Application of the recursion method to the calculation of the optical absorption of double-walled carbon nanotubes

Valentin N. Popov
Faculty of Physics, University of Sofia, BG-1164 Sofia, Bulgaria
(Dated: May 15, 2020)

The calculation of the absorption spectrum of double-walled carbon nanotubes within the microscopic approach is hindered by their low symmetry. Here, we propose an efficient approach for tackling this problem by using the recursion method with non-orthogonal tight-binding basis functions. The application of this approach is illustrated in the case of a double-walled carbon nanotube, for which experimental optical data are available for comparison. Our study shows that the interlayer interaction can give rise to major changes in the electronic structure of the considered nanotube, manifesting themselves with shifts of the optical transitions and appearance of new optical transitions. The derived absorption spectrum is found to be in excellent agreement with the experimental data. It has to be noted that the experimental data can be explained satisfactorily assuming only shifts of the transitions, while however predicting incorrectly the origin of some of the optical resonances. Therefore, calculations within the microscopic approach can be crucial for the correct assignment of the measured optical spectra of double-walled carbon nanotubes.

I. INTRODUCTION

The double-walled carbon nanotubes (DWNTs) consist of two coaxial cylindrical graphitic layers, interacting with each other by weak Van der Waals interactions. These structures have attracted much attention because they are ideal systems to study the influence of the interlayer interaction on the physical properties. The characterization of the DWNTs is usually performed by means of several high-precision experimental techniques including spectroscopic ones with laser excitation, such as optical absorption, Raman and Rayleigh spectroscopies.

The spectroscopic signal from nanotubes is usually observed for laser excitation close to their optical transitions. Therefore, the optical characterization of the nanotubes requires the precise theoretical modeling of the optical properties of the nanotubes, and, in particular, deriving their optical transitions. The presence of helical symmetry of the layers allows for the reduction of the computational efforts for calculation of their optical transitions. In the approximation of neglecting the interlayer interaction, the optical properties of the DWNTs are determined solely by those of the layers and, in particular, the optical transitions of a DWNT are those of the two layers. While this approximation can be used for the quick assignment of the optical spectra to DWNTs with specific layers, it is often observed that the optical transitions of DWNTs are shifted with respect to the corresponding ones of the layers, the deviations being attributed to the interlayer interaction. Since the observed shifts can be as large as several tens of meV, the mentioned approximation can yield incorrect identification of the layers.

The estimation of the effect of the interlayer interaction on the optical transitions of the DWNTs has turned out to be a difficult computational problem because of the low symmetry of these structures. The shift of the optical transitions has been calculated by perturbation theory. Using the effective theory and atomic structure mapping, it has been revealed that the electronic structure of the DWNTs can undergo a wide range of interlayer-interaction induced changes. Recently, a number of optical resonances have been observed in the Rayleigh spectra of individual (free-standing) DWNTs, some of which cannot be connected to transitions of the layers. As far as we are aware, no investigation of the effects of the interlayer interaction on the electronic structure of DWNTs, performed within a realistic non-perturbative microscopic approach, has been reported.

Here, we study the effect of the interlayer interaction on the optical transitions of a particular DWNT by calculating the electronic density of states (DOS) and the absorption coefficient using the recursion method with non-orthogonal tight-binding (NTB) basis functions.

The paper is organized as follows. The theoretical background is presented in Sec. II. The obtained results are presented and discussed in Sec. III. The paper ends up with conclusions, Sec. IV.

II. THEORETICAL BACKGROUND

A powerful method for solving the eigenvalue problem for large sparse symmetric matrices for various applications has been proposed by Lanczos. In this method, one selects an initial vector, constructs Krylov subspaces by matrix-vector products, and performs a three-term recurrence to finally obtain a new matrix in a tridiagonal form. This algorithm is faster than the direct diagonalization methods only for sparse matrices, for which the multiplication of the matrix and the vector can scale linearly with the dimension of the matrix.

