Magnetic impurity effects in metallic carbon nanotubes: local non-Fermi liquid theory

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Abstract. Magnetic impurity effects on metallic carbon nanotubes are studied theoretically. The resolvent method for the multichannel Kondo effect is applied to the band structure of the $k \cdot p$ perturbation Hamiltonian in the limit of infinite onsite repulsion at the impurity site. We discuss the local non-Fermi liquid behaviour at temperatures below the Kondo temperature $T_K$. The density of states of localized electrons has a singularity at about $|\omega|^{1/2}$, which gives rise to a pseudogap at the Kondo resonance at low temperatures. The temperature dependence of the electronic resistivity is predicted to be $T^{1/2}$, and the imaginary part of the dynamical susceptibilities is dependent on $|\omega|^{1/2}$. Possible experimental observations are discussed.

1. Introduction

Recently, carbon nanotubes with cylindrical graphite structures have been intensively studied. Many interesting experimental and theoretical investigations have been performed (see reviews [1, 2] for example), and the fundamental metallic and semiconducting behaviour of single-wall nanotubes predicted by theory [3]–[8] has been clarified in tunnelling spectroscopy experiments [9, 10].

Firstly, in a magnetoresistance study of metallic nanotubes [11], disorder gives rise to positive differential resistance at low temperatures due to weak localization effects [12]. Some samples are known to show negative resistance around the weak gate voltage region, which is
interpreted as possibly being due to the presence of the Kondo resonance as the result of the magnetic impurity effect. Therefore, a magnetic impurity might change the electronic structure of metallic carbon nanotubes.

The second candidate for the magnetic impurity is the fluorine (F) adatoms on the nanotubes. Recent experiments [13, 14] on nanographite doped with F show the appearance of electronic spin in the fluorine concentration range \([F]/[C] = 0–1.2\). The fluorine concentration is an order of magnitude greater than the carbon concentration. The computer simulation of F-doping effects on nanographite [15] supports the presence of a local spin at the fluorine atom bonded to the carbon atom.

Thirdly, it is known that pristine carbon nanotubes are found to coexist with amorphous carbon soots [1, 2]. Their effects are not of prime interest usually, however, we are aware that amorphous metals are modelled well by the two-level system [16, 17]. The low-temperature behaviour of resistivity in the two-level system is similar to that of the Kondo model of magnetic impurities [18–20]. So, the metallic nanotube with amorphous carbon soots may show behaviour similar to the effects of magnetic impurities at low temperatures. This viewpoint is very interesting as a possible realization of the results of low-temperature properties of the two-level system, or equivalently, magnetic impurity effects.

In this paper, we will study the effects of a magnetic impurity in metallic carbon nanotubes at low temperatures. Nonmagnetic impurity effects [21, 22] have also been studied by the present author. However, magnetic impurity effects are attractive also, when we look at our experience of the research of f electron systems [23]. There are two channels of electronic states at the Fermi energy in metallic carbon nanotubes. As known in magnetic systems such as heavy fermion systems [24], non-Fermi liquid behaviour, i.e., the singular density of states and the power-law temperature dependence of the electric resistivity, has been observed experimentally and explained theoretically by using the Kondo model or the Anderson model with multichannel scattering. Similar effects can occur in the carbon nanotubes when the presence of both scattering channels plays an important role.

We will use the \(k \cdot p\) method [25, 26] for the electronic states of carbon nanotubes. The method describes well the electronic states around the Fermi energy. The valence and conduction band states have linear dispersion at the Fermi energy in metallic nanotubes. It is assumed that there is one magnetic impurity at a carbon site. The magnetic impurity is modelled by the Anderson model where there is one localized electronic state, and strong onsite repulsion is assumed. For treatment of the Kondo effect, we use the resolvent method [27, 28] to discuss the infinite repulsion case. This is sufficient for the discussion of the low-temperature and low-energy behaviour. We will solve spectral functions of the resolvents, and derive analytic formulas of electronic density of states, resistivity, and dynamical susceptibilities. We will discuss the local non-Fermi liquid behaviour which might be observed at low temperatures. The density of states of localized electrons has a singularity at about \(|\omega|^{1/2}\). This singular behaviour gives rise to a pseudogap at the Kondo resonance at low temperatures. The temperature dependence of the electronic resistivity is predicted to be \(T^{1/2}\), and the imaginary part of the dynamical susceptibilities has a \(|\omega|^{1/2}\) dependence. Possible experimental observations are discussed.

