The quantum phase transition of phonons in single-walled nanotubes

2008 J. Phys.: Condens. Matter 20 095223

(http://iopscience.iop.org/0953-8984/20/9/095223)

J. Phys.: Condens. Matter **20** (2008) 095223 (4pp) doi:10.1088/0953-8984/20/9/095223

The quantum phase transition of phonons in single-walled nanotubes

Feng Peng

Physics Department, Beijing University of Science and Technology, Beijing 100083, People's Republic of China

Received 13 November 2007, in final form 30 January 2008
Published 14 February 2008
Online at stacks.iop.org/JPhysCM/20/095223

Abstract

A magnetic field not only changes the electronic states in a carbon nanotube, but also affects the atomic displacement fluctuation through the electron–phonon interaction. In the presence of a magnetic field, the fluctuation may be related to the magnetism due to the phonon excitations. In this work, we calculate the atomic displacement fluctuation for the nanotubes at different magnetic field strengths, and the magnetic moment per lattice point generated by the phonon excitations. Both the existence of the minimum fluctuation and the change of the magnetic moment direction indicate that there is a quantum phase transition of phonons.

(Some figures in this article are in colour only in the electronic version)

The phonon spectrum and the electron–phonon scattering in carbon nanotubes have been intensively investigated [1–7]. However, little attention was paid to the effect of the external magnetic field on the phonons. It is known that a high magnetic field may lead to a metal–insulator transition [8–10]. If the high magnetic field is applied normal to the carbon nanotube axis, it can significantly modify the electronic energy spectrum and convert the electronic properties of the nanotube. The change of the electronic states would affect the lattice vibrations through the electron–phonon interaction. In order to clarify this problem, it is necessary to study the effect of the magnetic field on the atomic displacement fluctuation, for atomic displacement fluctuation is not only related to the phonons themselves, but also related to the electron–phonon interaction; larger fluctuation means the stronger electron–phonon interaction at a particular temperature and vice versa. On the other hand, when the atomic displacement fluctuation takes its minimum value, the phonon system is most stable for when the fluctuation is proportional to the mean phonon energy.

We adopt a single-orbital nearest-neighbour tight-binding model to describe the Hamiltonian, and use a modified functional integral approach to calculate the atomic displacement fluctuation [11–16]. In the Hamiltonian, the first-order term of atomic displacement in the expansion of the exchange integral represents the electron–phonon interaction. In the calculation of the generating function (partition function), the integral variables corresponding to the electrons are represented by the row matrix and the column matrix composed of the creation operators and the annihilation operators in the Wannier representation. We apply the classical string concept to calculate the functional integral over the atomic displacement variables [17].

In the next section, we first of all derive the generation function, and then calculate the atomic displacement fluctuation as well as the magnetic moment generated by phonon excitations. Finally we give a conclusion.

The magnetic field applied normal to the nanotube axis is described by the vector potential $\vec{A} = -Bz\vec{e}_y$, where B is the magnetic field strength, z the coordinate along the nanotube axis, and $\vec{e}_y$ the unit vector in the y-axis direction. In practice, only when the magnetic field is along this direction will a significant Aharonov–Bohm effect occur. The structure of the nanotube with armchair ends is shown in figure 1. There are two types of atom, denoted by $A_{m,n}$ and $B_{m,n}$. Here m is the row index along the tube axis and n the periodic index of atomic arrangement along the circumference. The nanotube is assumed to be composed of M rows along the axis and N periods along the circumstance. Then the diameter of the nanotube is $d = (\sqrt{3}+2)Na/\pi$, while the length is $l = \sqrt{3}Ma/2$. In what follows, we use N and M to denote the diameter and the length, respectively. The Peierls phase due to the application of the magnetic field is incorporated in the exchange integral defined as [18, 19] $V_{m,n,i;m',n',j} \to V_{m,n,i;m',n',j} \exp(\frac{ie}{\hbar c}\int_{m,n,i}^{m',n',j}\vec{A}\cdot d\vec{l})$, where e is the electronic charge, c the light speed in the vacuum, and $\hbar$ the Planck constant divided by 2π. In the Wannier representation, the Hamiltonian of the system is

