NAND gate response in a mesoscopic ring: an exact result

Santanu K Maiti\textsuperscript{1,2}

\textsuperscript{1} Theoretical Condensed Matter Physics Division, Saha Institute of Nuclear Physics, 1/AF, Bidhannagar, Kolkata-700 064, India
\textsuperscript{2} Department of Physics, Narasinha Dutt College, 129, Belilious Road, Howrah-711 101, India

E-mail: santanu.maiti@saha.ac.in

Received 10 April 2009
Accepted for publication 2 October 2009
Published 4 November 2009

Abstract

NAND gate response in a mesoscopic ring threaded with a magnetic flux $\phi$ is investigated by using Green’s function formalism. The ring is attached symmetrically to two semi-infinite one-dimensional metallic electrodes and two gate voltages, namely, $V_a$ and $V_b$, are applied in one arm of the ring, these are treated as the two inputs of the NAND gate. We use a simple tight-binding model to describe the system and numerically compute the conductance–energy and current–voltage characteristics as functions of the gate voltages, ring-to-electrode coupling strength and magnetic flux. Our theoretical study shows that, for $\phi = \phi_0/2$ ($\phi_0 = ch/e$, the elementary flux quantum) a high output current (1) (in the logical sense) appears if one or both the inputs to the gate are low (0), while if both the inputs to the gate are high (1), a low output current (0) appears. It clearly exhibits the NAND gate behavior and this feature may be utilized in designing an electronic logic gate.

PACS numbers: 73.23.–b, 73.63.Rt

(Some figures in this article are in colour only in the electronic version.)

1. Introduction

Electronic transport in quantum confined geometries has attracted much attention since these simple looking systems are promising building blocks for designing nanodevices especially in electronic as well as spintronic engineering. A mesoscopic metallic ring is one such promising example where electronic motion is restricted. The recent progress in nanoscience and technology has allowed us to investigate the electron transport through a mesoscopic ring in a very tunable way. Using a mesoscopic ring we can make a device that can act as a logic gate, which may be used in nanoelectronic circuits. To explore this phenomenon we design a bridge system where the ring is attached to two external electrodes, the so-called electrode–ring–electrode bridge. The ring is then subjected to a magnetic flux $\phi$, the so-called Aharonov–Bohm (AB) flux, which is the key controlling factor for the whole logical operation in this particular geometry. The theoretical description of electron transport in a bridge system made much progress following the pioneering work of Aviram and Ratner [1].

Later, many excellent experiments [2–4] have been done in several bridge systems to understand the basic mechanisms underlying the electron transport. Although in the literature both theoretical [5–13] as well as experimental [2–4] works on electron transport are available, yet a lot of controversies are still present between the theory and experiment, and the complete knowledge of the conduction mechanism in this scale is not very well established even today. The interface geometry between the ring and the electrodes significantly controls the electronic transport in the ring. By changing the geometry, one can tune the transmission probability of an electron across the ring which is solely due to the effect of quantum interference among the electronic waves passing through different arms of the ring. Furthermore, the electron transport in the ring can be modulated in another way by tuning the magnetic flux, that threads the ring. The AB flux threading the ring may change the phases of the wave functions propagating along the different arms of the ring leading to constructive or destructive interferences, and therefore, the transmission amplitude changes [14–18]. Besides these factors, ring-to-electrode coupling is another
important issue that controls the electron transport in a meaningful way [18]. All these are key factors, which regulate the electron transmission in the electrode–ring–electrode bridge system and these effects have to be taken into account properly to reveal the transport mechanisms.

The main focus of the present work is to describe the NAND gate response in a mesoscopic ring threaded by a magnetic flux. The ring is contacted symmetrically to the electrodes, and the two gate voltages $V_a$ and $V_b$ are applied in one arm of the ring (see figure 1); these are treated as the two inputs of the NAND gate. A simple tight-binding model is used to describe the system and all the calculations are done numerically. Here, we address the NAND gate behavior by studying the conductance–energy and current–voltage ($I$–$V$) characteristics as functions of the ring–electrodes coupling strengths, magnetic flux and gate voltages. Our study reveals that for a particular value of the magnetic flux, $\phi = \phi_0/2$, a high output current (1) (in the logical sense) is available if one or both the inputs to the gate are low (0), while if both the inputs to the gate are high (1), a low output current (0) appears. This phenomenon clearly shows the NAND gate behavior. To the best of our knowledge the NAND gate response in such a simple system has yet not been addressed in the literature.

