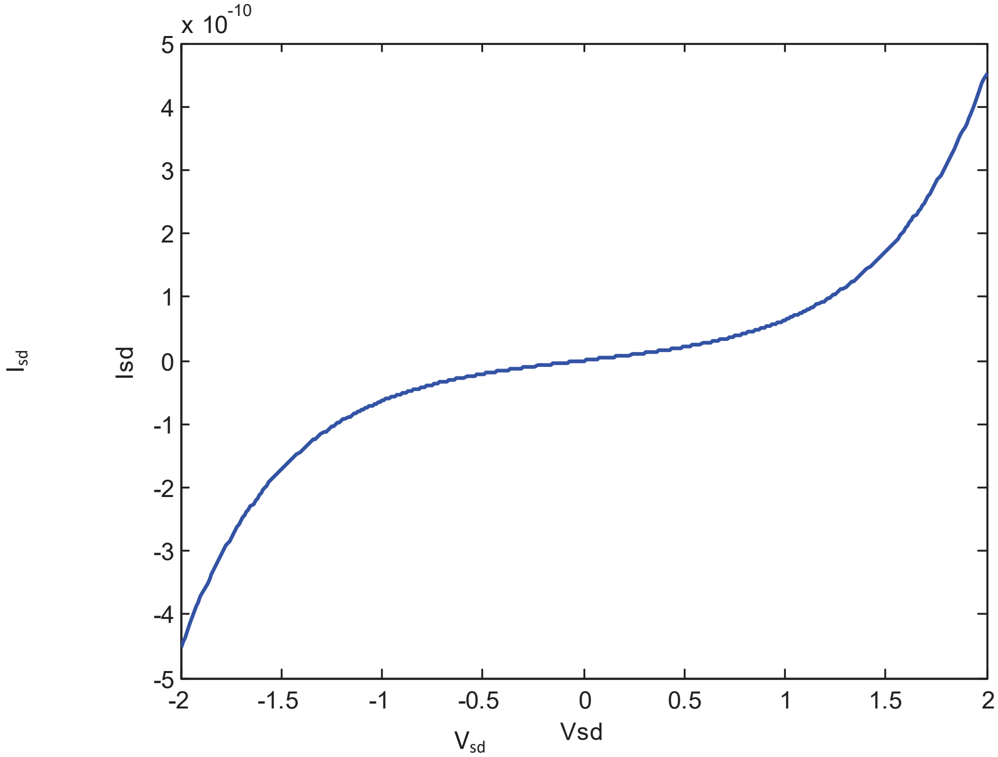

Fig.(4) The current source-drain as functions of the source-drain voltage of DNA molecule as single electron transistor with gate voltage($V_g = +2\ eV$) at temperature(300K).

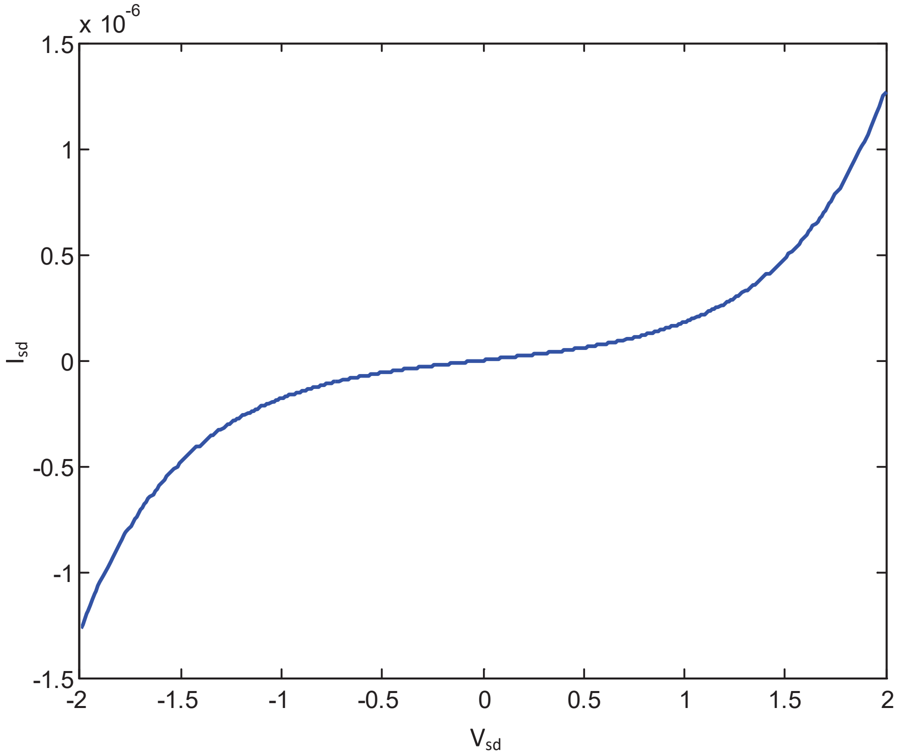

Fig. (5) The current source-drain as functions of the source-drain voltage of DNA molecule as single electron transistor with gate voltage($V_g = 0\ eV$) at temperature(300K).

