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J. Phys.: Condens. Matter 19 (2007) 026216 (9pp)

# Sub-terahertz photoconduction induced by interlayer transition in an InAs/GaSb-based type II and broken-gap quantum well system

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Received 14 September 2006, in final form 29 November 2006 Published 15 December 2006 Online at stacks.iop.org/JPhysCM/19/026216

#### Abstract

In this paper, we demonstrate theoretically that, when an InAs/GaSb-based type II and broken-gap quantum well is subjected to a light field, conductance can be observed along the growth direction due to charge transfer between electron and hole layers which are spatially separated. A peak profile can be observed in the conductance within sub-terahertz bandwidth. The peak shifts to the lower frequency (red-shift) with increasing temperature and a more broadened peak structure can be observed at lower temperatures. Our results suggest that InAs/GaSb-based quantum well systems are of potential to be applied as sub-terahertz photovoltaic devices working at relatively low temperatures.

#### 1. Introduction

The InAs/GaSb-based type II and broken-gap quantum well (QW) structure has a unique electronic subband structure. In such a novel device, the valence subband in the GaSb layer can be significantly higher than the conduction subband in the InAs layer and holes and electrons are separated spatially in the GaSb and InAs layers respectively [1, 2]. Motivated by many proposals dealing with advanced electronic and optical devices, type II and broken-gap QW systems have been investigated very intensively ever since such a device was realized experimentally in 1987 [3]. In recent years, this unique QW structure has been applied in advanced optical devices such as uncooled infrared detectors [4], negative persistent photoconductors [5, 6], etc. Very recently, it has also been realized that InAs/GaSb based electron–hole bilayer systems can also be used as photodiodes [4] and photovoltaic devices. In this work, we explore theoretically the possibility to apply InAs/GaSb based

type II and broken-gap QW systems as photocurrent devices working at terahertz  $(10^{12} \text{ Hz} \text{ or THz})$  or sub-THz bandwidth which lies between electronic and optical phenomena. This proposal is mainly based on the fact that in such systems the electrons and holes can be excited by the linearly polarized light fields into different layers due to the overlap of electron and hole wavefunctions. This can lead to a situation where the charge numbers in different layers are modified by the applied light fields through optical absorption scattering and a current circuit can therefore be achieved. Thus, the photocurrent can be generated along the growth direction. Such a mechanism is electrically equivalent to the admittance spectroscopy in which the conductance and capacitance are induced by charge transfer from bound to continuum states under the action of the ac fields [8].

In this paper, on the basis of a Boltzmann equation we develop a simple and transparent theoretical approach to calculate the photoconductance in a type II and broken-gap quantum well. The details of the analytical work and theoretical considerations are presented in section 2. The obtained analytical and numerical results are presented, analysed and discussed in section 3. The main conclusions obtained from this study are summarized in section 4.

#### 2. Theoretical approaches

In this study, we consider a type II QW structure in which a two-dimensional electron gas (2DEG) and a two-dimensional hole gas (2DHG) are separated spatially in two layers. When a linearly polarized light field is applied to such a system, the Hamiltonian to describe such a two-body system can be written as

$$H = H_{\rm e} + H_{\rm h} + H_{\rm e-o}' + H_{\rm h-o}'.$$
 (1)

Here,  $H_e = \mathbf{P}_e^2/2m_e^* + U_e(z_e)$  and  $H_h = -\mathbf{P}_h^2/2m_h^* + U_h(z_h)$  are the single-particle Hamiltonians for respectively an electron and a hole, where the energy is measured from the bottom of the conduction band in the electron layer,  $\mathbf{P}_i = (p_{x,i}, p_{y,i}, p_{z,i})$  (with i = e or h) is the momentum operator,  $\mathbf{R}_i = (\mathbf{r}_i, z_i) = (x_i, y_i, z_i)$  is the electron or hole coordinates,  $m_i^*$  is the effective mass for the electron or hole, and  $U_i(z_i)$  is the confining potential energy for an electron or a hole along the growth direction. Furthermore, in equation (1),

