Effects of anisotropy on quantum fluctuation of a three-layer system with mutisublattice*

Jiang Wei(姜 伟)[a)b)†], Zhang Fan(张 凡)[a)], Guan Hong-Yu(关宏宇)[a)], and Liang Ji-Yan(梁吉艳)[a)]

[a)] *School of Sciences, Shenyang University of Technology, Shenyang* 110870, *China*
[b)] *Key Laboratory for Magnetism and Magnetic Materials of the Ministry of Education, Lanzhou University, Lanzhou* 730000, *China*

(Received 15 May 2010; revised manuscript received 8 July 2010)

The quantum fluctuations of a three-layer Heisenberg model with six sublattices are studied by the retarded Green's function method and the spin-wave theory. The effects of anisotropy on the quantum fluctuations at zero temperature are discussed. The results show that the interlayer anisotropy plays an important role in balancing the quantum competitions.

Keywords: multisublattice, three-layer, quantum fluctuation, effects of anisotropy

PACC: 7550G, 7540F, 7550R

1. Introduction

Much interest has focused on the layered materials, because their magnetic properties are greatly different from those of their bulk counterparts. A multi-sublattice model consisting of different sites in a unit cell, was purposed to describe the magnetic properties of rare-earth transition — metal intermetallics compounds.[1−3] As is well known, the quantum fluctuations have been found to be important for physical properties of different materials, for instance, ferromagnetic nanoparticles, layers/multilayers, large single crystals, etc. The quantum fluctuations are so important in the magnetic systems with anisotropy that they affect seriously the magnetic properties of the ferromagnets (ferrimagnets) at low and zero temperatures and they can also change the ground-state spin structures.[4−7] In our previous work, the magnetic properties of the double-layer Heisenberg model with four sublattices have been investigated in detail.[8] In the present work, we study a three-layer Heisenberg model with six sublattices on a square lattice. It is understood that the circumstance in six-sublattice system is much more complicated than that in the three- or four-sublattice one. Emphasis will be put on the effects of the anisotropy constants on the quantum fluctuations by employing retard Green's functions in the framework of the liner spin wave approximation.

A schematic diagram of the three-layer Heisenberg model with six sublattices is illustrated in Fig. 1.[9] The lattices of sites are the interpenetrating six sublattices A, B, C, D, E and F that are distributed among these sites. The spin values of six sublattices are S_1, S_2, S_3, S_4, S_5 and S_6, respectively.

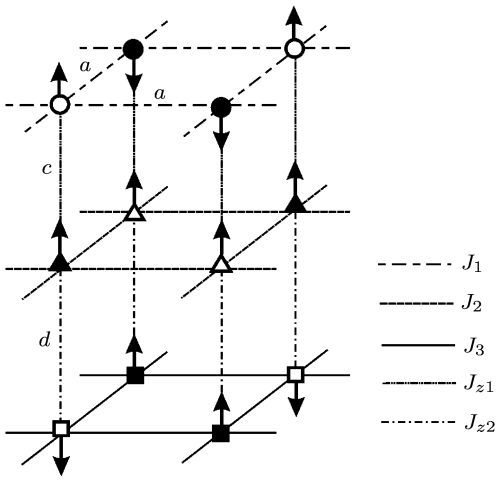


Fig. 1. The schematic diagram of the six-sublattice model.

The Hamiltonian is expressed as follows:

*Project supported by the Open Project of Key Laboratory for Magnetism and Magnetic Materials of the Ministry of Education, Lanzhou University, China (Grant No. LZUMMM2010010), the Scientific Foundation of the Educational Department of Liaoning Province, China (Grant No. L2010390), the Natural Science Foundation of Liaoning Province of China (Grant No. 20102171), the Scientific Technology Plan of Shenyang, China (Grant No. F10-205-1-33) and the Excellent Talents Program of the University of Liaoning Province, China (Grant No. LR201031).

