Semi-analytical theory of exciton fine structure in carbon nanotubes

Goupalov S.V.*[1,2]

[1]*Jackson State University, Jackson, MS 39217, USA*
[2]*Ioffe Institute, 194021, St.Petersburg, Russia*
**e-mail: serguei.goupalov@jsums.edu, goupalov@coherent.ioffe.ru*

Optical properties of single-walled carbon nanotubes (CNTs) are dominated by the excitonic effects. The high spin and subband (valley) degeneracy of the electron-hole pair ground state in the absence of the Coulomb interaction leads to a fine structure of excitonic levels when this interaction is taken into account.

It has been realized that both the long-range and the short-range parts of the Coulomb interaction are essential for a description of the exciton fine structure in CNTs. It has long been believed [1,2] that the best way to account for the short-range part of the Coulomb interaction in CNTs within the tight-binding method is to replace the Coulomb potential by the phenomenological Ohno potential of the form $V(r) = \frac{U}{\sqrt{\left(\frac{rU}{e^2}\right)^2 + 1}}$, where U is the energy cost to place two electrons on a single site.

We present an alternative approach whereby the matrix elements of the Coulomb potential are expanded into a series over CNT's one-dimensional reciprocal lattice vectors, $g_n = 2\pi n/|\boldsymbol{T}|$, where $\boldsymbol{T}$ is the CNT translational vector [3]. We show that, in order to make a non-vanishing contribution to this expansion, the reciprocal lattice vector g_n must satisfy the condition $|n| < N/M$, where N and M are the chirality-specific integers relating the chiral, $\boldsymbol{C}_h$, symmetry, $\boldsymbol{R}$, and translational, $\boldsymbol{T}$, vectors of the CNT by $N\boldsymbol{R} = \boldsymbol{C}_h + M\boldsymbol{T}$ [2] (N has meaning of the number of hexagons within the CNT unit cell).

We obtain analytical expressions for the Coulomb matrix elements which provide an insight into exciton physics which cannot be gained using a formalism based upon the phenomenological Ohno potential [1,2]. The calculated splittings between the dark and bright exciton states are in good agreement with the results of recent measurements [4,5].

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