

Formation of quantum dots in monolayer graphene with an energy gap

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1 Introduction

Graphene quantum dots might be used in spintronics and they might also allow relativistic effects to be probed in solid state. Graphene's quasi-particles are described by a Dirac-like equation and because of the Klein tunneling effect it is nontrivial to confine them and thus define a dot. Theoretical studies have shown that the combination of an external electrostatic potential and a uniform magnetic field leads to conditional confinement [1]. Here an alternative scheme is proposed to form a dot: a spatial modulation of the energy gap in graphene, that is called the Dirac gap, gives rise to confined states with discrete energy levels [2, 3]. The Dirac gap can be introduced experimentally and its spatial modulation might be induced via substrate engineering.

The gap in the energy spectrum of monolayer graphene suppresses the Klein tunneling and thus enables charge confinement by an electrostatic quantum well and formation of quantum dots. By solving the two-dimensional Dirac-like equation in the continuum limit we show that when the gap has a local minimum confined states with discrete energy levels can be formed, without applying external electric and/or magnetic fields [2]. This is one basic advantage of this type of dot which cannot be achieved in a graphene sheet with a constant energy gap.

The interplay of a gap-induced graphene dot with an electrostatic potential well leads to quantum states, with energies within the gap, whose localization region is tunable with the potential depth. Anti-crossing points in the energy levels of confined states reflect

this property which is related to the Dirac equation and the Klein tunneling effect [3]. Such anti-crossing points are not present in the energy spectrum of the dot system when the graphene sheet has a constant energy gap.

2 Results and conclusions

First the general conditions for confinement in the presence of a spatially modulated Dirac gap, an external electrostatic potential, and a magnetic vector potential are analysed. When the gap and/or the vector potential rises asymptotically, while the electrostatic potential is zero (constant), the resulting states are confined regardless of angular momentum, valley and eigenenergy.

When the Dirac gap is zero within a disc area and constant outside that area confinement is energy-dependent, thus the choice of angular momentum and valley is important. Confined states are localised inside the disc area provided their energies lie in the gap [Figure 1(a)]. Otherwise the states are deconfined. The energy spectrum of the confined states consists of two sets of discrete levels separated by a gap. Numerical calculations of the density of states suggest that states with small angular momentum lie in a region of low density and hence they could be probed using standard techniques such as scanning tunneling microscopy.

The interplay of the gap-induced dot with an electrostatic potential well leads to tunable states, that is from confined to deconfined and vice-versa. This can only happen provided the potential and the mass term

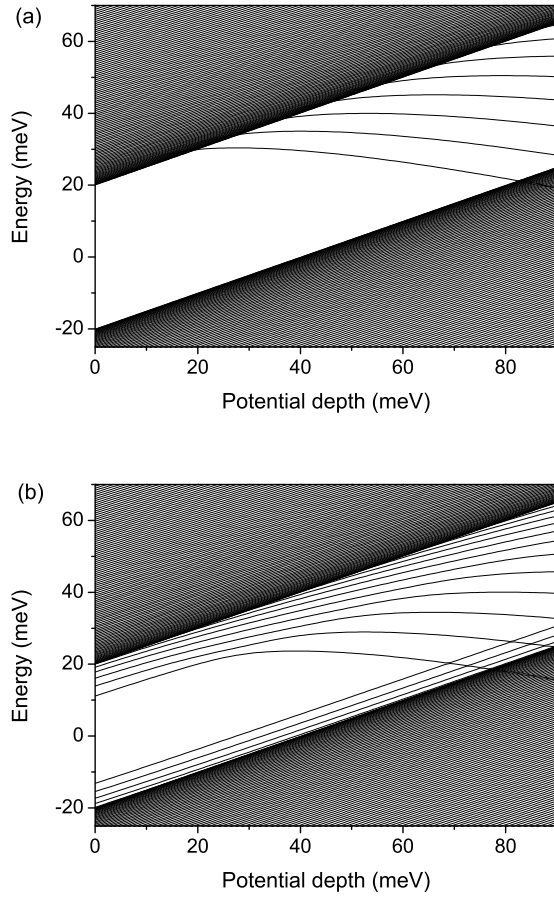


Figure 1: (a) Energy levels of a circular graphene quantum dot as a function of the potential depth for angular momentum $6\hbar$ and a constant energy gap of 40 meV. (b) The same as in (a) but for a spatially-dependent energy gap with an asymptotic value of 40 meV.

in the Hamiltonian, which generates the Dirac gap, have the same spatial forms asymptotically, while the magnetic field is zero. In this case the states can be tuned with the strength of the potential: the states are deconfined when the electrostatic potential is stronger than the mass term and confined in the opposite regime.

The states induced by the quantum well potential, which may be generated by a gate electrode, can coexist and couple to gap-induced dot states. When the coupling is weak the states retain their character, whereas in the opposite regime the states are strongly

hybridised. The signature of this coupling in the energy spectrum is the appearance of a series of anti-crossing points [Figure 1(b)]. This coupling property offers a way of tuning the spatial region, in which the hybridised states are localized, with the strength of the potential. Moreover, the states can have a large oscillatory amplitude in the barrier region, due to Klein tunneling, before they eventually decay asymptotically. Calculations of the density of states indicate that these quasi-relativistic effects could be probed.

References

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