Local Non-Fermi Liquid Theory of Magnetic Impurity Effects in Carbon Nanotubes

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Abstract. Magnetic impurity effects in carbon nanotubes are studied theoretically. The multi channel Kondo effect is investigated with the band structure of the metallic nanotubes. The local non-Fermi liquid behavior is realized at temperatures lower than the Kondo temperature $T_K$. The density of states of localized electron has a singularity $\sim |\omega|^{1/2}$ which gives rise to a pseudo gap at the Kondo resonance in low temperatures. The temperature dependence of the electronic resistivity is predicted as $T^{1/2}$, and the imaginary part of dynamical susceptibilities has the $|\omega|^{1/2}$ dependence.

INTRODUCTION

Recently, carbon nanotubes with cylindrical graphite structures have been intensively investigated. Many interesting experimental as well as theoretical researches have been performed (1,2), and the fundamental metallic and semiconducting behaviors of single wall nanotubes predicted by theories have been clarified in tunneling spectroscopy experiments.

In this paper, we will study effects of a magnetic impurity, for which several experimental works have been reported (3,4). Two channels of electronic states are present at the Fermi energy in metallic carbon nanotubes. In the magnetic systems (5), the non-Fermi liquid behaviors, i.e., the singular density of states and the power law temperature dependence of the electric resistivity, have been observed experimentally and explained theoretically by using the Kondo model or the Anderson model with multi channel scatterings. The similar effects can occur in the carbon nanotubes when the presence of the two scattering channels plays an important role.

SPECTRAL FUNCTIONS AND DENSITY OF STATES

The set of integral equations for the multi channel Kondo problem can be solved analytically in the limit of low frequency and low temperatures (6,7). We look at the
spectral functions for the empty states at $\omega > E_0$, $A^{(\pm)}_{d,b}(\omega)$, and those for the occupied states at $\omega < E_0$, $A^{(-)}_{d,b}(\omega)$, where $E_0$ is the ground state energy of the magnetic impurity at zero temperature.

After calculations following Ref. (6), we find the following formula at low frequency:

$$A^{(\pm)}(\omega) \sim |\Theta(\omega)|^{-\gamma}$$

and

$$A^{(\pm)}_b(\omega) \sim |\Theta(\omega)|^{-1},$$

where $\Theta(\omega) \equiv [(1 + \gamma)/\gamma \times (E_0 - \omega)/T_K]^{1/(1+\gamma)}$ with $\gamma = M/N$, $M$ is the scattering channel number, $N$ is the spin degeneracy, and $T_K$ is the Kondo temperature: $T_K = D(\gamma \tilde{\Gamma}/\pi D)^{\gamma} \exp(\pi E_d/\tilde{\Gamma})$. Here, $E_d$ is the localized level energy, $\tilde{\Gamma}$ is its broadening, and $D$ is the band cutoff.

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

$$A^{(\pm)}_d(\omega) \sim A^{(\pm)}_b(\omega) \sim |E_0 - \omega|^{\frac{1}{2}},$$

(1)

Next, the density of states of the localized electron is calculated by the convolution of spectral functions $A^{(\pm)}_{d,b}(\omega)$ (6,7). The explicit form of the density of states for spin $\sigma$ and the channel $\alpha$ at $T = 0$ becomes $\rho^{(\sigma,\alpha)}(\omega, 0) \approx [\pi N \tilde{\Gamma} / (1 + \gamma)^2][1 + \frac{\theta(\omega)f_+(\bar{\omega}) + \theta(-\omega)f_-(\bar{\omega})}{|\mathcal{D}_{ch}\Delta_{sp} + b_\pm|}]$, where $f_\pm(\bar{\omega}) = a_\pm|\bar{\omega}|^{\Delta_{sp} + b_\pm|\bar{\omega}|^{\Delta_{ch}}}$.

Here, $\bar{\omega} \equiv [1 + \gamma]/[|\omega/T_K]|$, and $a_\pm$ and $b_\pm$ are functions of the scaling dimensions of spin and channel fields, $\Delta_{sp} \equiv 1/(1 + \gamma)$ and $\Delta_{ch} \equiv \gamma/(1 + \gamma)$. Both quantities determine the degree of singularities of electronic density of states and physical quantities at low frequencies.

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

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

(2)

Such the singular functional form implies that a pseudo gap develops at the top of the Kondo resonance peak which appear at temperatures much lower than $T_K$. There appears a dip in the density of states at the Fermi energy. This is the local non-Fermi liquid behavior discussed in detail in the literature (5). If it is possible to measure the local density of states of a metallic atom attached to the carbon nanotubes, for example, by scanning tunneling microscope, we could observe such the pseudo gap behavior when role of the multi channel scatterings is dominant.

