Spin Excitation in Nano-Graphite Ribbons with Zigzag Edges

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Spin excitation in a nano-graphite ribbon with zigzag edges is investigated theoretically. Due to the strongly localized nature of the states near Fermi energy, the effective Hamiltonian for the low energy physics is given by Heisenberg Hamiltonian with the nearest neighbor exchange coupling. The action corresponding to the effective Hamiltonian is mapped to that of the $O(3)$ nonlinear sigma model. It is shown that the spin excitation has a gap when the number of the zigzag lines is even, whereas the excitation becomes gapless in case of the odd number of the zigzag lines.

KEYWORDS: nano-graphite ribbon, spin excitation, nonlinear sigma model

Recently, the graphite-based one-dimensional materials with nano-meter sizes have been attracting much attention in both the fundamental sciences and the application sides. One of the most remarkable characteristics in these materials is that the electronic properties depend strongly on their geometrical structure. For example, the carbon nanotubes, which are made by rolling up a graphite sheet, can be either a metal or a semiconductor depending on the chiral vector specifying the way of wrapping.

A nano-graphite ribbon (NGR) is the nano-meter size graphite fragment. It has been clarified that the edge regions play important roles for the electronic structure in this material. The calculation based on the tight-binding model revealed that a NGR with zigzag-shaped edges, which is called as a zigzag NGR in the following and shown in Fig.1, has strongly localized one-particle states around the edges. The same conclusion is obtained also by the first-principle calculation. Since the localized states appear near the Fermi energy, it is expected that the mutual interaction between electrons affects the electronic states more strongly compared to the ordinary systems with extended states near the Fermi energy. Then it may be necessary for clarifying the electronic properties to utilize the different approach from the method for the ordinary system.

The effects of the mutual interaction on the zigzag NGR have been investigated by applying the mean-field theory to the Hubbard model with the on-site repulsive interaction and the hopping energy between the nearest neighbor atoms. It has been shown that the infinitesimal on-site repulsion induces spontaneous magnetic moments; the conclusion is different from that of two-dimensional graphite sheet, where the finite value is needed for appearance of the magnetic order. In addition, the large magnetic moments appear at the edges (1A and NB sites in Fig.1). Based on this spin structure, the effective spin ladder model is proposed and the existence of the spin gap is claimed. However, since it is considered that, in one-dimensional systems, the effects of the mutual interaction are not sufficiently taken into account in the mean-field treatment, the conclusion obtained by it has to be reexamined. In the present work, we investigate the spin excitation of the zigzag NGR with $N$ (number of the zigzag lines from one side to the other, see Fig.1) based on the renormalization group analysis and by mapping the $O(3)$ nonlinear sigma model (NLSM). Quite recently, Hikihara et al. investigated the ground state and the excitation around it of the zigzag NGR by both the bosonization theory and the density matrix renormalization group method. The bosonization theory insists that the ground state is a spin-singlet Mott insulator with finite charge and spin gap. The numerical calculation supports the conclusion in case of $N = 2$. We compare our result with the above conclusions obtained by the previous studies.

Fig. 1. The structure of the zigzag NGR with $N = odd$. Here the close (open) circle shows the A (B) sublattice and the rectangle with the dashed-dotted line indicates the unit cell.
As a model of the interacting electrons in the zigzag NGR, we consider the Hubbard Hamiltonian used in refs. 4, 8 and 9. At first we derive the effective Hamiltonian describing the low energy excitations. As was already discussed above, the states near $K_F = \pi/a$ (a : lattice spacing) have the strongly localized nature around the edges, and then the energy dispersion near $K_F$ are given as $E(K) \simeq \pm (Ka - \pi)^N$ as was shown in Fig.2.\(^6\) When the charge degree of freedom is frozen, the system behaves as Mott insulator. Thus, we consider the states near $\pi/a$ and the system behaves as Mott insulator. Thus, we discuss the fluctuation around the classical solution by discussing the fluctuation around the classical solution by the Heisenberg model with the nearest neighbor exchange term.

![Fig. 2. The band structure of the zigzag NGR with $N = 2$ (a) and $N = 3$ (b). Here $t$ is the hopping energy between the nearest neighbor sites and $a$ is the lattice spacing. The thin dashed curve express the Fermi energy and the asymptotic behaviors near Fermi energy, $E(K)/t \sim \pm (Ka - \pi)^N$ are written by the thick dotted curves.](image)

