

# Tight-binding and $\mathbf{k} \cdot \mathbf{p}$ Methods in Carbon Nanotubes: Comparison, Results, and Improvements

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## INTRODUCTION

Carbon nanotubes are a very promising material for nanoelectronic applications, due to their very small size and to their peculiar physical properties. A carbon nanotube can be described as a graphene sheet rolled into a cylindrical shape. Its dispersion relations can be found from those of 2D graphite by enforcing a closure boundary condition.

## METHODS

The graphene energy bands can be found either using global methods (such as tight-binding), which provide results over the whole  $k$ -space, or local methods (such as  $\mathbf{k} \cdot \mathbf{p}$ ), which yield the correct energy bands only near their extrema, but with less computational effort. In particular, using the tight-binding method [1] and considering only the effect of the  $2p_z$  atomic orbitals (the most relevant for transport) as well as only nearest-neighbor interaction, we find the graphene energy dispersion relations reported in Fig. 1. Alternatively, if we insert the slowly varying electronic envelope functions into the tight-binding equations, around the extrema we obtain a  $\mathbf{k} \cdot \mathbf{p}$  Hamiltonian matrix, the eigenvalues of which give the  $\mathbf{k} \cdot \mathbf{p}$  dispersion relations of graphene [2]. Enforcing closure periodic boundary condition for graphene corresponds to considering cross-sections of the graphene energy bands along parallel segments; if we replot the thus found cross-sections in the nanotube Brillouin zone, we obtain the nanotube dispersion relations (Fig. 2). By differentiating the thus computed dispersion relations, it is then possible to obtain the density of states (DOS).

## COMPARISON AND IMPROVEMENTS

In Figs. 3-6 we show the results obtained with the two methods, in terms of energy bands and DOS, for two nanotubes with different circumference. The  $\mathbf{k} \cdot \mathbf{p}$  method yields quite good results for the bands obtained by cross-sectioning the graphene dispersion relations near their extrema. In particular, for nanotubes with larger circumference, the bands closer to the graphene extrema are better reproduced, due to the smaller distance between the parallel segments on which we take the cross sections of the graphene energy bands. Analogously, the DOS obtained with the  $\mathbf{k} \cdot \mathbf{p}$  method is very close to the one computed with the tight-binding approach for small values of the energy, corresponding to the energies for which the  $\mathbf{k} \cdot \mathbf{p}$  method provides a good approximation of the graphene energy bands. In these calculations  $\mathbf{k} \cdot \mathbf{p}$  is faster than tight-binding, not only because of the reduced complexity of the calculations, but also because in the  $\mathbf{k} \cdot \mathbf{p}$  approach (in which calculations are made relatively to the graphene extrema points) we can eventually limit ourselves to the determination of only the bands closest to the graphene extrema (which are the most interesting for transport analysis), while with tight-binding this choice of bands can be much more difficult. We propose an innovative procedure that, adopting an unusual choice of unit vectors in the reciprocal space, allows to easily select such bands in the tight-binding method.

## REFERENCES

- [1] R. Saito, G. Dresselhaus, and M. S. Dresselhaus, *Physical Properties of Carbon Nanotubes* (Imperial College Press, London, 1998).
- [2] T. Ando, *Theory of Electronic States and Transport in Carbon Nanotubes*, J. Phys. Soc. Jpn. **74**, 777 (2005).

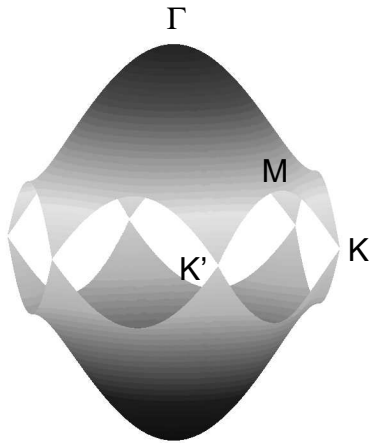


Fig. 1. Energy dispersion relations of the graphene within its Brillouin zone.

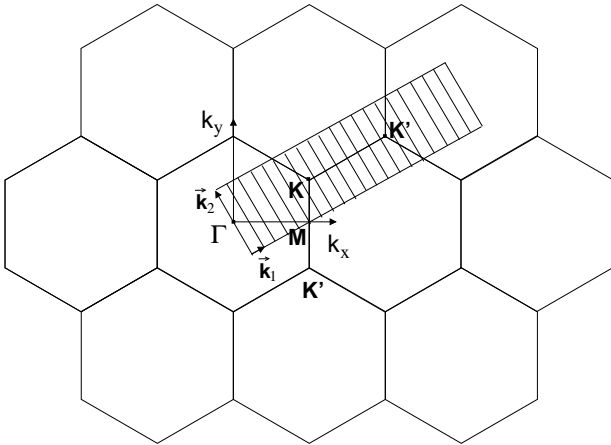


Fig. 2. The energy dispersion relations of the nanotube can be obtained from the ones of the graphene cross-sectioning them in correspondence of parallel segments.

