OPTIMIZED TECHNIQUE FOR THE CALCULATION OF CARBON NANOTUBE DISPERSION RELATIONSHIPS

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Carbon nanotubes are a very promising material for applications in many different fields, due to their small dimensions and to their remarkable physical properties. Indeed, the fact that they can have either a metallic or a semiconducting behavior, depending on their geometrical structure and on the applied magnetic field, together with the high current densities that they can handle and with their direct bandgap, makes them quite a promising material for electronics and optoelectronics. On the other hand, their large Young modulus, tensile strength and thermal conductivity, as well as their notable sensitivity to chemical interactions, make them suitable also for mechanical, thermal and chemical applications.

Since a single-wall carbon nanotube can be seen as a graphene sheet rolled up in a cylindrical shape along one of its lattice translational vectors (the chiral vector), many of its physical properties can be obtained from those of graphene, with the addition of a closure boundary condition along the chiral vector. This implies a discretization of the allowed graphene wave vectors along parallel segments of the reciprocal space; sectioning the graphene physical relations along these segments and folding them onto the nanotube Brillouin zone (located along the nanotube axis) we can obtain the correspondent nanotube relations. Such a technique (the so-called zone folding technique) is usually applied to the rectangular region of the graphene reciprocal space containing all the inequivalent graphene wave vectors and having an edge parallel to the nanotube axis and coincident with the nanotube Brillouin zone, in such a way as to easily fold the graphene relations.

Here we illustrate how this useful rectangular region, which can be taken as alternative primitive unit cell of the graphene reciprocal lattice, is related to the overall graphene reciprocal space. Since the usual unit vectors $\vec{b}_1$ and $\vec{b}_2$ in the graphene reciprocal space, corresponding to the commonly used graphene unit vectors $\vec{a}_1$ and $\vec{a}_2$ in the direct space, do not have a direct correspondence with such a rectangular region, we introduce an alternative choice of graphene unit vectors, which depends on the considered nanotube and which clarifies how the rectangular zone is repeated inside the graphene reciprocal space.

This choice of unit vectors allows to obtain, from any graphene wave vector, the equivalent vector inside the rectangular region in a computationally very inexpensive way. This can be fruitfully applied to significant graphene wave vectors, such as the ones corresponding to the graphene degeneration points. For example, when determining the nanotube dispersion relations from those of graphene through the zone folding technique, knowledge of the wave vectors equivalent to the graphene degeneration points, and located inside the rectangular zone where the zone-folding technique is applied, makes it possible to limit the computation only to the most interesting bands, thereby reducing the computational effort. In particular, we present an example of application of this technique to the computation of the graphene dispersion relations by means of the tight-binding method, with the inclusion of the contributions from up to the third-nearest neighbor atoms.