The scheme of the paper is as follows. Following the introduction (section 1), in section 2, we describe the model and the theoretical formulations for the calculation. Section 3 explores the results, and finally, we conclude our study in section 4.

2. Model and synopsis of the theoretical background

Let us begin by referring to figure 1. A mesoscopic ring, threaded by a magnetic flux $\phi$, is attached symmetrically (upper and lower arms have equal number of lattice points) to two semi-infinite one-dimensional (1D) metallic electrodes. The atoms $a$ and $b$ in the upper arm of the ring are subjected to the gate voltages $V_a$ and $V_b$, respectively; these are treated as the two inputs of the NAND gate. On the other hand, two additional voltages $V_a$ and $V_b$ are applied in the atoms $a$ and $b$, respectively, in the lower arm of the ring.

At very low temperature and bias voltage the conductance $g$ of the ring can be expressed from the Landauer conductance formula $[19, 20],$

$$g = \frac{2e^2}{h} T,$$

(1)

where $T$ gives the transmission probability of an electron across the ring. This ($T$) can be represented in terms of the Green’s function of the ring and its coupling to the two electrodes by the relation $[19, 20],$

$$T = \text{Tr} \left[ \Gamma_S G_R \Gamma_D G_D^a \right]$$

(2)

where $G_R$ and $G_D$ are, respectively, the retarded and advanced Green’s functions of the ring including the effects of the electrodes. Here, $\Gamma_S$ and $\Gamma_D$ describe the coupling of the ring to the source and drain, respectively. For the complete system, i.e. the ring, source and drain, the Green’s function is defined as

$$G = (E - H)^{-1},$$

(3)

where $E$ is the injecting energy of the source electron. To evaluate this Green’s function, the inversion of an infinite matrix is needed since the complete system consists of the finite ring and the two semi-infinite electrodes. However, the entire system can be partitioned into submatrices corresponding to the individual subsystems and the Green’s function for the ring can be effectively written as

$$G_R = (E - H_R - \Sigma_S - \Sigma_D)^{-1}$$

(4)

where $H_R$ is the Hamiltonian of the ring that can be expressed within the non-interacting picture as

$$H_R = \sum_i (\epsilon_i + V_a \delta_{ia} + V_b \delta_{ib} + V_a \delta_{ia} + V_b \delta_{ib})$$

$$+ \sum_{ij} t (c_i^c c_j + h.c.).$$

(5)

In this Hamiltonian $\epsilon_i$’s are the site energies for all the sites $i$ except the sites $i = a, b, \alpha$ and $\beta$, where the gate voltages $V_a$, $V_b$, $V_a$ and $V_b$ are applied; these are variable. These gate voltages can be incorporated through the site energies as expressed in the above Hamiltonian. $c_i$ ($c_i^c$) is the creation (annihilation) operator of an electron at the site $i$ and $t$ is the nearest-neighbor hopping integral. The phase factor $\theta = 2\pi \phi / N \phi_0$ is due to the flux $\phi$ threaded by the ring, where $N$ corresponds to the total number of atomic sites in the ring. In equation (4), $\Sigma_S = h_{SR} g_{SR} h_{SR}$ and $\Sigma_D = h_{DR} g_{DR} h_{TR}$ are the self-energy operators due to the two electrodes, where $g_{SR}$ and $g_{DR}$ are the Green’s functions for the source and drain, respectively. $h_{SR}$ and $h_{TR}$ are the coupling matrices and they will be nonzero only for the adjacent points of the ring and the electrodes as shown in figure 1. The coupling terms $\Gamma_S$ and $\Gamma_D$ for the ring can be calculated through the expression $[19, 21],$

$$\Gamma_S (D) = \text{Tr} \left[ \Sigma_S (D) - \Sigma_S^a (D) \right],$$

(6)

where $\Sigma_S (D)$ and $\Sigma_S^a (D)$ are the retarded and advanced self-energies, respectively, and they are conjugate to each other. Datta et al $[19, 21]$ have shown that the self-energies can be expressed as

