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Explanation of the Nano Quantum Electron Transport From Populated Occupied Higher Bound Energy States to Unoccupied Lower States

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Abstract: Maxwell's electric equation and Schrödinger quantum equation are used to find useful expressions for the probability of electrons existence and the electrons transport. The first expression which uses special relatively also shows that the probability of the electrons existence is higher for lower energy states compared to higher energy states where the probability is low. This means that electrons transport takes place from higher energy states to lower states. This conforms to the laws of chemistry where the atom tends to be stable by forcing electrons to occupy lower energy states. The second expression used the momentum velocity relation instead of special relatively. This expression shows also electrons transport from higher to lower states. It also shows that the probability of the electrons existence is higher for lower electrons density regions and lower for higher electrons density regions. This means that the electrons transport is from higher density regions to lower density regions. This conforms to the diffusion law.

Keywords: Maxwell's electric equation; Schrödinger equation; probability; transport; electron; energy states; diffusion; stable atom

1. Introduction:

Human needs for energy is one of the oldest known problems. Energy it is used for lighting, heating, cooking, and operating electric and electronic devices. It is also used for operating machines like factories, cars, trains and airplanes. The world energy demand is continuously increasing and the world power consumption, which is 13 terawatts (TW) currently, is expected to reach about 23 TW in 2050 [13]. The most popular energy sources are petroleum fuel and electric energy generated by the water falls [1,2].Despite the wide spread of using these sources, petroleum fuels were found to cause environmental pollution that is responsible for many severe diseases that are very dangerous for humans [1]. The electric energy generated by river waterfalls are not available everywhere. To solve the energy problem one needs pollution free energy source which is available everywhere. The most available energy source that satisfy the two requirements is the solar radiation energy [3].The most suitable energy from is the electric energy since it can be easily converted to other useful energy forms. Thus, one needs energy transducer that is capable of converting solar energy to electricity. Solar cells can convert solar energy into electric energy [4,5]. There are many types of cells fabricated from crystalline silicon, multi-crystalline, mono-crystalline, amorphous silicon [4, 5].The silicon solar cells till now are the most commercially available cells [6].They have long life and stability time which may extend some times to about 20 years. Despite these remarkable successes, solar cells suffer from many setbacks . Unfortunately, silicon solar cells have low efficiency, and high cost in addition to their complex fabrication processes [7]. This forces scientists to search for new alternatives to fabricate more efficient, low cost solar cells that can be easily fabricated. One of the most recently promising cells are the Nano solar cells [8, 9]. Nano solar cells can be fabricated from different Nano materials. Nano materials are the materials in the form of a large number of isolated particles having sizes in the range of 1up to 300 nm (1nm = 1 Nano meter =1/1000000000 m). These small particles cannot be described by classical laws but they obey quantum laws. Thus, their electrical and optical properties can be changed to satisfy the required needs by adjusting their particle size, geometry, orientation and structure [9]. Many types of Nano solar cells are now under development. These include polymers, while others can be fabricated using dyes, zinc or copper oxides [10,11,12].

The petroleum energy, which is now widely, used causes severe environmental pollution, which affects severely human health.

Owing to growing energy demand, exhaustion of oil resources, and global warming issues, there is a need for clean and renewable energy technologies. The other main energy sources like the electric energy generated by rivers are not available everywhere. The e silicon solar cells, which are commercially available, are expensive and have low efficiency, beside its complex fabrication processes. There are no well-known physical models that explain the behavior of Nano solar cells.

The aim of this work is to fabricate Nano solar cells using polymers and chemical beside natural dyes and explain their behavior using quantum Nano models.

Quantum Theoretical Explanation of the Electron Transport Trough Diffusion and From HoMo to LUMO.

Consider an electromagnetic wave having electric field E moving in a medium having magnetic permeabilityμ, electric permittivityε, and conductivityσ. The electric equation is given by:

$$-\nabla^2 E - \mu\varepsilon \frac{\partial^2 E}{\partial t^2} - \mu\sigma \frac{\partial E}{\partial t} = 0 \qquad (1)$$

This equation can be solved by using the conventional solution

$$E = E_0 e^{i(kx-wt)}$$

$$\partial E/\partial t = -iwE, \qquad \partial^2 E/\partial t^2 = +\omega^2 E \qquad \nabla^2 E = -k^2\psi \qquad (2)$$

