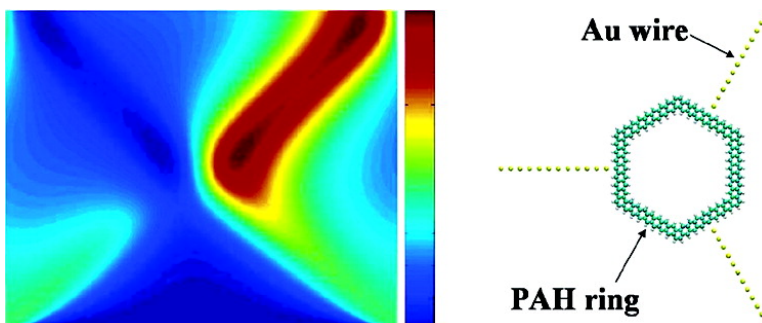


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## A Parallel Electromagnetic Molecular Logic Gate

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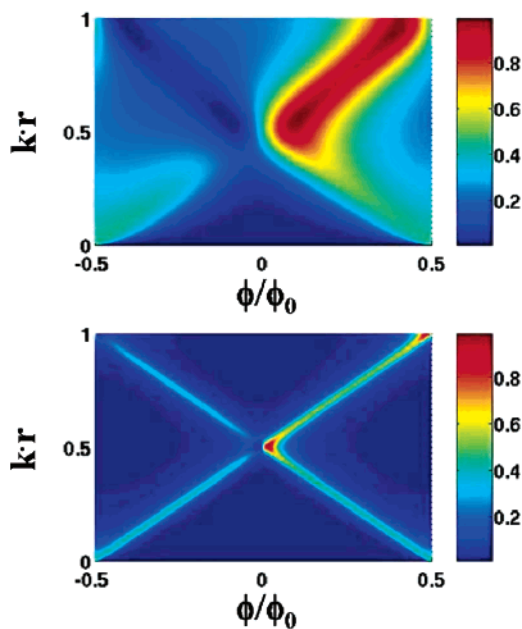
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Cyclic molecules have vast importance both in biological systems and in molecular electronics.<sup>1</sup> Such organic molecules have been pointed out as promising candidates for the fabrication of molecular wires and molecular electronic devices.<sup>2</sup> In particular, ring-shaped molecules have been suggested as model systems for coherent quantum molecular interferometry.<sup>3</sup> Recently, we have shown<sup>4,5</sup> how the conductance can be controlled in nanometer-scale rings by exploiting the Aharonov–Bohm (AB) effect.<sup>6</sup> Despite the fact that unrealistically large magnetic fields are required to establish a full AB period, moderate fields can have a dramatic effect on the conductance.

In this communication, we show how cyclic molecules (rings) can be used as parallel magnetoresistance logic gates (in contrast to our previous study on switching devices). The basic idea is to couple the cyclic molecular system to *three* leads, creating a three-terminal device, and to apply an external magnetic field. By carefully selecting a narrow resonance through which conductance occurs we show that such a setup can be used to simultaneously switch one channel “on” and at the same time switch the other channel “off”. A proper combination of a gate potential and a realistic magnetic field can be used to obtain parallel logic operations such as AND and AND+NOT. We demonstrate this for a molecular system composed of conjugated benzene rings and discuss the results in terms of a single-channel continuum model.

Consider a model of a ballistic three-terminal Aharonov–Bohm (AB) interferometer.<sup>7</sup> A homogeneous magnetic field is applied perpendicular to the plane of the ring. The electrons are assumed to travel freely along the conducting channels and to scatter elastically at the three junctions. Each junction is assigned with a scattering amplitude ( $\epsilon$ ) which represents the probability amplitude for an electron approaching the junction from one of the leads to transmit into the ring and vice versa. Following the lines of Gefen et al.,<sup>8</sup> the total transmittance probability for an electron originating at the input channel ( $I$ ) to emerge at one or both of the output channels ( $O_1$  and/or  $O_2$ ) can be calculated exactly as a function of the threading magnetic flux for a given ring diameter. We find, as expected, that the transmittance is periodic with the magnetic flux with a period given by  $\phi_0 = \hbar/e$  where  $\hbar$  is Planck’s constant divided by  $2\pi$  and  $e$  is the electron’s charge. Two parameters control the shape of the magneto-transmittance curve: the wavenumber of the conducting electron, which dominates the position of the conductance resonances, and the coupling between the leads and the ring, which controls the width of the peaks.<sup>5</sup>

In Figure 1 we show the transmittance through  $O_1$  as a function of the magnetic flux and the conducting electron wavenumber ( $k$ ) for two values of  $\epsilon$ . As a result of the symmetry of our device, the transmittance through  $O_2$  is a mirror image of the result shown for  $O_1$  and, therefore, is not shown in the figure. When the coupling between the leads and the ring (represented by  $\epsilon$  in the current



**Figure 1.** Transmittance as a function of the magnetic flux ( $\phi$ ) and the electron’s wave vector ( $\mathbf{k}$ ) for  $\epsilon = 0.61$  (upper panel) and  $\epsilon = 0.3$  (lower panel).  $\mathbf{r}$  is the electron’s position vector.

