Journal of Atomic, Molecular, Condensate & Nano Physics
Vol. 1, No. 1, pp. 31–35, 2014
RGN Publications

http://www.rgnpublications.com

Effect of Magnetic Flux on the Quantum Transport in a Biphenyl Molecule

Research Article

Suman Dudeja[1], Aranya B. Bhattacherjee[2,*] and Narine Gevorgyan[3,4]

[1] *Department of Chemistry, ARSD College, University of Delhi* (*South Campus*), *New Delhi 110021, India*
[2] *Department of Physics, ARSD College, University of Delhi* (*South Campus*), *New Delhi 110021, India*
[3] *Institute for Physical Research, National Academy of Sciences, Ashtarak-2, 0203, Armenia*
[4] *The Abdus Salam International Centre for Theoretical Physics Strada Costiera, 11, I - 34151 Trieste, Italy*
***Corresponding author**: bhattach@arsd.du.ac.in

Abstract. We report influence of magnetic flux on the quantum transport in a aromatic π conjugate system made up of two phenyl rings separated by an insulator group. In the presence of a transverse magnetic field the transmission, the dipole moment and the energy of the system gives oscillatory behaviour with flux ϕ, threaded by the molecular ring showing flux quantum periodicity. This aspect may be utilized in designing nano-scale electronic devices.

Keywords. Quantum transpost; Biphenyl molecule; Magnetic flux

PACS. 73.23.-b; 73.63.Rt

Received: September 26, 2013 **Accepted:** November 13, 2013

1. Introduction

Electron transport in low-dimensional systems has drawn much attention in the field of theoretical as well as experimental research due to flourishing development in nanotechnology and nano-scale device modeling. Low dimensional model quantum systems are the basic building blocks for future generation of nano-electronic devices. Recent progress in experimental and theoretical techniques have triggered enormous possibilities of using organic molecules as a fundamental complement to silicon in semiconductors [1–3]. This has opened up possibilities of fabricating logical circuits at the single molecule level [4]. Such molecular state electronics requires the precise knowledge of electron transport in organic molecules. The finite size of atoms, molecules and clusters offers an advantage in designing tailor-made materials to

perform desired functions by exploiting the quantum mechanical phenomena of electrons in a confined space. Besides such exciting developments on the design and fabrication of molecular devices, experiments have been performed on the electrical properties of single molecules [5], and highly sophisticated simulation tools for charge transport through molecules have been developed [6–9]. Recently, using a single benzene molecule, the first molecular transistor was developed [10]. Several molecular device concepts are based on the existence of potential barriers within molecules, which prevent the free flow of electrons and thus create a tunable system [11–15]. Aviram and Ratner [16] proposed such a device in 1974 based on an organic molecule made of π-donor and π-acceptor moieties linked by a saturated spacer and sandwiched between two metallic electrodes. This concept has recently been verified experimentally [17]. The presence of potential barriers is essential also in devices which are closer to traditional electronic components.

In the present article we focus on the electron transport properties of a biphenyl molecule, where each benzene ring is threaded by a magnetic flux ϕ, the so-called Aharonov-Bohm (AB) flux. The molecular device under consideration is made up of two phenyl rings separated by an insulator group like $-CH_2-$. Quite interestingly we see that, keeping all the other parameters as invariant, the current amplitude across the molecule can be regulated very nicely simply by tuning the magnetic flux ϕ. Thus we can design an electronic circuit by using the biphenyl molecule and the electron transmission through the circuit can be regulated efficiently just by controlling the parameter ϕ. This phenomenon can be utilized in designing the future nano-electronic circuits. Here we provide a very simple analytical formulation of the transport problem through the biphenyl molecule using the tight-binding Hamiltonian and also treat the system numerically. The influence of magnetic flux on the transport properties of biphenyl and ring system has been studied theoretically in some recent works [18].