**RESISTIVITY AND MAGNETIC SUSCEPTIBILITY**

We consider the electric resistivity in low temperatures. The scattering rate $\tau$ is calculated from the scattering $t$ matrix: $\tau^{(\sigma,\alpha)}(\omega, T)^{-1} = -2 \text{Im}\rho^{(1)}(\omega + i\delta, T) = 2\tilde{\Gamma} \rho^{(\sigma,\alpha)}(\omega, T)/\rho N$, where $\rho$ is the density of states at the Fermi energy of the clean nanotube. The relation with the electronic resistivity $\bar{\rho}(T) \sim [\int d\epsilon(-\partial f/\partial \epsilon)\tau(\epsilon, T)]^{-1}$ gives the low temperature behavior: $\bar{\rho}(T)/\bar{\rho}(0) \sim 1 - c(T/T_K)^{\min(\Delta_{sp}, \Delta_{ch})} + ..., $ where $c$ is a constant, but it is difficult to obtain its explicit form only from the information of $\omega$-dependence of $\rho^{(\sigma,\alpha)}$. 
For the metallic carbon nanotubes, we already know $\Delta_{\text{sp}} = \Delta_{\text{ch}} = 1/2$. Therefore, the low temperature behavior

$$\frac{\bar{\rho}(T)}{\bar{\rho}(0)} \sim 1 - c\sqrt{\frac{T}{T_K}}$$

is expected from the above general formula.

Next, spin and channel susceptibilities are calculated by the linear response function. The spin susceptibility is the magnetic susceptibility in other words. The imaginary parts of dynamical susceptibilities are defined as $\tilde{\chi}_{\text{sp}}'' = (1/N)\text{Im}\chi_{\text{sp}}$ and $\tilde{\chi}_{\text{ch}}'' = (1/M)\text{Im}\chi_{\text{ch}}$.

The first term of $\tilde{\chi}_{\text{sp}}''$ at $T = 0$ is calculated to be $\tilde{\chi}_{\text{sp}}''(\omega, 0) \sim (C_{\text{sp}}/T_K) \text{sgn}\omega|\tilde{\omega}|(\Delta_{\text{sp}} - \Delta_{\text{ch}})$, where $C_{\text{sp}} = \gamma\Delta_{\text{sp}}^2\sin(\pi\Delta_{\text{sp}})B(\Delta_{\text{sp}}, \Delta_{\text{sp}})$, and $B(x, y)$ is the Beta function. The second correction gives the $\omega$ dependence: $\tilde{\chi}_{\text{sp}}''(\omega, 0) \sim |\tilde{\omega}|(2\Delta_{\text{sp}} - \Delta_{\text{ch}})$.

In the similar way, the dominant term of $\tilde{\chi}_{\text{ch}}''$ at $T = 0$ becomes $\tilde{\chi}_{\text{ch}}''(\omega, 0) \sim (C_{\text{ch}}/T_K) \text{sgn}\omega|\tilde{\omega}|(\Delta_{\text{ch}} - \Delta_{\text{sp}})$, where $C_{\text{ch}} = W_{\text{ch}}^2\Delta_{\text{sp}}\sin(\pi\Delta_{\text{ch}})B(\Delta_{\text{ch}}, \Delta_{\text{ch}})$. The second term has the $\omega$ dependence: $\tilde{\chi}_{\text{ch}}''(\omega, 0) \sim |\tilde{\omega}|(2\Delta_{\text{ch}} - \Delta_{\text{sp}})$.

The above general formulas reduce to that of metallic carbon nanotubes. The result of singular behavior is common for spin and channel susceptibilities:

$$\tilde{\chi}''(\omega, 0) \sim A\text{sgn}\omega(1 - B\sqrt{\frac{|\tilde{\omega}|}{T_K}} + ...),$$

where $A$ and $B$ are constants. We find $\sqrt{|\omega|}$ dependence at low frequencies.

**SUMMARY**

Magnetic impurity effects on metallic carbon nanotubes have been investigated theoretically. We have discussed the local non-Fermi liquid behavior at temperatures lower than the Kondo temperature $T_K$. The density of states of localized electron has a singularity $\sim |\omega|^{1/2}$. This singular behavior gives rise to a pseudo gap at the Kondo resonance in low temperatures. The temperature dependence of the electronic resistivity is predicted as $T^{1/2}$, and the imaginary part of dynamical susceptibilities has the $|\omega|^{1/2}$ dependence.

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