Magneto-Optical Properties of Antidot Lattices

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Periodic modulations of graphene, in the form of graphene antidot lattices, have been shown to produce sizable band gaps in the otherwise semimetallic graphene [1]. Such antidot lattices may be realized via, e.g., actual perforations of the graphene sheet [2], or using hydrogen adsorption [3]. We present theoretical results regarding the magneto-optical properties of such structures.

The individual antidots may be modelled in a variety of ways. As a first approximation, the effect of the antidots may be included by directly adding a band gap to graphene via a mass term in the Dirac equation (DE) or, equivalently, adding a staggered potential in a tight-binding (TB) description of graphene. We have compared the results of these two methods, and find that the inclusion of overlap between neighbouring pi-orbitals in a TB treatment has pronounced consequences for the optical Hall conductivity, that are entirely missed in a DE approach [4]. Further, we find that a sufficiently large band gap quenches the effect of the magnetic field.

To more accurately model the individual antidots, we have studied a DE model of a single graphene antidot, modelled via a circularly symmetric position-dependent mass term, in a magnetic field [5]. Here, analytical expressions can be derived for the spinor eigenstates, which in turn can be used to formulate an eigenvalue condition for the spectrum. In the limit of an infinite mass term, corresponding to, e.g., perforations in the graphene sheet, we present approximate analytical expressions for the energies. The resulting density of states exhibits a very rich structure, when the radius of the antidot is of the order of the magnetic length. The eigenstate stemming from the zeroth Landau level of ordinary graphene is localized predominantly at the edge of the antidot, regardless of the size of the mass term. By simulating STM measurements, we discuss the possibility of experimentally probing such localized states. Due to the nature of the spectrum at large negative values of the angular momentum, STM measurements will only indicate localized states for very specific, narrow energy ranges.

To treat the antidot lattices more accurately, we need to consider the exact atomic structure of the antidots. This is accomplished in a TB model, where a magnetic field is included via a Peierls substitution. However, the magnetic phase added to the overlap integrals in the TB model forces the calculations to be performed on a magnetic supercell which may contain several houndred antidot lattice unit cells. This results in structures with more than one million carbon atoms, for which direct diagonalization methods are unsuitable. Instead, we derive recursive relations for the diagonal optical conductivity and the density of states using recursive Greenôs functions, including periodic boundary conditions in both directions [6]. Using these methods, we discuss unique signatures of the graphene antidot lattices that are not captured in the simpler models.

References

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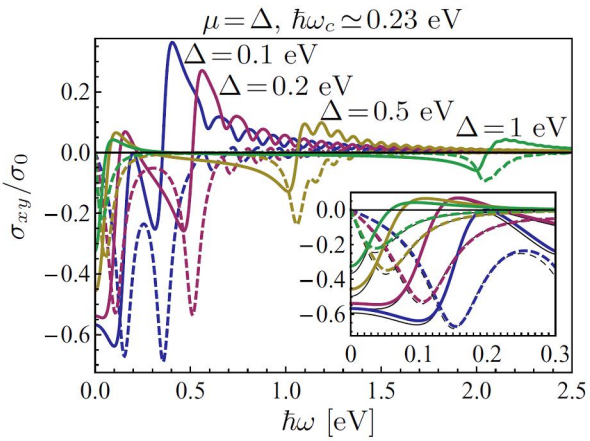
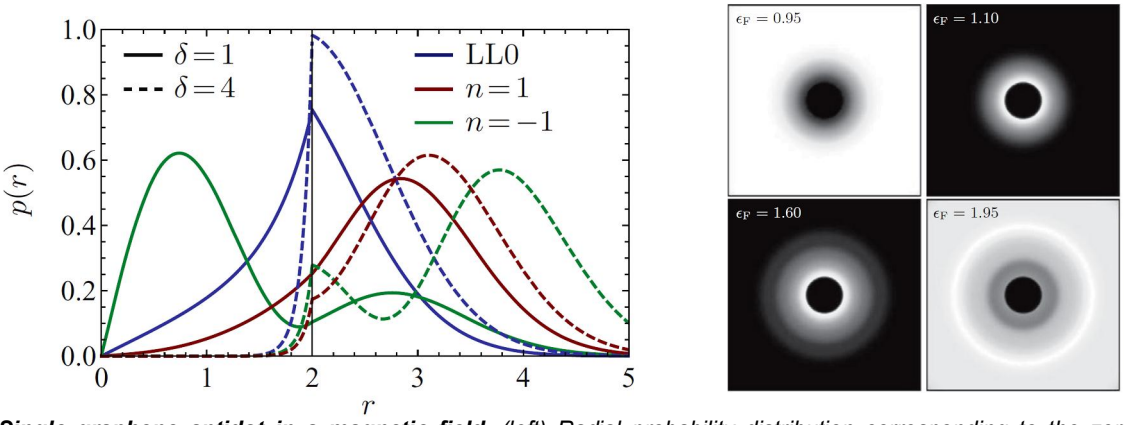
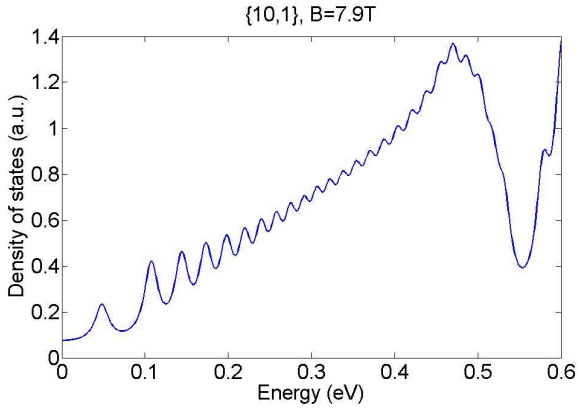
Figures



Gapped graphene in a magnetic field. *Optical Hall conductivity in units of the DC graphene conductivity. Results are shown for a magnetic field B = 78 T and for four different values of the mass term, all calculated using the TB model with overlap. The chemical potential is in each case fixed at the lowest Landau level. Full (dashed) lines indicate the real (imaginary) part of the conductivity. The inset shows a closer view of the first resonance. The results of the TB model without overlap are shown by thin, black lines, illustrating the slight discrepancies between the models in this regime. The DE results are practically identical to those of the TB model without overlap.*



Single graphene antidot in a magnetic field. *(left) Radial probability distribution corresponding to the zeroth Landau level (LL0) and the two states energetically above (n=1) and below (n=-1) the LL0 level. Results are shown for two different values of the mass term in units of the cyclotron energy. Note the unique behavior of the LL0 state, which remains localized near the antidot edge at r=2, measured in units of the magnetic length. (right) Simulated STM measurements, showing the tunneling current as a function of position for four different values of the Fermi energy.*



Graphene antidot lattice in a magnetic field. Density of states calculated for a structure containing roughly 1.2 million carbon atoms. The lower-energy features are well described by a gapped graphene model.