Symmetry restrictions in the chirality dependence of physical properties of single-wall nanotubes

Fei Ye,[1] Bing-Shen Wang,[2] and Zhao-Bin Su[3,1]
[1]*Center for Advanced Study, Tsinghua University, Beijing 100084, China*
[2]*National Laboratory of Semiconductor Superlattice and Microstructure and Institute of Semiconductor, Academia Sinica, Beijing 100083, China*
[3]*Institute of Theoretical Physics, Academia Sinica, Beijing 100080, China*
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We investigate the chirality dependence of physical properties of nanotubes which are wrapped by the planar hexagonal lattice including graphite and boron nitride sheet, and reveal its symmetry origin. The observables under consideration are of scalar, vector, and tensor types. These exact chirality dependences obtained are useful to verify the experimental and numerical results and propose accurate empirical formulas. Some important features of physical quantities can also be extracted by considering the symmetry restrictions without complicated calculations.

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I. INTRODUCTION

Since the discovery of the carbon nanotube (CNT),[1] there have been extensive investigations on the unusual physical properties of this novel nanomaterial. The simplest CNT is the single wall carbon nanotube (C-SWNT) consisting of only one rolled up graphite sheet, which was first synthesized in 1993[2,3] and now can be produced in large scale.[4,5] As an analogue to the graphite, the III-V layered compound, namely boron nitride (BN) sheet, also has the hexagonal lattice structure and can be wrapped into various nanotubes too. The single-wall BN nanotube (BN-SWNT) was synthesized in 1996,[6] which also attracted much attention very recently.[7,8] Unlike the nonpolar C-SWNT, which could be metallic or semiconducting with a moderate gap,[9] this heteropolar nanotube is expected always to be a wide gap semiconductor.[10,11] Both of these two kinds of nanotubes have similar descriptions of their chiral structures and constitute promising materials for wide applications.[12]

The properties of nanotubes are determined by their chiral structures. Therefore, investigating the chirality dependence of various physical quantities of nanotubes is always interesting. Particularly, analyzing the chiral composition of bulk samples will be helpful to the production of nanotubes with different species. Numerous experimental and theoretical investigations are devoted to this subject.[13–22] Most recently, it has been reported that detailed chirality distributions in the bulk samples of the separated C-SWNT can be obtained by the fluorescence measurement and by the resonant Raman spectroscopy.[13,14] Their assignments of the chiral numbers (n_1,n_2) to the observed spectra are based upon the comparison between the tight-binding (TB) calculations and the experimental data.

In the fluorescence experiment,[13] the authors also gave the empirical formulas of the measured Van Hove singularities with respect to the structures of C-SWNTs, which are expressed in terms of the chiral angle θ and chiral index ν defined as $\theta \equiv \mathrm{atan}\sqrt{3}n_2/(2n_1+n_2)$ and $\nu \equiv \mathrm{mod}(n_1-n_2,3)$. Actually, for the purpose of giving the dependence of physical observables on the chiral structure of nanotubes, it is more suitable and efficient to use ν and θ instead of the chiral numbers (n_1,n_2). Since there are some types of nanotubes not being observed in the experiments or numerical calculations due to various reasons, an appropriate empirical formula is quite useful and convenient to predict the properties of those unobserved ones. Generally speaking, there are two possible methods to obtain these empirical formulas for different physical quantities. One is through fitting the numerical and experimental data, the other is from the analytical expansion around the two K points of the hexagonal Brillouin zone based on various TB models and effective-mass approximations. However, there are technical difficulties with the second method with regard to getting higher-order terms, which are sometimes important.

In this paper, we show the symmetry restrictions on the general chirality dependence of physical quantities of various types, such as scalar, vector, and tensor. This leads to compact forms of the chirality dependence for these observables on θ and ν. Since our method is *model-independent* and exact, it not only can be used to propose accurate empirical formulas from the numerical or experimental data, but also can indicate some important features of physical quantities without complicated calculations. The idea was originated in our previous study of the natural optical activity of C-SWNT.[22] Here, we generalize it to include both nonpolar C-SWNT and heteropolar BN-SWNT with large ionicity; application to the latter will lead to more interesting results.

This paper is organized as following. In Sec. II, we give a general analysis about the symmetry restriction on the chirality dependence. In Sec. III, we illustrate through examples that the θ and ν dependence of observables will be dramatically reduced by applying the symmetry arguments. The examples examined include the excitation gap, electric polarization, dielectric tensor, and piezoelectricity, which cover the scalar, vector, and tensor types of observables. Section IV contains our conclusions.