$$\Sigma_S^a (D) = \Lambda_S (D) - i \Delta_S (D),$$

(7)
where $\Delta S_{(D)}$ are the real parts of the self-energies, which correspond to the shift of the energy eigenvalues of the ring, and the imaginary parts $\Delta S_{(D)}$ of the self-energies represent the broadening of these energy levels. This broadening is much larger than the thermal broadening, and accordingly, we restrict all our calculations to absolute zero temperature. These two self-energies $\Sigma_S$ and $\Sigma_D$ bear all the information of the coupling of the ring to the source and drain, respectively [19]. A similar kind of tight-binding Hamiltonian is also used, except the phase factor $\theta$, to describe the 1D perfect electrodes where the Hamiltonian is parameterized by constant on-site potential $\epsilon_{0}$ and nearest-neighbor hopping integral $t_0$. The hopping integral between the source and the ring is $t_S$, while it is $t_D$ between the ring and the drain.

The current $I$ passing through the ring is described as a single-electron scattering process between the two reservoirs of charge carriers. The current–voltage relation is evaluated from the following expression [19]:

$$I(V) = \frac{e}{\pi \hbar} \int_{E_F - \epsilon V/2}^{E_F + \epsilon V/2} T(E, V) \, dE,$$

where $E_F$ is the equilibrium Fermi energy. Here, we assume that the entire voltage drops across the ring–electrode interfaces, and it is examined that under such an assumption the $I$–$V$ characteristics do not change their qualitative features.

All the results in this communication are determined at absolute zero temperature, but they should be valid even for finite temperature ($\sim 300$ K), since the broadening of the energy levels of the ring due to its coupling to the electrodes becomes much larger than that of the thermal broadening [19]. For simplicity, we take the units $e = \hbar = 1$ in the present calculation.

### 3. Results and discussion

Let us start our discussion by mentioning the values of the different parameters used for the numerical calculation. In the ring, the on-site energy $\epsilon_{i0}$ is taken as 0 for all the sites $i$, except the sites $i = a, b, \alpha$ and $\beta$ where the site energies are taken as $V_{\alpha}, V_{\beta}, V_{\alpha}$ and $V_{\beta}$ respectively, and the nearest-neighbor hopping strength $t$ is set to 3. On the other hand, for the side attached electrodes the on-site energy ($\epsilon_{0})$ and the nearest-neighbor hopping strength ($t_0$) are fixed to 0 and 4, respectively. The voltages $V_a$ and $V_b$ are set to 2 and the Fermi energy $E_F$ is set at 0. Throughout the study, we focus our results for the two limiting cases depending on the strength of the coupling of the ring to the source and drain. In one case we use the condition $\tau_S < t$, which is the so-called weak-coupling limit. For this regime we choose $t_S = 0.5$. In the other case the condition $\tau_{S(D)} \sim t$ is used, which is named the strong-coupling limit. In this particular regime, the values of the parameters are set as $t_S = t_D = 2.5$. The key controlling parameter for all these calculations is the magnetic flux $\phi$ which is set to $\phi_0/2$, i.e. 0.5 in our chosen units.

