Peierls phase formulas for periodic systems under magnetic field

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The Peierls phase describes the orbital effect of a relatively weak magnetic field ***B***=∇×***A***, where ***A*** is the vector potential, on atomistic systems within a tight-binding-like Hamiltonian representation [1]. It is proportional to the line integral of ***A*** along the straight path between couple of orbitals and it changes under gauge transformations ***A***→***A***+∇χ, while its circulation and the physical observables are gauge independent. For periodic systems, under a generic gauge the Hamiltonian is not necessarily invariant under spatial translations, which could be inconvenient to allow the use of efficient techniques for electronic structure and transport simulations, as the so-called Sancho-Rubio algorithm [2] for determining the contact self-energies. In this contribution, I will provide a gauge choice and ready-to-use formulas to determine Peierls phase factors that preserve the translation symmetry of any periodic quasi-one-dimensional and two-dimensional systems under a homogeneous magnetic field [3]. I will show some interesting applications regarding a metallic carbon nanotube in high magnetic field and periodic 2D graphene with Gaussian bumps, where the induced strain makes Landau levels dispersive and lifts the valley degeneracy. The provided formulas represent a powerful tool for the simulation of electronic and transport properties of mesoscopic one- and two-dimensional systems in the presence of magnetic fields.

References

[1] R. Peierls, Zeitschrift für Physik, 80 (1933) 763
[2] M. P. Lopez Sancho et al., Journal of Physics F: Metal Physics, 15 (1985) 851
[3] A. Cresti, Physical Review B, 103 (2021) 045402

Figures

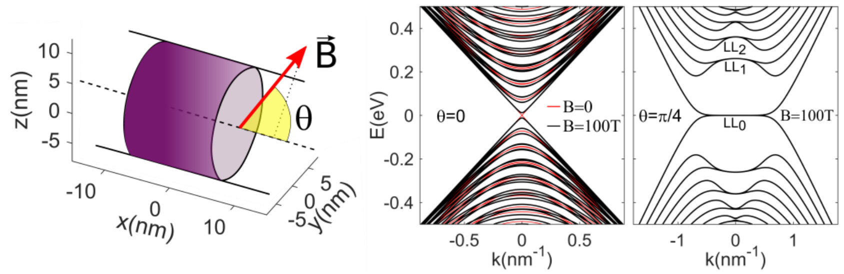

Figure 1: Sketch and band structure of a metallic carbon nanotube with 50 nm circumference in the presence of a magnetic field ***B*** at angle θ with the ribbon axis.

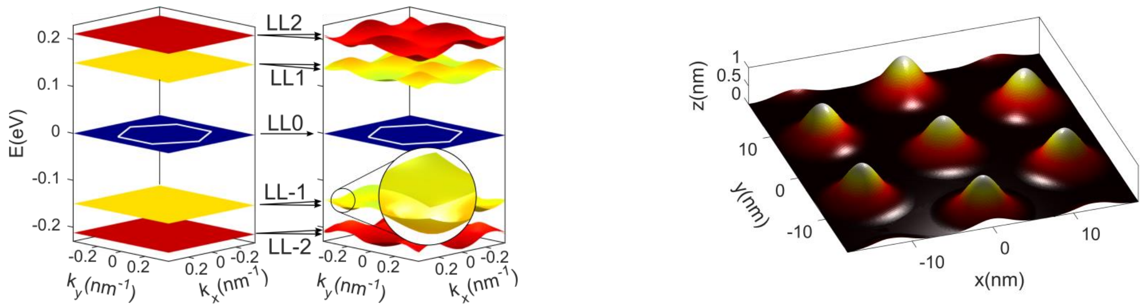

Figure 2: Low-energy bands in the absence (left) and in the presence (right) of the superlattice of a superlattice of bumps in two-dimensional graphene it (see sketch), under a 22.74 T orthogonal magnetic field. Strain makes Landau levels dispersive and removes the valley degeneracy, while the zero-energy Landau level does not change.