This paper is organized as follows. In the next section, we introduce the model and explain the theoretical formulations. In section 3, we report the low-temperature solution of the resolvents. In section 4, the electronic density of states is derived. In sections 5 and 6, resistivity and dynamical susceptibilities are explained. Section 7 is devoted to discussion, and the paper is closed with a summary in section 8.
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2. Model

We will study the metallic carbon nanotubes with one Anderson impurity at the A or B sublattice site. In the total Hamiltonian

\[ H = H_{\text{tube}} + H_{\text{imp}} \]

where \( H_{\text{tube}} \) represents the electronic states of the carbon nanotubes, and the model based on the \( k \cdot p \) approximation [25, 26] represents electronic systems on the continuum medium. The second term \( H_{\text{imp}} \) is the Anderson impurity where the onsite Coulomb interaction strength is taken as infinite in the course of calculation, and the resolvent formalism [27, 28] is introduced in order to take into account the infinite repulsion.

The Hamiltonian by the \( k \cdot p \) approximation [25, 26] in the secondly quantized representation has the following form

\[ H_{\text{tube}} = \sum_{k,\sigma} \Psi_{k,\sigma}^\dagger E_k \Psi_{k,\sigma} \]

where \( E_k \) is an energy matrix

\[ E_k = \begin{pmatrix}
    0 & \bar{\gamma}(k_x - ik_y) & 0 & 0 \\
    \bar{\gamma}(k_x + ik_y) & 0 & 0 & 0 \\
    0 & 0 & 0 & \bar{\gamma}(k_x + ik_y) \\
    0 & \bar{\gamma}(k_x - ik_y) & 0 & 0
\end{pmatrix} \]

with \( \mathbf{k} = (k_x, k_y) \), and \( \Psi_{k,\sigma} \) is an annihilation operator with four components. In the operator \( \Psi \), the first and second columns indicate electrons at the A and B sublattices around the Fermi point \( K \) of the graphite. The third and fourth columns represent electrons at the A and B sublattices around the Fermi point \( K' \). The quantity \( \bar{\gamma} \) is defined as \( \bar{\gamma} \equiv (\sqrt{3}/2)a\gamma_0 \), where \( a \) is the bond length of the graphite plane and \( \gamma_0 (\approx 2.7 \text{ eV}) \) is the resonance integral between neighbouring carbon atoms. When the above matrix is diagonalized, we obtain the dispersion relation \( E_{\pm} = \pm \bar{\gamma} \sqrt{k_y^2 + \kappa_{\nu \phi}^2(n)} \), where \( k_y \) is parallel with the axis of the nanotube, \( \kappa_{\nu \phi}(n) = (2\pi/L)(n + \phi - \nu/3) \), \( L \) is the circumference of the nanotube, \( n (= 0, \pm 1, \pm 2, \ldots) \) is the band index, \( \phi \) is the magnetic flux in units of the flux quantum, and \( \nu (= 0, 1, 2) \) specifies the boundary condition in the \( x \) direction. The metallic and semiconducting nanotubes are characterized by \( \nu = 0 \) and \( \nu = 1 \) (or 2), respectively. Hereafter, we consider the case \( \phi = 0 \) and metallic nanotubes with \( \nu = 0 \).

The second term in equation (1), \( H_{\text{imp}} \), is the impurity model

\[ H_{\text{imp}} = E_d \sum_{\sigma} d_{\sigma}^\dagger d_{\sigma} + \frac{U_d}{2} \sum_{\sigma} n_{d,\sigma} n_{d,-\sigma} + V \sqrt{\frac{2}{N_s}} \sum_{k,\sigma} [d_{\sigma}^\dagger (e^{i(k+\mathbf{K}) \cdot \mathbf{r}_0} \Psi_{k,\sigma}^{(1)} + e^{i\eta (k+\mathbf{K}) \cdot \mathbf{r}_0} \Psi_{k,\sigma}^{(3)}) + \text{h.c.}] \]

where \( d \) is a localized electron operator with spin \( \sigma \); its site energy is \( E_d \); \( U_d \) is the onsite repulsive interaction and \( n_{d,\sigma} = d_{\sigma}^\dagger d_{\sigma} \); \( V \) is the mixing interaction between the electrons on the nanotube and the localized orbital; \( N_s \) is the total number of lattice sites; \( \eta \) is the angle between the chiral vector of the present nanotube and the tube axis direction of the armchair-type nanotubes; and \( \Psi_{k,\sigma}^{(i)} (i = 1-4) \) is the \( i \)th component of the operator \( \Psi_{k,\sigma} \), assuming that the Anderson impurity is located at the site \( \mathbf{r}_0 \) of the A sublattice set. When the impurity is located at one of the B...
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sublattice sites, the second and fourth components of $\Psi_{k,\sigma}$ appear in $H_{\text{imp}}$. However, the result of the single-impurity system is exactly the same.