A direct insertion of (2) in

$$k^2 + iw\mu\sigma - \mu\varepsilon\omega^2 = 0 \qquad (3)$$

The interaction of the wave with the medium by exchanging energy and momentum can be represented by expressing k and σ in

$$k = k_1 + ik_2 \qquad (4)$$

$$\sigma = \sigma_1 + i\sigma_2 \qquad (5)$$

A direct substitution of (4) and (5) in (3) gives

$$(k_1 + ik_2)^2 - i\omega\mu(\sigma_1 + i\sigma_2) - \mu\varepsilon\omega^2 = 0 \qquad (6)$$

Therefore

$$k_1^2 - k_2^2 + 2k_1k_2 i - i\omega\mu\sigma_1 + i\omega\mu\sigma_2 - \mu\varepsilon\omega^2 = 0 \qquad (7)$$

Equation (7) can simplified by beating mind that

$$\mu\varepsilon\omega^2 = \frac{\omega^2}{v^2} = k_1^2 = \left(\frac{2\pi}{\lambda}\right)^2 \qquad (8)$$

$$2k_1k_2 i - k_2^2 - \omega\mu\sigma_1 i + \omega\mu\sigma_2 = 0 \qquad (9)$$

Equating the real and imaginary part

$$k_2^2 = \omega\mu\sigma_2 \qquad (10)$$

$$2k_1k_2 = \omega\mu\sigma_1 \qquad (11)$$

Dividing (10) by (11) gives

$$\frac{k_2}{2k_1} = \frac{\sigma_2}{\sigma_1} \qquad (12)$$

$$k_2 = 2\frac{\sigma_2}{\sigma_1}k_1 \qquad (13)$$

For very small rest mass, the energy – momentum relativistic relation become,

$$E = Pc \qquad (14)$$

Using De Broglie hypothesis

$$P = \hbar k_1 = \frac{E}{c} \qquad (15)$$

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$$k_2 = \frac{2\sigma_2}{\hbar\sigma_1} P = \frac{2\sigma_2 E}{\hbar c\sigma_1} \quad (16)$$

$$-\frac{\hbar^2}{2m}\nabla^2\psi + V\,\psi = E\,\psi \quad (17)$$

For a particle moving in a uniform crystal field, the potential V is given by:

$$V = V_0 \quad (18)$$

$$-\frac{\hbar^2}{2m}\nabla^2\psi = (E - V_0)\psi = E_0\,\psi \quad (19)$$

Where

$$E_0 = E - V_0 \quad (20)$$

This equation can be solved by suggesting

$$\psi = Ae^{ikx}$$

$$\nabla^2\psi = -k^2\,\psi \quad (21)$$

Thus substituting (21) in (19) gives

$$\frac{\hbar^2 k^2}{2m}\psi = E_0\psi$$

$$\frac{\hbar^2 k^2}{2m} = E_0 \quad (22)$$

When absorption takes place according to optical theorem, the potential can describe it if it is in a complex form

$$V_0 = V_1 + iV_2 \quad (23)$$

In this case, equation (20) becomes

$$E_0 = E - V_1 - iV_2 \quad (24)$$

According to equation (4), (22) and (24)

$$(k_1 + ik_2)^2 = k^2 = \frac{2m}{\hbar^2}(E - V_1 + iV_2)$$

$$k_1^2 - k_2^2 + 2ik_1k_2 = \frac{2m}{\hbar^2}(E - V_1) - \frac{2im}{\hbar^2}V_2 \quad (25)$$

Equating real and imaginary parts

$$k_1^2 - k_2^2 = \frac{2m}{\hbar^2}(E - V_1) \quad (26)$$

$$k_1k_2 = -\frac{2m}{\hbar^2}V_2$$

$$V_2 = -\frac{k_1k_2}{2m\hbar^2} \quad (27)$$

According to equation (11), equation (27) gives

$$V_2 = -\frac{\omega\mu\sigma_1}{4m\hbar^2} \quad (28)$$

In view of equations (4), (15), (16) and (21) the wave function becomes

$$\psi = Ae^{ikx} = Ae^{-k_2x}e^{ik_1x}$$

$$\psi = Ae^{\frac{-2\sigma_2}{\hbar c\sigma_1}Ex}e^{ik_1x} \quad (29)$$

Thus, the probability to occupy energy E is given by

$$P_E = |\psi|^2 = A^2 e^{\frac{-4\sigma_2}{\hbar c\sigma_1}Ex} \quad (30)$$

For higher energy states $(E \to \infty)$

$$P_E = |\psi|^2 \to 0 \quad (31)$$

However, for lower energy states $(E \to 0)$the probability is maximum, where

$$P_E = |\psi|^2 \to |A|^2 \quad (32)$$

Thus, the electrons tend to occupy the lowest energy state where the probability is maximum. In other words, it tends to move from the higher occupied molecular states (HOMO) where the energy is higher and the probability of existence is lower to the lower unoccupied molecular state (LUMO) where the energy is low.

