P:05 Characterization of topological phase transitions in silicene and other 2D gapped Dirac materials

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In this work, we have studied the time evolution of electron wave packets in a monolayer of silicene under perpendicular magnetic and electric fields to characterize the topologicalband insulator transitions. We have found that the periodicities exhibited by the wave packets dynamics (zitterbewegung, classical and revival times) reach maximum values at the charge neutrality points (CNP). Additionally, we have discovered that electron currents reflect the transitions from a topological insulator to a band insulator at CPN too. These results are valid for other 2D gapped Dirac materials analogous to silicene with a buckled honeycomb structure and a significant spin-orbit coupling [1-4].

[1] E. Romera, J. C. Bolívar, J. B. Roldán and F. de los Santos, Revivals of electron currents and topological-band insulator transitions in 2D gapped Dirac materials, EPL, 115, 20008 (2016).
[2] M. Calixto and E. Romera, Inverse participation ratio and localization in topological insulator phase transitions, Journal of Statistical Mechanics, P06029 (2015).
[3] E. Romera and M. Calixto. Uncertainty relations and topological-band insulator transitions in 2D gapped Dirac materials. Journal of Physics: Condensed Matter, 27, 175003 (2015).
[4] M. Calixto and E. Romera. Identifying topological-band insulator transitions in silicene and other 2D gapped Dirac materials by means of Rényi-Wehrl entropy. EPL, 109, 40003 (2015).

P:06 study of ballistic transport in phosphorene--nanoribbon-- FETs using empirical pseudopotentials

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Among the 2D materials currently being considered as possible channel materials for future field--effect transistors, mono-- and multi--layer phosphorous (phosphorene) stands out for its promising fabrication and electron--transport properties: Experimental FETs have shown a high on-off current ratio and with a field--effect carrier mobility of the order of 10^3 cm^2/Vs in few--layer phosphorene [1]. Here we present an empirical--pseudopotential study of ballistic quantum transport in monolayer phosphorene in order to assess its potential application in nanoelectronics, following the methodology we have developed before [2].

BAND STRUCTURE CALCULATION AND TRANSPORT SIMULATION

Monolayer phosphorene exhibits a band gap of 1.5 eV [3]. In order to reproduce correctly this experimental observation, we have considered a previously proposed functional form for the local empirical pseudopotential phosphorous [4],

$$V_P(q) = \sum^{4} a_j e^{-b_j(q-c_j)^2}[1 - d_j e^{-f_j q^2}]$$

and calibrated it obtaining the band structure shown in Fig. 1. The pseudopotential for the H required to terminate the P dangling bonds was taken from Ref. 5 without modifications:

$$V_H(q) = \begin{cases} b_0 + b_1 q + b_2 q^2 + b_3 q^3 & \text{for } (q \leq 2) \\ b_{-1}/q + b_{-2}/q^2 + b_{-3}/q^3 + b_{-4}/q^4 & \text{for } (q > 2) \end{cases}$$