The Lanczos method finds a particular application to electronic structure calculations for non-crystalline solids, where the algorithm is generally referred to as the Lanczos - Haydock method or the recursion method. In the case of short-range interactions, it is advantageous to
use the tight-binding approximation, where the Hamiltonian, arising from the expansion of the wave function as a linear combination of atomic orbitals, is obtained in the form of a sparse matrix. The electronic DOS, electron density, total number of electrons, etc., are expressed through the real-space Green’s function. In the recursion method, the tight-binding Hamiltonian is tridiagonalized by the Lanczos method and the evolving Green’s function is expressed as a Jacobi continued fraction expansion.

In this Section, theoretical details on the calculation of the electronic DOS and the absorption coefficient, as well as on the recursion method, are provided.

A. The electronic density of states

The quantum-mechanical description of a solid is usually based on the stationary wave equation\(^{12}\)

\[
\hat{H}\psi_\lambda(r) = E_\lambda\psi_\lambda(r)
\]

(1)

where \(\hat{H}\) is the spin-independent Hamiltonian, \(\psi_\lambda(r)\) is the wavefunction, \(E_\lambda\) is the energy, and the index \(\lambda\) enumerates the solutions of the wave equation. In the NTB approach, the wavefunction is expanded as a linear combination of atomic orbitals

\[
\psi_\lambda(r) = \sum_\alpha C_\alpha^\lambda \varphi_\alpha(r)
\]

(2)

where \(C_\alpha^\lambda\) are expansion coefficients, \(\varphi_\alpha\) are atomic orbitals, and the index \(\alpha\) runs over the atomic orbitals in the solid: \(\alpha = 1, 2, \ldots, N\). The substitution of Eq. (2) in Eq. (1) results in the matrix eigenvalue equation

\[
\sum_\beta (H_{\alpha\beta} - E_\lambda S_{\alpha\beta}) C_\beta^\lambda = 0
\]

(3)

Here

\[
H_{\alpha\beta} = \int \varphi_\alpha^*(r) \hat{H} \varphi_\beta(r) d\mathbf{r}
\]

(4)

are the Hamiltonian matrix elements with respect to the atomic orbitals and

\[
S_{\alpha\beta} = \int \varphi_\alpha^*(r) \varphi_\beta(r) d\mathbf{r}
\]

(5)

are the overlap matrix elements, arising from the non-orthogonality of orbitals on different atoms. From the normalization condition for \(\psi_\lambda\)

\[
\int \psi_\lambda^*(r) \psi_{\lambda'}(r) d\mathbf{r} = \delta_{\lambda\lambda'}
\]

(6)

one obtains

\[
\sum_{\alpha\beta} C_\alpha^\lambda S_{\alpha\beta} C_\beta^{\lambda'} = \delta_{\lambda\lambda'}
\]

(7)

where \(\delta_{\lambda\lambda'}\) is the Kronecker delta.

The electron density is given by

\[
\rho(r) = 2 \sum_\lambda^{\text{occ}} |\psi_\lambda(r)|^2
\]

\[
= 2 \int_{-\infty}^{E_F} \sum_\lambda \delta(E - E_\lambda) |\psi_\lambda(r)|^2 dE
\]

(8)

where the summation over \(\lambda\) is carried out over all occupied states up to the Fermi energy \(E_F\) and the factor 2 accounts for the spin degeneracy; \(\delta(E - E_\lambda)\) is the Dirac delta function. In the last line of Eq. (8), Eq. (2) is used and the following notation is introduced

\[
\rho_{\beta\alpha} = \int_{-\infty}^{E_F} \rho_{\beta\alpha}(E) dE
\]

(9)

where

\[
\rho_{\beta\alpha}(E) = 2 \sum_\lambda \delta(E - E_\lambda) C_\alpha^\lambda C_\beta^{\lambda'}
\]

(10)

