**Modeling Electronic Properties of Single-layer and Multilayer Graphene**

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Recent experimental realizations of bilayer and trilayer graphene have opened the possibility of exploring their intriguing electronic properties, which depend dramatically on the stacking sequence of the graphene layers. It has been demonstrated that the band gap can be tuned from 0 to several hundred meV by applying voltage to a dual-gate bilayer or ABC-stacked trilayer graphene field-effect transistor (FET) at room temperature. These experimental observations are important for the applications of graphene in future electronics.

Just like the single-layer graphene, the bilayer and trilayer graphene samples in the real experiments always have different kinds of disorder or impurities, such as ripples, adatoms, admolecules, etc. One of the most important problems in graphene physics is to understand the effect of these imperfections on the electronic structure and transport properties, especially for the cases of gap opening under the perpendicular electronic field. Motivated by recent experiments, we performed a systemic study of the effects of different types of disorder or impurities to the electronic properties of single-layer and (gated or ungated) multilayer (including bilayer and trilayer) graphene [1-9].

We study this issue by direct numerical simulations of electrons on a honeycomb lattice in the framework of full pi-band tight-binding model. The magnetic field is introduced by means of the Peierls substitution. Numerical calculations based on exact diagonalization can only treat samples with relative small number of sites. For large graphene sheet with millions of atoms, the numerical calculation of an important property, the density of states (DOS), is performed by the time-evolution method. The time-evolution method is based on numerical solution of time-dependent Schrödinger equation with additional averaging over random superposition of basis states. We further extend this method to the calculation of various quantities by using the Kubo formula, such as the static and dynamical conductivity, polarization function, dielectric function, response function, and energy loss function. The effect of electron-electron interaction is considered within the random phase approximation (RPA). Another extension of the time-evolution method yields the quasieigenstate, a superposition of degenerate energy eigenstates. The Klein tunneling and quantum interference (Aharonov-Bohm effect) are studied by direct simulation of the wave packet propagation. Our numerical method allow us to carry out calculations for rather large systems, up to hundreds of millions of sites, with a computational effort that increases only linearly with the system size.

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