Figure 2 shows the variation of the conductance ($g$) as a function of the injecting electron energy ($E$) in the limit of weak coupling for a mesoscopic ring with $N = 8$ and $V_a = V_{\beta} = 2$, where (a)–(d) correspond to the results for the different values of $V_a$ and $V_{\beta}$. When both the inputs $V_a$ and $V_{\beta}$ are identical to 2, i.e. both the inputs are high, the conductance $g$ becomes exactly zero (figure 2(d)) for all energies. This reveals that the electron cannot conduct from the source to the drain through the ring. While, for the cases where either one or both the inputs to the gate are zero (low), the conductance shows fine resonant peaks for some particular energies, as shown in figures 2(a)–(c), respectively. Thus, in all these three cases, the electron can conduct through the ring. From figure 2(a) it is observed that, at the resonances, the conductance $g$ approaches the value 2, and accordingly, the transmission probability $T$ becomes unity, since the expression $g = 2T$ is satisfied from the Landauer conductance formula (see equation (1) with $e = h = 1$). The height of the resonant peaks falls ($T < 1$) for the cases where one of the two inputs is high and the other is low (figures 2(b) and (c)). All these resonant peaks are associated with the energy eigenvalues of the ring, and thus, it can be predicted that the conductance spectrum manifests the electronic structure of the ring. This reveals that more resonant peaks are expected for the larger rings, associated with their energy spectra. Now we illustrate the dependences of the gate voltages on the electron transport for these four different cases. The probability amplitude of getting an electron across the ring depends on the quantum interference of the electronic waves passing through the two arms (upper and lower) of the ring. For the symmetrically connected ring, i.e. when the two arms of the ring are identical with each other, the probability amplitude is exactly zero ($T = 0$) for the flux $\phi = \phi_0/2$. This is due to the result of the quantum interference among the two waves in the two arms of the ring, which can be obtained in a very simple mathematical calculation. So, for the case when both the two inputs to the gate are identical to 2, i.e. $V_a = V_{\beta} = 2$, the upper and lower arms of the ring become exactly the same. This is due to the fact that the potentials $V_a$ and $V_{\beta}$ are also fixed to 2. Therefore, in this particular case the transmission probability drops to zero. If the two inputs $V_a$ and $V_{\beta}$ are different from the potentials applied in the sites $\alpha$ and $\beta$, then the two arms are not longer identical to each other and the transmission probability will not vanish.
we show the characteristics for a mesoscopic ring with $N = 8$, $V_α = V_β = 2$ and $φ = 0.5$. (a) $V_α = V_β = 0$, (b) $V_α = 2$ and $V_β = 0$, (c) $V_α = 0$ and $V_β = 2$ and (d) $V_α = V_β = 2$.

Hence, to get the zero transmission probability when both the inputs are high, we should tune $V_α$ and $V_β$ properly, observing the input potentials and vice versa. On the other hand, due to the breaking of the symmetry of the two arms (i.e. the two arms are no longer identical to each other) in the other three cases by making either one or both the inputs to the gate zero (low), nonzero value of the transmission probability is achieved which reveals the electron conduction across the ring. The reduction of the transmission probability from unity for the cases where either one of the two gates is high and the other is low compared to the case where both the gates are low is solely due to the quantum interference effect. Thus, it can be emphasized that the electron conduction takes place across the ring if either one or both the inputs to the gate are low, while if both the inputs are high, the conduction is no longer possible. This feature clearly describes the NAND gate behavior. In this context, we also discuss the effect of the ring-to-electrode coupling. As illustrative examples, in figure 3 we show the conductance–energy characteristics for the strong-coupling limit, where (a)–(d) are drawn, respectively, for the same conductance–energy characteristics for the strong-coupling limit. This is due to the broadening of the energy levels of the ring in the limit of strong coupling, where the contribution comes from the imaginary parts of the self-energies $Σ_S$ and $Σ_D$, respectively [19]. Therefore, by tuning the coupling strength, we can get the electron transmission across the ring for a wider range of energies and it provides important behavior in the study of $I–V$ characteristics.

All these properties of electron transfer can be much more clearly understood from our presented $I–V$ characteristics. The current across the ring is determined by integrating the transmission function $T$ as prescribed in equation (8). The transmission function varies exactly the same as that of the conductance spectrum, differing only in magnitude by the factor 2 since the relation $g = 2T$ holds from the Landauer conductance formula equation (1).