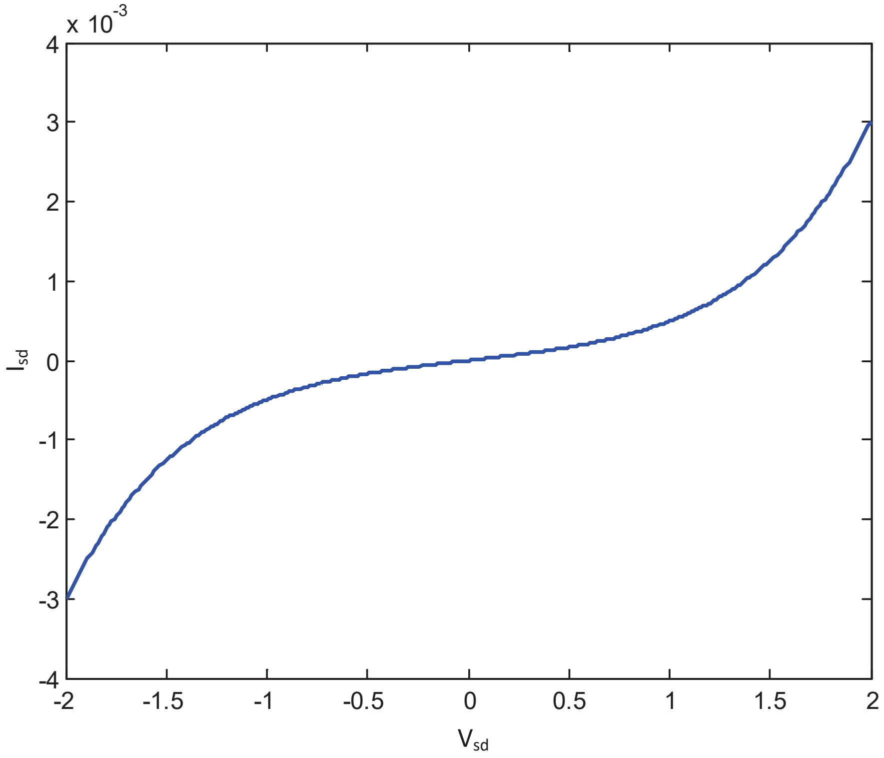

Fig. (6) The current source-drain as functions of the source-drain voltage of DNA molecule as single electron transistor with gate voltage($V_g = -2\ eV$) at temperature(300K).

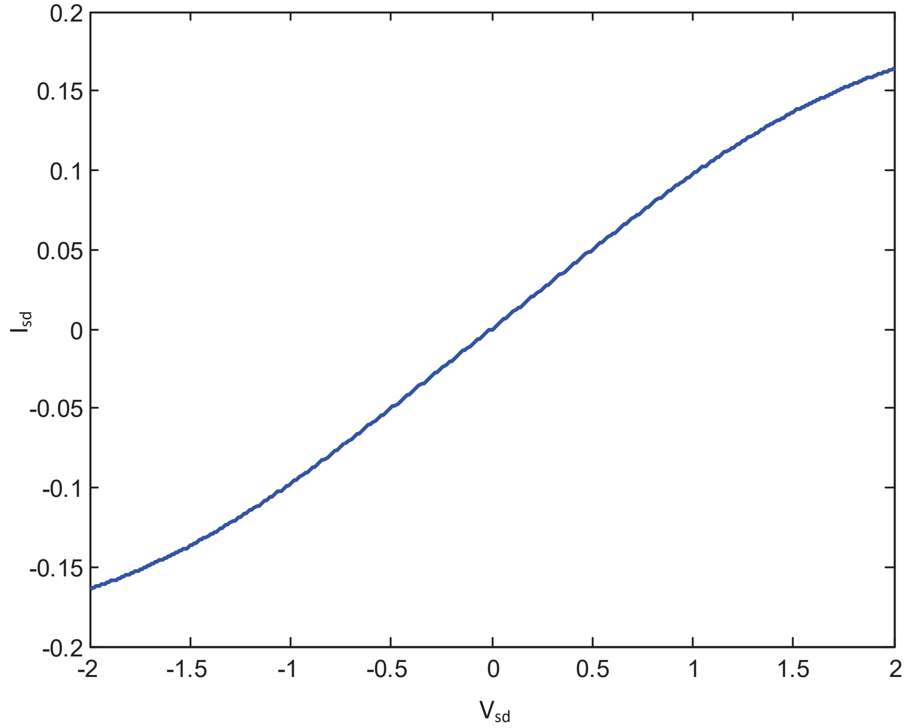

Fig.(7) The current source-drain as functions of the source-drain voltage of DNA molecule as single electron transistor with gate voltage($V_g = -4\ eV$) at temperature(300K).

