Induced Magnetic Moment in Defected Single-Walled Carbon Nanotubes

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Abstract. The existence of a large induced magnetic moment in defect single-walled carbon nanotube (SWNT) is predicted using the Green’s function method. Specific to this magnetic moment of defect SWNT is its magnitude which is several orders of magnitude larger than that of perfect SWNT. The induced magnetic moment also shows certain remarkable features. Therefore, we suggest that two pair-defect orientations in SWNT can be distinguished in experiment through the direction of the induced magnetic moment at some specific energy points.

1. Introduction
At the present stage, though intensive studies have been carried out to understand the deformed SWCNTs, there still exist many experimental and theoretical uncertainties about the intimate relationships between their electrical and mechanical properties. Also, how to measure the defect distribution and deformation degree remains a major challenge to the existing experimental techniques. Furthermore, only from the local densities of states (LDOS) and the corresponding conductance results, it is very difficult to clearly observe the structure of topological defects among many pair defect distributions in defected SWNT. Recently, Nakanishi et al. [1] suggested that the existence of large induced magnetic moment in a C_{60} molecular bridge. We think that the different quantum internal current caused by different defect will significantly produce different magnetic moment. Therefore, in this paper we first investigate the magnetic moment induced by quantum internal current in two types SWCNTs with different pair defect orientations — i.e., symmetric pair-defect and asymmetric pair-defect. The most interesting finding is that the magnetic moment could be increasing extensively, upto seven orders of the magnitude, due to the existence of pair defect, and obviously show different characteristics for two different pair defect orientations, which may provide a powerful experimental tool to measure precisely the defect distribution of defected SWCNTs.

We adopted a tight-binding Hamiltonian and follow the single-particle Green’s function formalism to obtain local density of states (LDOS), quantum conductance and induced magnetic moment within real-space renormalization techniques [2, 3, 4, 5]. This paper is organized as follows. In Sec.2, we present theoretical method and geometric structures. In Sec.3, we proceed numerical calculations and give discussions.
2. Theoretical Method and Model Geometry

We calculate the local density of states (LDOS) and quantum conductance to characterize the electronic properties within a tight binding description of the carbon bonds, which is given by

\[ H = \sum_{<i,j>,s} V_{pp\pi}(C^+_{i,s}C_{j,s} + C_{i,s}C^+_{j,s}). \]  

(1)

where the \(\sum_{<i,j>}\) is restricted to nearest-neighbor atoms, the two-center hopping integral \(V_{pp\pi}\) is \(-2.75\,eV\), on-site energies are set to zero, which means the Fermi energy is \(E = 0\,eV\). The internal current form site \(j\) to \(i\) is calculated from the Green’s function \(G^n\), usually referred to as a correlation function[1, 7]

\[ I_{ij} = \frac{4e}{\hbar} \text{Im}[H_{ij}G^n_{ij}]. \]  

(2)

The correlation function \(G^n\) is defined as \(G^n = G^R G^A\). The quantities \(G^a\) represent the retarded and advanced Green’s function of the heterojunction, and \(\Gamma_{L,R}\) are the couplings of the heterojunction to the left and right SWCNTs, respectively. The magnetic moment arising as a result of the quantum loop current also has interesting properties. Recall that the induced magnetic moment is expressed as

\[ M = \sum_{<i,j>} I_{ij}(\mathbf{r}_i \times \mathbf{r}_j)/2. \]  

(3)

where the summation is taken over each pair, \(ij\), whose corresponding Hamiltonian matrix element is nonzero, and \(\mathbf{r}_i\) indicates the coordinates of the site \(i\).

Figure 1. The geometry structures of two orientations of pair defect: the left two figures are \((5,5)\) tubes and the right figures are \((9,0)\) tubes, respectively. The top figures show symmetric orientation and the bottom figures show asymmetric orientation.

Here, we have studied two kinds of different chiral SWCNTs in detail, for which, for comparison, the original length of the central part is taken to be equal, containing three unit cells for the armchair tube \((5,5)\) and zigzag one \((9,0)\). On the base of our previous work [8], we had constructed the structures of pair defect through Stone-Whales transformation. In this work, all \(z\) axis is along the axis of tube, and the center of pair defect is taken on the \(x\)–\(axis.\)
3. Results and Discussion
Firstly, we calculate the electronic properties and quantum conductance of perfect (5,5) and (9,0) tube. According to our previous work[8], the propagating electron will be localized at sites near the pair defects: for symmetric pair defects this is mainly at sites 1 and 2, but for asymmetric pair defects the localized states are still very strong at sites 3-6. It is very difficult to distinguish the difference between these two types of defect orientations in (5,5) tube (or (9,0) tube) only from their LDOS and conductance.