$$H'_{i-0} = \pm \frac{e}{m_i^*} \mathbf{A} \cdot \mathbf{P}_i \tag{2}$$

is a perturbative Hamiltonian for an electron or a hole interaction with the applied electromagnetic (EM) field, which is polarized linearly along the growth direction [9], with **A** being the vector potential of the radiation field. In the present study, we have neglected the interaction between electrons and holes in different layers via the Coulomb potential, because such an excitonic effect in a type II QW is relatively weak due to relatively small overlap of the electron and hole wavefunctions at the interface. Suppose that the Schrödinger equation regarding  $H_e$  and  $H_h$  can be analytically solved respectively; the electron and hole wavefunctions along with the corresponding energy spectra are given respectively as  $|e\rangle = e^{i\mathbf{k}\cdot\mathbf{r}_e}\psi_n^e(z_e)$  and  $|h\rangle = e^{i\mathbf{k}\cdot\mathbf{r}_h}\psi_n^h(z_h)$ , and  $E_n^e(\mathbf{k}) = \hbar^2k^2/2m_e^* + \varepsilon_n^e$  and  $E_n^h(\mathbf{k}) = -\hbar^2k^2/2m_h^* + \varepsilon_n^h$ . Here  $\mathbf{k} = (k_x, k_y)$  is the electron or hole wavevector in the 2D plane, and  $\psi_n^i(z_j)$  with a corresponding subband energy  $\varepsilon_n^j$  are the solutions of the Schrödinger equation along the growth direction for an electron or a hole. Thus, the two-body wavefunction corresponding to  $H_e + H_h$  is  $|e, h\rangle = |e\rangle|h\rangle$ .

The steady-state electronic transition rate for scattering of an electron or a hole from a state  $\mathbf{k}$  in layer *i* to a state  $\mathbf{k}'$  in layer *j* can be derived using an approach akin to Fermi's golden rule,



**Figure 1.** The ground-state electron and hole wavefunctions obtained from self-consistent calculation for a fixed InAs layer thickness  $L_{\text{InAs}}$  and a fixed GaSb layer width  $L_{\text{GaSb}}$  as indicated. The interface between InAs and GaSb layers is taken at z = 0 and z is the growth direction.

which reads  $W_{ij}(\mathbf{k}, \mathbf{k}') = W_{ij}(\mathbf{k})\delta_{\mathbf{k}',\mathbf{k}}$  and

$$W_{ij}(\mathbf{k}) = \frac{2\pi}{\hbar} \left( \frac{e\hbar F_0}{m_i^* \omega} \right)^2 |X_{ij}|^2 \delta[E_n^i(\mathbf{k}) - E_{n'}^j(\mathbf{k}) + \hbar \omega], \tag{3}$$

where  $F_0$  and  $\omega$  are respectively the electric field strength and frequency of the EM field and  $X_{ij} = \int dz \psi_{n'}^{j*}(z) d\psi_n^i(z)/dz$ . It should be noted that although the overlap of the wavefunctions for an electron and a hole is relatively small in a type II QW structure (see figure 1)  $X_{ij}$  can be significant if  $d\psi_n^i(z)/dz$  is relatively large. Here we have taken  $H'_{i-0} = \pm (e\hbar F_0/m_i^*\omega)e^{i\omega t} d/dz$  for a weak radiation field so that only the one-photon absorption is a more possible channel for electronic transition.

In this work, we employ the semi-classical Boltzmann equation in degenerate statistics as the governing transport equation to study the consequence of applying an EM field to a type II and broken-gap QW structure. We consider a situation where only the lowest electron subband and the highest hole subband are occupied respectively by electrons and heavy holes. For electronic transition from a layer i to a layer j, the time-dependent Boltzmann equation is

$$\frac{\partial f_i(\mathbf{k},t)}{\partial t} = g_s \sum_{\mathbf{k}'} [F_{ji}(\mathbf{k}',\mathbf{k},t) - F_{ij}(\mathbf{k},\mathbf{k}',t)] + g_s \sum_{\mathbf{k}'} [F_{ii}(\mathbf{k}',\mathbf{k},t) - F_{ii}(\mathbf{k},\mathbf{k}',t)]$$
(4)

