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Hypothetical Quantum Wire of Hydrogen

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Abstract: *A one dimensional quantum nano-wire of hydrogen is hypothetically demonstrated. This nanostructure device has been designed to perform at nanoscale with more efficiency than existing semiconductor based devices. Because this device is smaller and fabrication process is simpler, which are the primary requirements of semiconductor industry. The device has achieved a very flexible physical structure. A framework has been developed in this work that a device of completely non-metal element can behaves like a pure conductor depending on the atomic arrangement and a semiconductor without any significant dopant species presents. Basis function has been used as a computational tool for solving the Schrödinger's Equation for periodic solid composed of hydrogen. By using MATLAB we will produce the E(k)diagram which will give us the expected eigenvalues of the dispersion relation of the wires. A base calculation has been developed to calculate the bandstructure of a quantum wire.*

Keywords: *Dispersion relation, eigenvalues, tight-binding model, Quantum wire, wavefunction, hamiltonian matrix, dispersion relation, E-k diagram*

I. Introduction

Hypothetical quantum wire of hydrogen is a one dimensional device designed in nanometer scale. Our main purpose is to illustrate the procedure for calculating the bandstructure for quantum wire by using the 1D model concept of quantum wire. Electronic structure of the hydrogen wire is demonstrated where numerical solution has been preferred instead of analytical solution for the device. The wire is a one dimensional solid composed of N hydrogen atoms which are actually a lattice of finite range whose unit cell is consisting one atom each. In this structure electrons are free to move only in the x direction and confined in both y- and z-directions.[1] This type of atomic arrangement simply forms a quantum wire of hydrogen atoms. The bandstructure has been calculated by solving Hamiltonian matrix eigenvalue equation. Finite difference method followed to find the eigenvalues of the matrix.[2] In this paper we have developed a quantum wire to investigate its conducting properties with help of the E-k diagram. We have plotted the E-k diagram from dispersion relation which shows the eigenvalues by using MATLAB. The resulting bandstructures of the quantum wire of hydrogen atom and quantum wire of hydrogen dimer establish the solid-state like material property. A model structure for nano-wire transistor of quantum wire of hydrogen has been proposed in this research.

II. Device Structure

The Quantum wire of hydrogen atom is composed of repeating unit cell containing one Atom each. Consider each atom is separated by a lattice constant 'a'.[2] This nano wire is a single dimensional periodic arrangement of hydrogen atom. In this work, we have developed a hypothetical electronic structure of the quantum wire of hydrogen atom.

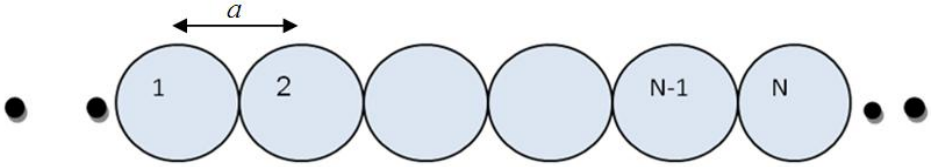

Fig. 1: A one dimensional array of hydrogen atoms

The wire is actually an array of hydrogen atoms and we have used periodic boundary conditions to make the calculation simple. For this one orbital per atom model we can write down a (N×N) Hamiltonian matrix by using 1st neighbor approximation [3]:

$$H = \begin{array}{c|cccccc} & 1 & 2 & \dots & N-1 & N \\ 1 & \varepsilon_0 & t_{ss} & & 0 & t_{ss} \\ 2 & t_{ss} & \varepsilon_0 & \dots & 0 & 0 \\ \vdots & & & & & \\ N-1 & 0 & 0 & \dots & \varepsilon_0 & t_{ss} \\ N & t_{ss} & 0 & \dots & t_{ss} & \varepsilon_0 \end{array} \quad (1)$$

In (1), ε_0 and t_{ss} are 1st and 2nd neighbor tight binding model parameter respectively. According to the periodic boundary condition (PBC) where we are assuming that the last point N is connected back to the first point 1, so that there are no ends. We can also say that the N^{th} atom warps around and overlaps the first atom as in a ring. This leads to non-zero values for the elements $H_{(1,N)}$ and $H_{(N,1)}$ which would normally be zero if the solid were abruptly truncated [2]. The PBC is usually not realistic, because real solids usually have "ends" where periodicity is lost. But if we are discussing the bulk properties of a large solid then the precise boundary condition at the surface does not matter [2].

