Method of Time Evolution of Quantum States in Real Space for Calculation of Electronic and Optical Properties of Twisted Bilayer Graphene

H. A. Le[1] and V.-N. Do[2,3]

Abstract: A computational method based on the time evolution of quantum states in real space is formulated to calculate the density of states and optical conductivity of twisted bilayer graphene systems with arbitrary twist angles. These two physical quantities are reformulated as the Fourier transform of relevant time-correlation functions which are defined as the scalar products of two state vectors generated by appropriately manipulating and developing in time initial random states. The Chebyshev polynomial expansion scheme is used to realize the time evolution and a stochastic technique is invoked to calculate the trace of large scale matrices. We demonstrate that the developed formulation is general and efficient to explore the electronic properties of the twisted bilayer graphene with small twist angles which are hardly accessed by Bloch's theorem-based methods. By investigating a series of configurations with the twist angle θ ranging from extremely tiny to large values we show that the commensurability is not the essential factor governing the physics of the twisted bilayer graphene. Particularly, when decreasing the twist angle to zero the unique van Hove singularity characteristic of the electronic structure can be realized when $\theta > 0.01^\circ$ and in the limit of $\theta \to 0$ the properties of the configurations continuously approach those of the original ($\theta = 0^\circ$) configuration.

[1,2] International Institute for Computational Science and Engineering,
Hanoi University of Science and Technology, 01 Dai Co Viet Street, Hai Ba Trung District, Hanoi, Vietnam
hoanganh.le@hust.edu.vn

[3] Advanced Institute for Science and Technology, Hanoi University of Science and Technology, 01 Dai Co Viet Street, Hai Ba Trung District, Hanoi, Vietnam
vannam.do@gmail.com