II. GENERAL ANALYSIS

In this section, we give a general description of our symmetry analysis for both the nonpolar (C-SWNT) and het-

eropolar (BN-SWNT) nanotubes. Considering a hexagonal lattice with base vectors $\vec{a}_1$ and $\vec{a}_2$, it can be rolled up into a nanotube along the chiral vector $\vec{R}=n_1\vec{a}_1+n_2\vec{a}_2$,[9] so that each nanotube can be simply represented by a pair of chiral numbers (n_1,n_2) and the chiral angle θ is just the angle between $\vec{R}$ and $\vec{a}_1$. We can then establish a mapping from the space of chiral vectors on the planar sheet to that of the nanotube structure in a fixed way of wrapping,

$$f:\{\text{chiral vector set}\} \mapsto \{\text{nanotube set}\}.$$

However this mapping is not one-to-one. For a given chiral vector $\vec{R}_0$ with chiral angle θ on the BN sheet with C_{3v} symmetry, there are two other equivalent vectors, obtained by rotating $\vec{R}_0$ by $2\pi/3$ successively, corresponding to the same nanotube. These vectors have the explicit forms

$$\vec{R}_0 = n_1\vec{a}_1 + n_2\vec{a}_2,$$

$$\vec{R}_2 = -(n_1+n_2)\vec{a}_1 + n_1\vec{a}_2,$$

$$\vec{R}_4 = n_2\vec{a}_1 - (n_1+n_2)\vec{a}_2. \quad (1)$$

All of them constitute an invariant subspace of the threefold symmetry of the BN sheet with the same chiral index ν. Another three relevant chiral vectors $\vec{R}_1$, $\vec{R}_3$, and $\vec{R}_5$ have chiral angle $\theta+\pi/3$, $\theta+\pi$, and $\theta+5\pi/3$, respectively, and can be written as

$$\vec{R}_1 = -n_2\vec{a}_1 + (n_1+n_2)\vec{a}_2,$$

$$\vec{R}_3 = -n_1\vec{a}_1 - n_2\vec{a}_2,$$

$$\vec{R}_5 = (n_1+n_2)\vec{a}_1 - n_1\vec{a}_2. \quad (2)$$

The nanotube mapping from $\vec{R}_1$ can be related to that from $\vec{R}_0$ by rotating the latter one around the horizontal x axis by π. In this paper, for convenience of discussion, the x axis is defined as passing through the center of the curved hexagon on the tube surface, the tube axis as the z axis, and the y axis is thus determined by the right-hand rule. Note that with this choice, the x axis, also known as the U axis (see Ref. 23 for details), is in fact a C_2 rotation symmetry axis for C-SWNT, but not for the heteropolar BN-SWNT.

In addition, there is another special chiral vector $\vec{R}_0'$, which is the reflection of $\vec{R}_0$ about the base vector $\vec{a}_1$ on the BN sheet and has the same chiral index ν of $\vec{R}_0$. When mapping onto a nanotube, it corresponds to the mirror image of that from $\vec{R}_0$ with respect to the section along the tube axis. For the graphite sheet, since the two atoms in one unit cell are the same, it has a higher symmetry C_{6v}. The six vectors $\vec{R}_i$ $(i=0,\ldots,5)$ all correspond to the same nanotube, which means that a C-SWNT may be represented by opposite chiral indices, ν and $-\nu$.

Briefly, through the mapping f the manipulations on $\vec{R}$ in the chiral vector set lead to the change of the structure in the nanotube set, and we have the following three observations:

(i) When $\theta \to \theta+2\pi/3$, the nanotube remains unchanged, and ν is also unchanged.

(ii) When $\theta \to \theta+\pi/3$, the nanotube is rotated around the horizontal x symmetry axis by π, and $\nu \to -\nu$.

(iii) When $\theta \to -\theta$, the nanotube is reflected with respect to the section along the tube axis, and ν is unchanged. According to the first observation, we know that the physical quantities of the nanotube can always be expanded in the Fourier series of θ with respect to each class of ν,

$$Q^{(\nu)}(\theta) = \sum_{n=0}^{\infty} a_n^{(\nu)}\cos(3n\theta) + b_n^{(\nu)}\sin(3n\theta). \quad (3)$$

Q is some physical quantity. The coefficients $a_n^{(\nu)}$ and $b_n^{(\nu)}$ are functions of those chirality-independent variables, such as the chiral vector length and some external parameters. Our analysis will reveal *the characteristic role of the chiral index ν in classifying the chirality dependence*. In the next section, we will consider some examples to show that the second and third observations together with features of the physical quantity under consideration will reduce the above chiral expressions Eq. (3).