The propagator of the electrons on the nanotube is defined in matrix form as

$$G(k, \tau) = -\langle T_{\tau} \Psi_{k,\sigma}(\tau) \Psi_{k,\sigma}^\dagger(0) \rangle$$  \hspace{1cm} (5)$$

where $T_{\tau}$ is the time ordering operator with respect to the imaginary time $\tau$ and $\Psi_{k,\sigma}(\tau) = \exp(H\tau)\Psi_{k,\sigma}\exp(-H\tau)$. The Fourier transform of $G$ is calculated as

$$G^{-1}(k, i\omega_n) = \begin{pmatrix} G_{K}^{-1}(k, i\omega_n) & 0 \\ 0 & G_{K'}^{-1}(k, i\omega_n) \end{pmatrix}$$  \hspace{1cm} (6)$$

where $\omega_n = (2n + 1)\pi T$ is the odd Matsubara frequency for fermions. The components of $G$ are written explicitly

$$G_{K}^{-1}(k, i\omega_n) = \begin{pmatrix} i\omega_n - \bar{\gamma}(k_x + ik_y) & -\bar{\gamma}(k_x - ik_y) \\ -\bar{\gamma}(k_x - ik_y) & i\omega_n \end{pmatrix}$$  \hspace{1cm} (7)$$

and

$$G_{K'}^{-1}(k, i\omega_n) = \begin{pmatrix} i\omega_n - \bar{\gamma}(k_x + ik_y) & -\bar{\gamma}(k_x - ik_y) \\ -\bar{\gamma}(k_x - ik_y) & i\omega_n \end{pmatrix}.$$  \hspace{1cm} (8)

There are several theoretical characteristic parameters. We will explain them as follows

(i) The total carbon number $N_s$ is given by

$$N_s = A \times L \div \left( \frac{\sqrt{3}}{2} a^2 \right) \times 2 = \frac{4AL}{\sqrt{3}a^2}$$  \hspace{1cm} (9)$$

where $A$ is the length of the nanotube, and $(\sqrt{3}/2)a^2$ is the area of the unit cell. There are two carbons in one unit cell, so the factor 2 is multiplied.

(ii) The density of states near the Fermi energy $E = 0$ is calculated as

$$\rho(E) = \frac{A}{2\pi} \int_{-\infty}^{\infty} dk_y \delta(E - \bar{\gamma}k_y) = \frac{aN_s}{4\pi L\gamma_0}.$$  \hspace{1cm} (10)$$

Because two sites in the discrete model correspond to one site in the continuum $k \cdot p$ model, the density of sites in the continuum model is given by

$$\rho(E) = \frac{a}{2\pi L\gamma_0}.$$  \hspace{1cm} (11)$$

(iii) In the Kondo effect theory, it is necessary to define the band cutoff $D$ in order that $\rho(E = 0) = 1/2D$. Thus, the quantity $D$ is written explicitly

$$D = \frac{\pi L}{a}\gamma_0.$$  \hspace{1cm} (12)$$

Table 1 shows several combinations of parameters, $D$ and $E_1 \equiv \bar{\gamma}k_{00}^2(n = 1) = (\sqrt{3}\pi a/L)\gamma_0$, as a reference for realistic parameter values of nanotubes. We find that $D$ is a fairly large cutoff for typical single-wall nanotubes. The energy $E_1$ at the bottom of the conduction band $n = 1$ is apparently larger than the energy scale which corresponds to room temperature or low temperatures. This would mean that the effects of the upper or lower bands which do not cross the Fermi energy are small enough to neglect their contributions to the multichannel Kondo behaviour at low temperatures.