$$H = \Psi^{+}_{m,n} E_{m,n} \Psi_{m,n}, \tag{1}$$

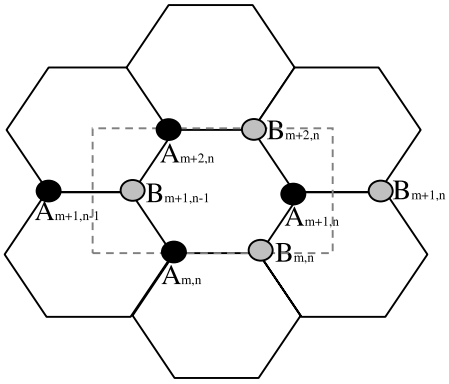

Figure 1. The atomic arrangement of the nanotube with armchair ends. The rectangle with the dashed line is a larger unit cell used as calculating the atomic displacement fluctuation of nanotubes. The magnetic field is applied normal to the nanotube axis.

where $E_{m,n}$ is a 7×7 matrix, its non-zero elements are

$$(E_{m,n})_{1,1} = 3(E_{m,n})_{2,2} = \frac{2}{1+\delta_{m,1}}(E_{m,n})_{3,3} = \frac{2}{1+\delta_{m,M-2}}(E_{m,n})_{4,4} = \frac{2}{1+\delta_{m,M-2}}(E_{m,n})_{5,5} = \frac{2}{1+\delta_{m,1}}(E_{m,n})_{6,6} = \frac{3}{2}(E_{m,n})_{7,7} = \varepsilon_0 \tag{2}$$

$$(E_{m,n})_{1,2} = (E_{m,n})^*_{2,1} = \tfrac{1}{4}[V_0 + \vec{\alpha}\cdot(\vec{u}_{m+1,n,B} - \vec{u}_{m+1,n,A})]\mathrm{e}^{\mathrm{i}\phi^1_{m,n}}, \tag{3}$$

$$(E_{m,n})_{1,3} = (E_{m,n})^*_{3,1} = \tfrac{1}{4}[V_0 + \vec{\alpha}\cdot(\vec{u}_{m,n,B} - \vec{u}_{m,n,A})]\mathrm{e}^{\mathrm{i}\phi^2_{m,n}}, \tag{4}$$

$$(E_{m,n})_{1,4} = (E_{m,n})^*_{4,1} = \tfrac{1}{4}[V_0 + \vec{\alpha}\cdot(\vec{u}_{m+1,n,A} - \vec{u}_{m+2,n,B})]\mathrm{e}^{\mathrm{i}\phi^3_{m,n}}, \tag{5}$$

$$(E_{m,n})_{3,6} = (E_{m,n})^*_{6,3} = \tfrac{1}{4}[V_0 + \vec{\alpha}\cdot(\vec{u}_{m,n,B} - \vec{u}_{m,n,A})]\mathrm{e}^{\mathrm{i}\phi^1_{m-1,n}}, \tag{6}$$

$$(E_{m,n})_{4,5} = (E_{m,n})^*_{5,4} = \tfrac{1}{4}\delta_{m,M-2}[V_0 + \vec{\alpha}\cdot(\vec{u}_{m+2,n,B} - \vec{u}_{m+2,n,A})]\mathrm{e}^{\mathrm{i}\phi^1_{m+1,n}}, \tag{7}$$

$$(E_{m,n})_{5,7} = (E_{m,n})^*_{7,5} = \tfrac{1}{4}[V_0 + \vec{\alpha}\cdot(\vec{u}_{m+2,n,A} - \vec{u}_{m+1,n-1,B})]\mathrm{e}^{\mathrm{i}\phi^4_{m,n}}, \tag{8}$$

$$(E_{m,n})_{6,7} = (E_{m,n})^*_{7,6} = \tfrac{1}{4}[V_0 + \vec{\alpha}\cdot(\vec{u}_{m,n,A} - \vec{u}_{m+1,n-1,B})]\mathrm{e}^{\mathrm{i}\phi^5_{m,n}}, \tag{9}$$

and other elements are all zeros, where

$$\phi^1_{m,n} = 2m\gamma\cos\left(\frac{\pi}{N}\left|\sin\left(m\frac{\pi}{2}\right)\right| + \frac{2\pi(n-1)}{N} - \frac{\pi}{3N}\right)\sin\left(\frac{\pi}{3N}\right), \tag{10}$$