The DOS \(\rho(E) = 2 \sum_\lambda \delta(E - E_\lambda)\) can be written as

\[
\rho(E) = \sum_{\alpha\beta} \rho_{\alpha\beta}(E) S_{\alpha\beta}
\]

(11)

The matrix \(\rho_{\beta\alpha}(E)\) can be connected to the Green’s function \(G_{\beta\alpha}(E)\) \((\tilde{E} = E + i\eta, \eta \to 0^+)\)

\[
G_{\beta\alpha}(\tilde{E}) = \sum_\lambda (\tilde{E} - E_\lambda)^{-1} C_\alpha^\lambda C_\beta^{\lambda'}
\]

(12)

namely,

\[
\rho_{\beta\alpha}(E) = -(2/\pi) \text{Im} G_{\beta\alpha}(\tilde{E})
\]

(13)

Therefore, the knowledge of the Green’s function allows for the calculation of the DOS, Eq. (11).

B. The optical absorption coefficient

The one-photon optical absorption in nanotubes is usually observed for light polarization along the nanotube. The optical absorption coefficient can be expressed via the imaginary part of the frequency-dependent dielectric function \(\epsilon_2(\omega)\), given by\(^{12}\)

\[
\epsilon_2(\omega) \propto \frac{1}{\omega^2} \sum_{\lambda} \sum_{\lambda'} |p_{\lambda'\lambda}|^2 \delta(E_{\lambda'} - E_\lambda - \hbar\omega)
\]

(14)

where \(p_{\lambda'\lambda}\) is the momentum matrix element

\[
p_{\lambda'\lambda} = \int \psi_\lambda^*(r) \hat{p} \psi_\lambda(r) d\mathbf{r}
\]

(15)
and \( \hat{p} \) is the component of the momentum operator along the nanotube; \( \lambda \) runs over the occupied states and \( \lambda' \) runs over the unoccupied states.

Here, using Eq. (2), we cast the matrix element \( p_{\lambda'\lambda} \) in the form

\[
   p_{\lambda'\lambda} = \sum_{\alpha\beta} C_{\alpha}^{\lambda'} C_{\beta}^{\lambda} p_{\alpha\beta} \quad (16)
\]

where

\[
   p_{\alpha\beta} = \int \varphi_{\alpha}^*(\mathbf{r}) \hat{p} \varphi_{\beta}(\mathbf{r}) d\mathbf{r} \quad (17)
\]

In view of \( p_{\lambda'\lambda} = -p_{\lambda\lambda'} \), we get

\[
   |p_{\lambda\lambda'}|^2 = p_{\lambda\lambda'}^* p_{\lambda\lambda'} = - \sum_{\alpha\gamma\delta} C_{\alpha}^{\lambda'} C_{\gamma}^{\lambda} p_{\gamma\delta} C_{\delta}^{\lambda} p_{\delta\alpha} \quad (18)
\]

Introducing \( \rho_{\alpha\beta}(E) \), Eq. (10), \( \epsilon_2(\omega) \) becomes

\[
   \epsilon_2(\omega) \propto \frac{1}{\omega^2} \int dE \int dE' \sum_{\alpha\beta} p_{\alpha\beta}(E) p_{\beta\alpha}(E') \delta(E' - E - \hbar\omega) \quad (19)
\]

where \( p_{\alpha\beta}(E) = \sum_{\gamma} \rho_{\alpha\gamma}(E) p_{\gamma\beta} \). The integration is performed over the occupied states with energy \( E \) and the unoccupied states with energy \( E' \). It is clear that the calculation of \( \epsilon_2(\omega) \) requires the knowledge of \( \rho_{\alpha\beta}(E) \), but not of the wavefunction.