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In the resolvent method [27, 28], we consider mainly the limit $U_d \to \infty$ so that double occupancy at the localized level is forbidden. The empty state and the singly occupied state at the magnetic impurity are taken into account in the formalism. The spin degeneracy $N$ and the number of scattering channels $M$ of the band states are generalized to take an arbitrary integer value. In the limit of $M, N \to \infty$ with $\gamma \equiv M/N$ fixed, the single-impurity problem is represented by the coupled integral equation

$$
\Sigma_d(\omega) = \frac{\gamma \tilde{\Gamma}}{\pi} \int d\epsilon f(\epsilon) \Phi_b(\epsilon + \omega)
$$

(13)

$$
\Pi_b(\omega) = \frac{\tilde{\Gamma}}{\pi} \int d\epsilon f(\epsilon) \Phi_d(\epsilon + \omega)
$$

(14)

where $\tilde{\Gamma} \equiv \pi \rho N V^2$, $f(\epsilon) = 1/[\exp(\epsilon/T) + 1]$,

$$
\Phi_d(i\omega_n) = \frac{1}{i\omega_n - E_d - \Sigma_d(i\omega_n)}
$$

(15)

is the resolvent for the singly occupied d state, and

$$
\Phi_b(i\nu_n) = \frac{1}{i\nu_n - \Pi_b(i\nu_n)}
$$

(16)

is the resolvent for the empty d state. Here, we denote the even Matsubara frequency as $\nu_n$.

The validity of the multichannel problem for the application of metallic nanotubes can be understood easily by looking at the formula of the self-energies. In the case $U_d = 0$, the self-energy of the d electron is

$$
\Sigma_d(i\omega_n) = V^2 \frac{2}{N_s} \sum_k \left[ G^{(1)}_K(k, i\omega_n) + G^{(3)}_K'(k, i\omega_n) \right]
$$

(17)

where $G^{(1)}_K$ is the first diagonal component of the propagator equation (6) and $G^{(3)}_K'$ is the third component. After inserting their explicit forms, we obtain

$$
\Sigma_d(i\omega_n) = V^2 \frac{2}{N_s} \sum_k \frac{2i\omega_n}{(i\omega_n)^2 - \gamma^2(k_x^2 + k_y^2)}
$$

$$
= V^2 \frac{2}{N_s} \sum_k \left( \frac{1}{i\omega_n - \gamma \sqrt{k_x^2 + k_y^2}} + \frac{1}{i\omega_n + \gamma \sqrt{k_x^2 + k_y^2}} \right)
$$

$$
\simeq MV^2 \frac{2}{N_s} \sum_k \frac{1}{i\omega_n - \epsilon_k}
$$

(18)

where the scattering channel number is expressed as $M$ and $-D < \epsilon_k < D$ with the density of states $\rho = 1/2D$ ($D$ is defined by equation (12)). Only the two bands which cross the Fermi energy are retained in the sum of the last line, because the characteristic energy $E_1$ is fairly large, as discussed above. Similarly, in the limit $U_d \to \infty$, the self-energy of the resolvent $\Phi_d$ is

$$
\Sigma_d(i\omega_n) = -MV^2 \frac{2}{N_s} \sum_k T \sum_{\omega_{n'}} \frac{1}{\omega_{n'} - \epsilon_k} \Phi_b(i\omega_n - i\omega_{n'}). 
$$

(19)

The difference from the $U_d = 0$ case is that the resolvent $\Phi_b$ appears in the right-hand side. After taking the frequency sum, we obtain the integral form equation (13). Therefore, we have shown that the set of integral equations of the multichannel Kondo problem is valid for a magnetic impurity in metallic carbon nanotubes.
We note that we can derive an exchange-type interaction Hamiltonian by applying the Schrieffer–Wolff transformation. The result is written as

\[ H_{SW} = -J \sum_{k, k', \alpha} (\chi_{d,k}^\dagger S \chi_{d,k}) \cdot (\chi_{d,k'}^\dagger S \chi_{d,k'}) \]

where \( J = 2V^2/E_d \), \( \alpha \) is a channel index, \( S = (1/2)\sigma \), \( \chi_{d,k}^\dagger = (d_{\uparrow}, d_{\downarrow}) \), and \( \chi_{d,k}^\dagger = (\Psi_{\alpha,k}^\dagger \Psi_{\alpha,k}^\dagger) \).

The conformal field theory and other methods teach us that we can obtain the power exponent of \( 1/2 \) of the singular density of states of the localized electron (see [29], for example). Therefore, the results of the present paper by the resolvent method do not depend on whether we use the exchange-type Hamiltonian or the exact theoretical method.