where  $F_{ij}(\mathbf{k}, \mathbf{k}', t) = f_i(\mathbf{k}, t)[1 - f_j(\mathbf{k}', t)]W_{ij}(\mathbf{k}, \mathbf{k}')$ ,  $f_i(\mathbf{k}, t)$  is the momentum-distribution function for an electron or a hole, and  $g_s = 2$  counts for spin-degeneracy. In equation (4),  $F_{ij}(\mathbf{k}, \mathbf{k}', t)$  corresponds to an inter-layer transition and  $F_{ii}(\mathbf{k}', \mathbf{k}, t)$  to an intra-layer transition. Furthermore, the effect of the EM field has been included within the time-dependent electron/hole distribution functions and within the electronic transition rate. Thus, to avoid double counting, the force term induced by the EM field does not appear on the left-hand side of the Boltzmann equation. It is known that there is no simple and analytical solution to equation (4). For the first moment, the mass-balance equation [10] can be derived by multiplying  $\sum_{\mathbf{k}}$  to both sides of the Boltzmann equation. In doing so, we obtain a rate equation

$$\frac{\mathrm{d}Q_{\mathrm{e}}\left(t\right)}{\mathrm{d}t} = \frac{\mathrm{d}Q_{\mathrm{h}}\left(t\right)}{\mathrm{d}t} = -Q_{\mathrm{h}}(t)\lambda_{\mathrm{he}} - Q_{\mathrm{e}}(t)\lambda_{\mathrm{eh}},\tag{5}$$

3

where  $Q_e$  and  $Q_h$  are respectively the charge numbers for electrons and holes and  $\lambda_{ij}$  is the scattering rate from a layer *i* to a layer *j*. We have used the definition that the electron and hole densities are respectively  $n_e(t) = g_s \sum_k f_e(\mathbf{k}, t)$  and  $n_h(t) = g_s \sum_k f_h(\mathbf{k}, t)$  and  $Q_e(t) = en_e(t)S$  and  $Q_h(t) = -en_h(t)S$ , with *S* being the area of the 2D plane. As expected, equation (5) reflects a fact that only the inter-layer transition can result in a change of the charge numbers in different layers. Equation (5) also gives a condition of total charge number conservation  $d[Q_e(t) - Q_h(t)]/dt = 0$ , which implies that the change of the charge numbers in a certain layer is due to the formation and separation of the electron-hole pairs. Furthermore,  $\lambda_{eh} = \lambda_E$  is the emission rate and  $\lambda_{he} = \lambda_C$  is the capture rate with respect to electrons, which are

$$\lambda_{\rm E} = \frac{4}{n_{\rm e}} \sum_{\mathbf{k}', \mathbf{k}} f_{\rm e}(\mathbf{k}, t) [1 - f_{\rm h}(\mathbf{k}', t)] W_{\rm eh}(\mathbf{k}, \mathbf{k}'), \tag{6}$$

and

$$\lambda_{\rm C} = \frac{4}{n_{\rm h}} \sum_{\mathbf{k}', \mathbf{k}} f_{\rm h}(\mathbf{k}, t) [1 - f_{\rm e}(\mathbf{k}', t)] W_{\rm he}(\mathbf{k}, \mathbf{k}').$$
(7)

In the calculation of the emission and capture rates under the condition of a weak EM field, we can neglect the influence of the EM field on the momentum distribution function and employ the statistical energy distribution as the distribution function. We take  $f_e(\mathbf{k}, t) \simeq f_e(E_0^e(\mathbf{k}))$ and  $f_h(\mathbf{k}, t) \simeq f_h(E_0^h(\mathbf{k}))$  with  $f_i(x)$  being the Fermi–Dirac function for an electron or a hole. Thus, the emission and capture rates become

$$\lambda_{\rm E} \simeq \frac{4}{n_{\rm e}} \sum_{\mathbf{k}, \mathbf{k}'} f_{\rm e}(E_0^{\rm e}(\mathbf{k})) [1 - f_{\rm h}(E_0^{\rm h}(\mathbf{k}))] W_{\rm eh}(\mathbf{k}, \mathbf{k}'), \tag{8}$$

and

$$\lambda_{\rm C} \simeq \frac{4}{n_{\rm h}} \sum_{\mathbf{k}, \mathbf{k}'} f_{\rm h}(E_0^{\rm h}(\mathbf{k})) [1 - f_{\rm e}(E_0^{\rm e}(\mathbf{k}))] W_{\rm he}(\mathbf{k}, \mathbf{k}'), \tag{9}$$

which are time independent when taking  $n_e$  and  $n_h$  as their values at the steady state.