III. APPLICATIONS: SEVERAL EXAMPLES

A. Excitation gap Δ

We can treat the band gap for the C-SWNT and BN-SWNT as a scalar since its value does not change under rotation or mirror reflection of the nanotube. Hence, its chiral angle dependence must satisfy

$$\Delta^{(\nu)}\left(\theta+\frac{\pi}{3}\right) = \Delta^{(-\nu)}(\theta),$$

$$\Delta^{(\nu)}(-\theta) = \Delta^{(\nu)}(\theta). \quad (4)$$

Notice that in the first expression in Eq. (4), ν becomes $-\nu$ when $\theta \to \theta+\pi/3$. Then, from Eq. (3) the chirality dependence of Δ reads

$$\Delta^{(\pm)}(\theta) = a_0 \pm a_1\cos(3\theta) + a_2\cos(6\theta) + \cdots,$$

$$\Delta^{(0)}(\theta) = a_0 + a_1\cos(6\theta) + a_2\cos(12\theta) + \cdots. \quad (5)$$

Clearly, the coefficients of $\cos(3\theta)$ for $\nu=\pm1$ should have the same value but opposite signs.

For the semiconducting C-SWNT with $\nu=\pm1$, the longitudinal optical excitation can be measured in the fluorescence experiment[13] and is quite useful in analyzing the chiral composition of bulk samples. In Ref. 13, the authors fitted the experimental data of the Van Hove singularities for $\nu=1$ and -1 separately. According to their fitting function, the absolute values of a_1 are quite different for $\nu=1$ and $\nu=-1$, which does not agree with the symmetry analysis Eq. (5) and suggests that it may need to consider higher-order terms like $\cos(6\theta)$ for more accurate fitting functions. In fact, we have tried to fit all their data for both $\nu=\pm1$ by just one four-parameter formula with a $\cos(6\theta)$ term

$$\frac{p_1}{R}+\frac{p_2}{R^2}+\nu\frac{p_3\cos 3\theta}{R^2}+\frac{p_4\cos 6\theta}{R^3}$$

which satisfies the symmetry restriction Eq. (5). It turns out that the result has a smaller root-mean-square deviation than that in Ref. 13.

Recently, an interesting temperature dependence of band gap $\Delta(T)$ was reported for the semiconducting C-SWNT in Ref. 24, that is, when θ is small, the temperature dependence of the gap is monotonic for $\nu=1$ and nonmonotonic for $\nu=-1$. This could be understood by assuming that both a_0 and a_1 are decreasing functions of temperature. Then from Eq. (5), it is clear that the band gap for $\nu=1$ is monotonically decreasing with temperature. For $\nu=-1$ and small chiral angle, the sign of a_1 is negative, so Δ can be nonmonotonic with temperature increasing as a result of the interplay between $a_0(T)$ and $a_1(T)$. However, when θ is close to $\pi/6$, the $\cos(3\theta)$ is nearly vanishing and only a_0 takes the dominant role, so that the temperature dependence of the band gap should behave similarly for both $\nu=1$ and -1.

B. Electric polarization (EP) $\vec{P}$

The macroscopic electric polarization along the nanotube axis is a consequence of the broken sublattice symmetry of BN-SWNT, which was studied as a geometric phase in Ref. 25. They found the sign and size of the longitudinal polarization are dramatically dependent on the chiral structure of the nanotube. This in fact has its symmetry origin, and we will show below that some remarkable properties of EP can be extracted by the symmetry analysis.

Due to the helical symmetry of the nanotube,[23,26,27] this EP vector only exists in the tube axis direction (z axis) and vanishes in the cross section (xy plane),[23,27,28] i.e., $P_z\neq 0$ and $P_{x,y}=0$. According to observations (ii) and (iii) and the vector nature of EP, we have

$$P_z^{(\nu)}\left(\theta+\frac{\pi}{3}\right)=-P_z^{(-\nu)}(\theta),$$

$$P_z^{(\nu)}(-\theta)=P_z^{(\nu)}(\theta), \tag{6}$$

which leads to the chirality dependence of P_z,

$$P_z^{(0)}(\theta)=a_1\cos(3\theta)+a_3\cos(9\theta)+\cdots,$$

$$P_z^{(\pm)}(\theta)=\pm a_0+a_1\cos(3\theta)\pm a_2\cos(6\theta)+\cdots. \tag{7}$$