†Corresponding author. E-mail: jiang_wei63@yahoo.com.cn

© 2010 Chinese Physical Society and IOP Publishing Ltd

$$
\begin{aligned}
H = & -2\sum_{ij}\left[(J_1+D_1)S_i^z\cdot S_j^z+\frac{1}{2}J_1(S_i^+\cdot S_j^-+S_i^-\cdot S_j^+)\right]-2\sum_{kl}\left[(J_2+D_2)S_k^z\cdot S_l^z+\frac{1}{2}J_2(S_k^+\cdot S_l^-+S_k^-\cdot S_l^+)\right]\\
& -2\sum_{mn}\left[(J_3+D_3)S_m^z\cdot S_n^z+\frac{1}{2}J_2(S_m^+\cdot S_n^-+S_m^-\cdot S_n^+)\right]-2\sum_{ik}\left[(J_{z1}+D_{z1})S_i^z\cdot S_k^z\right.\\
& \left.+\frac{1}{2}J_{z1}(S_i^+\cdot S_k^-+S_i^-\cdot S_k^+)\right]+2\sum_{jl}\left[(J_{z1}+D_{z1})S_j^z\cdot S_l^z+\frac{1}{2}J_{z1}(S_j^+\cdot S_l^-+S_j^-\cdot S_l^+)\right]\\
& -2\sum_{km}\left[(J_{z2}+D_{z2})S_k^z\cdot S_m^z+\frac{1}{2}J_{z2}(S_k^+\cdot S_m^-+S_k^-\cdot S_m^+)\right]\\
& +2\sum_{\ln}\left[(J_{z2}+D_{z2})S_l^z\cdot S_n^z+\frac{1}{2}J_{z2}(S_l^+\cdot S_n^-+S_l^-\cdot S_n^+)\right], \qquad (1)
\end{aligned}
$$

where the summation runs over all the nearest-neighbour spin pairs only; J_1 (D_1) J_2 (D_2) and J_3 (D_3) are the exchange integrals (anisotropy) in the first layer, the second layer and the third layer, respectively; J_{z1} (D_{z1}) is the interlayer exchange integral (anisotropy) between the first layer and the second layer; J_{z2} (D_{z2}) is the interlayer exchange integral (anisotropy) between the second layer and the third layer. There are N sites on each sublattice, and a total of $6N$ sites for the system.

The rest of the present paper is organized as follows. In Section 2, the Hamiltonian and calculation procedure are presented. The calculation results and discussion are given in Section 3. Finally, the summary is presented in Section 4.

2. Theory

Using the following Holstein–Primakoff transform and the spin-wave approximation:

$$
\begin{aligned}
&\begin{cases} S_i^+=\sqrt{2S_1}a_i, \\ S_i^-=\sqrt{2S_1}a_i^\dagger, \\ S_i^z=S_1-a_i^\dagger a_i, \end{cases}
\quad \begin{cases} S_j^+=\sqrt{2S_2}b_j^\dagger, \\ S_j^-=\sqrt{2S_2}b_j, \\ S_j^z=b_j^\dagger b_j-S_2, \end{cases}\\
&\begin{cases} S_k^+=\sqrt{2S_3}c_k, \\ S_k^-=\sqrt{2S_3}c_k^\dagger, \\ S_k^z=S_3-c_k^\dagger c_k, \end{cases}
\quad \begin{cases} S_l^+=\sqrt{2S_4}d_l, \\ S_l^-=\sqrt{2S_4}d_l^\dagger, \\ S_l^z=S_4-d_l^\dagger d_l, \end{cases}\\
&\begin{cases} S_m^+=\sqrt{2S_5}e_m^\dagger, \\ S_m^-=\sqrt{2S_5}e_m, \\ S_m^z=e_m^\dagger e_m-S_5, \end{cases}
\quad \begin{cases} S_n^+=\sqrt{2S_6}f_n, \\ S_n^-=\sqrt{2S_6}f_n^\dagger, \\ S_n^z=S_6-d_n^\dagger d_n, \end{cases} \qquad (2)
\end{aligned}
$$

and introducing the spin-wave operators $a_k(a_k^\dagger)$, $b_k(b_k^\dagger)$, $c_k(c_k^\dagger)$, $d_k(d_k^\dagger)$, $e_k(e_k^\dagger)$ and $f_k(f_k^\dagger)$ of the six-sublattice A, B, C, D, E and F, we rewrite Hamiltonian (1) as follows:[9]