### 3. Low temperature solution of resolvents

The set of integral equations (13) and (14) can be solved analytically in the limit of low frequency and low temperatures [27, 28]. Before discussing physical quantities, we derive analytic forms of resolvents. As the resolvents mean singly occupied states and empty states physically, the analytic property is not the same as that of the usual propagators. We define spectral functions for the empty states at \( \omega > E_0 \)

\[ A_{d,b}^{(+)\dagger}(\omega) \equiv -\frac{1}{\pi} \text{Im} \Phi_{d,b}(\omega + i\delta) \]

and spectral functions for the occupied states at \( \omega < E_0 \),

\[ A_{d,b}^{(-)} \equiv \lim_{T \to 0} \left[ -\frac{1}{\pi} \text{Im} \Phi_{d,b}(\omega + i\delta) \right] \exp[\beta(E_0 - \omega)] \]

where \( E_0 \) is the ground state energy of the magnetic impurity at zero temperature, \( \delta \) is the positive infinitesimal, and \( \beta = 1/T \).

After some calculations following [27], we find the following formula at low frequency

\[ A_d^{(+)} \sim |\Theta(\omega)|^{-\gamma} \]

and

\[ A_b^{(+)} \sim |\Theta(\omega)|^{-1}. \]

Here,

\[ \Theta(\omega) \equiv \left[ \left( \frac{1 + \gamma}{\gamma} \right) \left( \frac{E_0 - \omega}{T_K} \right) \right]^{1+\gamma} \]

with \( \gamma = M/N \), and where \( T_K \) is the Kondo temperature

\[ T_K = D \left( \frac{\gamma \Gamma}{\pi D} \right)^{\gamma} \exp \left( \frac{\pi E_d}{\Gamma} \right). \]

For the special case of metallic nanotubes, \( M = 2 \) and \( N = 2 \). Therefore, we find the singular frequency dependence around the ground state energy \( E_0 \)

\[ A_d^{(\pm)}(\omega) \sim A_b^{(\pm)}(\omega) \sim |E_0 - \omega|^{-\frac{1}{2}}. \]

This singular dependence is the main conclusion of this section. The frequency dependence is shown schematically in figure 1.

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Figure 1. The singular behaviour of the spectral functions $A_{d,b}^{(\pm)}(\omega)$. The figure is drawn schematically.

4. Density of states

The local density of states of d electrons is calculated by the convolution of spectral functions $A_{d,b}^{(\pm)}(\omega)$ [27, 28]. The explicit form of the density of states for spin $\sigma$ and the channel $\alpha$ at $T = 0$ becomes

$$\rho_{\sigma,\alpha}(\omega, 0) \simeq \left[ \frac{\pi}{(1 + \gamma)^2 \tilde{\Gamma}} \right] [1 + \theta(\omega)f_+ (\tilde{\omega}) + \theta(-\omega)f_- (\tilde{\omega})]$$

where

$$f_\pm (\tilde{\omega}) = a_\pm |\tilde{\omega}|^{\Delta_{sp}} + b_\pm |\tilde{\omega}|^{\Delta_{ch}}$$

with

$$a_- = - \left( \frac{4\gamma}{2 + \gamma} \right) \sin(\pi \Delta_{ch}) B(2\Delta_{sp}, \Delta_{ch})$$

$$a_+ = - \cos(\pi \Delta_{ch}) a_-$$

$$b_+ = - \left( \frac{4W_{ch}}{1 + 2\gamma} \right) \sin(\pi \Delta_{ch}) B(2\Delta_{ch}, \Delta_{sp})$$

$$b_- = \cos(\pi \Delta_{ch}) b_+.$$  

Here, $\tilde{\omega} \equiv [(1 + \gamma)/\gamma](\omega/T_K)$, $B(x, y)$ is the beta function, and $W_{ch} \equiv \pi T_K/\tilde{\Gamma}$ is the weight of channel fluctuations. Further, $\Delta_{sp} \equiv 1/(1 + \gamma)$ and $\Delta_{ch} \equiv \gamma/(1 + \gamma)$ are the scaling dimensions of spin and channel fields, respectively. As $\Delta_{ch} \propto M$, this measures the magnitude of fluctuations from the channel degree of freedom. Also, $\Delta_{sp} \propto N$ means that this is a measure of the contributions from the spin degree of freedom. Both quantities determine the degree of singularity of the electronic density of states and physical quantities at low frequencies. They are the most important parameters introduced in this section.