3.2.2. Temperature effects:

Fig.(8) exhibited the estimation of the $(IV)_{sd}$-characteristics for V_g=-4 eV for an option of temperatures (5, 50 and 300) K. With increasing temperature the Coulomb blockade region shrinks until at about 300 K the Coulomb blockade is totally vanished and the IV characteristic gets approximately linear. Fig.(8) shows that the relationship between the drain current and the source-drain voltage is greatly affected by the change in temperature, as it was observed that the curves (IV) drain-source whose temperature is relatively low (5 and 50) K, we find that there is a gap In the (I V) curve, where it was found that the current values are close to zero in the region confined between (-0.2, +0.2) eV at the temperature 5K. So that this gap shrinks when the temperatures rise until it reaches (50) K, the value of this gap that is confined between (-0.09 and +0.09) eV is shrinking more , and when the temperatures continue to rise, this gap continues to shrink gradually until it completely disappears at a temperature (300) K, and the reason for this is due to the HOMO and LUMO levels, where the electrons in the molecular orbitals are of low energy at low temperatures so the electrons in the molecular levels need an occupation function or a threshold voltage to contribute to the formation or creation of the electric current between the source and the drain. The threshold voltage decreases with increasing temperature so that it completely vanishes at high temperatures (300) K, and this is due to the fact that the electrons have sufficient energy thermally so that when any bias voltage is applied to the source and drain sides, a current is generated directly.It was also observed from Fig.(8) that the (IV) curves for low values of temperatures (5 and 50) K have a non-linear relationship between them, and perhaps the reason for this is due to a state of imbalance with the surroundings, while at high temperatures (300) K it was observed that this the relationship is almost linear and the linear behavior of the system at high temperatures is attributed to the state of balance between the molecular system and the environment in which this molecular system resides. Accordingly, the behavior of the molecular system changes clearly and explicitly with the change of temperatures that affecting on this molecular system.

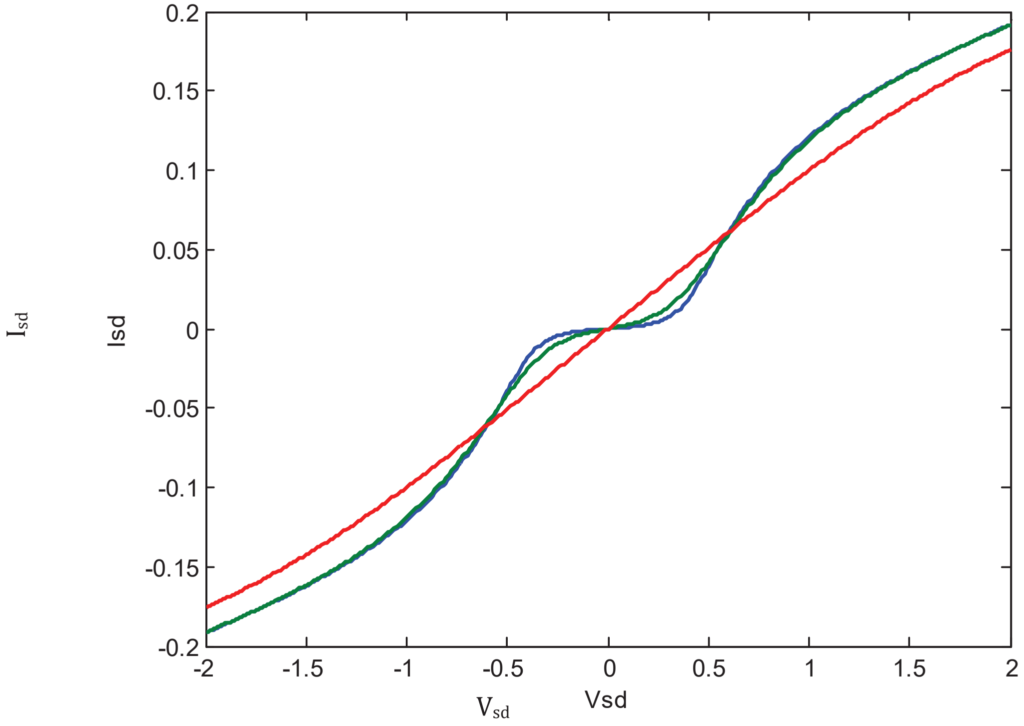

Fig. (8) The current source-drain as functions of the source-drain voltage of DNA molecule as single electron transistor with gate voltage($V_{\mathrm{g}} = -4\ eV$) at temperature(5K(blue), 50K(green) and 300K(red)).