$$\phi^2_{m,n} = \gamma\left[\frac{6N}{\pi}\sin\left(\frac{\pi}{N}\left(2n-\frac{7}{6}\right)\right) \times \sin\left(\frac{\pi}{N}\left(\frac{1}{2}\left(-1\right)^m - \frac{1}{3}\right)\right) - (m-3+3(-1)^m) \times \sin\left(\frac{\pi}{N}\left(\left|\sin\left(m\frac{\pi}{2}\right)\right| + 2n - 2\right)\right) + (m-1)\sin\left(\frac{\pi}{N}\left(\left|\cos\left(m\frac{\pi}{2}\right)\right| + 2n - \frac{4}{3}\right)\right)\right], \tag{11}$$

$$\phi^3_{m,n} = \gamma\left[\frac{6N}{\pi}\sin\left(\frac{\pi}{N}\left(2n-\frac{7}{6}\right)\right) \times \sin\left(\frac{\pi}{N}\left(\frac{1}{2}\left(-1\right)^m - \frac{1}{3}\right)\right) - (m-2+3(-1)^m) \times \sin\left(\frac{\pi}{N}\left(\left|\cos\left(m\frac{\pi}{2}\right)\right| + 2n - \frac{4}{3}\right)\right) + m\sin\left(\frac{\pi}{N}\left(\left|\sin\left(m\frac{\pi}{2}\right)\right| + 2n - 2\right)\right)\right], \tag{12}$$

$$\phi^4_{m,n} = \gamma\left[\frac{6N}{\pi}\sin\left(\frac{\pi}{N}\left(2n-\frac{13}{6}\right)\right) \times \sin\left(\frac{\pi}{N}\left(\frac{1}{2}\left(-1\right)^m - \frac{2}{3}\right)\right) + (m+4-3(-1)^m) \times \sin\left(\frac{\pi}{N}\left(\left|\cos\left(m\frac{\pi}{2}\right)\right| + 2n - 2\right)\right) - m\sin\left(\frac{\pi}{N}\left(\left|\sin\left(m\frac{\pi}{2}\right)\right| + 2n - \frac{10}{3}\right)\right)\right], \tag{13}$$

$$\phi^5_{m,n} = \gamma\left[\frac{6N}{\pi}\sin\left(\frac{\pi}{N}\left(2n-\frac{13}{6}\right)\right) \times \sin\left(\frac{\pi}{N}\left(\frac{1}{2}\left(-1\right)^m - \frac{2}{3}\right)\right) + (m+3-3(-1)^m) \times \sin\left(\frac{\pi}{N}\left(\left|\sin\left(m\frac{\pi}{2}\right)\right| + 2n - \frac{10}{3}\right)\right) - (m-1)\sin\left(\frac{\pi}{N}\left(\left|\cos\left(m\frac{\pi}{2}\right)\right| + 2n - 2\right)\right)\right], \tag{14}$$

and

$$\gamma = \frac{3\sqrt{3}eBNa^2}{4\pi\hbar c}, \tag{15}$$

where ε_0 is the free atomic energy, $\vec{u}_{m,n,i}$ $(i = A, B)$ the atomic displacement, N the total period number along the circumstance, and a the atomic separation.

The partition function of the system is

$$Z = \prod_{m,n,i} D\Psi^*_{m,n} D\Psi_{m,n} D\vec{u}_{m,n,i} \times \mathrm{e}^{-\int_0^\beta \mathrm{d}\tau[\Psi^*_{m,n}(\partial_\tau - \mu + E_{m,n})\Psi_{m,n} + \sum_i \frac{1}{2}M_c((\partial_\tau \vec{u}_{m,n,i})^2 + (\omega_\mathrm{p}\sigma_i\vec{u}_{m,n,i})^2)]}, \tag{16}$$

where $\beta = 1/(kT)$, with k the Boltzmann constant, T the temperature; μ is the electronic chemical potential, M_c is the atomic mass, ω_p is the phonon frequency, and σ_i $(i = A, B)$ is the auxiliary coefficient. The functional integral over the electronic variables is calculated using the Grassmann algebra rules [11–15], and the functional integral over the displacement variables is calculated using the classical string concept [17]. On the basis of the partition, we obtain the atomic displacement