Finally, the absorption coefficient \( \alpha(\omega) \) can be evaluated approximately as

\[
   \alpha(\omega) \propto \omega \epsilon_2(\omega) \quad (20)
\]

### C. The recursion method

For the calculation of \( \text{Im} G_{\alpha\beta}(\hat{E}) \), the Hamiltonian \( H \) is tridiagonalized by the modified three-term recurrence

\[
   b_{i+1} u_{i+1} = (H' - a_{i} I) u_{i} - b_{i} u_{i-1} \quad (21)
\]

Here, \( H' = S^{-1} H \) is an \( N \times N \) matrix, \( I \) is an \( N \times N \) unit matrix, \( u_i \) are \( S \)-orthonormal column-vectors of size \( N \); \( u_i^T S u_j = \delta_{ij} \), \( \delta_{ij} \) is the Kronecker delta; \( a_i \) and \( b_i \) \( (i = 1, 2, \ldots, n, n \leq N, n \) is the number of iterations) are elements of the tridiagonal \( n \times n \) matrix

\[
   H_{TD} = \begin{pmatrix}
   a_1 & b_2 & \cdots & 0 \\
b_2 & a_2 & \cdots & 0 \\
   \vdots & \vdots & \ddots & \vdots \\
   0 & 0 & \cdots & a_n
   \end{pmatrix} \quad (22)
\]

During the recurrence procedure, partial reorthogonalization of \( u_i \) is performed to avoid the loss of orthogonality and appearance of ghost states due to the finite-precision arithmetic.

The recurrence, Eq. (21), can be written as the matrix equation

\[
   H' U = U H_{TD} \quad (23)
\]

where \( U \) is an \( N \times n \) matrix consisting of the column-vectors \( u_i \). The orthonormality condition for \( u_i \) can be written concisely as \( U^T S U = I \), where \( I \) is an \( n \times n \) unit matrix and \( U^+ \) is the Hermitian conjugate of \( U \).

Next, using Eq. (23), the following relation between the Green’s functions \( G = (\hat{E} S - H)^{-1} \) and \( G_{TD} = (\hat{E} I - H_{TD})^{-1} \) is readily derived

\[
   U^+ S G = G_{TD} U^+ \quad (24)
\]

The Green’s function \( G_{TD} \) is expressed as a Jacobi continued fraction expansion, which is terminated at the \( n \)th recursion level and the square-root terminator is used for the remainder of the expansion.

Equation Eq. (24) with a starting vector \( u_{1\beta} = \delta_{\alpha\beta} \) is reduced to \( G'_{\alpha\beta} = G_{TD,1\gamma} U'_{\gamma\beta} \), where \( G' = S G \). After evaluating \( G' \), the Green’s function \( G \) is found as \( G = S^{-1} G' \).

The overlap matrix \( S \) can be inverted by the recursion method as well. Indeed, the inverse of the overlap matrix can be written as \( S^{-1} = \text{Re} R(0) \), where \( \text{Re} \hat{E} = (S - \hat{E} I)^{-1} \) and \( I \) is an \( N \times N \) unit matrix.

### III. Results and Discussion

The calculations of the DOS and the absorption coefficient are performed with NTB parameters taken over from ab-initio calculations on carbon dimers. These parameters are used for deriving the Hamiltonian and overlap matrix elements between the \( s \), \( p_x \), \( p_y \), and \( p_z \) orbitals of the four valence electrons of the carbon atoms. Previously, the parameters have been used for the successful prediction of the electronic structure and optical absorption of single-walled carbon nanotubes (SWNTs) and twisted bilayer graphene. For better agreement with experiment, the transition energies of the SWNTs have been rigidly upshifted by 0.44 eV for transitions \( S_{33}, \ S_{34}, \ldots \). This correction is implied everywhere below.