3.3.Source-Drain current vs. Gate Voltage:

3.3.1. Source-Drain voltage effects:

It is a tremendous defiance to produce smallish single electron transistors as field effect transistors due to too arduous to a smallish pole of the molecule to the source-drain electrodes and to add a third gate on it to achieve the required gate field. They are used as an electrochemical gate to get a high gate field on a molecule lead to gold electrodes (source and drain) via gold-molecule nexus. In their putting up, the gate potential is applied between the source and a gate. I_{sd} during the molecule can be reflectable governed with a gate electrode over approximate ranks of the value of temperatures. Figs.((9) to (11)) illustrate the relationship between the source-drain current and the gate voltage values. It was found that the current values in the negative and positive directions are as high as possible at the highest values of the gate voltage in the negative direction and decrease dramatically and suddenly at the gate voltage values from the negative towards the positive little by little until it was approached a specific value, this value depends on the value of the source-drain voltage so that it increases for both the negative and positive sides and symmetrically with the increase in the absolute value of the source-drain voltage in the negative and positive directions. After this value, the value of the current begins to increase slowly as it was progressed from the negative values to the positive values of the gate voltage. After this value, the current is fixed and reaches the state of saturation, whereas the value of the gate voltage increases in the positive direction, the value of the source-drain current remains constant and does not change. Where the value of the saturation current relies largely on the value of the source-drain voltage, so that the higher value of the source-drain voltage for the negative and positive polarities gives the greater value of the saturation current for both the negative and positive sides, and this behavior is very similar to the behavior of the (FET) transistor in the case of pinch-off voltage. It was observed that both voltages (V_g and V_{sd}) have a major role in influencing on the values of the current (I_{sd}), but the effect of the gate voltage values on the current (I_{sd}) value begins to decrease as it has been progressed from the specific value of the gate voltage of the negative direction to the positive direction values to certain values that have not any an effect of the gate voltage on the source-drain current (I_{sd}). The reason for this is due to the effect of the gate voltage, as well as the source-drain voltage, on the molecular levels of the molecule, as well as on the electrodes, but when the gate voltage reaches a certain value, the electrons in the molecular levels reach a certain level so that the value of energy obtained by gate voltage for the electron is not sufficient to affect the increase in the number of electrons present in the LUMO region, and therefore the value of the current is stay fixed and is not affected after that by increasing the values of the gate voltage.It was noticed that the effect of temperature on the curves in Figs.((9) to (11)) is the occurrence of some ripples at low temperatures (5-50) K, but at high temperatures(300)K, these ripples disappear and fade completely. This can be explained by the effect of temperature on the electrodes, as well as the energy gap between the HOMO and LUMO levels.

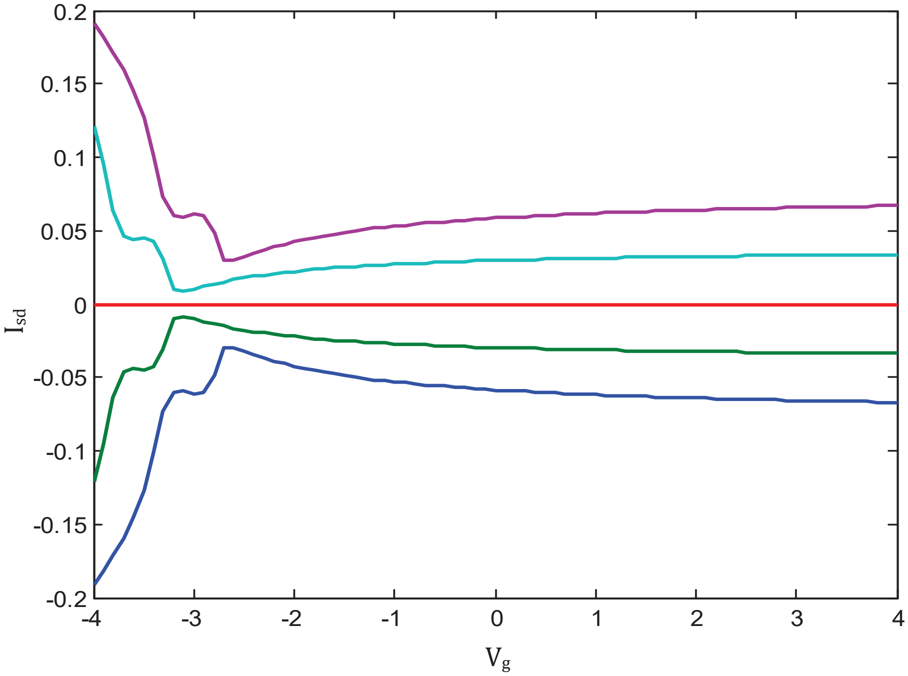

Fig. (9) The current source-drain as functions of the gate voltage of DNA molecule as single electron transistor at temperature (5K) with source-drain voltage(V_{sd}=-2 eV(dark blue), -1eV(green), 0 eV(red), 1eV(bright blue) and 2eV(violet)).

