Shaping Dirac fermions in graphene / h-BN layered systems

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Combining graphene and hexagonal boron nitride (h-BN) allows to construct multilayer structures [1] with amazing electronic properties, which are promising both for fundamental studies and novel applications. Since in most electronic devices the band gap is required, many approaches have been proposed to tailor the band structure of graphene for specific applications, especially to tune the energy gap in a controllable way, as in the Bernal stacked bilayer graphene (BLG). Recently, BLG transistors have been fabricated, but still graphene devices on SiO_2 substrate are highly disordered which limits the carrier mobility and suppresses the graphene unique properties. Moreover, in the unbiased bilayer graphene the low energy bands are parabolic, not cone-shaped, which leads to a finite value of the effective mass. The linear dispersion of pristine graphene can be preserved in one of the graphene/h-BN tunable systems, which offers new possibilities based on the properties of massless Dirac fermions.

It emerges in a natural way that structural similarities of graphene and h-BN layers allows to create heterostructures geometrically similar to pristine graphene multilayers with properties depending on number of layers, stacking order, configurations of boron, carbon and nitrogen atoms and on the lattice mismatch. By means of tight binding method and density functional theory, it is demonstrated that in graphene/h-BN analogue of AB bilayer graphene a substrate induced energy gap of about 50 meV should be opened in the spectrum [2, 3]. Using external electric field perpendicular to the layers, the band-gap can be continuously tuned up to 130 or 250 meV depending on the atomic configuration.

In contrast, in the unbiased ABC h-BN/graphene/h-BN sandwich the Dirac cones are exactly preserved in the band structure. It originates from the symmetry between A and B sublattices: it is not broken because both carbon atoms in the unit cell have identical neighbors (boron or nitrogen) either in the top or in the bottom layer. The external electric field breaks the structural symmetry and lifts the degeneracy of energy levels in the K/K' points, thus the band gap can be created in the biased system [4]. This unique mechanism of energy gap tuning in graphene-based systems seems to become useful in modern electronic devices.

Graphene is claimed to be a bridge between condensed matter physics and quantum electrodynamics (QED), in particular the Klein tunneling phenomenon provides the important knowledge of electron propagation through potential barriers [5, 6]. Since graphene/h-BN heterostructures are described in terms of tight binding Hamiltonians constructed in the same manner as for graphene layers, we will discuss the existence of massless or massive Dirac fermions, the chirality and charge conjugation symmetry. We will show that graphene/h-BN hybrids are interesting as complementary systems which should indicate features related to anomalies in Klein tunneling phenomenon.

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References

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Figures

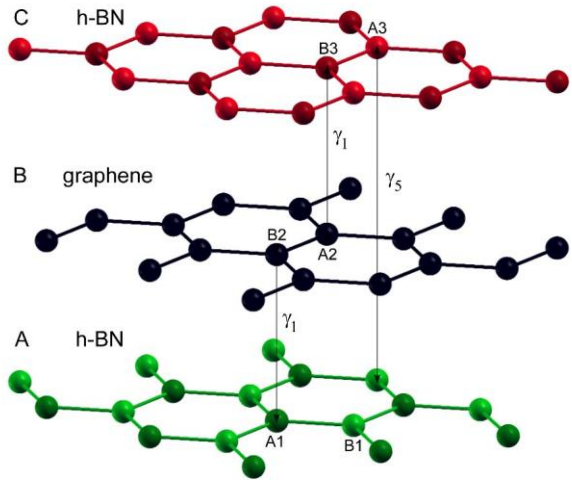

Fig. 1

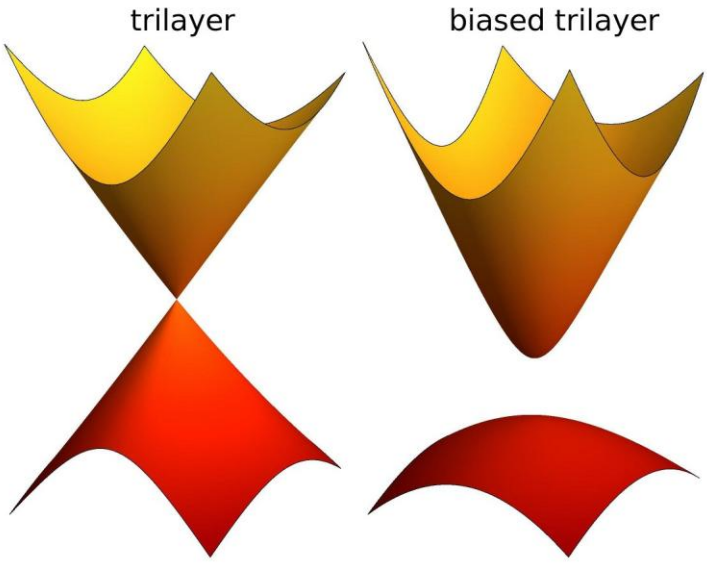

Fig. 2

Fig. 1 Geometry of ABC stacked h-BN/graphene/h-BN trilayer

Fig. 2 Energy gap tuning in ABC stacked h-BN/graphene/h-BN trilayer