2. Analytical Model

Figure 1 shows the schematic representation of the system we are investigating here. Two phenyl rings are attached by an insulator X. Here X could be $-CH_2-$. The onsite energies of the left and the right phenyl ring is E_{-1} and E_{+1} respectively. The channel X has an extra potential U_o/a apart from the onsite energy E_o. The distance between the phenyl ring and X is a. Here t_o is the tunneling matrix element. $\psi_j(\psi_j^\dagger)$ corresponds to the creation (annihilation) operator of an electron at the site j. We now apply a magnetic field perpendicular to the plane of the molecule. This gives a phase factor to the tunneling. On going from the left phenyl ring to X, the e^- will pick up a phase $e^{-i\phi}$. As a result $t_o \to t_o e^{-i\phi}$ and when going from right to left $t_o \to t_o e^{i\phi}$. The phase factor $\phi = 2\pi\Phi/N$ is due to the magnetic flux Φ measured in the units of $\Phi_o = ch/e$, the elementary flux quantum. Here N corresponds to the total number of carbon-type sites in each benzene ring. The factor U_o appears due to the repulsive potential $U(z) = U_o\delta(z)$ at $z = 0$. The general Hamiltonian of the system for M sites is

$$H = \sum_j E_j \psi_j^\dagger \psi_j - t_o \sum_j \left[e^{i\phi} \psi_j^\dagger \psi_{j+1} + e^{-i\phi} \psi_{j+1}^\dagger \psi_j \right]. \tag{1}$$

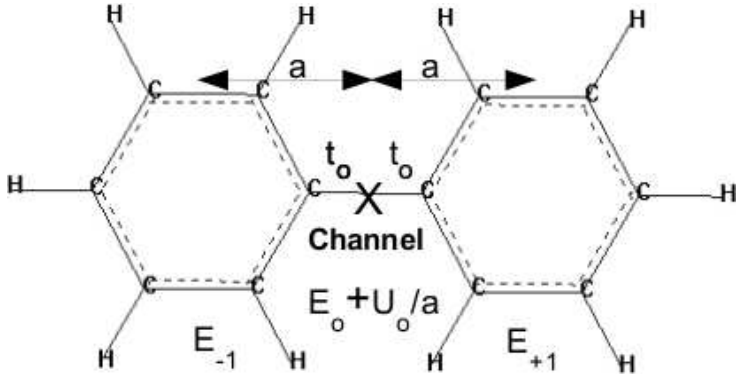

Figure 1. Schematic representation of the system we are investigating here. Two phenyl rings are attached by an insulator X. Here X could be $-CH_2-$. The onsite energies of the left and the right phenyl ring is E_{-1} and E_{+1} respectively. The channel X has an extra potential U_o/a apart from the onsite energy E_o. The distance between the phenyl ring and X is a. Here t_o is the tunneling matrix element.

The Heisenberg equation of motion for ψ is derived as $i\hbar\dot{\psi}_j = [\psi_j, H]$.

$$i\hbar\dot{\psi}_j = E_j\psi_j - t_o e^{i\phi}\psi_{j+1} - t_o e^{-i\phi}\psi_{j-1}. \tag{2}$$

This is the discrete lattice version. We now look for solution for the eigenvalue equation by substituting $\psi_j \to \psi_j e^{-iEt/\hbar}$. This yields for $j = 0$

$$E\psi_0 = [E_0 + U_0/a]\psi_0 - t_0 e^{i\phi}\psi_{+1} - t_0 e^{-i\phi}\psi_{-1}. \tag{3}$$

We choose $\psi_0 = 1 + r = t$, $\psi_{+1} = te^{ika}$ and $\psi_{-1} = e^{-ika} + re^{ika}$.
So that $\psi_{+1} = \psi_0 e^{ika}$, $\psi_{-1} = \psi_0 e^{ika} - 2i\sin ka$.
This gives

$$\left[E - E_0 - \frac{U_0}{a} + 2t_0 e^{ika}\cos\phi\right]\psi_0 = 2it_0 e^{-i\phi}\sin ka. \tag{4}$$

