Substrate Modulated Graphene Quantum Dot

Qiong Ma, Zhi-Rong Lin, Tao Tu, Guang-Can Guo, and Guo-Ping Guo

Key Laboratory of Quantum Information,
University of Science and Technology of China,
Chinese Academy of Sciences, Hefei, 230026, P.R.China

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Abstract

We propose a new method to use gapped graphene as barrier to confine electrons in gapless graphene and form a good quantum dot, which can be realized on an oxygen-terminated SiO$_2$ substrate partly H-passivated. In particular, we use ferromagnetic insulators deposited on top of barrier which give rise to a spin related energy spectrum and transport properties. Compared to the complexity of etched quantum dots in graphene, the setup suggested here is a promising candidate for practical applications.

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Introduction. Graphene has attracted a lot of research interest because of its unique electronic properties which make it a promising candidate for future nanoelectronics \[1, 2, 3, 4, 5\]. However, there are still many barriers in the way of making effective uses out of it. For example, due to the absence of gap between conductance and valance bands in the carrier spectrum and the phenomenon of Klein tunnelling, it is hard to confine electrons within a small region to form quantum dot using electrostatic potential barriers \[6\]. Alternative strategies have been proposed to solve this difficulty by etching graphene into nanostructures \[7, 8\], using non-zero transverse momentum in armchair nano ribbon \[9, 10\], considering bilayer structure \[11\], or applying inhomogeneous magnetic fields \[12\]. Here, we propose a new and easier method to use gapped graphene as barrier to confine electrons in gapless graphene and form a good quantum dot.

Setup. It is well known that electron in ideal graphene behaves as a massless Dirac-fermion whose energy spectrum has no gap between conduction and valance bands. Recently, the electron in epitaxially grown graphene monolayer on a SiC substrate is found to be massive close to the Dirac point because of the symmetry breaking of sublattice caused by substrate and lattice interaction \[13\]. Further, there are also some experiments carried on widely used SiO$_2$ substrate \[14\]. Ref. \[15\] points out that if a single layer graphene is deposited onto a SiO$_2$ surface, the electronic energy spectrum of the monolayer graphene depends strongly on the surface characteristic, i.e. a finite energy gap will open between conduction and valence bands for an oxygen-terminated surface, but close when the oxygen atoms on the substrate are passivated with hydrogen atoms. Thus if an oxygen terminated SiO$_2$ substrate is fully exposed to hydrogen atoms atmosphere within a small region in the middle, then a single layer graphene is deposited on it, and we will get a gapless part confined by gapped parts, which can serve as barriers, as shown in Fig. 1. Moreover, when we make the barrier region also exposed to hydrogen atoms atmosphere but in a different degree from the dot, the gap will not close completely, and we can tune the barrier height in this system. It is realizable in experiment by using PMMA to cover the region which doesn’t need to be passivated.

For simplicity and clarity, we put our discussion in the setup of metallic armchair shaped graphene nanoribbon. In the present case, we use the substrate induced energy gap as barrier to confine electrons, therefore the realization of quantum dot will not depend much on the boundary conditions. More remarkably, we consider adding ferromagnetic insulator such as EuO upon the two gapped graphene barriers. Ferromagnetic insulators deposited on graphene can induce ferromagnetic correlations in graphene and the induced exchange interaction is estimated to achieve 5 meV by using EuO \[16\]. We find that it will lead to spin dependent energy spectrum and conductance phenomenon in the proposed graphene dot.

Bound States and Energy Spectrum. The electron waves in graphene system are usually described by four component spinor envelop wavefunction $\Psi = (\psi_A^{(K)}, \psi_B^{(K)}, -\psi_A^{(K')}, -\psi_B^{(K')})$ and their behaviors will be governed by $4 \times 4$ Dirac equation for massless or massive particles,
FIG. 1: Schematic illustration of a graphene quantum dot. (a) The substrate and graphene interaction when hydrogen-passivated (right) and non hydrogen passivated (left). (b) The light part is the dot region, which is fully hydrogen-passivated and gapless. The dark part is the barrier region, which is non hydrogen-passivated or slightly hydrogen-passivated and gapped. (c) The energy spectrum of this system.