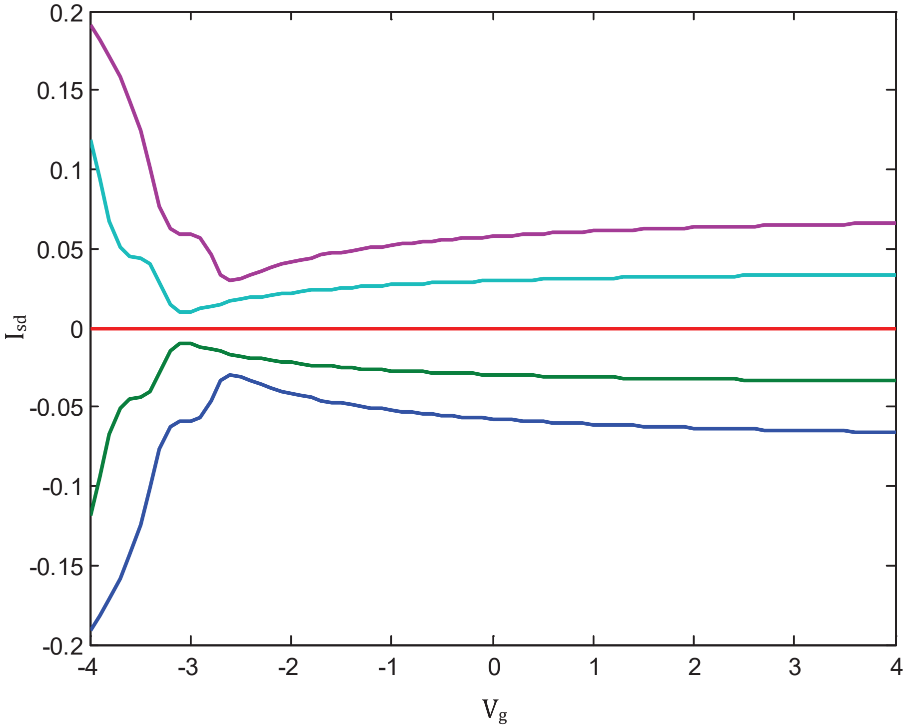

Fig. (10) The current source-drain as functions of the gate voltage of DNA molecule as single electron transistor at temperature (50K) with source-drain voltage(V_{sd}=-2 eV(dark blue), -1eV(green), 0 eV(red), 1eV(bright blue) and 2eV(violet)).

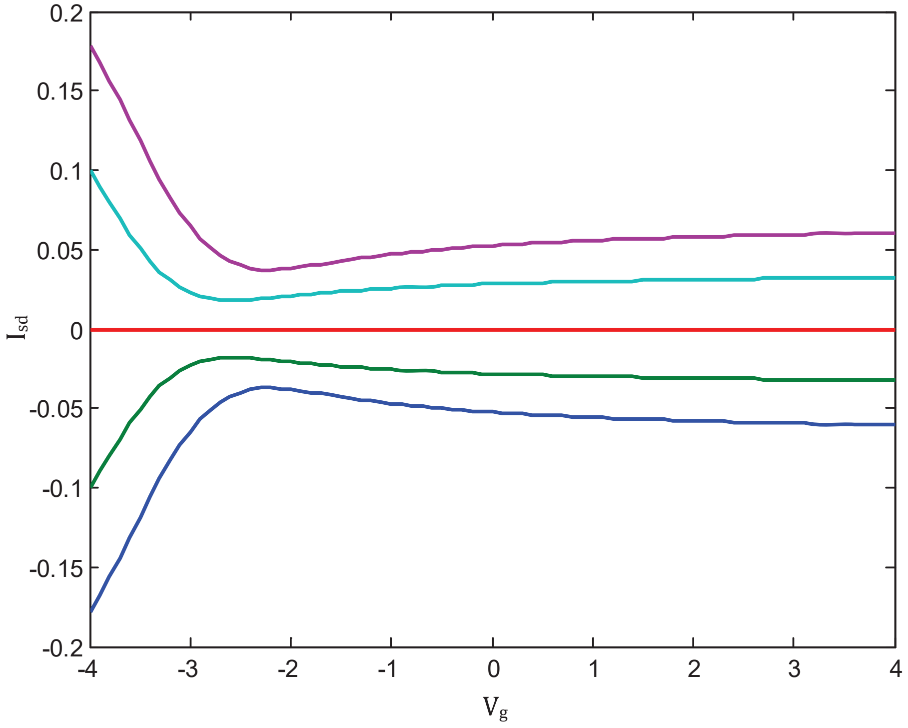

Fig. (11) The current source-drain as functions of the gate voltage of DNA molecule as single electron transistor at temperature (300K) with source-drain voltage(V_{sd}=-2 eV(dark blue), -1eV(green), 0 eV(red), 1eV(bright blue) and 2eV(violet)).

