Coupled nano-rings: strain and magnetic field effects

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INTRODUCTION

Over the past two decades, remarkable advances have been made in the field of quantum transport in mesoscopic systems. Much study has been put into the different geometries of quantum wires and their effect on electron propagation. Of particular note are the transmission properties of coupled molecular and mesoscopic rings [1], and the electron-spin transport in semiconductor nanostructures and nanoscale electronic devices [2]. Graphene nanoribbons are an example of a system composed of coupled molecular rings which have demonstrated interesting electronic properties [3].

MODEL

We investigate a series of coupled nano-rings with a total of six quantum dot (QD) sites around each ring. Two of the six sites couple to nearest-neighbor rings or to the source/drain leads. The number of rings in series is a variable parameter in our model and the system represents a single-molecule graphene nanoribbon of arbitrary length, as depicted in Fig. 1. The hopping integrals between QD sites and the QD site energy values are parameters which can be varied to study the effects of physical strain and site defects on the system. We also incorporate a variable external magnetic field into the computational system in order to study the effects of energy-level separation via the Zeeman effect and resonance interference modulation via the Aharonov-Bohm (AB) effect. Using the tight-binding approximation to the Schrödinger equation (1), we solve for the transmission through the entire system for arbitrary numbers of rings in series.

$$-\sum_{m} V_{n,m}\Psi_m + \varepsilon_n \Psi_n = E\Psi_n \qquad (1)$$

SELECTED RESULTS

The effect of a magnetic field on the electron transport is considered via the AB effect and Zeeman splitting of the QD quasi-bound states. The effects of longitudinal strain on the nanoribbon are investigated through a relative variation in the inter-ring couplings, V_m. As shown in Fig. 2, increasing V_m relative to V_{QD} results in closing the transmission bandgap, thereby producing a semiconductor to metallic transition. In a graphene nanoribbon, the ratio of the coupling strengths, V_{QD}/V_m is a function of strain [3]. With the electron energy set equal to ε_{QD}, the resonant transmission, $T(\varepsilon_{QD})$, is varied as a function of V_m, the system-leads coupling, V_{leads}, and the number of rings in series, N. In Fig. 3, V_{leads}=0.775 and $T(\varepsilon_{QD})$ is plotted vs. N for 6 different values of V_m. Exponential decay of the $T(\varepsilon_{QD})$ occurs as N increases, except for when V_m=0.6, or twice V_{QD}=0.3. At V_m=0.6 and V_{leads}=0.775, the transmission remains at 100%, independent of N. Resonance saturation (Fig. 4) occurs for specific values of inter-ring and system-leads coupling constants. A non-zero magnetic flux through the plane of the rings splits the transmission bands and produces a shifting and narrowing of the resonances along the energy axis (Fig. 5), until complete destructive interference occurs at half a flux quantum. Zeeman effects are shown in Fig. 6.

REFERENCES

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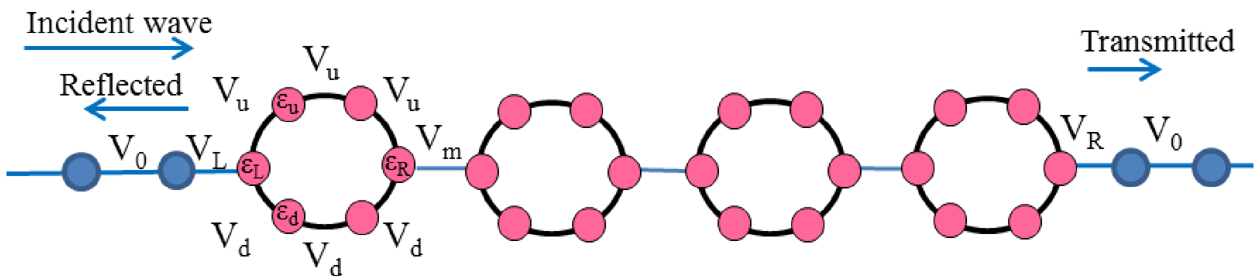

Fig. 1. Schematic of a 4-ring system comprised of 6-QD rings coupled so as to represent a graphene nanoribbon in the armchair configuration. Coupling constants (V_i) and QD site energy values (ε_i) are illustrated as labeled. In subsequent results, $V_u = V_d \equiv V_{QD}$, and $\varepsilon_u = \varepsilon_d \equiv \varepsilon_{QD}$.