III. Numerical solution for eigenvalues

To find the eigenvalues of the matrix [H] given in equation (3.4.1) numerically the finite difference method is used. Because of the periodicity in the electronic structure the matrix equation is E(ψ)=[H](ψ) consists of a set of N equations that are all identical in form and can be written as:[4]

$$E\psi_n = \varepsilon_0\psi_n + t_{ss}\psi_{n-1} + t_{ss}\psi_{n+1} \quad ; \text{unit cell, n=1,2,3,…,N} \quad (2)$$

This set of equations can be solved analytically by the wavefunction:

$$\psi_n = \psi_0 e^{ikna} \quad (3)$$

Now (2) can be written as:

$$E\psi_0 = \varepsilon_0\psi_0 + t_{ss}e^{-ika}\psi_0 + t_{ss}e^{ika}\psi_0$$

Thus finally got,

$$E = \varepsilon_0 + 2t_{ss}\cos(ka) \quad (4)$$

As we have found the eigenvalues from (4) so it can be written in form,

$$E_\alpha = \varepsilon_0 + 2t_{ss}\cos(k_\alpha a), \quad \text{(where α is an integer)} \quad (5)$$

This is the expected 1-D dispersion relation of quantum wire of hydrogen atoms, where k has only a finite number of allowed values equal to the number of unit cells in the solid.

IV. Analysis Of Dispersion Relation And E-K Diagram

Let's take a sample array of N=40 hydrogen atoms and by using the dispersion relation of equation (5) we can find the expected eigenvalues from an E-k diagram with help of MATLAB.

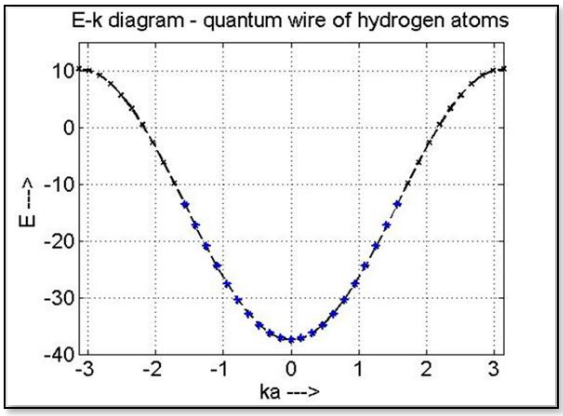

Fig. 2: Bandstructure of quantum wire of hydrogen atoms. The crosses denote the eigenvalues of the matrix [H] with N=40, where black ××× curve specify the conduction band and blue ××× curve specify valence band

The E-k diagram shows that the eigenvalue numbers are restricted to a finite number. This is a result of two factors. Firstly, the use of periodic boundary conditions is equivalent to envisioning the lattice to be in the form of a closed N-atom ring. So, for an N-atom ring with interatomic spacing a, so according to the Bloch theorem:

$$ka = \frac{2\pi\alpha}{N},\ \alpha = 0,\pm1,\pm2,.....,\pm\frac{N}{2}$$

Thus, for a finite solid k can only assume a set of discrete values and the total number of distinct k values is equal to N.

Secondly, values of ka differing by 2π do not represent distinct states on a discrete lattice.

From Fig. 2 we observed that the values of $k_\alpha a$ limited from $-\pi$ to $+\pi$ and are spaced by $2\pi/N$. In principle any range of the size 2π is acceptable, but it is common to restrict the values of $k_\alpha a$ to the range called first Brillouin zone. Black ××× curve represents the conduction band. It can be shown from the Fig. 2 that for the discrete lattice system, two and only distinct values of $k_\alpha a$ exist for each and every allowed values of E_α. In Fig. 2 where values of $k_\alpha a$limited from $-\frac{\pi}{2}$ to $\frac{+\pi}{2}$ and blue ××× curve represents the valance band. From E-k diagram we get the following energy states for conduction band.