Equation (7) shows that the armchair tubes ($n_1=n_2=N$) with $\theta=\pi/6$ and $\nu=0$ have no electric polarization. Other types of achiral tube, namely zigzag tubes ($n_1=N, n_2=0$), show different pictures. If we assume reasonably the coefficients of higher-order terms are small enough compared to the zero order term a_0, we then obtain $P_z^{(0)}\approx 0$ for $\mathrm{mod}(N,3)=0$ and $P_z^{(\pm)}\approx\pm a_0$ for $\mathrm{mod}(N,3)=\pm 1$, i.e., when N is increasing, the EP is oscillating among 1, 0, and -1, which is just the striking result of BN-SWNT found in Ref. 25.

For the C-SWNT, the sixfold C_{6v} symmetry in the chiral vector set guarantees $P_z^{(\nu)}(\theta+\pi/3)=P_z^{(-\nu)}(\theta)$, which combined with Eq. (6) leads to $P_z^{(\nu)}=0$, i.e., *no EP in C-SWNT*. This is consistent with the symmetry analysis of nanotubes.[23,27]

C. Dielectric tensor ϵ

This second-rank tensor is restricted to have the following form by the helical symmetry of nanotube:[23,27,28]

$$\epsilon=\begin{pmatrix}\epsilon_{xx} & \epsilon_{xy} & 0\\ \epsilon_{yx} & \epsilon_{yy} & 0\\ 0 & 0 & \epsilon_{zz}\end{pmatrix} \tag{8}$$

with $\epsilon_{xx}=\epsilon_{yy}$ and $\epsilon_{xy}=-\epsilon_{yx}$. The diagonal matrix elements of ϵ, denoted by ϵ_{ii} with $i=x,y,z$, have the same chirality dependence. Similar to the analysis of the EP vector, we obtain

$$\epsilon_{ii}^{(\nu)}\left(\theta+\frac{\pi}{3}\right)=\epsilon_{ii}^{(-\nu)}(\theta),$$

$$\epsilon_{ii}^{(\nu)}(-\theta)=\epsilon_{ii}^{(\nu)}(\theta),$$

$$\epsilon_{xy}^{(\nu)}\left(\theta+\frac{\pi}{3}\right)=-\epsilon_{xy}^{(-\nu)}(\theta),$$

$$\epsilon_{xy}^{(\nu)}(-\theta)=-\epsilon_{xy}^{(\nu)}(\theta) \tag{9}$$

by noticing that the diagonal term is unchanged when the tube is reversed or reflected, and the off-diagonal term gets its sign changed. Then

$$\epsilon_{ii}^{(\pm)}(\theta)=a_0\pm a_1\cos(3\theta)+a_2\cos(6\theta)+\cdots,$$

$$\epsilon_{ii}^{(0)}(\theta)=a_0+a_2\cos(6\theta)+a_4\cos(12\theta)+\cdots,$$

$$\epsilon_{xy}^{(\pm)}(\theta)=b_1\sin(3\theta)\pm b_2\sin(6\theta)+\cdots,$$

$$\epsilon_{xy}^{(0)}(\theta)=b_1\sin(3\theta)+b_3\sin(9\theta)+\cdots. \tag{10}$$

The coefficients a_n' and b_n' in the above four expressions have no direct relationships. Obviously, the diagonal and off-diagonal terms have quite different chirality dependence and the off-diagonal terms vanish for the zigzag tube, whose chiral angle is 0.

The discussion above is for the heteropolar BN-SWNT. For the C-SWNT, the higher symmetry requires $\epsilon_{xy}^{(\nu)}(\theta+\pi/3)=\epsilon_{xy}^{(-\nu)}(\theta)$, which together with Eq. (9) leads to $\epsilon_{xy}^{(\nu)}=0$ *for any kind of C-SWNT*.