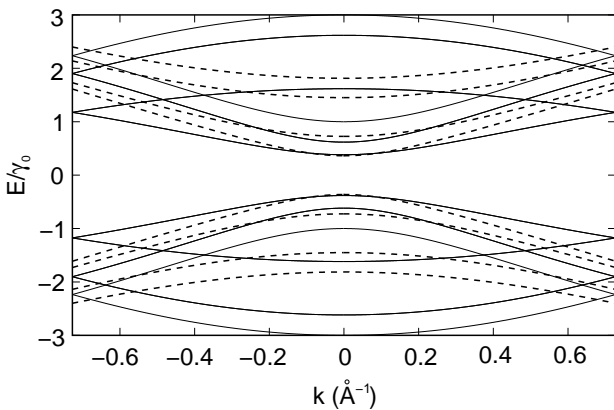


Fig. 3. Dispersion relations of the nanotube (5,0) computed with the tight-binding method (solid lines) and with the  $\mathbf{k} \cdot \mathbf{p}$  method (dashed lines);  $\gamma_0$  is the absolute value of the transfer integral between nearest-neighbor atomic orbitals.

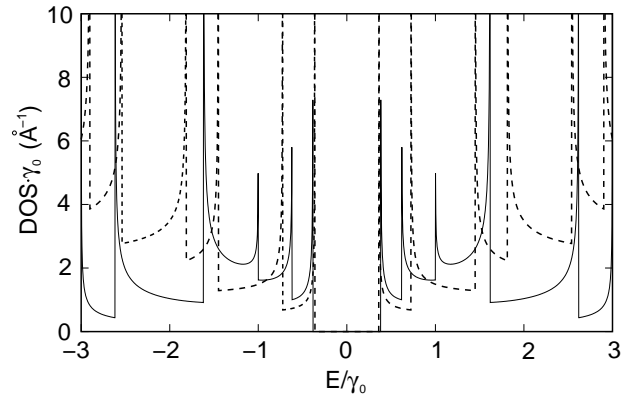


Fig. 4. Density of states of the nanotube (5,0) computed with the tight-binding method (solid lines) and with the  $\mathbf{k} \cdot \mathbf{p}$  method (dashed lines).

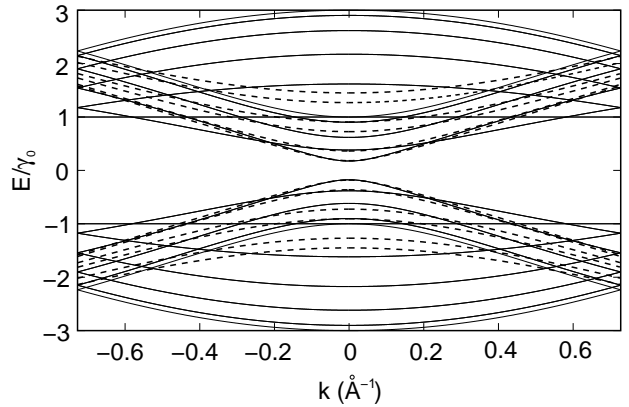


Fig. 5. Dispersion relations of the nanotube (10,0) (which has a circumference twice that of the nanotube (5,0)), computed with the tight-binding method (solid lines) and with the  $\mathbf{k} \cdot \mathbf{p}$  method (dashed lines).

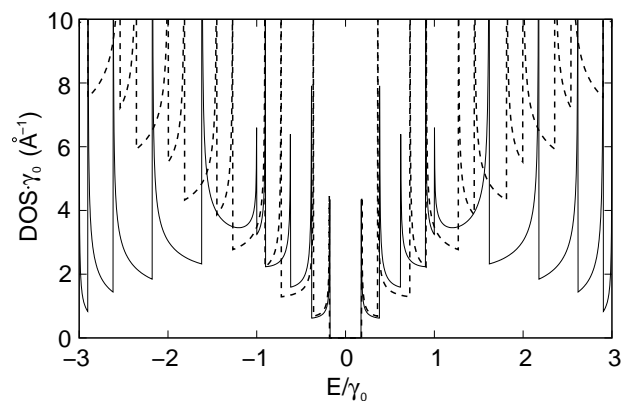


Fig. 6. Density of states of the nanotube (10,0) computed with the tight-binding method (solid lines) and with the  $\mathbf{k} \cdot \mathbf{p}$  method (dashed lines).