The action $A = A_{WZ} + A_0$ corresponding to the above Hamiltonian is expressed by the coherent state path integral as,\(^\text{10}\)

$$A_{WZ} = iS \sum_{i} \sum_{l} \{ w[n_iA(l)] + w[n_iB(l)] \},$$

$$A_0 = \frac{JS^2}{2} \int_0^\beta d\tau \sum_{l} \left[ \sum_{\text{codd}} \{ (n_{iA}(l) + n_{iB}(l))^2 ight.$$  
$$+ (n_{iB}(l - 1) + n_{iA}(l))^2 + (n_{iA}(l) + n_{iB}(l - 1))^2 \} 
$$  
$$+ \sum_{i \ge \text{even}} \{ (n_{iB}(l) + n_{iA}(l))^2 + (n_{iA}(l) - n_{iB}(l))^2 \} \right].$$

where $\beta = 1/(k_B T)$ ($T$ : temperature) and the constraint $n_{iA/B}(l) = 1$ is imposed. The quantity, $w[n_{iA/B}(l)]$ is the solid angle which $n_{iA/B}(l)$ forms in the period $0 \le \tau \le \beta$.

In the classical limit, the Hamiltonian (1)-(3) has the ground state with $S_{iA}(l) = S_{iB}(l) = -S$ where $e_z$ is the unit vector along the $z$-direction. Here we discuss the fluctuation around the classical solution by expanding as $S_{iA}(l) = S_{iB}(l) + S_{iA}(l)$ and $S_{iB}(l) = -S_{iB}(l)$. The equations of motion of the fluctuation in the linearized approximation are given as follows,

$$s_{iA}(l) = -iJS \left\{ 2s_{iA}(l) + s_{iB}(l) + s_{iB}(l - 1) \right\},$$

$$s_{iB}(l) = -iJS \left\{ 3s_{iA}(l) + s_{iB}(l) + s_{iB}(l) \right\} + s_{iB}(l) + (-1)^i), \quad \text{for } i = 2 \sim N,$$

$$s_{iB}(l) = iJS \left\{ 3s_{iB}(l) + s_{iA}(l) + s_{iA}(l) + s_{iA}(l) \right\} + s_{iB}(l) + (-1)^i), \quad \text{for } i = 1 \sim N - 1,$$

$$s_{iB}(l) = iJS \left\{ 2s_{iB}(l) + s_{iA}(l) + s_{iA}(l) \right\},$$

where $s_{iA/B}(l) = s_{iA/B}(l) + i s_{iA/B}(l)$. By introducing the Fourier transformation, $s_{iA}(l) = (N_L)^{-1/2} \sum_{k} e^{i(k(l+1)/4) - \omega t} s_{iA}(k)$ and $s_{iB}(l) = (N_L)^{-1/2} \sum_{k} e^{i(k(l-1)/4) - \omega t} s_{iB}(k)$, the eqs.(6)-(9) are rewritten as,

$$\omega s_{iA}(k) = 2s_{iA}(k) + 2\cos(ka/2)s_{iB}(k),$$

$$\omega s_{iB}(k) = 3s_{iA}(k) + s_{i-1B}(k) + 2\cos(ka/2)s_{iB}(k),$$

for $i = 2 \sim N,$

$$\omega s_{iB}(k) = -\{3s_{iB}(k) + s_{i+1A}(k) + 2\cos(ka/2)s_{iA}(k)\},$$

for $i = 1 \sim N - 1,$

$$\omega s_{iB}(k) = -\{2s_{iB}(k) + 2\cos(ka/2)s_{iA}(k)\}.\quad \text{(13)}$$

The above equations have the two Goldstone modes.
whose frequencies are given by \( \tilde{\omega} = \omega/JS = \pm 2|\sin(ka/2)| \sim \pm |ka| \equiv \omega_k(k)/JS \) (see Fig.3). Since the eigenvectors for the modes are obtained up to the \( k \)-linear as

\[
s_iA(k) = -i + 1/2 |ka|, \\
s_iB(k) = 1 + N - i/2 |ka|, \\
\]

the fluctuation, \( s_i^+(l) \), can be written as follows,

\[
s_iA(l) = \frac{1}{\sqrt{Nl}} \sum_k e^{i(k(l+(-1)^i)/4)a} \left\{ (-1 + N - i/2 |ka|) \right\}, \\
s_iB(l) = \frac{1}{\sqrt{Nl}} \sum_k e^{i(k(l-(-1)^i)/4)a} \left\{ (1 + N - i/2 |ka|) \right\},
\]

where \( \alpha(k) = i\omega_+(k)\alpha(k) \) and \( \beta(k) = -i\omega_-(k)\beta(k) \). Then, we introduce the spatially slowly varying functions made from the Goldstone modes,

\[
F(x_l) = \frac{1}{\sqrt{NL}} \sum_k e^{i(k(l+(-1)^i)/4)a} \left\{ (-1 + N - i/2 |ka|) \right\}, \\
G(x_l) = \frac{1}{\sqrt{NL}} \sum_k e^{i(k(l-(-1)^i)/4)a} \left\{ (1 + N - i/2 |ka|) \right\},
\]

with \( x_l = la \), eqs.(16) and (17) are written as follows, for \( i = \text{odd} \),

\[
s_iA^+(l) = F(x_l) + (N - i + 1/2)G(x_l), \\
s_iB^+(l) = -F(x_l + a/2) - (N - i - 1/2)G(x_l + a/2),
\]

and for \( i = \text{even} \),

\[
s_iA^+(l) = F(x_l + a/2) + (N - i + 1/2)G(x_l + a/2), \\
s_iB^+(l) = -F(x_l) - (N - i - 1/2)G(x_l).
\]