As representative examples, in figure 4 we plot the $I–V$ characteristics for a mesoscopic ring with $N = 8$ in the limit of weak coupling, where (a)–(d) correspond to the results for the different cases of the input voltages. Quite interestingly we see that when both the inputs to the gate are identical to 2 (high), the current $I$ becomes zero (see figure 4(d)) for the entire bias voltage $V$. This feature is clearly understood from the conductance spectrum, figure 2(d), since the current is computed from the integration method of the transmission function $T$. In all the other three cases of the input voltages, a nonzero value of the current is obtained, this is clearly presented in figures 4(a)–(c). These figures show that the current exhibits staircase-like structure with fine steps as a function of the applied bias voltage. This is due to the existence of the fine resonant peaks in the conductance spectra in the weak-coupling limit. With the increase of the bias voltage $V$, the electrochemical potentials on the electrodes are shifted gradually, and finally cross one of the quantized energy levels of the ring. Accordingly, a current channel is opened up which provides a jump in the $I–V$ characteristic curve. Here, it is also important to mention that the nonzero value of the current appears beyond a finite value of the bias voltage $V$, the so-called threshold voltage ($V_{th}$). This $V_{th}$ can be changed by controlling the size ($N$) of the ring. From these $I–V$ curves, the NAND gate behavior of the ring can be observed very nicely. To make it much clearer, in table 1, we show a quantitative estimate of the typical current amplitude determined at the bias voltage $V = 6.02$. It is observed that, when either one of the two gates is high and the other is low, the current gets the value 0.157, and for the case when both the two inputs are low, it ($I$) achieves the value 0.339. While, for the case when both the two inputs are high ($V_α = V_β = 2$), the current becomes exactly zero. On the same footing as above, here we also describe the $I–V$ characteristics for the strong-coupling limit.

![Figure 3](image)

![Figure 4](image)

**Figure 3.** $g–E$ curves in the strong-coupling limit for a mesoscopic ring with $N = 8$, $V_α = V_β = 2$ and $φ = 0.5$. (a) $V_α = V_β = 0$, (b) $V_α = 2$ and $V_β = 0$, (c) $V_α = 0$ and $V_β = 2$ and (d) $V_α = V_β = 2$.

**Figure 4.** $I–V$ curves in the weak-coupling limit for a mesoscopic ring with $N = 8$, $V_α = V_β = 2$ and $φ = 0.5$. (a) $V_α = V_β = 0$, (b) $V_α = 2$ and $V_β = 0$, (c) $V_α = 0$ and $V_β = 2$ and (d) $V_α = V_β = 2$.

**Table 1.** NAND gate behavior in the limit of weak coupling. The current $I$ is computed at the bias voltage 6.02.

| Input-I ($V_α$) | Input-II ($V_β$) | Current ($I$) |
|-----------------|------------------|--------------|
| 0               | 0                | 0.339        |
| 2               | 0                | 0.157        |
| 0               | 2                | 0.157        |
| 2               | 2                | 0            |
In this limit, the current varies almost continuously with the applied bias voltage and gets much larger amplitude than the weak-coupling case as presented in figure 5. The reason is that, in the limit of strong coupling all the energy levels get broadened which provide larger current in the integration procedure of the transmission function $T$. Thus, by tuning the strength of the ring-to-electrode coupling, we can achieve very large current amplitude from the very low one for the same bias voltage $V$. All the other properties, i.e. the dependences of the gate voltages on the $I-V$ characteristics are exactly the same as those given in figure 4. In this strong-coupling limit we also make a quantitative study of the typical current amplitude, given in table 2, where the current amplitude is determined at the same bias voltage ($V = 6.02$) as earlier. The response of the output current is exactly the same as that given in table 1. Here the current achieves the value $1.174$ in the cases where either one of the two gates is high and other is low, and it ($I$) becomes 4.018 for the case where both the two inputs are low. On the other hand, the current becomes exactly zero for the case where $V_a = V_b = 2$. The nonzero values of the current in this strong-coupling limit are much larger than the weak-coupling case, as expected. From these results we can clearly manifest that a mesoscopic ring exhibits the NAND gate response.

### 4. Concluding remarks

In this work, we have explored the NAND gate response in a mesoscopic metallic ring threaded by a magnetic flux $\phi$ in the Green’s function formalism. The ring is attached symmetrically to the electrodes and two gate voltages $V_a$ and $V_b$ are applied in one arm of the ring; these are taken as the two inputs of the NAND gate. A simple tight-binding model is used to describe the system and all the calculations are exact and performed numerically. We have computed the conductance–energy and $I-V$ characteristics as functions of the gate voltages, ring-to-electrode coupling strength and magnetic flux. Very interestingly we have observed that, for the half flux-quantum value of $\phi$ ($\phi = \phi_0/2$), a high output current (1) (in the logical sense) appears if one or both the inputs to the gate are low (0). On the other hand, if both the inputs to the gate are high (1), a low output current (0) appears. It clearly manifests the NAND gate behavior and this aspect may be utilized in designing a tailor made electronic logic gate.