Here, the proposed computational scheme is applied to the case of the DWNT (15, 13)@(21, 17), for which Rayleigh spectrum has been reported recently. In the usual DWNT notation, \( (15, 13) \) are the indices of the inner layer and \( (21, 17) \) are the indices of the outer layer. A long piece of the DWNT of length \( L \) and number of orbitals \( N \) (number of atoms \( N/4 \)) is considered. The atomic structure of the DWNT is relaxed as in Ref. Indeed, the recursion procedure is carried out with a number of iterations \( n \). In the calculations of the DOS and absorption coefficient, different values of \( L \), \( N \), and \( n \) are used, which are sufficient for deriving converged results in the energy interval between 1.5 and 2.9 eV. The large size of the considered piece of the DWNT ensures negligible influence of the edge states on the DOS and absorption coefficient.
A. The electronic density of states

Figure 1 presents the results for the DOS of the DWNT, obtained with $L = 2000$ Å, $N = 430000$, and $n = 5000$, in comparison with the DOS of the non-interacting layers. According to the selection rules for optical transitions for light polarization along the nanotube, the optical transitions take place between mirror spikes of DOS. The so-derived optical transitions of the inner ($i$) and outer ($o$) layers, denoted by $S^i$ and $S^o$, respectively, correspond within 0.01 eV to the already derived within the NTB model by solving Eq. 3 with direct diagonalization.

It is clear from Fig. 1 that the DOS of the DWNT undergoes major changes, most of the spikes being red or blue shifted with respect to those of the non-interacting layers. Since the number of spikes of the DOS of the DWNT corresponds to that of the layers, it is tempting to derive the optical transition of the DWNT similarly to the layers and adopt the same notation of the transitions. The so-derived optical transitions of the DWNT are given in Table I in comparison with those for the non-interacting layers and the experimentally measured ones. It is seen from Table I that the transitions of the DWNT are generally only slightly shifted with respect to those of the non-interacting layers except for $S_{44}^i$ and $S_{55}^o$, where the shifts are as large as $-0.18$ eV and $0.15$ eV, respectively.

Such a straightforward approach for derivation of the optical transitions of the DWNT rules out the appearance of additional optical transitions. On the other hand, the electronic structure of the DWNT is significantly modified with respect to that of the layers due to the interlayer interaction and, therefore, new transitions cannot be excluded a priori. For elucidating this problem, we plot in Fig. 2 the DOS of the DWNT in comparison with the contributions of the layers. It is seen in Fig. 2 that most of the spikes of DOS of the DWNT can be connected to one of the layers. However, the spikes, marked by vertical lines, have non-negligible contribution from both layers, which can be interpreted as a significant mixing of the electronic states of the two layers.

For understanding the mixing of the electronic states and the consequences of it, let us consider a pair of electronic states of the non-interacting inner and outer layers with wavefunctions $\psi^i$ and $\psi^o$, and close energies $E^i$ and $E^o$, respectively. The interlayer interaction will give rise to new pair of wavefunctions $\psi_k = \alpha_k \psi^i + \beta_k \psi^o$ with energies $E_k$, where $\alpha_k$ and $\beta_k$ are coefficients, $k = 1, 2$. Consider now pairs of wavefunctions $\psi^i$, $\psi^i$, and $\psi^o$, $\psi^o$ of occupied $(o)$ and unoccupied $(c)$ states of the non-interacting layers, between which optical transitions are allowed: $E^o_i \rightarrow E^c_i$ and $E^o_o \rightarrow E^c_o$. In the DWNT, because of the interlayer interaction, the latter two optical transitions will be doubled to $E_{o,1} \rightarrow E_{c,1}$, $E_{o,1} \rightarrow E_{c,2}$, $E_{o,2} \rightarrow E_{c,1}$, and $E_{o,2} \rightarrow E_{c,2}$.

It can be seen from Table I that the transitions $S_{44}^i$ and $S_{55}^o$ of the layers are very close, differing only by 60 meV. Therefore, in view of the arguments above, it can be expected that between the four spikes, connected to these transitions, there could be four transitions in the DWNT marked by the horizontal arrows and labeled by 1 to 4 in Fig. 2: two transitions between “mirror” spikes and two additional cross transitions with energies 2.26 eV and 2.31 eV (black arrows). Below, we identify the contribution of the four transitions to the calculated optical absorption coefficient of the DWNT.