Table 1: energy state values of conduction band

Values of $k_\alpha a$ $(-\pi \le ka < +\pi)$	Conduction band Energy(E_c)(eV)	Values of $k_\alpha a$ $(-\pi \le ka < +\pi)$	Conduction band Energy(E_c)(eV)
3.142	**10.26**	**2.356**	**3.272**
2.985	**9.966**	**2.199**	**0.4246**
2.827	**9.092**	**2.042**	**−2.768**
2.670	**7.659**	**1.885**	**−6.227**
2.513	**5.703**	**1.728**	**−9.867**
Interatomic distance a= $1 \times e^{-10}$			

From the E-k diagram we get the following energy states for valance band.

Table 2: energy state values of valance band

Values of $k_\alpha a$ $(-\pi/2 < ka < +\pi/2)$	Valance band Energy(E_v)(eV)	Values of $k_\alpha a$ $(-\pi/2 < ka < +\pi/2)$	Valance band Energy(E_v)(eV)
1.571	**−13.6**	**0.7854**	**−30.47**
1.414	**−17.33**	**0.6283**	**−32.9**
1.257	**−20.97**	**0.4712**	**−34.86**
1.1	**−24.43**	**0.3142**	**−36.29**
0.9425	**−27.62**	**0.1571**	**−37.17**
Interatomic distance a= $1 \times e^{-10}$			

V. Conductive properties of quantum wire

As we see from the E-k diagram Fig.2 is a bandstructure of 40 atoms hydrogen wire, where we got 40 energy states. Let's do a simple calculation. These 40 hydrogen atoms have total 40 valance electrons. It is easy to say that first 20 energy states are completely filled with 40 electrons and form the valance band, where two hydrogen atoms made a covalent bond. Other 20 energy states left empty and form the conduction band. Now as we see that bottom of the conduction band and top of the valance band overlaps which means that there is no energy band gap between two bands. This is similar to the bandstructure of a conductor.[5] So according to the conducting properties it is a metallic quantum wire.

VI. Conclusion

A hypothetical quantum wire of hydrogen has been developed. We have showed a numerical model for solving the one dimensional Schrödinger equation for the quantum wire of hydrogen by finite difference method using MATLAB. In order to obtain the numerical solution for the quantum wire of hydrogen we have taken into

account some assumptions as: the mass of an electron is very small compared to a proton, the nucleus is not moving and it's fixed at the center of the atom. No relativistic correction and Quantum Electrodynamic calculations were done in this work. The atomic orbitals can be used as a basis to write down a matrix representation for the Hamiltonian operator, which can then be diagonalized to find the energy eigenvalues.[6] This numerical model of solution can be used as a base calculation for any infinite periodic solid system to calculate the energy eigenvalues. An array of infinite periodic solid where atoms are spaced by equal distance from each other, acts like conductor, and we can say that an array of infinite periodic solid where pair of atoms [7] separated by an equal distance, would acts like a semiconductor. Based on this conception a one dimensional solid composed of N hydrogen dimer whose unit cell consists of two atoms can form quantum wire of hydrogen di-mer [8]. A hypothetical transistor of hydrogen can be developed by using these two types of hydrogen wires. [1] Such development will be done elsewhere in future. Results obtained from this atom model can be used to calculate the I/V characteristics of hydrogen wire and thereby very significant quantum phenomena such as quantum tunneling can be investigated.

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References

[1]. Colinge, Jean-Pierre; Lee, Chi-Woo; Afzalian. A; Akhavan, D, N; Yan. R; Ferain, Razavi. P; O'Neill. B; Blake. A; White. M; Kelleher. A. M.; McCarthy. B; and Murphy. R. Nanowire transistors without junctions, DOI: 10.1038/ NNANO.2010.15, 21 Feb 2010
[2]. Datta, S. Quantum Transport: Atom to Transistor. (Cambridge, Cambridge University Press, 2005).
[3]. Omar, Ali M. Elementary solid state physics. 4th edition. (Pearson Education India, 1999).
[4]. Bandstructure, in Datta, S. Quantum Transport: Atom to Transistor. (Cambridge, Cambridge University Press, 2005).
[5]. Beiser, Arthur. Concepts of modern physics. (Tata McGraw-Hill edition,2003)
[6]. Basis Functions, in Datta, S. Quantum Transport: Atom to Transistor. (Cambridge, Cambridge University Press, 2005).
[7]. Harker, A H. Physics and Astronomy. UCL. TIGHT BINDING MODEL.
[8]. Griffiths, David J. Introduction to Quantum Mechanics.(New Jersey, Prentice Hall,1995)