3.3.2. Temperature effects:

The source-drain current (I_{sd}) shows a non-stationary reliance on the gate voltage when the source drain voltage (V_{sd}) is set to (-2, -1, 0, 1 and 2) eV, see Figs.(12) to (16)) that the relation between the gate voltage and the source-drain current are also significantly replenished by the computations. To get a sense of this demeanor the permeability spectra of the device was plotted under the influence of gate voltage (-4, -2, 0, 2 and 4) eV respectively, with V_{sd} (-2, -1, 0, 1, and 2) eV, it should be noted indicates that the current flow at V_{sd} (-2, -1, 1 and 2) eV is determined by the tail of the conductive bands while at ($V_{sd} = 0$ eV) there is no current flow. At gate voltage $V_g = 4$ eV, the first conducting band is above the Fermi level. At $V_g = -4$eV, the first conductive band shifted to -0.5 eV and became much wider, see Fig.(7). The permeability density at a gate voltage of 4 eV increased in terms of value compared to the case of gate voltage $V_g = -4$ eV. This explains well the big gate effects illustrated in Figs. ((12) to (16). It is noted that between these two voltages, the energy shift of the orbitals, 8.5 eV on the scale of the energy spectra of the system, is much higher than the gate voltage increase of −4 eV, which indicates that the molecular orbitals are hugely affected by the electric field strength, rather than the voltage itself. By increasing the temperature the electrons tunneling increase to molecules but electrons accrual occurs in molecules, so electrons transport decrease, therefore the current decreases in the high temperature.Where it was found that the value of the saturation current of the source-drain current at low temperatures is higher than its value at high temperaturesfor the aforementioned reason. Also, the value of the saturation current of the source-drain current is greatly affected by the value of the voltage of the source-drain.The permeability density is confirmed under the action of the gate voltage close to resonant effects. The molecular orbitals are not linearly shifted with respect to the increase in the gate voltage, thus theoretical computations get very useful for cognizing the microscopic operation of a single electron transistor.

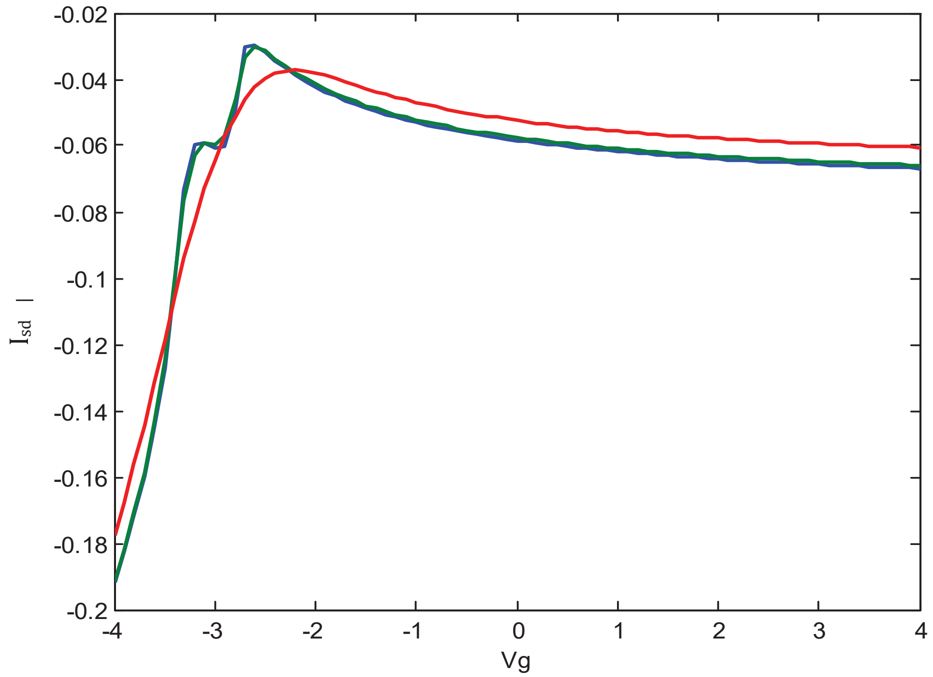

Fig. (12) The current source-drain as function he gate voltage of DNA molecule as single electron transistor at source-drain voltage($V_{sd} = -2\ eV$) with temp re(300K(red), 50K(green) and 5 K (blue)).