### Table I. Optical transition energies (in eV) of the DWNT (first line) and the non-interacting layers (second line), derived from the separation between the “mirror” spikes of DOS, together with the shift of the former with respect to the latter (fourth line). Available experimental values are provided for comparison (third line).

| Layer | $S_{33}^i$ | $S_{44}^i$ | $S_{55}^o$ | $S_{66}^o$ |
|-------|-------------|-------------|-------------|-------------|
| DWNT  | 1.63        | 1.81        | 1.97        | 2.09        |
| layer | 1.54        | 1.83        | 1.95        | 2.27        |
| layer | 1.44        | 1.82        | 1.94        | 2.28        |
| shift | 0.09        | -0.02       | 0.02        | -0.18       |

B. The optical absorption coefficient

Figure 3 shows the calculated absorption coefficient of the DWNT, obtained with $L = 400$ Å, $N = 86000$, and $n = 1000$, in comparison with the volume-weighted av-
FIG. 2. The DOS of the DWNT (15,13)@(21,17) (black line) in comparison with the contributions of the inner layer (15,13) (blue line) and outer layer (21,17) (red line). The graph shows strong mixing of electronic states of the two layers at certain energies, marked by vertical lines. The red and blue horizontal arrows show transitions between “mirror” spikes related to transitions $S_{44}$ and $S_{55}$ of the layers, while the black horizontal arrows show cross transitions, induced by the mixing of the electronic states.

FIG. 3. The absorption coefficient of the DWNT (15,13)@(21,17) (thick black line) in comparison with that for a DWNT without interlayer interaction (thin red line). The red vertical lines mark the transitions of the layers. The black vertical line mark the transitions of the DWNT. The numbers 1 to 4 label the four transitions, shown in Fig. 2.

IV. CONCLUSIONS

We have applied the recursion method to the calculation of the DOS and absorption coefficient of the DWNT (15,13)@(21,17). This method has the advantage to describe the effect of the interlayer interaction within the quantum-mechanical picture without resorting to the perturbation theory. The recursion method is used with ab-initio derived NTB parameters, which yield realistic prediction of the optical transitions of layered carbon structures.

We have shown that the use of the recursion method with NTB basis functions allows predicting the absorption coefficient of the DWNT in excellent agreement with the experimental data. In particular, the calculations reveal that the interlayer interaction gives rise to strong mixing of certain electronic states of the layers and to major changes of the electronic structure, which may be accompanied by appearance of new optical transitions. Strong mixing of the electronic states can be expected if the two non-interacting layers have close optical transitions and there is a strong interaction between the electronic states of the layers. However, if the strong mixing of the states is not accounted for and a simpler explanation based on the transitions of the layers is adopted, the example, the resonance around 2.3 eV is predicted here to arise from such new transitions, rather than from shifted transitions of the layers.
conclusions for the origin of the related resonances may not be correct.

Finally, the presented computational scheme can be applied to other DWNTs and to twisted few-layer graphene.

**ACKNOWLEDGMENTS**

V.N.P. acknowledges financial support from the National Science Fund of Bulgaria under grant KP-06-N38/10-06.12.2019. V.N.P. thanks Profs. M. Paillet and J.-L. Sauvajol for useful discussions.