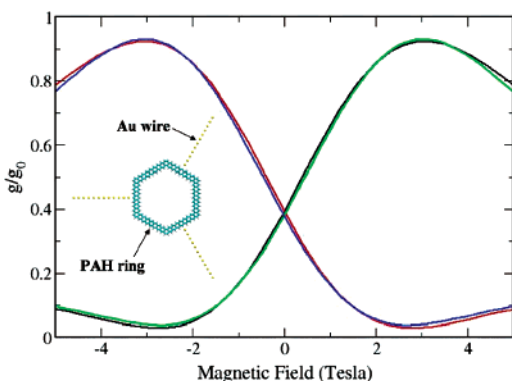
model) is high (upper panel of Figure 1), the system is characterized by a wide range of high transmittance which can be shifted along the AB period by changing the electron’s wavenumber. Switching  $O_1$  “on” while at the same time switching  $O_2$  “off” at this value of  $\epsilon$  requires high magnetic fields, since the transmittance peaks are quite wide.

As the coupling between the ring and the leads decreases (lower panel of Figure 1), a narrow resonant tunneling is formed on the ring, and the transmittance probability becomes very sensitive to the magnetic flux. This is translated to sharper peaks that develop in the magnetoresistance curve. For the parameters studied in the lower panel of Figure 1 we find that both output channels show negligible transmittance for all values of  $k$  at zero magnetic field. The position of first maximum in the transmittance depends linearly on the value of  $\phi$  and  $k$ . By carefully selecting the wavenumber of the conducting electrons,  $k \cdot \mathbf{r} = 0.5$ , it is possible to shift the transmittance peak toward low magnetic fields, such that at a finite, relatively small magnetic flux, a sharp transmittance peak is obtained for both outputs. The peak appears at positive magnetic fields for  $O_1$  and at negative magnetic fields for  $O_2$  (not shown). Thus, switching is obtained at low values of  $B$ .

Now the discussion shifts to the plausibility of developing a realistic nanometer-scale molecular device based on the concepts discussed above. We consider a polycyclic aromatic hydrocarbon (PAH) hexagonal ring composed of 48 conjugated benzene units. PAH molecules have been synthesized<sup>9</sup> and studied theoretically.<sup>10</sup>

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**Figure 2.** Comparison of magnetoconductance for the molecular switch (shown in the inset) and the continuum model.

Furthermore, the conductance of organic molecules attached to gold wires has recently been measured.<sup>11</sup> The molecule is coupled to three gold atomic wires (see the inset of Figure 2), and the geometry of the entire system is optimized using Fletcher–Reeves/Polak–Ribiere conjugate-gradient algorithm applied to the MM+ force field on the HyperChem 6.02 software. The electronic structure of the systems is described within the magnetic extended Hückle theory (MEHT).<sup>5</sup> We assume a homogeneous magnetic field in the direction perpendicular to the molecule surface. The conductance is calculated using the Landauer formalism,<sup>12</sup> and the transmittance is computed using absorbing potentials<sup>13</sup> and within the Seidman–Miller formalism.<sup>14</sup>

In Figure 2 we plot the zero bias conductance of the molecular switch as a function of the magnetic field intensity for both output channels (black and red curves). We focus on the region of realistic magnetic fields (much smaller than the field required to complete a full AB period which is  $2\pi\hbar/eS \approx 470$  T for a ring with a cross section area of  $S \approx 8.75$  nm<sup>2</sup>). The gate voltage applied in the calculation is  $V_{\text{gate}} = 1.854$  V. For zero magnetic field, both channels are “half”-opened and conduct with a value of  $\sim 0.4g_0$  ( $g_0 = 2e^2/h$  is the quantum conductance) at the selected gate voltage. When a relatively small magnetic field is applied, we observe that one output channel conducts while the other does not conduct. As the polarity of the field changes sign, the two output channels interchange their role. Exactly the same characteristics are captured by the continuum model (e.g. green and blue curves of Figure 2).

On the basis of these results it is possible to design a molecular logic gate which processes two different logic operation in parallel.

This can be achieved by choosing one input signal as the current in the incoming channel ( $I$ ) and the other input signal as the magnetic field ( $B$ ). For the bias input signal  $I$  we mark as 0 the case where  $I = 0$  and as 1 the case where a small bias is applied. For the magnetic field input signal we mark as 0 the case where  $B \approx -3$  T and as 1 the case where  $B \approx 3$  T. For a given gate voltage, the output  $O_1$  gives the logic operation  $I \text{ AND } B$  while the output  $O_2$  gives the logic operation  $I \text{ AND } \bar{B}$ . Shifting the conductance peaks via the change of the gate potential will give rise to different logic operations of the same setup.

Summarizing, in this communication we have shown that single cyclic molecules are promising candidates for the fabrication of magnetoresistance parallel switching and gating devices at feasible magnetic fields. The essential procedure is to weakly couple the system to the conducting contacts to narrow the conductance resonances while at the same time control the position of the resonances by the application of a gate potential. A careful fine-tuning of these two parameters allows the selective switching of only one output channel. This feature allows the design of a molecular logic gate, processing two logic operations in parallel.

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