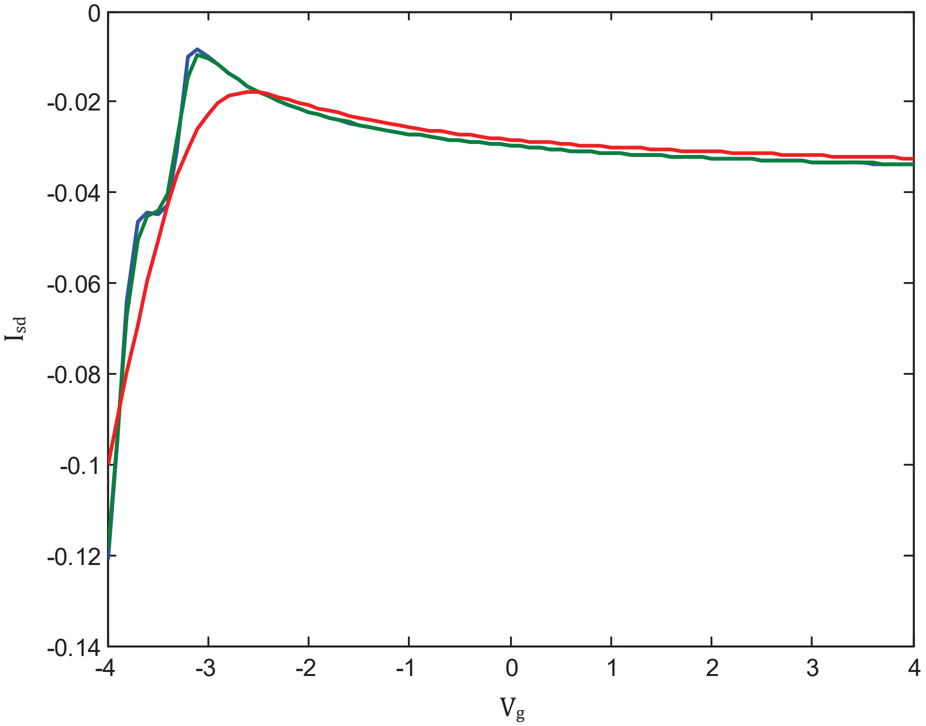

Fig. (13) The current source-drain as functions of the gate voltage of DNA molecule as single electron transistor at source-drain voltage($V_{sd} = -1\ eV$) with temperature(300K(red),50K(green) and 5 K (blue)).

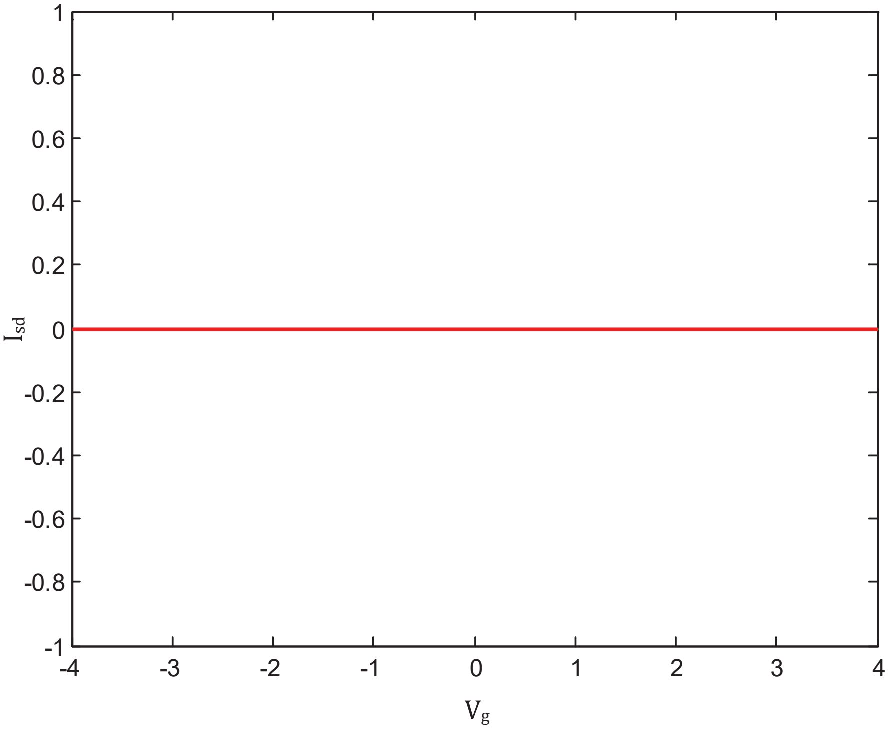

Fig. (14) The current source-drain as functions of the gate voltage of DNA molecule as single electron transistor at source-drain voltage($V_{sd} = 0\ eV$) without any effect of temperature(300K,50Kand 5 K) or gate voltage.