---

1. R. Pfeiffer, T. Pichler, Y.-A. Kim, and H. Kuzmany, Double-wall carbon nanotubes, in Carbon Nanotubes: Advanced Topics in the Synthesis, Structure, Properties and Applications, edited by A. Jorio, G. Dresselhaus, and M. S. Dresselhaus (Springer Berlin Heidelberg, Berlin, Heidelberg, 2008) pp. 495–530.
2. K. Liu, C. Jin, X. Hong, J. Kim, A. Zettl, E. Wang, and F. Wang, Van der Waals-coupled electronic states in incommensurate double-walled carbon nanotubes, Nature Physics 10, 737 (2014).
3. H. N. Tran, J.-C. Blancon, R. Arenal, R. Parret, A. A. Zahab, A. Ayari, F. Vallée, N. DelFatti, J.-L. Sauvajol, and M. Paillet, Quantum interference effects on the intensity of the g modes in double-walled carbon nanotubes, Phys. Rev. B 95, 205411 (2017).
4. D. Levshov, T. X. Than, R. Arenal, V. N. Popov, R. Parret, M. Paillet, V. Jourdain, A. A. Zahab, T. Michel, Y. I. Yuzyuk, and J.-L. Sauvajol, Experimental evidence of a mechanical coupling between layers in an individual double-walled carbon nanotube, Nanolett. 11, 4800 (2011).
5. K. Liu, X. Hong, M. Wu, F. Xiao, W. Wang, X. Bai, J. W. Ager, S. Aloni, A. Zettl, E. Wang, and F. Wang, Quantum-coupled radial-breathing oscillations in double-walled carbon nanotubes, Nature Communications 4, 1375 (2013).
6. S. Zhao, T. Kitagawa, Y. Miyauchi, K. Matsuda, and R. Kitaura, Rayleigh scattering studies on inter-layer interactions in structure-defined individual double-walled carbon nanotubes, Nano Res. 7, 1548 (2014).
7. S. Zhao, P. Moon, Y. Miyauchi, T. Nishihara, K. Matsuda, M. Koshino, and R. Kitaura, Observation of drastic electronic-structure change in a one-dimensional moiré superlattice, Phys. Rev. Lett. 124, 106101 (2020).
8. V. N. Popov and L. Henrard, Comparative study of the optical properties of single-walled carbon nanotubes within orthogonal and nonorthogonal tight-binding models, Phys. Rev. B 70, 115407 (2004).
9. M. Koshino, P. Moon, and Y.-W. Son, Incommensurate double-walled carbon nanotubes as one-dimensional moiré crystals, Phys. Rev. B 91, 035405 (2015).
10. C. Lanczos, An iteration method for the solution of the eigenvalue problem of linear differential and integral operators, J. Res. Natl. Bur. Stand. 45, 255 (1950).
11. R. Haydock, V. Heine, and M. J. Kelly, Electronic structure based on the local atomic environment for tight-binding bands: II, J. Phys. C: Solid State Phys. 8, 2591 (1975).
12. G. Grosso and G. P. Parravicini, Solid State Physics (Academic Press, Amsterdam, 2000) p. 857.
13. R. Jones and M. W. Lewis, Electronic charge densities and the recursion method, Phil. Mag. B 49, 95 (1984).
14. T. Ozaki, Efficient recursion method for inverting an overlap matrix, Phys. Rev. B 64, 195110 (2001).
15. V. N. Popov and C. VanAlsenoy, Low-frequency phonons of few-layer graphene within a tight-binding model, Phys. Rev. B 90, 245429 (2014).
16. T. Michel, M. Paillet, D. Nakabayashi, M. Picher, V. Jourdain, J. C. Meyer, A. A. Zahab, and J.-L. Sauvajol, Indexing of individual single-walled carbon nanotubes from raman spectroscopy, Phys. Rev. B 80, 245416 (2009).
17. V. N. Popov, Raman bands of twisted bilayer graphene, J. Raman Spectrosc. 49, 31 (2017).
18. V. N. Popov, D. I. Levshov, J.-L. Sauvajol, and M. Paillet, Computational study of the shift of the g band of double-walled carbon nanotubes due to interlayer interactions, Phys. Rev. B 97, 165417 (2018).
19. K. Liu, J. Deslippe, F. Xiao, R. B. Capaz, X. Hong, S. Aloni, A. Zettl, W. Wang, X. Bai, S. G. Louie, E. Wang, and F. Wang, An atlas of carbon nanotube optical transitions, Nature Nanotechnology 7, 325 (2012).