Throughout our work, we have addressed the conductance–energy and $I-V$ characteristics for a quantum ring with total number of atomic sites $N = 8$. In our model calculations, this typical number ($N = 8$) is chosen only for the sake of simplicity. Here it is important to note that for a larger ring with more atomic sites, one can also apply input voltages to the other atomic sites, preserving the symmetry between the upper and lower arms of the ring. Although the results presented here change numerically with the ring size ($N$) and the distance between the input positions, all the basic features remain exactly invariant since the results solely depend on the quantum interference effect of the electronic waves passing through the two arms of the ring. To be more specific, it is important to note that, in a real situation, the experimentally achievable rings have typical diameters within the range $0.4–0.6 \mu m$. In such a small ring, unrealistically very high magnetic fields are required to produce a quantum flux. To overcome this situation, Hod et al have studied extensively and proposed how to construct nanometer scale devices, based on Aharonov–Bohm interferometry, that can be operated in moderate magnetic fields [22–25].

In the present paper, we have done all the calculations by ignoring the effects of the temperature, electron–electron correlation, disorder, etc. Owing to these factors, any scattering process that appears in the arms of the rings would influence the electronic phases, and, in consequence can disturb the quantum interference effects. Here we have assumed that in our sample all these effects are too small, and accordingly, we have neglected all these factors in this particular study.

The importance of this article is concerned with (i) the simplicity of the geometry and (ii) the smallness of the size. To the best of our knowledge the NAND gate response in such a simple low-dimensional system that can be operated even at finite temperature ($\sim 300 K$) has not been addressed earlier in the literature.

### References

[1] Aviram A and Ratner M 1974 *Chem. Phys. Lett.* 29 277
[2] Chen J, Reed M A, Rawlett A M and Tour J M 1999 *Science* 286 1550
[3] Reed M A, Zhou C, Muller C J, Burgin T P and Tour J M 1997 *Science* 278 252
[4] Dadash T, Gordin Y, Krahnse R, Khivrich I, Mahalu D, Frydman V, Sperling J, Yacoby A and Bar-Joseph I 2005 *Nature* 436 677
[5] Nitzan A 2001 *Ann. Rev. Phys. Chem.* 52 681
[6] Nitzan A and Ratner M A 2003 *Science* 300 1384
[7] Orellana P A, de Guevara M L L, Pacheco M and Latge A 2003 Phys. Rev. B 68 195321
[8] Orellana P A, Dominguez-Adame F, Gomez I and de Guevara M L L 2003 Phys. Rev. B 67 085321
[9] Mujica V, Kemp M and Ratner M A 1994 J. Chem. Phys. 101 6849
[10] Mujica V, Kemp M, Roitberg A E and Ratner M A 1996 J. Chem. Phys. 104 7296
[11] Walczak K 2004 Phys. Status Solidi b 241 2555
[12] Walczak K 2003 arXiv:0309666
[13] Cui W Y, Wu S Z, Jin G, Zhao X and Ma Y Q 2007 Eur. Phys. J. B 59 47
[14] Baer R and Neuhauser D 2002 J. Am. Chem. Soc. 124 4200
[15] Walter D, Neuhauser D and Baer R 2004 Chem. Phys. 299 139
[16] Tagami K, Wang L and Tsukada M 2004 Nano Lett. 4 209
[17] Walczak K 2004 Cent. Eur. J. Chem. 2 524
[18] Baer R and Neuhauser D 2002 Chem. Phys. 281 353
[19] Datta S 1997 Electronic Transport in Mesoscopic Systems (Cambridge: Cambridge University Press)
[20] Nardelli M B 1999 Phys. Rev. B 60 7828
[21] Tian W, Datta S, Reifenberger R, Henderson J I and Kubiak C I 1998 J. Chem. Phys. 109 2874
[22] Hod O, Baer R and Rabani E 2004 J. Phys. Chem. B 108 14807
[23] Hod O, Baer R and Rabani E 2008 J. Phys.: Condens. Matter 20 383201
[24] Hod O, Baer R and Rabani E 2005 J. Am. Chem. Soc. 127 1648
[25] Hod O, Rabani E and Baer R 2006 Acc. Chem. Res. 39 109