The dispersion relation is

$$E = E_0 - 2t_0\cos ka + \phi. \tag{5}$$

The transmission function $T = |\psi_0|^2$ is derived as:

$$T = \frac{E'^2}{U_0^2 + E'^2 - 2U_0\sin\phi}. \tag{6}$$

Where $E' = 2at_0\sin ka$. A plot of the transmission function T of eqn. (6) as a function of the phase ϕ is shown in Figure 2. When the electron waves passes through different paths of the given molecular system, destructive and constructive interference takes place leading to stronger or weaker transmission probability across the molecule. Applying the magnetic flux, the interference condition of the electron waves among the different pathways can be controlled, and accordingly the transmission spectrum gets modified. Consequently, the transmission probability oscillates with the magnetic phase ϕ with a periodicity of 2π. Thus the quantum interference effect plays an important role in the study of the electron transport in molecular electronics.

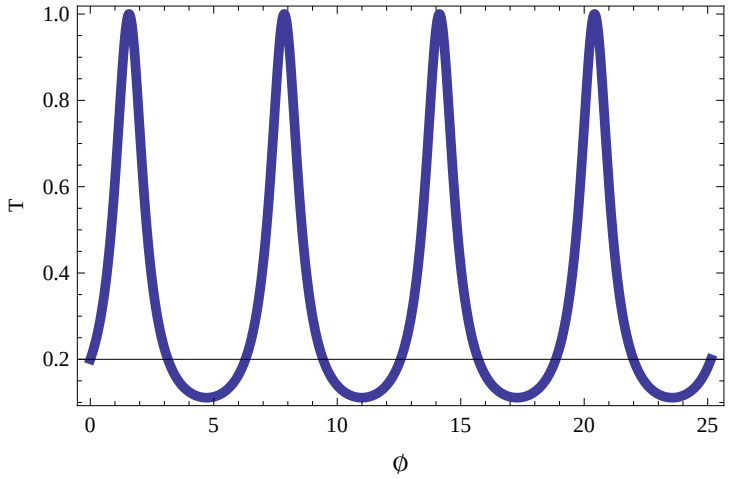

Figure 2. A plot of the transmission function T of eqn. (6) as a function of the phase ϕ.

3. Numerical Results

All calculations were performed using HYPERCHEM 7.0 software. To obtain good starting geometries, the initial configurations were optimized at the Hartree-Fock (HF) level. The density functional theory (DFT) method was used on the optimized geometries obtained from HF calculations. We have used the $6-31G^*$ basis and hybrid functional $B3PW91$, which combines the Becke exchange (B) functional, and the Perdew-Wang-91 correlation functional, both of which are nonlocal generalized gradient-approximated functionals. Note that for each value of magnetic field used, we have optimized the geometry of the molecules before calculating the energy levels and the spatial structure of the energy levels. We found that there was no appreciable change in the bond length and the bond angles in the presence of the magnetic fields used in this study compared to the zero field case. Absence of appreciable geometry change in the presence of magnetic field is also a good indicator of the stability of the molecule to external perturbation.

We particularly focus on two physical parameters, dipole moment along the long axis of the molecule μ_X (in atomic units) and the energy gap ΔE (in electron volts) as a function of the magnetic field (B_Z) (in atomic units). As expected oscillations in μ_X and ΔE as a function of B_Z is observed in Figure 3.

4. Conclusions

In conclusion, we have used an analytical approach based on the tight binding model and numerical approach to investigate the electron transport properties of a molecular system consisting of two phenyl rings connected by an insulating spacer in the presence of a transverse magnetic field. In particular, we have shown that the transmission coefficient, the electric dipole moment and the band gap shows oscillatory behaviour as the magnetic field/flux changes.Our results indicate that the conduction property of the molecule can be regulated by controlling the magnetic flux. This aspect maybe utilized in designing a tailor made nano-scale electronic device.