The calculated magnetic moment along the three axes, x, y and z, are shown in Fig. 2 and Fig.3. Firstly, for all these two perfect tubes without any defect do not have the x component of magnetic moment. For perfect (9,0) tube, there is y component of magnetic moment only, which increases step-like with the increasing of energy. For perfect (5,5) tube, the y and z components of magnetic moment only show some large peaks near the corresponding energies of LDOS peaks. Furthermore, if the unit of magnetic moment is taken as AÅ², the induced magnetic moment in perfect tube is very small, only about $10^{-9}$ for (5,5) tube and $10^{-7}$ in magnitude for (9,0) tube, respectively. In contrast, the magnetic moment of defected tubes is several orders of magnitude larger than the perfect ones, i.e., about seven orders higher for

![Figure 2](image.png)  
**Figure 2.** The induced magnetic moment in (5,5) tube having pair defect with two orientations, respectively.

![Figure 3](image.png)  
**Figure 3.** The induced magnetic moment in (9,0) tube having pair defect with two orientations, respectively.
defected (5,5) tubes and five orders for defected (9,0) tube, respectively. It shows that in perfect metallic tube the localization length of electron is very long and almost have not quantum internal current, which is in good agreement with the result of ballistic transport of electron in perfect metallic SWNT[9, 10].

However, when there is pair defect, the propagating electron will be scattered near the defect region and some will be bounded in this region. Due to the bounded electrons and the scattering, quantum internal current can be generated near the defect region. Furthermore, the different defect structure causes different localization behaviors of propagation electrons near it. These effect can be obviously seen in the induced magnetic moment(see in Fig.2 and Fig.3). For symmetric pair-defect orientation in (5,5) tube, not only do the sharp peaks disappear in magnetic moment along three axis compared with perfect tube, but also the x and z components of magnetic moment both disappear. Comparing with the magnetic moment in these two pair defect orientations, one remarkable difference is the behavior near −3.64eV. For symmetric situation, only y-component has nonvanishing value and shows one peak, but for asymmetric situation, both z- and y-components have one peak near this energy. Thus, through the experiment value and direction of magnetic moment around the energy −3.64eV we can distinguish these two types of pair-defect in (5,5) tube. From Fig.3, the different features between these induced magnetic moment are also obvious in two defected (9,0) tubes. One remarkable difference between them is the peak of magnetic moment z component near energy 3.7eV: for symmetric situation of pair defect the z components is negative, but for asymmetric situation, the z component is positive.

In summary, the magnetic moment induced by quantum internal current and the influence of pair-defect orientation on magnetic moment are studied in defected SWNT. The most interesting finding is that the magnetic moment could increase extensively by several orders of the magnitude due to the existence of pair defect, and obviously show different characteristics for two different pair-defect orientations. We suggest that two pair defect orientations can be distinguished by the direction and value of the induced magnetic moment at some specific energy points, which may provide a powerful experimental tool to measure precisely the defect orientation of defected SWCNTs.

Although the calculated magnetic moment is related to the coordinates of atoms in models, we find the main results and characteristics based on the optimized models by using Universal Force Field(UFF)[11] will not change.

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References
[1] Nakanishi S and Tsukada M 2001 Phys. Rev. Lett. 87 126801
[2] Kubo R 1957 J. Phys. Soc. Jpn. 12 570
[3] Nardelli M B 1999 Phys. Rev. B 60 7828
[4] Ferreira M S, Dargam T G, Muniz R B and Latge A 2000 Phys. Rev. B 62 16040
[5] Ferreira M S, Dargam T G, Muniz R B and Latge A 2001 Phys. Rev. B 63 245111
[6] Nardelli M B and Bernholc J 1999 Phys. Rev. B 60 16338
[7] Datta S 1995 Electronic Transport in Mesoscopic Systems (Cambridge: Cambridge University Press)
[8] Liu H, Chen J W and Yang H T 2004 Phys. Stat. Sol. B 241 127
[9] Tans S J, Devoret M H, Dai H, Thess A, Smalley R E, Geerligs L J, and Dekker C 1997 Nature (London) 386 474
[10] Bockrath M et al. 1997 Science 275 1922
[11] Yao N, Lordi V 1998 J. Appl. Phys. 84 1939