In particular, for metallic carbon nanotubes, we know that $\Delta_{sp} = \Delta_{ch} = 1/2$. This implies the singularity around the Fermi energy $\omega = 0$

$$\rho(\omega, 0) \sim 1 + \theta(\omega)|\omega|^\frac{1}{2} + \theta(-\omega)|\omega|^\frac{1}{2} \sim \sqrt{|\omega|}.$$  

Such a singular functional form implies that a pseudogap develops at the top of the Kondo resonance peak, which appears at temperatures much lower than $T_K$. A dip appears in the density of states at the Fermi energy. The dip structure of the density of states is shown schematically in figure 2. This is the local non-Fermi liquid behaviour discussed in detail in the literature [24, 29]. If it becomes possible to measure the local density of states of a metallic atom attached
The dip structure of the density of states \( \rho(\omega) \). The figure is drawn schematically.

to the carbon nanotubes, for example, by scanning tunnelling microscopy, we could observe such pseudogap behaviour when the role of the multichannel scattering is dominant.

5. Resistivity

In this section, we consider the electric resistivity in order to look at how the singular behaviour will be observed. The scattering rate \( \tau \) is calculated from the scattering \( t \) matrix

\[
\tau_{\sigma,\alpha}(\omega, T)^{-1} = -2\text{Im} t^{(1)}_{\sigma,\alpha}(\omega + i\delta, T) = \frac{2\tilde{\Gamma}_{\sigma,\alpha}(\omega, T)}{\rho N}. \tag{34}
\]

The relation with the electronic resistivity

\[
\bar{\rho}(T) \propto \left[ \int d\epsilon \left( -\frac{\partial f}{\partial \epsilon} \right) \tau(\epsilon, T) \right]^{-1} \tag{35}
\]
gives the low-temperature behaviour

\[
\frac{\bar{\rho}(T)}{\bar{\rho}(0)} \simeq 1 - c \left( \frac{T}{T_K} \right)^{\min(\Delta_{sp}, \Delta_{ch})} + \ldots \tag{36}
\]

where \( c \) is a constant, but it is difficult to obtain its explicit form from only information about the \( \omega \) dependence of \( \rho_{\sigma,\alpha} \). Here, we stress that the above singular functional form agrees with that obtained from the conformal field approach [30, 31]. Therefore, the temperature dependence of the leading term \( (T/T_K)^{\min(\Delta_{sp}, \Delta_{ch})} \) is a general result, which is independent of the theoretical treatment method.

For the metallic carbon nanotubes, we already know that \( \Delta_{sp} = \Delta_{ch} = 1/2 \). Therefore, the low-temperature behaviour

\[
\frac{\bar{\rho}(T)}{\bar{\rho}(0)} \simeq 1 - c \sqrt{\frac{T}{T_K}} \tag{37}
\]
is expected from the above general formula.

6. Magnetic susceptibility

Spin and channel susceptibilities are calculated by the linear response function. The spin susceptibility means the magnetic susceptibility, in other words. The imaginary parts of the
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dynamical susceptibilities are defined as
\[ \tilde{\chi}''_{\text{sp}} = \frac{1}{N} \text{Im} \chi_{\text{sp}} \]  
(38)
and
\[ \tilde{\chi}''_{\text{ch}} = \frac{1}{M} \text{Im} \chi_{\text{ch}}. \]  
(39)

The first term of \( \tilde{\chi}''_{\text{sp}} \) at \( T = 0 \) is calculated to be
\[ \tilde{\chi}''_{\text{sp}}(\omega, 0) \sim \frac{C_{\text{sp}}}{T_K} sgn \omega |\tilde{\omega}|(\Delta_{\text{sp}} - \Delta_{\text{ch}}) \]  
(40)
where
\[ C_{\text{sp}} = \gamma \Delta_{\text{sp}}^2 \sin(\pi \Delta_{\text{sp}}) B(\Delta_{\text{sp}}, \Delta_{\text{sp}}). \]  
(41)

The second correction gives the \( \omega \) dependence
\[ \tilde{\chi}''_{\text{sp}}(\omega, 0) \sim |\tilde{\omega}|^{(2\Delta_{\text{sp}} - \Delta_{\text{ch}})}. \]  
(42)