$$
\begin{aligned}
H = & \ 8NS_1S_2(J_1+D_1)-8NS_3S_4(J_2+D_2)+8NS_5S_6(J_3+D_3)\\
& +2N(J_{z1}+D_{z1})(S_2S_4-S_1S_3)+2N(J_{z2}+D_{z2})(S_3S_5-S_4S_6)\\
& -8(J_1+D_1)\left[S_1\sum_k b_k^\dagger b_k+S_2\sum_k a_k^\dagger a_k\right]-2J_1\sqrt{S_1S_2}\left[\sum_k\gamma_k a_k b_k+\sum_k\gamma_k a_k^\dagger b_k^\dagger\right]\\
& +8(J_2+D_2)\left[S_3\sum_k d_k^\dagger d_k+S_4\sum_k c_k^\dagger c_k\right]-2J_2\sqrt{S_3S_4}\left[\sum_k\gamma_k c_k d_k^\dagger+\sum_k\gamma_k c_k^\dagger d_k\right]\\
& -8(J_3+D_3)\left[S_6\sum_k e_k^\dagger e_k+S_5\sum_k f_k^\dagger f_k\right]-2J_3\sqrt{S_5S_6}\left[\sum_k\gamma_k e_k^\dagger f_k^\dagger+\sum_k\gamma_k e_k f_k\right]\\
& +2(J_{z1}+D_{z1})\left[S_1\sum_k c_k^\dagger c_k+S_3\sum_k a_k^\dagger a_k\right]-2J_{z1}\sqrt{S_1S_3}\left[\sum_k p_k a_k c_k^\dagger+\sum_k p_{-k}a_k^\dagger c_k\right]\\
& -2(J_{z1}+D_{z1})\left[S_2\sum_k d_k^\dagger d_k+S_4\sum_k b_k^\dagger b_k\right]-2J_{z1}\sqrt{S_2S_4}\left[\sum_k p_k b_k^\dagger d_k^\dagger+\sum_k p_{-k}b_k d_k\right]\\
& -2(J_{z2}+D_{z2})\left[S_3\sum_k e_k^\dagger e_k+S_5\sum_k c_k^\dagger c_k\right]-2J_{z2}\sqrt{S_3S_5}\left[\sum_k p'_k c_k e_k+\sum_k p'_{-k}c_k^\dagger e_k^\dagger\right]\\
& +2(J_{z2}+D_{z2})\left[S_4\sum_k f_k^\dagger f_k+S_6\sum_k d_k^\dagger d_k\right]-2J_{z2}\sqrt{S_4S_6}\left[\sum_k p'_k d_k f_k^\dagger+\sum_k p'_{-k}d_k^\dagger f_k\right], \qquad (3)
\end{aligned}
$$

where

$$\gamma_k = 2(\cos k_x a + \cos k_y a), \tag{4}$$

$$p_{\pm k} = \cos k_z c \pm \mathrm{i} \sin k_z c, \tag{5}$$

$$p'_{\pm k} = \cos k_z d \pm \mathrm{i} \sin k_z d \tag{6}$$

with a, c and d being the lattice constants.

Using the method of Refs. [8] and [9], we obtain the equation of the Green's function

$$G(k,\omega) = \frac{1}{\det(D(\omega_i))}[M_{i,j}]_{6\times 6}[N_{i,j}]_{6\times 6}. \tag{7}$$

The matrix elements in the six-order matrix $\boldsymbol{M}$ are $M_{i,j} = (i,j = 1\text{–}6)$. $N_{i,j} = (i,j = 1\text{–}6)$ is the unit matrix, where $N_{11} = 1$, $N_{22} = -1$, $N_{33} = 1$, $N_{44} = 1$, $N_{55} = -1$, $N_{66} = 1$. ω_i correspond to six branches of the spin-wave spectrum, equaling the number of sublattices.

By employing the spectral theorem, the magnetizations per site (the unit is taken to be $g\mu_{\mathrm{B}}$, a normalized unit) of sublattices at zero temperature are correspondingly as follows:

$$M_i = S_i + \frac{1}{\pi^2}\iint\left[\frac{M_{ii}(\omega_5)}{\omega_{\mathrm{AB}}} + \frac{M_{ii}(\omega_6)}{\omega_{\mathrm{CD}}}\right]\mathrm{d}k_x\mathrm{d}k_y, \quad (i = 1,3,4,6), \tag{8}$$

$$M_j = -1 - S_j + \frac{1}{\pi^2}\iint\left[\frac{M_{jj}(\omega_5)}{\omega_{\mathrm{AB}}} + \frac{M_{jj}(\omega_6)}{\omega_{\mathrm{CD}}}\right]\mathrm{d}k_x\mathrm{d}k_y, \quad (j = 2,5), \tag{9}$$

where $\omega_{\mathrm{AB}} = \prod_{l\neq 5}^{6}(\omega_5 - \omega_i)$, and $\omega_{\mathrm{CD}} = \prod_{l\neq 6}^{6}(\omega_6 - \omega_i)$.