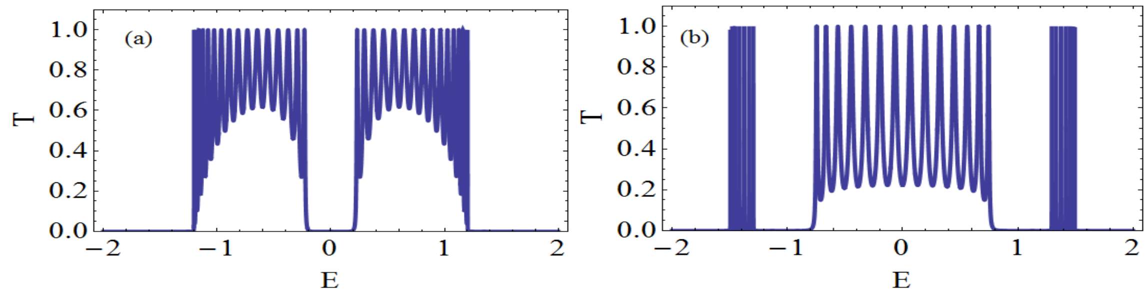

Fig. 2. Transmission through N=8 rings, with $\varepsilon_{QD} = 0.0$, $V_L=V_R=V_{QD}=0.5$, for different inter-ring couplings: (a) Vm = 0.5, and (b) Vm = 1.0.

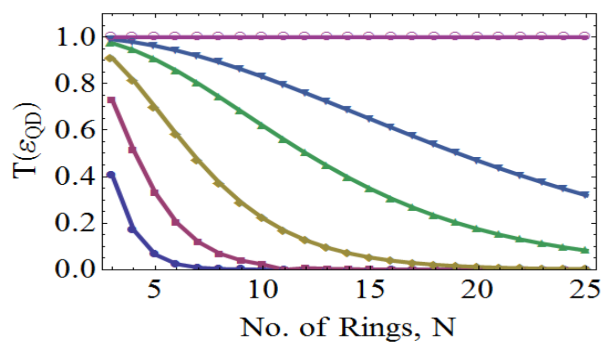

Fig. 3. Resonant transmission at $E=\varepsilon_{QD}$ vs. number of rings in series for 6 different values of inter-ring coupling. Vm = 0.60, 0.63, 0.65, 0.7, 0.8, and 1.0 (top to bottom curves). V_{leads}=0.775.

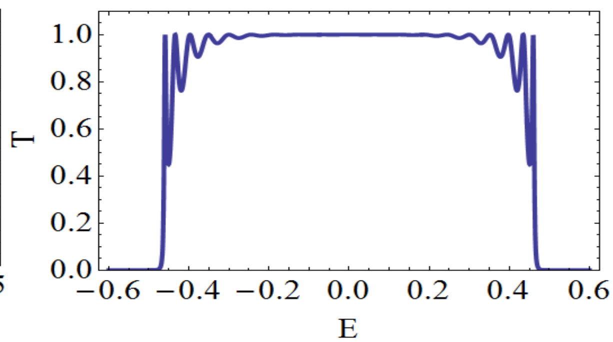

Fig. 4. Resonance saturation occurs for Vm = 0.60 and V_{leads}=0.775, giving nearly flat 100% transmission across the energy range. Shown above for N=10 rings.

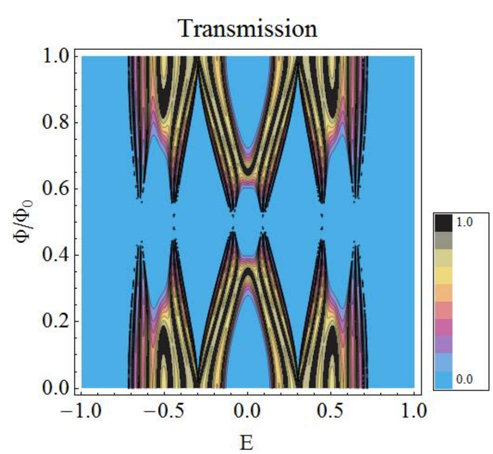

Fig. 5. Variation in transmission as a function of magnetic flux. $V_{leads}=V_{QD}=V_m$=0.3.

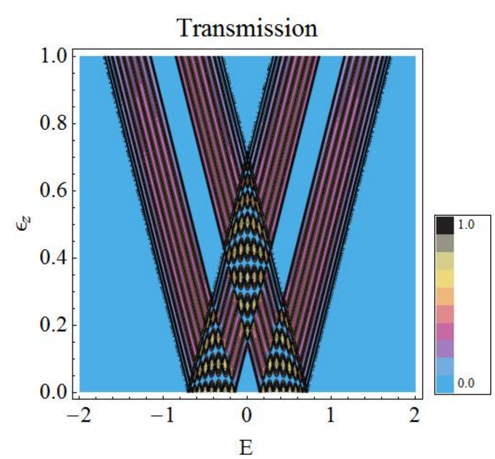

Fig. 6. Variation in transmission as a function of Zeeman splitting of the QD energy levels.