which can be written as: in the dot region (where $0 \leq y \leq L$),

$$-i\hbar v_F \begin{pmatrix} \sigma_x \partial_x + \sigma_y \partial_y & 0 \\ 0 & -\sigma_x \partial_x + \sigma_y \partial_y \end{pmatrix} \Psi = E\Psi,$$

and in the barrier region (where $y < 0$ or $y > L$),

$$-i\hbar v_F \begin{pmatrix} \sigma_x \partial_x + \sigma_y \partial_y & 0 \\ 0 & -\sigma_x \partial_x + \sigma_y \partial_y \end{pmatrix} \Psi + \Delta \begin{pmatrix} \sigma_z & 0 \\ 0 & \sigma_z \end{pmatrix} \Psi - \eta V_0 \Psi = E\Psi,$$
where $\hbar$ is the Planck constant divided by $2\pi$, $v_F \approx 10^6$ m/s is the analog of the Dirac electron speed of light, $\sigma_x$, $\sigma_y$, $\sigma_z$ are Pauli matrices acting on two-spinor states related to the two triangular sublattices of graphene, $\eta = \pm 1$ stands for the two spin indexes. $2\Delta$ is the induced gap by the substrate, $2V_\sigma$ is the spin splitting energy due to the correlation with ferromagnetic contacts.

We consider metallic armchair boundaries and the quantized transverse momentum $q_n = n\pi$ keeps the same during the movement of electron, but the wave vector in the $y$ direction must satisfy different conditions as

$$E = \pm \sqrt{(\hbar v_F q_n)^2 + (\hbar v_F k)^2},$$

in the dot and

$$E = \pm \sqrt{(\hbar v_F q_n)^2 + (\hbar v_F k')^2 + \Delta^2 - \eta V_\sigma},$$

in the barriers, where $k$ is the wave vector in the dot and $k'$ in the ferromagnetic barrier with $\pm$ signs referring to conduction band $(+)$ and valence band $(-)$ respectively. The bound state requires that $k'$ is a pure imaginary, which means the bound state energy should satisfy

$$|E| \geq \hbar v_F |q_n|, \quad |E + \eta V_\sigma| < \sqrt{(\hbar v_F q_n)^2 + \Delta^2}.$$ 

After matching the wavefunctions in different regions at $y = 0$ and $y = L$, we can get the energy levels of the bound states. We set the parameters of this system as $L = 100$ nm and $W = \pi L \approx 300$ nm. Then if we use $1/L$ as the unit of $q_n$, $q_n = n$. The characteristic energy $\hbar v_F/L$, which is about 7 meV in this case, will be used as the energy unit below. In Fig. 2, we show the energy spectrum as a function of the substrate induced interaction $\Delta$ for different transverse momentums $(q_n)$ and spin indexes $(\eta)$ where $V_\sigma$ is assumed to be 5 meV according to Ref. [16]. Fig. 2a plots the energy spectrum for $q_n = 0, 1, 2, 3$ and $\eta = 1$ above the Dirac point. When $\Delta$ increases, the number of bound states is increasing at the same time, which can be deduced from Eq. 5. Bound states are formed even when the transverse momentum is zero, which is distinguished from the former results [10]. The result lies at the heart of our approach where the dot levels (bound states) are located in the gap of the barrier regions induced by the interaction with substrate, which is schematically illustrated in the Fig. 1c. More interestingly, we find that for a particular spin index, the energy spectrum is unsymmetrical relative to the zero energy point, as shown in Fig. 2b for $\eta = 1$ and Fig. 2c for $\eta = -1$. Non-zero $V_\sigma$ shift the potential for a certain spin orientation only in the barrier region, therefore the symmetry of the spectrum in the dot region shown in Fig. 1c are broken. However the chirality between electron and hole remains if the two spin indexes are considered together, as shown in Fig. 2d and Fig. 2e. What should be emphasized is that symmetric states here belong to opposite spin indexes. Besides, we can find that with the increase of $\Delta$, the difference between energy of different spins is suppressed, and each energy level becomes spin degenerate again.