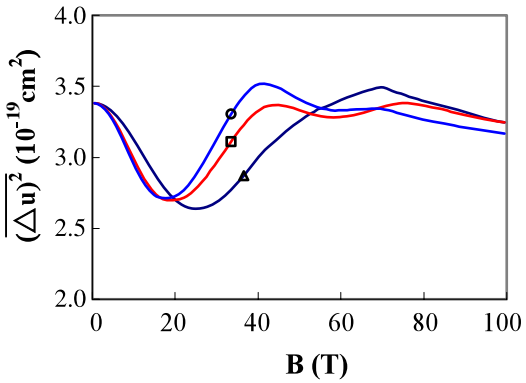

Figure 2. The atomic displacement fluctuation versus the magnetic field strength for the nanotube with the length $M = 900$ and the three different diameters $N = 5$ (triangle), $N = 10$ (square), and $N = 15$ (circle) at temperature 4.2 K.

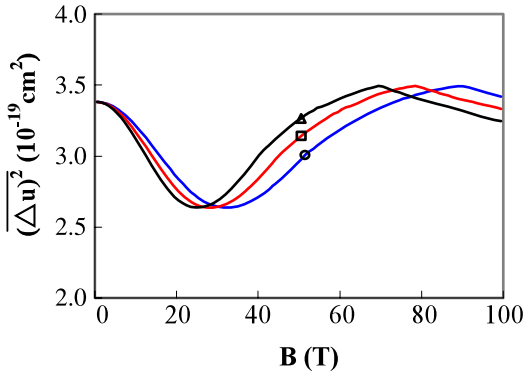

Figure 3. The atomic displacement fluctuation versus the magnetic field strength for the nanotubes with the diameter $N = 5$, and the three different lengths $N = 700$ (circle), $N = 800$ (square), and $N = 900$ (triangle) at temperature 4.2 K.

fluctuation per lattice point

$$\overline{(\Delta u)^2} = \overline{u^2} - \bar{u}^2 = \overline{u^2} = -\frac{2}{N_c M_c \omega_{\rm p}^2 \beta}\frac{\partial}{\partial \sigma_A}\ln Z\Big|_{\substack{\sigma_A=1\\ \sigma_{\rm B}=1}}$$
$$= \frac{\hbar}{M_c\omega_{\rm p}}\left(1+\frac{2}{{\rm e}^{\beta\hbar\omega_{\rm p}}-1}\right)+\frac{\alpha^2}{196M_c^2\omega_{\rm p}^4 N_c}$$
$$\times \sum_{m,n}[\cos(\phi^2_{m-1,n})+\cos(\phi^3_{m-1,n})$$
$$+\ \cos(\phi^4_{m-2,n})+\cos(\phi^5_{m,n})$$
$$-\ (2+\delta_{m,M})\cos(\phi^1_{m-1,n})]^2(1+{\rm e}^{\beta(\varepsilon^{m,n}_{\rm eff}-\mu)})^{-1}, \qquad (17)$$

where

$$\varepsilon^{m,n}_{\rm eff} = \frac{\varepsilon_0}{7}(4+\delta_{m,1}+\delta_{m,M})+\frac{V_0}{14}[\cos(\phi^1_{m,n})$$
$$+\cos(\phi^2_{m,n})+\cos(\phi^3_{m,n})+\cos(\phi^4_{m,n})$$
$$+\ \cos(\phi^5_{m,n})+(1+\delta_{m,M})\cos(\phi^1_{m-1,n})]$$
$$-\frac{\alpha^2}{392M_c\omega_{\rm p}^2}\{[\cos(\phi^2_{m-1,n})$$
$$+\ \cos(\phi^3_{m-1,n})+\cos(\phi^4_{m-2,n})+\cos(\phi^5_{m,n})$$
$$-\ (2+\delta_{m,M})\cos(\phi^1_{m-1,n})]^2$$
$$+[\cos(\phi^2_{m,n})+\cos(\phi^3_{m-2,n})$$
$$+\ \cos(\phi^4_{m-1,n+1})+\cos(\phi^5_{m-1,n+1})$$
$$-\ (2+\delta_{m,M})\cos(\phi^1_{m-1,n})]^2\}, \qquad (18)$$

is the effective energy of single electron, and $N_c = M \times N$. In equation (15), the first term represents the fluctuation due to the lattices themselves, and the second term represents the fluctuation led by the electron–phonon interaction. For the phase $\phi^i_{m,n}$ $(i = 1, 2, 3, 4, 5)$ proportional to the magnetic field strength and the fluctuation related to the phase, the magnetic field can effectively tune the fluctuation. In order to make the phase vary obviously, a higher magnetic field is required.

