A practical Peierls phase recipe for periodic atomistic systems under magnetic fields

Alessandro Cresti[1]

[1] *Univ. Grenoble Alpes, Univ. Savoie Mont Blanc, CNRS, Grenoble INP, IMEP-LAHC, 38000 Grenoble, France*
alessandro.cresti@grenoble-inp.fr

The Peierls phase conveniently describes the orbital effect of a relatively weak magnetic field $\mathbf{B}$ on atomistic systems represented by a tight-binding-like Hamiltonian [1]. The phase multiplies the Hamiltonian elements between couples of atomic orbitals and is proportional to the line integral of the vector potential $\mathbf{A}$ (with $\mathbf{B} = \nabla \times \mathbf{A}$) along the straight path between them. The Peierls phase changes under gauge transformations $\mathbf{A} \rightarrow \mathbf{A} + \nabla\chi$, but its circulation as well as the physical observables are gauge independent.

For periodic systems, or systems with periodic components (as contacts and probes in a Hall bar), a generic gauge will not guarantee the Hamiltonian to be invariant under spatial translations. However, this invariance is desirable to allow the use of convenient techniques for electronic structure and transport simulations, as the Bloch theorem for the Hamiltonian diagonalization, or the Sancho-Rubio algorithm [2] for determining the contact self-energies.

In this contribution, by a proper gauge choice, I will provide general ready-to-use formulas to determine Peierls phase factors that preserve the translation symmetry of any periodic quasi-one-dimensional or two-dimensional system under a homogeneous magnetic field [3]. Some examples of applications will be briefly illustrated, see figures. First, I will present the case of a metallic carbon nanotube in high magnetic fields. Depending on the angle between field and nanotube axis, the electronic structure exhibits a rich physics ranging from Landau states to Aharonov-Bohm effect. Then, based on Green's function transport simulations, we will discuss the importance of disorder for the observation of extended Hall resistance plateaus in 2DEG Hall bars. Finally, I will present the case of periodic 2D graphene with Gaussian bumps, where the induced strain makes Landau levels dispersive and lifts the valley degeneracy.

The provided formulas represent a practical and useful tool for the simulation of electronic and transport properties of mesoscopic systems in the presence of magnetic fields.

[1] R. Peierls, Z. Phys., **80**, 763 (1933).
[2] M. P. Lopez Sancho et al., J. Phys. F, **15**, 851 (1985).
[3] A. Cresti, Phys. Rev. B., **103**, 045402 (2021).

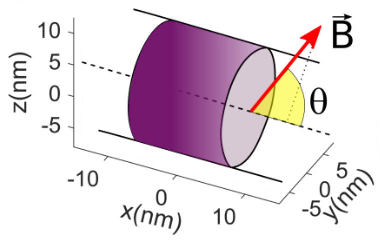

*Fig.1: Sketch of a metallic carbon nanotube with chirality (204,0), corresponding to a circumference of 50 nm. The homogeneous magnetic field **B** forms an angle θ with the nanotube axis.*

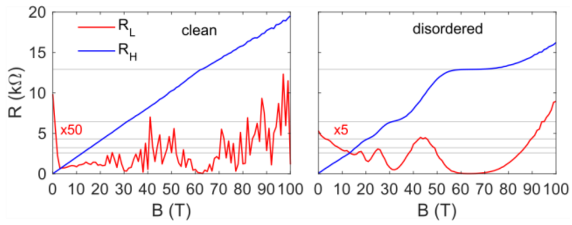

Fig.4: Longitudinal R_L and Hall R_H resistances as a function of the magnetic field B in clean and disordered Hall bars with the geometry illustrated in Fig. 3, for average charge density $3x10^{13}$ e/cm^2, temperature 77.36 K and drain current 0.1 μA. Hall plateaus are observed in the disordered case, in correspondence of the R_L dips. The horizontal lines indicate the resistance quantum $h/(2e^2)≈12.9$ kΩ and its submultiples.