**Coulomb Blockade Behaviors.** In the following part, we will study the transport properties of the system above [17]. If a bias voltage $V_{sd}$ is applied between left and right reservoirs, a current $I$ can pass through the dot. The number of electrons in the dot, and hence its energy
FIG. 2: Bound-state energy levels in the assumption $V_0 = 5\text{meV}$. Both axe labels are in the characteristic energy unit of $\hbar v_F/L$. $L$ is the length of dot, and if $L$ equals 100 nm, then the characteristic energy unit is about 7 meV. (a) for $q_n = 0, 1, 2, 3$ and $\eta = 1$, blue: $q_n = 0$, red: $q_n = 1$, yellow: $q_n = 2$, green: $q_n = 3$. (b) $q_n = 0$ and $\eta = 1$, (c) $q_n = 0$ and $\eta = -1$, (d) $q_n = 0$, the blue line and red line respectively stand for $\eta = 1$ and $\eta = -1$, (e) $q_n = 1$, the blue line and red line respectively stand for $\eta = 1$ and $\eta = -1$.5.
FIG. 3: (a) Coulomb Blockade oscillation at different $\Delta$ values when $V_\sigma = 0.7$ and $k_B T = 0.01$. The gate voltage is in a unit of meV and the conductance is in a unit of $\frac{e^2}{4k_B T} \Gamma_1$. (a) $\Delta = 0.5$, (b) $\Delta = 1$, (c) $\Delta = 1.5$. The up arrow stands for $\eta = 1$, and the down arrow stands for $\eta = -1$. $\Delta$, $kT$, and $V_\sigma$ are all in a unit of $\hbar v_F/L$. 


is varied by an applied gate voltage. In the liner conductance response regime ($V_{sd} \approx 0$), we will observe the Coulomb Blockade of single tunneling process, which will lead to a series of sharp peaks, as long as heat fluctuation cannot compete with the energy separation $e^2/C \approx 1$ in a unit of $\hbar v_F/L$, where $e$ is the charge of the electron. Then we use the method described in Ref. [18] to discuss in detail this single electron tunneling phenomenon at low temperature. The linear response conductance is

$$G = -\frac{e^2}{2k_B T} \sum_N \Gamma_N f'(E_N + U(N) - U(N-1) - E_F)$$

where $f(x) = \frac{1}{1+e^{x/k_BT}}$ is the Fermi-Dirac distribution function, $E_N$ is the energy of the top filled single electron state for a $N$ electron dot, and $U(N) = (Ne^2)/2C - Ne\phi_{ext}$, in which $\phi_{ext} = \phi_0 + \alpha V_{gate}$. The width of localized energy $\Gamma$ in the above equation is determined by tunneling though the classically forbidden region [19],

$$T = \exp \left(-\int_L^{L+d} |k'| dy \right)$$

where $k' = i \sqrt{\frac{q_n^2 + (\Delta / \hbar v_F)^2 - (E + \eta V_{\sigma} \hbar v_F)^2}{L + d}}$ is the vanishing wave vector in the barrier region and $d$ is the width of each barrier. Here, we assume $d = L$. It must be emphasized that the tunneling rate is not precisely gained theoretically, so the amplitude of Coulomb Blockade peaks can only show a general pattern. Inversely, the tunneling rate can be measured from experiment by studying the amplitude of Coulomb Blockade peaks. Fig. 3 shows the obtained conductance as a function of gate voltage at different $\Delta$ values assuming that energy levels below the Dirac point have already been filled up. Here, the up arrow stands for $\eta = 1$ and the down arrow stands for $\eta = -1$. From Fig. 3, we can see that when $\Delta$ is very small, all the conductance peaks for up spin have been suppressed, only down spin peaks remain. When $\Delta$ increases, peaks for up spin appear. This simply derives from the fact that for $\Delta < V_{\sigma}$, there is no bound states for spin up case and for $\Delta > V_{\sigma}$, the spin up energy level appears later than spin down, as shown in Fig. 2d and Fig. 2e. Here, the spin down or up is relative, and they can be exchanged if we change the direction in which the ferromagnetic insulator is deposited.

**Conclusion.** In this paper, we propose a new method to form a quantum dot in graphene without electrostatic barrier. By using oxygen-terminated $SiO_2$ substrate which is partly passivated by Hydrogen atom, we can realize to make gapped graphene around gapless graphene. The gapped graphene serves as a natural barrier for gapless graphene due to its substrate induced opening energy gap. In particular, we use ferromagnetic insulators deposited on top of gapped graphene to induce a energy splitting between spin up and down levels. We systematically investigate the bound states of the dot and get the energy spectrum for different spins as a function of substrate induced energy gap. We also study
the transport behavior in the system and show how the linear response conductance for different spins is modified by the change of substrate induced energy gap. Compared to the complexity of experiments on etched quantum dots in graphene [7,8], the setup suggested here has potential to become a well tunable nanodevice using today’s fabrication techniques, and can be directly developed to array of many quantum dots. This unique feature is of practical importance for future applications in quantum computations [10].

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