Similarly, the dominant term of \( \tilde{\chi}''_{\text{ch}} \) at \( T = 0 \) becomes
\[ \tilde{\chi}''_{\text{ch}}(\omega, 0) \sim \frac{C_{\text{ch}}}{T_K} sgn \omega |\tilde{\omega}|(\Delta_{\text{ch}} - \Delta_{\text{sp}}) \]  
(43)
where
\[ C_{\text{ch}} = W_{\text{ch}}^2 \Delta_{\text{sp}} \sin(\pi \Delta_{\text{ch}}) B(\Delta_{\text{ch}}, \Delta_{\text{ch}}). \]  
(44)

The second term has \( \omega \) dependence
\[ \tilde{\chi}''_{\text{ch}}(\omega, 0) \sim |\tilde{\omega}|^{(2\Delta_{\text{ch}} - \Delta_{\text{sp}})}. \]  
(45)

The above general formulas (40)–(45) reduce to that of metallic carbon nanotubes. The result of singular behaviour is common for spin and channel susceptibilities
\[ \tilde{\chi}''(\omega, 0) \sim A sgn \omega \left( 1 - B \sqrt{\frac{|\omega|}{T_K}} + \ldots \right) \]  
(46)

where \( A \) and \( B \) are constants. We find \( \sqrt{|\omega|} \) dependence at low frequencies. We note that the term \( sgn \omega \) is related with the real part
\[ \tilde{\chi}'(\omega, T) \sim -\log \left[ \max(\omega, T) \right]. \]  
(47)

7. Discussion

We have discussed the solutions of the integral equations in the limit \( M, N \to \infty \) in this paper. The higher-order corrections of \( O(1/N) \) [27, 28] are known to change the coefficients of the leading terms of singular behaviour, but they do not affect the powers of the singularities (i.e. \( \Delta_{\text{sp}} \) and \( \Delta_{\text{ch}} \) in (28)). Therefore, the non-Fermi liquid behaviour is not affected by the higher-order corrections in the \( O(1/N) \) expansion.

In the course of the investigation, we have neglected the valence and conduction band states which do not cross the Fermi energy. This approximation applies well at low energies.
Table 1. Parameters $D$ and $E_1$ for typical metallic carbon nanotubes.

| Nanotube | $D (\gamma_0 = 2.7 \text{ eV})$ | $E_1$  |
|----------|---------------------------------|--------|
| (5,5)    | 8.60 $\gamma_0 = 23.2 \text{ eV}$ | 1.99 $\gamma_0 = 5.37 \text{ eV}$ |
| (10,10)  | 12.2 $\gamma_0 = 32.9 \text{ eV}$ | 1.40 $\gamma_0 = 3.78 \text{ eV}$ |
| (15,15)  | 14.9 $\gamma_0 = 40.2 \text{ eV}$ | 1.15 $\gamma_0 = 3.11 \text{ eV}$ |
| (6,0)    | 16.3 $\gamma_0 = 44.0 \text{ eV}$ | 1.05 $\gamma_0 = 2.84 \text{ eV}$ |
| (9,0)    | 24.5 $\gamma_0 = 66.2 \text{ eV}$ | 0.698 $\gamma_0 = 1.88 \text{ eV}$ |

$|\omega| \sim T_K \ll E_1$. Typical magnitudes of $E_1$ have been shown in table 1. However, at higher energies or at high temperatures, such deep bands will give some correction to low-energy singular behaviour. Furthermore, functional forms of spectral functions at entire frequencies can be affected by the presence of deep bands. In order to treat the deep band effects, we have to solve the resolvent equations numerically at least, even though it is beyond the scope of this paper.

There are two scattering channels when the impurity interacts with the single-wall metallic nanotube. Is it possible that there are more scattering channels? When two metallic carbon nanotubes are present and one impurity interacts with both nanotubes, four scattering channels are realized as long as the interactions between electrons of two nanotubes are negligible. The powers of the singularities of the density of states and physical quantities become different from those in the case of the single nanotube. By putting $M = 4$ and $N = 2$, the general formulas of this paper can be applied to one magnetic impurity which interacts with two aligned metallic nanotubes. If the impurity interacts with more nanotubes, such general formulas are useful for predicting singular behaviour, which depends on the scattering channel number.

In the literature, for example in [32], the power-law temperature dependences of electronic resistivity have been interpreted by the Luttinger liquid picture of the correlated one-dimensional systems. The Kondo effect in the Luttinger liquid has been studied by Furusaki and Nagaosa [33]. A further study of the Kondo impurity with two scattering channels in the presence of conduction bands with Luttinger liquid properties would be a fascinating extension of the present work.