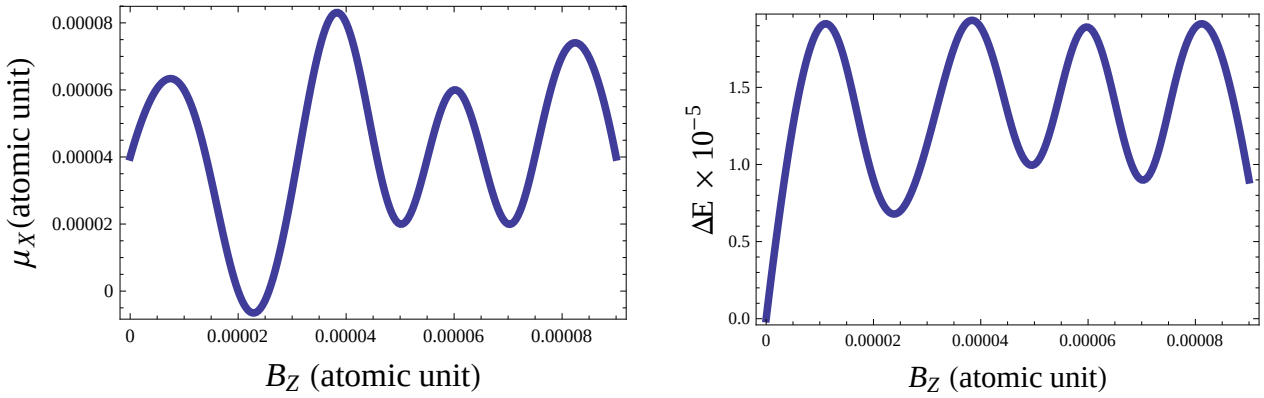

Figure 3. Dipole moment μ_X and energy band gap ΔE as a function of the applied magnetic field B_Z.

Acknowledgements

Suman Dudeja thanks the University Grants Commission, New Delhi for the financial support for carrying out this work under grant number 8-1(203)/(MRP/NRCB). Narine Gevorgyan thanks the Abdus Salam ICTP, Trieste, Italy for the facilities under the Junior Associateship Programme.

References

[1] L.A. Bumm *et al.*, Science **271**, 1705 (1996).

[2] L. Jones *et al.*, J. Org. Chem. **62**, 1388 (1997).

[3] M.A. Reed *et al.*, Science **278**, 252 (1997).

[4] R. Wu *et al.*, J. Org. Chem. **61**, 6906 (1997).

[5] C. Kergueris *et al.*, Phys. Rev. B **59**, 12505 (1999).

[6] M. Brandbyge *et al.*, Mater. Res. Soc. Symp. **636**, D9.25 (2000).

[7] M. Di Ventra *et al.*, Phys. Rev. Lett. **84**, 979 2000.

[8] P.S. Damle *et al.*, Phys. Rev. B **64**, 201403 (2001).

[9] J. Taylor *et al.*, Phys. Rev. Lett. **63**, 245407 (2001).

[10] H. Song, Y. Kim, Y.H. Jang, H. Jeong, M.A. Reed and T. Lee, Nature **462**, 1039 (2009),

[11] J.M. Seminario *et al.*, J. Am. Chem. Soc. **120**, 3970 (1998).

[12] J.M. Seminario *et al.*, J. Am. Chem. Soc. **122**, 3015 (2000).

[13] Y. Karzazi *et al.*, Nanotechnology **13**, 336 (2002).

[14] C. Majumder *et al.*, Jpn. J. Appl. Phys. **41**, 2770 (2002).

[15] M. Girlanda and M. Macucci, J. Phys. Chem A **107**, 706 (2003).

[16] A. Aviram and M.A. Ratner, Chem. Phys. Lett. **29**, 277 (1974).

[17] R.M. Metzger *et al.*, J. Am. Chem. Soc. **119**, 10455 (1997).

[18] S.K. Maiti, Chemical Physics **331**, 254 (2007), arXiv:0908.2884.