The quantum fluctuations of the six-sublattice magnetizations at zero-temperature are defined as

$$\Delta M = S_{i(j)} - M_{i(j)}, \quad i(j) = 1,3,4,6(2,5). \tag{10}$$

3. Results and discussion

In the following discussion, we shall take $J_2 = 1$ as unit and treat other parameters as being relative to J_2, the lattice constants $a = c = 1.0$, $d = 1.2c$, $S_1 = S_3 = S_4 = S_6 = 1.0$, $S_2 = S_5 = 0.5$, $J_1 = -0.8$, $J_3 = -1.2$, $D_1 = -0.1$, $D_2 = 0.2$, $D_3 = -0.3$, $J_{z1} = 0.3$, and $J_{z2} = -0.5$. The parameters mentioned above are different from those in Ref. [9], in which sublattices have different values of the spins: $S_1 = S_3 = S_4 = S_6 = 0.5$, and $S_2 = S_5 = 1.0$ without considering the interlayer anisotropies (D_{z1} and $D_{z2} = 0$). The effects of the interlayer anisotropy D_{z1} on the quantum fluctuation of spins for the three-layer system with six-sublattice system at zero-temperature are plotted in Figs. 2(a) and 2(b), where the D_{z2} is fixed as $D_{z2} = -0.8$, –0.2; D_{z1} and D_{z2} are the interlayer anisotropies between sublattices A and C, sublattices C and E, respectively; D_{z1} is positive while D_{z2} is negative. As marked in the figures, these curves actually belong to the sublattices A, B, C, D, E and F, respectively. In Figs. 2(a) and 2(b), the quantum fluctuation ΔM of the sublattice B is stronger than that of A in the first layer. It can be explained as the fact that a stronger zero-point quantum fluctuation is achieved because the value of the spin-1/2 in the sublattice B is smaller than that of spin-1 in the sublattice A if the rest of the parameters are the same. Likewise, F is smaller than E in the second layer. With the increase of anisotropy D_{z1}, the quantum fluctuations of sublattices C and D decrease monotonically and change slightly, due to the interaction between sublattices C and D that are in ferromagnetic exchange coupling. Because of the enhancement of the anisotropy D_{z1} between the sublattices A and C, curves A and B drop off monotonically and obviously. There is a crossover between curves $A(B)$ and $E(F)$ which is affected by the interlayer anisotropies D_{z1} and D_{z2}. The position of the crossover shifts toward weaker region of the anisotropy D_{z1} when the value of D_{z2} increases from -0.8 to -0.2. Comparing Figs. 2(a) and 2(b) shows that the region of the anisotropy D_{z1} is narrow for the case of $|D_{z2}| = 0.2$, where the quantum fluctuation of the sublattice A(B) is stronger than that of the sublattice E(F). Note that the quantum fluctuations in the sublattices C and D are lower than those in the sublattices A(E) and B(F). It can be understood that the quantum fluctuation in a layer with ferrimagnetic interaction is affected more strongly than that in a ferromagnetic layer.