8. Summary

Magnetic impurity effects on metallic carbon nanotubes have been investigated theoretically. The resolvent method for the multichannel Kondo effect has been applied to the band structure of the $k \cdot p$ model in the limit of the infinite onsite repulsion at the impurity site. We have discussed the local non-Fermi liquid behaviour, which might be observed at temperatures below the Kondo temperature $T_K$. The density of states of localized electrons has a singularity at about $|\omega|^{1/2}$. This singular behaviour gives rise to a pseudogap at the Kondo resonance at low temperatures. The temperature dependence of the electronic resistivity is predicted to be $T^{1/2}$, and the imaginary part of the dynamical susceptibilities is dependent on $|\omega|^{1/2}$. 

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References

[1] Dresselhaus M S, Dresselhaus G and Eklund P C 1996 Science of Fullerenes and Carbon Nanotubes (San Diego: Academic)
[2] Saito R, Dresselhaus G and Dresselhaus M S 1998 Physical Properties of Carbon Nanotubes (London: Imperial College Press)
[3] Mintmire J W, Dunlap B I and White C T 1992 Phys. Rev. Lett. 68 631
[4] Hamada N, Sawada S and Oshiyama A 1992 Phys. Rev. Lett. 68 1579
[5] Saito R, Fujita M, Dresselhaus G and Dresselhaus M S 1992 Appl. Phys. Lett. 60 2204
[6] Tanaka K, Okahara K, Okada M and Yamabe T 1992 Chem. Phys. Lett. 193 101
[7] Harigaya K 1992 Phys. Rev. B 45 12071
[8] Harigaya K and Fujita M 1993 Phys. Rev. B 47 16563
[9] Wildöer J W G, Venema L C, Rinzler A G Smalley R E and Dekker C 1998 Nature 391 59
[10] Odom T W, Huang J L, Kim P and Lieber C M 1998 Nature 391 62
[11] Avouris P 1999 in Electronic Properties of Novel Materials: Science and Technology of Molecular Nanostructures ed H Kuzmany (New York: American Institute of Physics) p 393
[12] Bergmann G 1984 Phys. Rep. 11
[13] Shibayama Y et al 1998 Mol. Cryst. Liq. Cryst. 310 273
Shibayama Y et al 2000 Phys. Rev. Lett. 84 1744
[14] Takai K et al Mol. Cryst. Liq. Cryst. to be published
[15] Saito R, Yagi M, Kimura T, Dresselhaus G and Dresselhaus M S 1999 J. Phys. Chem. Sol. 60 715
[16] Phillips W A 1971 J. Low Temp. Phys. 7 161
[17] Anderson P W, Halperin B I and Varma C M 1972 Phil. Mag. 25 1
[18] Kondo J 1976 Physica B 84 207
[19] Black J L and Gyorffy B L 1978 Phys. Rev. Lett. 41 1595
[20] Vladar K and Zawadowski A 1983 Phys. Rev. B 28 1564
Vladar K and Zawadowski A 1983 Phys. Rev. B 28 1956
[21] Harigaya K 1998 cond-mat/9810341
[22] Harigaya K 1999 Phys. Rev. B 60 1452
[23] The slave boson method has been used for the heavy fermion (f electron) systems in:
Harigaya K 1990 J. Phys.: Condens. Matter 2 3259
Harigaya K 1990 J. Phys.: Condens. Matter 2 4623
[24] Degiorgi L 1999 Rev. Mod. Phys. 71 687
[25] Ajiki H and Ando T 1993 J. Phys. Soc. Japan 62 1255
[26] Ando T and Nakanishi T 1998 J. Phys. Soc. Japan 67 1704
[27] Müller-Hartmann E 1984 Z. Phys. B 57 281
[28] Coleman P 1984 Phys. Rev. B 29 3035
[29] Cox D I and Zawadowski A 1998 Adv. Phys. 47 599
[30] Affleck I and Ludwig A W W 1991 Nucl. Phys. B 352 849
Affleck I and Ludwig A W W 1991 Nucl. Phys. B 360 641
[31] Ludwig A W W and Affleck I 1991 Phys. Rev. Lett. 67 3160
[32] Bockrath M et al 1999 Nature 397 598
[33] Furusaki A and Nagaosa N 1994 Phys. Rev. Lett 72 892

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