One can also use equation (11) to find another expression for ψ, where

$$k_2 = \frac{\omega\mu\sigma_1}{2k_1} = \frac{2\pi f\mu\sigma_1\lambda}{4\pi} = \frac{\mu\sigma_1}{2}f\lambda = \frac{\mu\sigma_1}{2}v \quad (33)$$

A summing that the velocity v of the wave is the same as that of the electron, one gets its momentum in the form

$$P = mv \quad (34)$$

Using relation

$$v = \frac{P}{m} = \frac{E}{mc} \quad (35)$$

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Thus equation (33) gives

$$k_2 = \frac{\mu \sigma_1 E}{2mc} \quad (36)$$

Thus according to equation (29)

$$\psi = Ae^{-k_2 x} e^{ik_1 x}$$

$$\psi = Ae^{\frac{-\mu \sigma_1}{2mc} Ex} e^{ik_1 x} \quad (37)$$

Thus, the transition probability is given by

$$P_E = |\psi|^2 = |A|^2 \, e^{\frac{-\mu \sigma_1}{mc} Ex} \quad (38)$$

In view of equations (30), (31) and (32) the electrons tend to move from higher levels HOMO to lower energy levels LUMO, let us now see what happen to occupied and non-occupied orbits. To do this one have to bear in mind that the orbital electrons contribute also to conductivity through the polarization term, where the application of an electric field causes atoms to be polarized. The electric dipole moment P_e is given by

$$P_e = enx = \chi E \quad (39)$$

Thus, the current generated due to the vibrating bounded atoms is given by

$$J = \frac{dP_e}{dt} = nev = \sigma E = -i\omega \, \chi E$$

$$= -i\omega(\chi_1 + i\chi_2)E = (-i\omega\chi_1 + \omega\chi_2)E \quad (40)$$

Hence

$$\sigma_1 = \omega\chi_2 \qquad \sigma_1 = -\omega\chi_1 \quad (41)$$

According to equations (40) and (41) the real conductivity σ_1 is proportional to the electrons density n. for non-occupied levels

$$n \to 0 \qquad P_E \to max \quad (42)$$

While for occupied level

$$n \to \infty \qquad P_E \to 0 \quad (43)$$

Since electrons tend to occupy levels with higher probability, thus they tend to move from highly populated levels having low probability to low populated levels having high probability to low populated levels having high probability. This can explain the hole transport as in Hubbard model where electrons moves from occupied bound energy states to unoccupied bound energy states.

2. Discussion:

Maxwell's electric equation (1-3) were used to relate the wave number K to the conductivity. The wave number and the conductivity are assumed to be complex as shown in equations (4)and (5).The imaginary part of K which is related to the absorption coefficient is expressed in terms of the real part in equation (13).Using special relativistic and quantum expressions for the momentum in equations (14)and (15) the imaginary part is expressed in term of the energy E in equation (16).This complex form of the wave number K is used in the solution of the Schrodinger quantum equation (21) for constant bulk matter internal field. This makes the probability exponentially energy dependent as shown by equation (30).According to the probability expression the electrons have higher probability to occupy lower states than higher ones as equations (31)and (32) indicates. This means that electrons transport takes place from higher states. This conforms with the fact that the atom prefer to be stable by forcing electrons to return to their ground states. The probability was found also by using the momentum velocity relation in equation (34).This makes the probability depending on the energy E and the density of electrons through the conductivity term as shown in equation (38).The probability expression indicates that the electrons transfer takes place from the higher level to the lower level as before. It also shows that electrons transport is from higher density regions where the probability is low to the lower density regions where the probability is higher as shown in equations (42)and (43).This result conforms with the diffusion law, where particles move from higher density to lower density regions.

3. Conclusion:

Using Maxwell's electric equation and assuming the wave number and the conductivity to be complex , then using special relatively a useful expression of the quantum probability was found using Schrodinger equation. This expression indicates that the electrons transport takes place from high to low energy states. This conforms with the laws of chemistry, where the atom tends to be stable by forcing electrons to occupy lower energy levels. Another useful expression for the probability was also obtained by using the momentum velocity relation. This expression shows that the electrons transport takes place from higher levels to lower ones. It also shows that the electrons transport is from higher density regions to lower density regions.

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