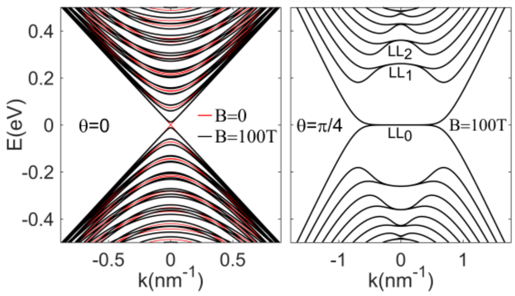

Fig.2: Band structure of the metallic carbon nanotube of Fig. 1 in the absence and in the presence of a 100 T magnetic field with θ=0 and 45°. The magnetic field along the nanotube axis opens a small gap due to Aharonov-Bohm effect. When the magnetic field is not along the nanotube axis, dispersive Landau levels appear.

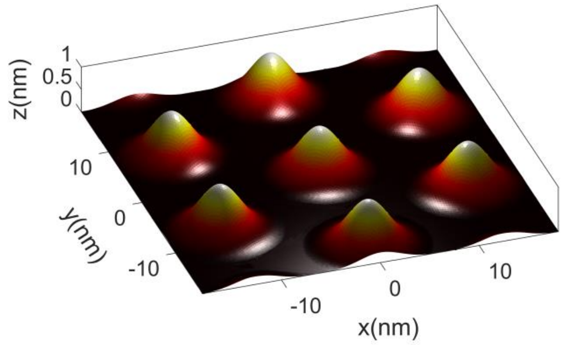

Fig.5: Superlattice of bumps in two-dimensional graphene. The bumps have a Gaussian profile with a height of 1 nm. This results in a tensile strain on the sides of the bumps. The superlattice is triangular and thus has a hexagonal Brillouin zone.

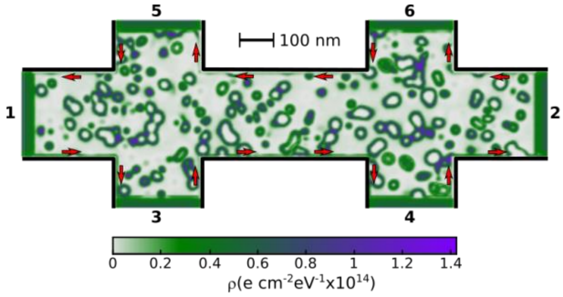

Fig.3: Six-terminal Hall bar obtained in a GaAs/AlGaAs 2DEG with effective mass 0.068 m_e. Terminals 1 and 2 are source and drain contacts, while terminals 3-6 are voltage probes. In the presence of impurities (here with density $7x10^{10}$ cm^{-2} and Gaussian potential profile with maximum height 150 meV) and under high magnetic fields, the current flows along the edges, while localized states form around the impurities, thus pinning the Fermi energy and leading to extended Hall resistance plateaus, see Fig. 4. The color map represents the density of states in such a situation. The red arrows indicate the current flow.

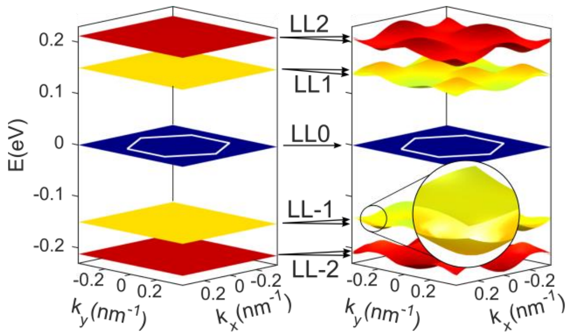

Fig.6: Low-energy band structure for 2D graphene in the absence (left) and in the presence (right) of the superlattice of periodic bumps described in Fig. 1, under a 22.74 T orthogonal magnetic field. The first Brillouin zone is indicated by a white hexagon. In flat graphene, the usual sequence of Landau levels appears. Strain makes Landau levels dispersive and removes the valley degeneracy. Only the Landau level with zero energy is unchanged, since its value is independent of the Fermi velocity of low energy electron, which is affected by strain.

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