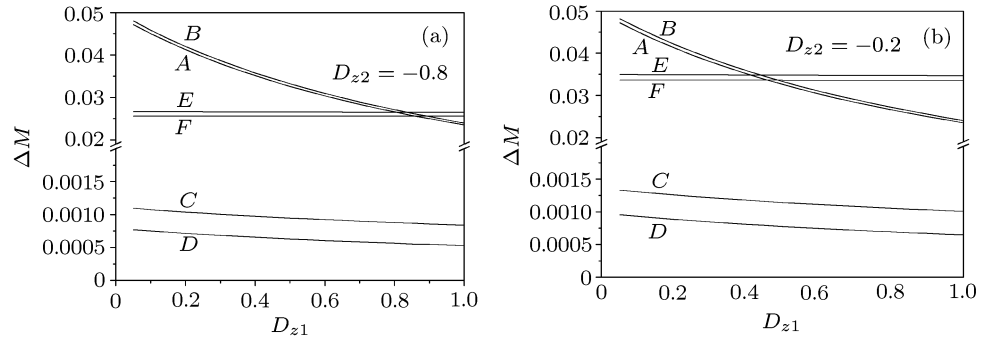


Fig. 2. D_{z1} dependences of the quantum fluctuation of spins at zero-temperature with $S_1 = S_3 = S_4 = S_6 = 1.0$, $S_2 = S_5 = 0.5$, $J_1 = -0.8$, $J_3 = -1.2$, $D_1 = -0.1$, $D_2 = 0.2$, $D_3 = -0.3$, $J_{z1} = 0.3$, $J_{z2} = -0.5$, and $D_{z2} = -0.8$ (a), and -0.2 (b).

In order to better understand the influence of the anisotropy on quantum fluctuation, we plot the quantum fluctuations in the three-dimensional parameter space (ΔM, D_{z1}, D_{z2}) at zero-temperature in Figs. 3(a)–3(f) for the three-layer system with six-sublattice system.