Next, we try to map the action given by eqs.(4) and (5) to that of the \( O(3) \) NLSM. Eqs. (20)-(23) suggest the following ansatz, for \( i = \text{odd} \),

\[
n_iA(l) = \Omega(x_l) + (N - i + 1/2)\frac{a}{S}l(x_l), \\
n_iB(l) = -\Omega(x_l + a/2) - (N - i - 1/2)\frac{a}{S}l(x_l + a/2),
\]

and for \( i = \text{even} \),

\[
n_iA(l) = \Omega(x_l + a/2) + (N - i + 1/2)\frac{a}{S}l(x_l + a/2), \\
n_iB(l) = -\Omega(x_l) - (N - i - 1/2)\frac{a}{S}l(x_l).
\]

The constraint \( |n_{iA/B}| = 1 \) leads to \( |\Omega| = 1 \) and \( \Omega = 0 \) to the first order of \( a/S \). By substituting eqs.(24)-(27) into eq.(4), we obtain in the continuum limit,

\[
A_{WZ} = i\theta Q + iN \int d\tau d\Omega(\partial_x \Omega \times \Omega)_l, \\
\]

where \( \theta = 2\pi S \) for \( N = \text{odd} \) and \( \theta = 0 \) for \( N = \text{even} \). The quantity \( Q \) is the winding number of the Euclidean space configuration \( \{\Omega(x, \tau)\} \) and written as,

\[
Q = \frac{1}{4\pi} \int d\tau d\Omega(\partial_x \Omega \times \partial_\tau \Omega)\Omega.
\]

On the other hand, the quantity \( A_0 \) is expressed as

\[
A_0 = \frac{JS^2N}{2} \int d\tau d\Omega \left\{ \frac{1}{2} (\partial_\tau \Omega)^2 + \frac{2}{S^2} l^2 \right\},
\]

By integrating the field \( l \) in eqs.(28) and (30), we obtain the following effective action of the NLSM as

\[
A_{\text{eff}} = i\theta Q + \frac{1}{2g} \int d^2x (\partial_\tau \Omega)^2.
\]

where \( x_1 = x, x_2 = \nu t \) with \( \nu = JSa \) and \( g = 2/(NS) \). The above effective action is the same as that for spin ladder systems\(^{11-13} \) and the excitation is gapless (gapped) for \( N = \text{odd (even)} \) in case of \( S = 1/2 \). The conclusion is different from the result based on the mean-field theory and that by the bosonization theory where there is the spin gap irrespectively of the number, \( N \). The discrepancy is considered to be due to the following facts. The effects of the interaction are difficult to be taken into account sufficiently in the mean-field theory starting from the band picture and the consistent mapping from the Fermionic theory to the bosonic one is
not done in the present case without the linear dispersion across the Fermi energy. In ref. 9, the spin excitation has been calculated for \( N = 3 \) numerically. It seems to us that the result indicates that the excitation for \( N = 3 \) is gapless, which is identical with our conclusion, though the authors do not insist it because of lack of the enough system size for extrapolation.

We note that the velocity of the excitation \( v \) is identical with that obtained by the spin wave analysis. In addition, in case of \( N = 1 \), the present results are identical with that with one-dimensional spin chains\(^{14}\) with \( a \to 2a \) because the lattice spacing becomes a half.

The coupling constant, \( g \), for \( N = 2 \) obtained here is smaller than that for the two-leg spin ladders with the isotropic coupling.\(^{12,13}\) Then the spin gap of the present system is expected to be smaller than that of the spin ladders. This fact is considered to be due to the lack of the exchange coupling between \( eg \), 1A and 2B. In deriving the effective action, eq.(31), the modes with high frequencies have been neglected. We have derived the effective action with taking account of both the Goldstone modes and the high frequency modes in case of \( N = 2 \). The conclusion is the same as eq.(31) with \( N = 2 \). Thus, it is expected that the high frequency modes do not play an important role for the analysis presented here.

In summary, we investigated the spin excitation of the zigzag NGR with the width \( N \). We concluded that the spin excitation is gapless for \( N = \text{odd} \), whereas the excitation has a gap in case of \( N = \text{even} \).

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