In our numerical calculation, the material parameters are chosen as $\varepsilon_0 - \mu = 0.0$ eV, $V_0 = 2.50$ eV, $\alpha = 6.31$ eV Å^{-1}, and $\omega_{\rm p} = 2.72 \times 10^{14}$ s^{-1} [20]. Figure 2 shows the curves of the atomic displacement fluctuation versus the magnetic field strength corresponding to the tube length $M = 900$, and three different tube diameters $N = 5$ (triangle), $N = 10$ (square), and $N = 15$ (circle) at temperature 4.2 K. The curves show that there are the minimum values for the atomic displacement fluctuations changing with the magnetic field. The minimum fluctuation is observed at $B = 26$ T for the nanotube with the diameter $N = 5$, and its value decreases with the nanotube diameter decreasing; it is independent of the nanotube length, as shown in figure 3. The magnetic field strength corresponding to the minimum fluctuation decreases with increasing tube diameter. Although the change of the fluctuation amplitude is very small, it reflects that the vibrational modes of the phonons undergo a transition in the vicinity of the minimum fluctuation. On either side of the minimum point, there are two different phonon phases. It is known that the phonon energy is proportional to the atomic displacement fluctuation, namely $E_{\rm p} = M_c\omega_{\rm p}^2\overline{(\Delta u)^2}/4$. When the fluctuation takes its minimum value, the mean phonon energy is lowest.

We define the magnetic moment generated by the phonon excitations:

$$\bar{\mu} = -\partial E_{\rm p}/\partial B = \bar{\eta}\mu_{\rm B}, \qquad (19)$$

where $\mu_{\rm B}$ is the Bohr magneton. We observe that in the vicinity of the minimum fluctuation there is a change of the magnetic moment sign, as shown in figures 4 and 5, The phonon system may undergo a transition from the paramagnetic phase to the diamagnetic phase or the inverse process. For the nanotube with the diameter $N = 5$ and the length $M = 900$, the maximum magnetic moment is $19.7\mu_{\rm B}$ per lattice point at $B = 12$ T and the minimum one is $-14.6\mu_{\rm B}$ per lattice point at $B = 40$ T. Such a large change of the magnetic moment shows that the externally magnetic field can induce the observable phonon magnetic effect as well as the phonon phase transition. Figure 4 shows the curves of the magnetic moment generated by the phonon excitations versus the magnetic field strength corresponding to the tube length $M = 900$, and the three different tube diameters $N = 5$ (triangle), $N = 10$ (square), and $N = 15$ (circle) at temperature 4.2 K. We can see that when the nanotube length is taken at a definite value,

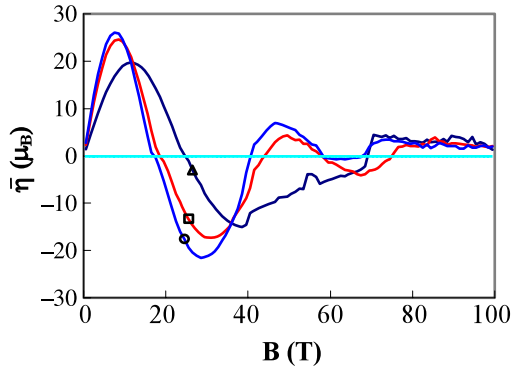

Figure 4. The effective magnetic moment versus the magnetic field strength for the nanotubes with the length $M = 900$, and the three different diameters $N = 5$ (triangle), $N = 10$ (square), and $N = 15$ (circle) at temperature 4.2 K.