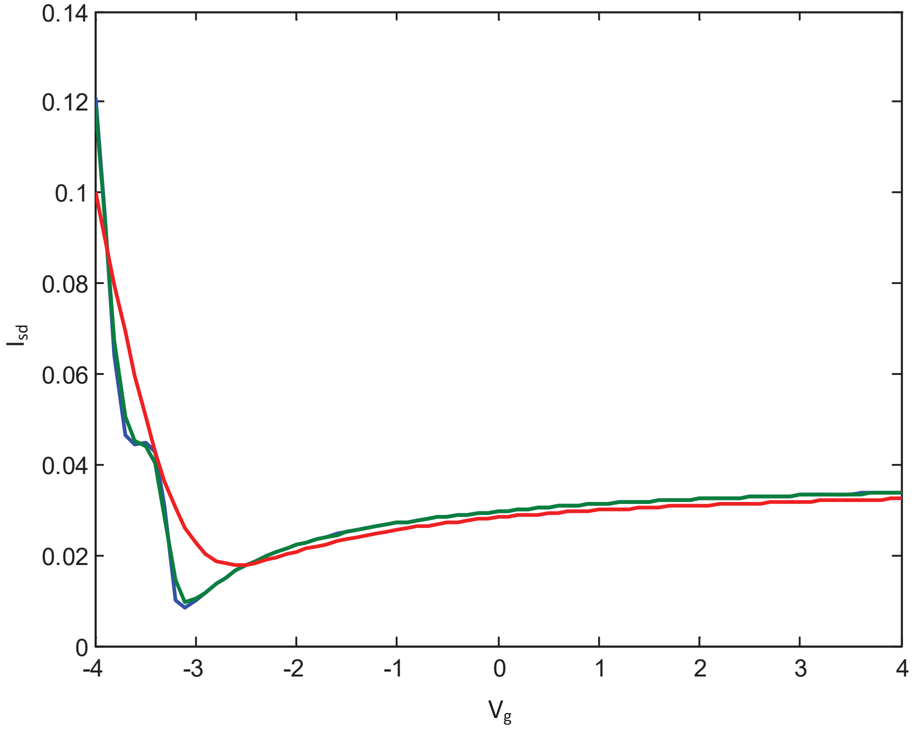

Fig. (15) The current source-drain as functions of the gate voltage of DNA molecule as single electron transistor at source-drain voltage($V_{sd} = +1\ eV$) with temperature(300K(red),50K(green) and 5 K (blue).

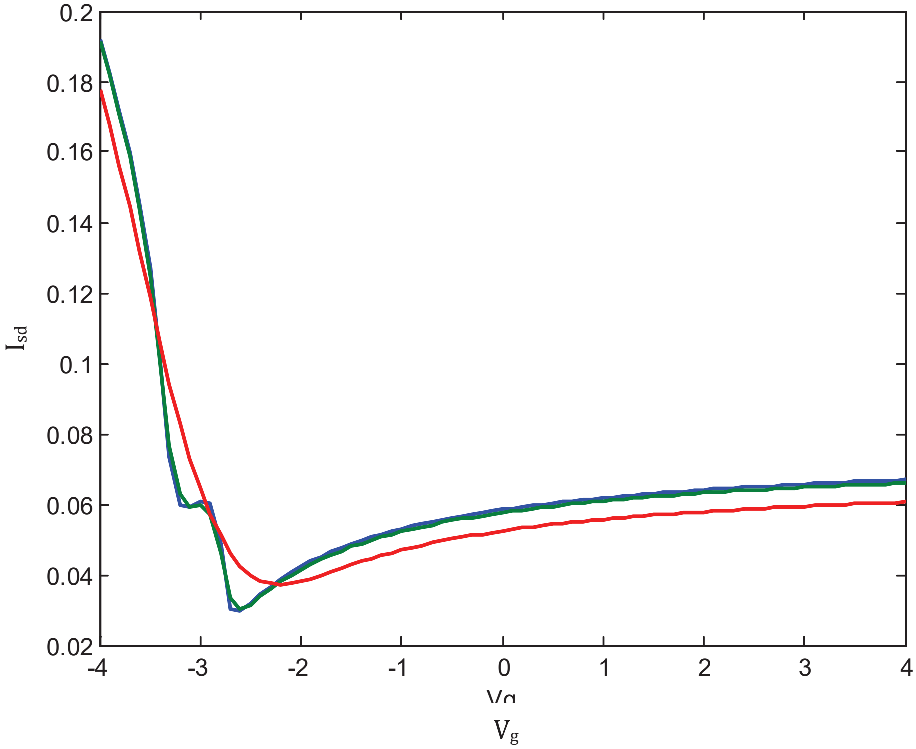

Fig. (16) The current source-drain as functions of the gate voltage of DNA molecule as single electron transistor at source-drain voltage($V_{sd} = +2\ eV$) with temperature(300K(red),50K(green) and 5 K (blue)

4. Conclusion

In this paper, a single electron transistor is presented and designed based on the placement of DNA molecules between source and drain. The effect of the gate voltage on the permeability spectrum of this system was studied, and it had a significant effect in shifting the permeability peaks towards positive regime power spectrum values, which had a pivotal role in controlling the electronic properties of the single electron transistor. Among these electronic properties are studied, source-drain (IV) curves for different gate voltages and at different temperatures. In addition to studying the source-drain current curves as a function of the gate voltage with different temperatures and source-drain voltages. It was found that the results of this pattern are in good agreement with the experimental data. Therefore, it must be taken into account that this pattern is useful in approaching more and more SET manufacturing with high flexibility.

5. Acknowledgements

Many thanks and gratitude to Dr. JenanMajeed Al Mukh and Dr. Shakir Ibrahim Issa from the College of Education for Pure Sciences at the University of Basra for their useful guidance and instructions. Thanks are also extended to the Ministry of Higher Education and Scientific Research for its support and encouragement of scientific research.

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