Using equation (5), the current in the circuit is given by

$$I(t) = -\frac{\mathrm{d}Q_{\mathrm{e}}(t)}{\mathrm{d}t} = Q_{\mathrm{e}}(t)\lambda_{\mathrm{E}} + Q_{\mathrm{h}}(t)\lambda_{\mathrm{C}}.$$
(10)

It is known that under the action of an EM driving field  $\delta V_t = V_0 e^{i\omega t}$ , with  $\omega$  being the frequency of the EM field, the electron number in the quantum well  $Q_e(t)$  is the difference between the mobile electron number  $\delta Q_e(t)$  and the emitted electron number  $\int_0^t dt I(t)$ , namely,

$$Q_{\rm e}(t) = \delta Q_{\rm e}(t) - \int_0^t \mathrm{d}t \, I(t). \tag{11}$$

For the case of a weak EM field so that a linear response is achieved, we have

$$\delta Q_{\rm e}(t) = \kappa \, \delta V_{\rm t} = \kappa \, V_0 {\rm e}^{{\rm i}\omega t} \qquad \text{and} \qquad I(t) = I_0 {\rm e}^{{\rm i}\omega t}.$$
 (12)

Here a coefficient

$$\kappa = \frac{\delta Q_{\rm e}(t)}{\delta V_{\rm t}} = \frac{\mathrm{d}Q_{\rm e}(t)}{\mathrm{d}V_{\rm t}} = 2eS\sum_{\mathbf{k}}\frac{\partial f_{\rm e}(E_{\rm e}(\mathbf{k}))}{\partial \mu_{\rm t}}\frac{\partial \mu_{\rm t}}{\partial V_{\rm t}}$$

can be evaluated by assuming that the effect of the EM field is mainly on the Fermi energy of the system. We note that for a weak radiation field so that a linear response is achieved we have

$$\partial \mu_{\rm t} / \partial V_{\rm t} = e$$

4

and consequently

$$\kappa = \frac{2e^2 S}{k_{\rm B}T} \sum_{\mathbf{k}} f_{\rm e}(E_0^{\rm e}(\mathbf{k}))[1 - f_{\rm e}(E_0^{\rm e}(\mathbf{k}))].$$
(13)

This result reflects the fact that the emission and capture of electrons or holes are mainly achieved for transitions around the Fermi level.

Inserting equations (11) and (12) into equation (10), we get

$$I(t) = \left(\kappa V_0 e^{i\omega t} - \int_0^t I(t) dt\right) \lambda_{\rm E} + Q_{\rm h}(t) \lambda_{\rm C}$$

and, as a result,

$$\dot{I}(t) = \left[i\omega\kappa V_0 e^{i\omega t} - I(t)\right] \lambda_{\rm E} + \dot{Q}_{\rm h}(t) \lambda_{\rm C}.$$
(14)

When the system is in equilibrium, the total charge number should be conserved so that  $\dot{Q}_{\rm h}(t) = \dot{Q}_{\rm e}(t) = -I(t)$ . Thus, equation (14) can be solved analytically. After using the definition for conductance  $\mathcal{G} = I_0/V_0$ , we obtain

$$G = \frac{i\kappa\omega\lambda_E}{\lambda_E + \lambda_C + i\omega}$$
 and  $G = \operatorname{Re} G = \frac{\kappa\omega^2\lambda_E}{(\lambda_E + \lambda_C)^2 + \omega^2}.$  (15)

After using the Fermi–Dirac function as the energy distribution function for an electron or a hole, we obtain for the electron emission and capture rates

$$\lambda_{\rm E} = C \frac{m_{\rm h}^* |X_{\rm eh}|^2}{m_{\rm e}^* n_{\rm e}} f_{\rm e}(x_{\rm h}^+) [1 - f_{\rm h}(x_{\rm e}^-)]$$
(16)

and

$$\lambda_{\rm C} = C \frac{m_{\rm e}^* |X_{\rm he}|^2}{m_{\rm h}^* n_{\rm h}} f_{\rm h}(x_{\rm e}^+) [1 - f_{\rm e}(x_{\rm h}^-)], \tag{17}$$

where  $C = 4(eF_0)^2 / [\hbar\omega^2 (m_e^* + m_h^*)]$ ,  $x_i^{\pm} = (m_e^* \varepsilon_0^e + m_h^* \varepsilon_0^h \pm m_i^* \hbar \omega) / (m_e^* + m_h^*)$ ,  $f_e(x) = [e^{(x-E_F)/k_BT} + 1]^{-1}$  and  $f_h(x) = [e^{(E_F-x)/k_BT} + 1]^{-1}$  with  $E_F$  being the Fermi energy. Furthermore, the coefficient  $\kappa = m_e^* e^2 S f_e(\varepsilon_0^e) / (\pi \hbar^2)$ .