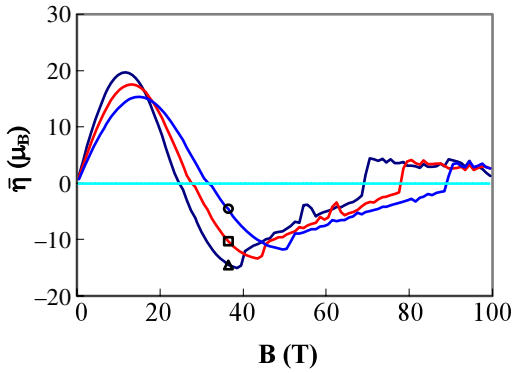

Figure 5. The magnetic moment versus the magnetic field strength for the nanotubes with the diameter $N = 5$, and the three different lengths $N = 700$ (circle), $N = 800$ (square), and $N = 900$ (triangle) at temperature 4.2 K.

the critical magnetic field of the generating phonon phase transition decreases with the increasing tube diameter. The critical magnetic field is also related to the nanotube length, as shown in figure 5. The longer the nanotube is, the lower the critical magnetic field will be. Our numerical calculations indicate that the point of minimum fluctuation basically does not change its position as the temperature increases. This shows that the phonon phase transition is a quantum phase transition induced by the magnetic field.

It is known that the phonons have various vibrational modes. Now the phonon magnetism shows that besides the intrinsic vibration modes of phonons, much more complicated modes may be induced by external magnetic fields in the carbon nanotubes. It should be pointed out that it is just due to the particular cylindrical geometry of the nanotubes that the electrons move along a closed circumference orbital and generate the induced magnetism. Also it is just due to this structure that the phonons generate the induced magnetism through the electron–phonon interaction. Now that the atomic displacement fluctuation is related to the electron–phonon interaction, the minimum fluctuation should correspond to weaker electron–phonon scattering. Thus it is expected that there is minimum resistivity if the system is in a state of minimum atomic displacement fluctuation. When the external magnetic field is weaker, this effect is too weak to be observed. However, when the external field is strong enough, this effect cannot be disregarded.

In conclusion, we have calculated the atomic displacement fluctuation as well as the magnetic moment of the phonons for nanotubes using a modified functional integral method. The calculation results exhibit that there is the minimum value for the fluctuation. From the point of view of the magnetization due to the phonon excitations, there is a quantum phase transition from the paramagnetic phase to the diamagnetic phase in the vicinity of the minimum fluctuation point. The critical magnetic field strength for achieving the phonon quantum phase transition falls within the current experimental capability range.

Acknowledgment

This work was supported by the National Natural Science foundation of China.

References

[1] Reich S, Thomsen C and Ordejon P 2001 *Phys. Rev.* B **64** 195416
[2] Maultzsch J, Reich S and Thomsen C 2001 *Phys. Rev.* B **64** 121407
[3] Maultzsch J, Reich S, Schlecht U and Thomsen C 2003 *Phys. Rev. Lett.* **91** 087402
[4] Hertel T and Moos G 2000 *Phys. Rev. Lett.* **84** 5002
[5] Rols S, Benes Z, Anglaret E, Sauvajol J L, Fischer J E, Goddens G, Schober H and Dianoux A J 2000 *Phys. Rev. Lett.* **85** 5222
[6] Mahan G D 2003 *Phys. Rev.* B **68** 125409
[7] Machon M, Reich S and Thomsen C 2006 *Phys. Rev.* B **74** 205423
[8] Roche S and Saito R 1999 *Phys. Rev.* B **59** 5242
[9] Fujiwara A, Tomiyama K, Suematsu H, Yumura M and Uchida K 2001 *Physica* B **298** 541
[10] Zaric S, Ostojic G N, Kono J, Shaver J, Moore V C, Strano M S, Hauge R H, Smalley R E and Wei X 2004 *Science* **304** 1129
[11] Florencio J and Goodman B 1986 *Phys. Rev.* B **34** 3634
[12] Florencio J 1987 *Phys. Rev.* B **35** 452
[13] Faddeev L D and Slavnov A A 1991 *Gauge Fields, Introduction to Quantum Theory* (California: Addison-Wesley)
[14] Potz W and Zhang J 1992 *Phys. Rev.* B **45** 11496
[15] Peng F 1997 *Phys. Rev.* E **56** 2663
[16] Peng F 2007 *Physica* B **389** 324
[17] Tsvelik A M 1995 *Quantum Field Theory in Condensed Matter Physics* (Cambridge: Cambridge University Press)
[18] London F 1937 *J. Phys. Rad.* **8** 397
[19] Harigaya K 1992 *Phys. Rev.* B **45** 12071
[20] Figge M T, Mostovoy M and Knoester J 2002 *Phys. Rev.* B **65** 125416