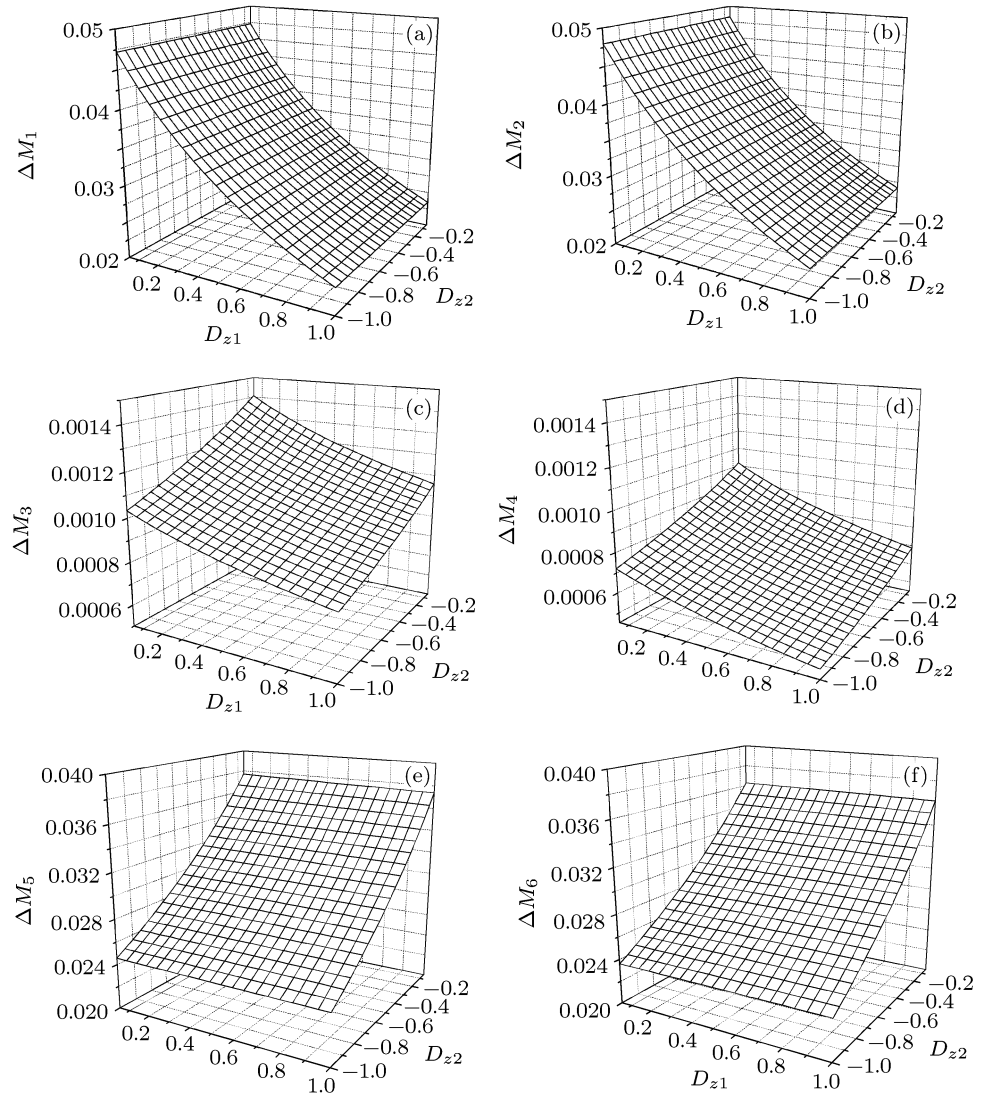


Fig. 3. Three-dimensional quantum fluctuations of spins at zero-temperature with $S_1 = S_3 = S_4 = S_6 = 1.0$, $S_2 = S_5 = 0.5$, $J_1 = -0.8$, $J_3 = -1.2$, $D_1 = -0.1$, $D_2 = 0.2$, $D_3 = -0.3$, $J_{z1} = -J_{z3} = 0.3$, $J_{z2} = -J_{z4} = -0.5$ for the sublattices (a) A, (b) B, (c) C, (d) D, (e) E, and (f) F.

Figures 3(a) and 3(b) show the anisotropies D_{z1} and D_{z2} dependences of quantum fluctuations ΔM_1 and ΔM_2 for the two sublattices on the first layer, respectively. The anisotropies D_{z1} and D_{z2} have the same contributions to ΔM_1 for the sublattice A and ΔM_2 for the sublattice B. But the former is weaker than the later ($\Delta M_2 > \Delta M_1$). The anisotropies D_{z1} and D_{z2} dependences of the quantum fluctuations ΔM_3 and ΔM_4 for the two sublattices C and D on the second layer are plotted in Figs. 3(c) and 3(d). As shown in the figures, there exists $\Delta M_3 > \Delta M_4$, owing to the fact that the interlayer ferrimagnetic exchange integral is stronger between sublattices C and E than that between sublattices D and B. The D_{z1} and the D_{z2} dependence of the quantum fluctuations ΔM_5 and ΔM_6 are illustrated in Figs. 3(e) and 3(f) for the two sublattices E and F on the third layer. Note that the quantum fluctuation ΔM_5 changes more obviously than ΔM_6. This indicates that the interlayer ferrimagnetic exchange integral strongly affects the quantum fluctuations of the system.

4. Summary

By employing the linear spin-wave method and the retarded Green's function technique, we have investigated the quantum fluctuations at zero temperature for a six-sublattice three-layer Heisenberg system, which affect strongly the physical properties of system at zero and low temperatures. Numerical results show that the quantum fluctuations of the sublattices in the ferrimagnetic interaction are affected more strongly than that of the sublattices in the ferromagnetic layer for any values of the interlayer anisotropies. The interlayer anisotropy plays an important role in the quantum fluctuations of the system. As the interlayer anisotropy D_{z1} (or D_{z2}) increases, the quantum fluctuations of the sublattices A and B (E and F) decrease obviously, while the quantum fluctuations of the sublattices C, D, E and F (A, B, C and D) decrease slightly for the fixed D_{z2} (D_{z1}). We have also discussed the position of the crossover between the quantum fluctuation curves which is affected strongly by the interlayer anisotropy

References

[1] Zhang Z D 1996 *Phys. Rev.* B **53** 2569.

[2] Moschel A, Usadel K D and Hucht A 1993 *Phys. Rev.* B **47** 8676

[3] Zhou X, Liang B Q, Wang H, Liu H, Zhang Z R, Fan J H, Ji S Y, Chen L R, Han B S, Wang Y J and Tang Y J 2001 *Acta Phys. Sin.* **50** 159 (in Chinese)

[4] Liu W M, Wang X B, Pu F C and Huang N N 1997 *Phys. Rev.* E **55** 1375

[5] Liu W M, Wang X B, Pu F C and Huang N N 2005 *Phys. Rev.* B **72** 064410

[6] Kim Y J, Aharony A, Birgeneau R J, Chou F C, Entin W O, Erwin R W, Greven M, Harris A B, Kastner M A, Korenblit I Y, Lee Y S and Shirane G 1999 *Phys. Rev. Lett.* **83** 852

[7] Barbara B, Sampaio L C, Wegrowe J E, Ratnam B A, Marchand A, Paulsen C, Novak M A, Tholence J L, Uehara M and Fruchart D1993 *J. Appl. Phys.* **73** 6703

[8] Jiang W, Zhu C B, Yu G H and Lo V C 2009 *Chin. Phys.* B **18** 3547

[9] Zhu C B, Jiang W, Lo V C, Yang J and Wang W 2010 *Physica* B **405** 1677