#### 3. Results and discussion

2

In the present study, we consider a typical InAs/GaSb QW in which the broken-gap structure can be achieved and has been verified experimentally [2]. The widths of the InAs and GaSb layers are taken respectively as  $L_{InAs} = 17$  and  $L_{GaSb} = 5$  nm. The electron and hole wavefunctions and subband energies along with the electron and hole densities are obtained by solving self-consistently the Schrödinger equation and Poisson equation, where the Schrödinger equations for an electron and for a hole are coupled through the Hartree potential determined by the Poisson equation<sup>3</sup>. Using the material parameters for InAs and GaSb and taking the energy gap between the bottom of the conduction band in the InAs layer and the top of the valence band in the GaSb layer to be  $E_g = 140$  meV, the results obtained from this calculation are  $n_e = 1.14 \times 10^{12}$  cm<sup>-2</sup>,  $n_h = 3.10 \times 10^{11}$  cm<sup>-2</sup>,  $\varepsilon_0^e = 32.0$  meV,  $\varepsilon_0^h = 106.3$  meV and  $E_F = 104.0$  meV. Here the energy is measured from the bottom of the conduction band in the InAs layer. In such a structure, only the lowest electron subband and the highest hole subband are occupied by electrons and holes. The electron and hole wavefunctions and the charge distribution in such a QW are shown respectively in figures 1 and 2. From these theoretical results, we see that (i) there is a significant overlap of the electron and hole

<sup>&</sup>lt;sup>3</sup> The scheme and details of the self-consistent calculation will be presented elsewhere.



Figure 2. Electron (solid curve) and hole (dotted curve) distributions in an InAs/GaSb quantum well. The results are obtained self-consistently for  $L_{InAs} = 17$  and  $L_{GaSb} = 5$  nm. The interface between InAs and GaSb layers is taken at z = 0.

wavefunctions at the interface between InAs and GaSb (see figure 1); (ii) the electrons and holes are located mainly in, respectively, the InAs and GaSb layers (see figure 2); and (iii) although the hole density  $n_h$  is lower than the electron density  $n_e$ , the hole distribution is more localized than the electron distribution. Thus, the overlap between the electron and hole distributions is mainly through the penetration of the electron wavefunction into the GaSb layer (see figure 1).

When such a type II and broken-gap quantum well is subjected to a linearly polarized radiation field, electronic transition occurs. This transition is accompanied by the absorption of a photon and by the charge transfer between different layers. The electrons and holes can absorb a photon and be excited to a higher energy state. Meanwhile, this process corresponds to the separation and combination of electron-hole pairs and, therefore, to a charge transfer in the device system. For example, if an electron-hole pair is formed within the first half circle of the light field, an electron-hole pair will be separated within the second half circle of the light field. In the former case, the electron and hole numbers in different layers will be reduced. In the latter case, the charge numbers in different layers will be increased. As a result, a current circuit can be formed in different material layers. In figure 3, the conductance in the current circuit is shown as a function of the radiation frequency at a fixed radiation intensity for different temperatures. A sharp peak of the conductance can be observed in the sub-THz regime  $\omega_p \sim 0.1$  THz. This implies that a strong photocurrent can be generated in the device by sub-THz radiation fields. With increasing temperature, the conductance peak is red-shifted and lowered. This suggests that this kind of photoconduction effect can be detected at relatively low temperatures. The dependence of the conductance on temperature at a fixed radiation intensity  $F_0 = 10 \text{ V cm}^{-1}$  for different radiation frequencies is shown in figure 4. Here we note that when the radiation frequency is higher than  $\omega_p$  (which gives the peak value of G shown in figure 3) the conductance decreases with increasing temperature, whereas when  $\omega < \omega_p$  the conductance can increase with T (e.g. at  $\omega = 0.08$  THz) or first increase then decrease with T (e.g. at  $\omega = 0.1$  THz).

In a type II and broken-gap QW structure, because both electron and hole states are occupied respectively by electrons and holes and the hole subband is higher than the electron subband, the additional channels open up for optical transition. In such a situation, optical



**Figure 3.** Conductance in the current circuit as a function of radiation frequency  $\omega$  at a fixed radiation intensity  $F_0$  for different temperatures *T*.  $L_{\text{InAs}}$  and  $L_{\text{GaSb}}$  are respectively the widths for the InAs and GaSb layers and  $G_0 = e^2/\hbar$ .