D. Piezoelectricity e

Piezoelectricity is the response of the EP of the material to the mechanical strain, which is a third-rank tensor defined by the derivative of the EP vector with respect to the elastic strain tensor u,

$$e_{i,jk}=\frac{\partial P_i}{\partial u_{jk}}. \tag{11}$$

For the quasi-one-dimensional nanotube, we are concerned with the response of EP along the z direction to uniaxial (s) and torsional (t) strains, i.e.,

$$e_s = \frac{\partial P_z}{\partial u_s}, \quad e_t = \frac{\partial P_z}{\partial u_t}. \tag{12}$$

u_s is the stretch strain along the tube, and u_t is the torsional strain around the tube circumference. They can be related to the second-rank tensor u_{ij} in the Cartesian coordinates system through the following equation:

$$u_s = u_{zz}, \quad u_t = \frac{1}{r^2}(xu_{zy} - yu_{zx}) \tag{13}$$

with $r^2 = x^2 + y^2$. Through Eq. (13), it is clear that u_s and u_t transform under the rotation around the x axis by π or the mirror reflection with respect to the section along the tube axis. Consequently, we have

$$e_s^{(\nu)}\left(\theta + \frac{\pi}{3}\right) = -e_s^{(-\nu)}(\theta),$$

$$e_s^{(\nu)}(-\theta) = e_s^{(\nu)}(\theta),$$

$$e_t^{(\nu)}\left(\theta + \frac{\pi}{3}\right) = -e_t^{(-\nu)}(\theta),$$

$$e_t^{(\nu)}(-\theta) = -e_t^{(\nu)}(\theta), \tag{14}$$

and the chirality dependence of piezoelectricity then reads

$$e_s^{(\pm)}(\theta) = \pm a_0 + a_1 \cos(3\theta) \pm a_2 \cos(6\theta) + \cdots,$$

$$e_s^{(0)}(\theta) = a_1 \cos(3\theta) + a_3 \cos(9\theta) + \cdots,$$

$$e_t^{(\pm)}(\theta) = b_1 \sin(3\theta) \pm b_2 \sin(6\theta) + b_3 \sin(9\theta) + \cdots,$$

$$e_t^{(0)}(\theta) = b_1 \sin(3\theta) + b_3 \sin(9\theta) + \cdots. \tag{15}$$

Equation (15) implies the zigzag ($\theta=0$) tube can only have piezoelectric response to the longitudinal stretch and no response to the torsion strain around the circumference. On the contrary, the armchair ($\theta=\pi/6$ and $\nu=0$) tube has response to torsion strain but not to stretch strain. These conclusions are in agreement with the numerical results of the *ab initio* and TB calculations in Ref. 29, where the chiral angle by definition has a difference $\pi/2$ from ours. Apart from this difference in the θ definition, in Ref. 29 only $\cos(3\theta)$ and $\sin(3\theta)$ terms appear in the chirality dependence of e_s and e_t, respectively, while there are extra terms according to our results, Eq. (15). In fact, their θ dependence of e_s and e_t does not agree with their numerical data very well. The reason for this difference is that in Ref. 29 the chirality dependence of e_t and e_s is inherited from the BN planar sheet,[30] so that only the 3θ terms are permitted by the C_{3v} symmetry of the BN sheet. However, when the sheet is rolled up, this planar C_{3v} symmetry is broken, therefore those C_{3v}-forbidden terms are not forbidden any more, although they should be small by the continuous argument from sheet to nanotube, i.e., they vanish when the tube radius tends to infinity.

For the C-SWNT, the symmetry leads to additional restriction $e_\alpha^{(\nu)}(\theta+\pi/3) = e_\alpha^{(-\nu)}(\theta)$, which, combined with Eq. (14), requires $e_\alpha^{(\nu)}(\theta)=0$ for both $\alpha=s$ and t, namely, *for C-SWNT there should be no piezoelectricity along the tube, i.e., e_s and e_t due to its nonpolar feature.*

In the above discussion, the expansion coefficients $a_n^{(\nu)}$ and $b_n^{(\nu)}$ cannot be determined by the symmetry argument, which in fact depends on the chirality-independent parameters, such as the chiral vector length, magnetic flux, temperature, and so on. By tuning the external parameters, one can adjust the magnitude of $a_n^{(\nu)}$ and $b_n^{(\nu)}$, which will be helpful to identify the chirality of the tubes. As examples, one could refer to Refs. 22 and 24 to find the different dependence of these coefficients on magnetic flux or temperature.

IV. CONCLUSION

As a conclusion, we give the explicit θ dependence of physical quantities for different values of ν by a symmetry analysis. It shows clearly that the chiral index ν plays a characteristic role in describing the chirality dependence. This model-independent method may be used to verify the numerical and experimental data and also can give rise to some important properties qualitatively without complicated calculations. In addition, this method is not restricted to the examples illustrated in this paper and could be extended to other situations.

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