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Modeling graphene layers and single-walled carbon nanotubes with regularized δ-function potentials HAN HSU, L.E. REICHL, Center for Studies in Statistical Mechanics and Complex Systems, The University of Texas at Austin — Using *ab initio* methods to study the interaction between strong electromagnetic fields and thin films or crystalline materials would be extremely difficult. A common way is to use simplified models with several fitting parameters to simulate real physical systems. In this paper, we propose a model to simulate the π electrons in a graphene layer and single-walled carbon nanotubes. We let the atomic potential of each carbon atom be replaced by a two-dimensional attractive regularized δ function and construct a honeycomb lattice of regularized δ function to reproduce the band structure of a graphen layer and nanotubes. We also use this model to calculate the electron wave functions of nanotubes with finite length. The results are in good agreement with first principle calculations. With the accuracy and simplicity provided by this model, it can be a good candidate to study the interaction between the π electrons of nanotubes and electromagnetic fields in nonperturbative regime.

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