Implications of time-reversal symmetry for band structure and optical properties of carbon nanotubes

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When single-particle electron states in single-walled carbon nanotubes (CNTs) are characterized by two-dimensional wave vectors with the components K_1 and K_2 along the CNT circumference and cylindrical axis, respectively, then two such vectors symmetric about a ***M***-point in the reciprocal space of graphene are shown to be related by the time-reversal operation. We show that to each CNT there correspond five relevant ***M***-points with the following coordinates [1]: $K_1^{(1)} = N/2R$, $K_2^{(1)} = 0$; $K_1^{(2)} = M/2R$, $K_2^{(2)} = -\pi/T$; $K_1^{(3)} = (2N-M)/2R$, $K_2^{(3)} = \pi/T$; $K_1^{(4)} = (M+N)/2R$, $K_2^{(4)} = -\pi/T$, and $K_1^{(5)} = (N-M)/2R$, $K_2^{(5)} = \pi/T$, where *N* and *M* are the integers relating the chiral, $\boldsymbol{C}_h$ symmetry, ***R***, and translational, ***T***, vectors of the CNT by $N\boldsymbol{R}=\boldsymbol{C}_h + M\boldsymbol{T}$ [2], $T=|\boldsymbol{T}|$, and *R* is the CNT radius. We show that the states at the edges of the one-dimensional Brillouin zone which are symmetric about the ***M***-points with $K_2 = \pm\pi/T$ are degenerate due to the time-reversal symmetry.

We also discuss implications of the time-reversal symmetry for optical properties of CNTs [3].

In addition to the ***M***-points, we obtain explicit expressions for the coordinates of the ***K***-points in the reciprocal space of graphene relevant to a given CNT. If for a (n,m) CNT, $(n-m)$ is not a multiple of $3d$, where d is the greatest common divisor of n and m, then the coordinates of the relevant ***K***-points (corresponding to the ***K*** and ***K'*** valleys, respectively) are $K_1 = N/3R$, $K_2 = 0$ and $K_1 = 2N/3R$, $K_2 = 0$. This case includes all semiconductor CNTs and some metal ones. In particular, all the zigzag CNTs ($m = 0$) belong to this case. For the armchair nanotubes $(n = m)$ one has $K_1 = n/R$, $K_2 = \pm 2\pi/3T$. For the rest of the metal CNTs the choice is to be made between the two cases: (i) $K_1 = (N-M)/3R$, $K_2 = 2\pi/3T$ and $K_1 = (2N+M)/3R$, $K_2 = -2\pi/3T$ and (ii) $K_1 = (N+M)/3R$, $K_2 = -2\pi/3T$ and $K_1 = (2N-M)/3R$, $K_2 = 2\pi/3T$. (Which case realizes for a particular chirality turns out to be a more subtle question.) Knowing the coordinates of the relevant ***K***-points greatly simplifies comparison of CNT descriptions within the zone-folding and effective-mass approaches.

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