**Figure 4.** Photo-conductance as a function of temperatures *T* at a fixed radiation intensity  $F_0$  for different radiation frequencies  $\omega$ . The other parameters are the same as in figure 3.

transition processes are in sharp contrast to those in a undoped conventional quantum well in which optical absorption scattering is mainly achieved through the excitation of electrons in the valence subbands across the forbidden zone into the conduction subband [11]. The electron and hole interactions with a light field via absorption scattering in a type II and broken-gap QW can be achieved in the following ways (see figure 5). In the small **k** case (processes 1 and 2 in figure 5) electrons in the InAs layer can be scattered into occupied and unoccupied states in the GaSb layer by the absorption of a photon. This corresponds to the emission of electrons in the InAs layer. However, in the large **k** case (processes 3 and 4 in figure 5) holes in the GaSb layer can be excited into occupied and unoccupied states in the InAs layer by photon absorption scattering. This corresponds to the capture of electrons. All these optical transition



**Figure 5.** Optical transition in a type II and broken-gap quantum well structure via absorption scattering in different subbands. The intrasubband optical scattering is forbidden. Note that the electron and hole subbands are located in spatially separated layers. Here  $E_e(\mathbf{k}) = \hbar^2 k^2 / 2m_e^* + \varepsilon_0^e$  and  $E_h(\mathbf{k}) = -\hbar^2 k^2 / 2m_h^* + \varepsilon_0^h$  are respectively the energy spectra for a 2DEG and a 2DHG and  $E_F$  is the Fermi level.

processes can contribute to electronic emission and capture and to the charge transfer between different layers. Consequently, although the overlap of the electron and hole wavefunctions at the interface is not as large as in a conventional quantum well (see figure 1), a strong photocurrent can be generated.

From the theoretical result given by equation (15) one can see that the peak of the conductance can be observed when the electronic emission and/or capture rates are comparable to the radiation frequency, i.e. when  $\lambda_{\rm E} + \lambda_{\rm C} \sim \omega$ . This implies that when the charge transfer rate is resonant with the radiation field a strong current can be generated in the circuit. Our numerical results indicate that for an InAs/GaSb type II quantum well at  $L_{\rm InAs} = 17$  and  $L_{\rm GaSb} = 5$  nm,  $\lambda_{\rm E} + \lambda_{\rm C} \sim 10^{11}$  Hz. Thus, a strong photocurrent can be generated by high-frequency microwave radiation from such a structure.

It is known that optical transition depends strongly on occupancy of the carriers in the system and, therefore, also depends on temperature sensitively (see figure 4). This has been reflected in the coefficient  $\kappa$  and emission and capture rates in equation (15). Because  $\lambda_E$  and  $\lambda_C$  are the functional forms of the temperature, the photoconductance of the device depends on *T* as indicated in figure 4. It should be noted that with decreasing temperature the *conventional* optical transition (i.e., transition between an occupied state and a unoccupied state) is more likely. Thus, at relatively low temperatures, processes 1 and 4 in figure 5 are more possible. This is one of the main reasons why the peak of the conductance lowers with increasing temperature and the red-shift can be observed at higher temperatures.

#### 4. Concluding remarks

In this work, we have demonstrated theoretically that when a linearly polarized sub-THz light field (such as high-frequency microwave radiation) is applied to an InAs/GaSb based type II and broken-gap quantum well, a current circuit can be formed and the photocurrent can be generated via optical absorption scattering accompanied by charge transfer between different layers. Thus, such a structure can be used as a sub-THz photovoltaic device working at relatively low temperatures ( $T \sim 10$  K). We have developed a simple and tractable theoretical approach to deal with such a situation and obtained theoretical results which can be related to experiments and experimental findings. We hope the interesting and important theoretical finding observed in this work can be verified experimentally. This work was supported by the Australia Research Council, the NSF of China under grant No 10374091, the special Funds for Major State Basic Research Project of China (973) under grant No 2005CB623603, the Knowledge Innovation Program of the Chinese Academy of Sciences and the Director Grants of Hefei Institutes of Physical Sciences. Part of the calculation was performed at the Center for Computational Science, Hefei Institutes of Physical Sciences.

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