The Effective Theory of Hole Doped Spin-1 Chain

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Abstract

An effective theory for the hole doped spin-1 antiferromagnetic chain is proposed in this paper. The two branches of low energy quasi-particle excitation is obtained by the diagrammic technique. In the large t limit (in which t is the hole hopping term), the lower band is essentially the bound state of one hole and one magnon and the other band is the single hole state. We find a critical value of t, \( t_c = 0.21\Delta_H \) (in which \( \Delta_H \) is the Haldane gap). For \( t > t_c \), with the decrement of t, the mixing of these two bands become stronger and stronger, and at the same time the effective band mass becomes larger and larger. When \( t < t_c \) the minimum of the lower band moves away from zero to another point between zero and \( \pi/2 \). The spin structure factor is also calculated in this paper, and we find that for large t limit the main contribution is from the inter-band transition which induce a resonant peak in the Haldane gap. While for small t limit the main contribution is from the intra-band transition which only cause a diffusion like broad bump in the Haldane gap.

Key words: spin-1 chain, free Boson model, Haldane gap

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I. INTRODUCTION

Since Haldane’s seminal paper on the quantum Heisenberg spin chains [1], it has been investigated by many theoretical and experimental studies. For spin-1 antiferromagnetic chain, it is now well established both experimentally [2] and theoretically [3,4] that there is an energy gap between the triplet excitation and the singlet ground state. The gap size is recently determined to be $0.41J$ by using density matrix renormalization group (DMRG) [5] and exact diagonalization [6]. It is known that the low energy behavior for the quantum antiferromagnetic spin chains can be described by the nonlinear sigma ($NL\sigma$) models [1,7] and additional topological terms are further needed for half integer spin chains. Particular for the spin-1 chain, a phenomenological model named as free boson model has been proposed by Ian Affleck et al [8–10] based on the large N expansion for the $NL\sigma$ model. It has been shown that the free boson model captures the basic physics of the spin-1 chain in low temperature and can be used to calculate many physical properties correctly.

There are mainly two families of compounds which exhibit the essential physics of the antiferromagnetic quantum spin-1 chain. One is the early discovered compound $CsNiCl_3$ [2] and the other is $Y_2BaNiO_5$. Replacing $Y$ by $Ca$ for $Y_2BaNiO_5$ [11,12] one can dope the spin-1 chains by holes. The electronic transport properties, polarized x-ray absorption and neutron scattering of $Y_{2-x}Ca_xBaNiO_5$ have been measured by J. F. DiTusa et al [13]. The result of electronic resistivity shows that the hole doping greatly reduces the resistivity which implies a considerably large mobility for the holes. The neutron scattering experiment confirms the existence of new states in the Haldane gap [13]. Theoretically the effect of doping in Haldane gap system is a very interesting problem and have been studied by several groups using both numerical [14] and analytical methods [15,16].

For case of static hole doping, by using the DMRG method [14] Sorensen and Ian Affleck studied the in-gap state caused by two kinds of doping. One is bond doping and the other is site doping. In bond doping case, the effect of doping is to perturb an antiferromagnetic bond with $J' \neq J$. It gives rise a localized state centered at the perturbed bond with a
discrete energy level appeared inside the Haldane gap for sufficiently strong or weak $J'$. In site doping case, a static hole is considered to be located on the O ion between two Ni ions. Therefore the super exchange process between these two spins is destroyed or partly destroyed by the hole. The bound states in the Haldane gap are found only when the coupling between the hole and the nearest spin is weaker than a critical value. Similar results were obtained by M.Kaburagi and et al using variational calculation [16].

Also one can consider a mobile hole doped in spin-1 chain. S.C. Zhang and D. P. Arovas [17] considered a spin-0 hole hopping in a background of spin-1 chain by using an effective model which is quite similar to the t-J model and found some exact single and multi-hole spin singlet wave functions. The problem of spin 1/2 hole moving in spin-1 chain has been considered by K. Penc and H. Shiba [18] in the limit of small hopping amplitude. In their approach, the holes are hopping between the O sites and destroy the corresponding super exchange processes completely when the O sites are occupied by the holes. They found one spin-3/2 band and two spin 1/2 bands either in the VBS model or in the Heisenberg model due to the interaction between hole and its nearest neighboring spins. But for the realistic Heisenberg model, their variational calculation can only treat the finite lattice up to 15 sites. Recently E. Dagotto proposed a t-J like model to study the hole doped spin-1 chain. Using numerical techniques [19], the dispersion of the effective hole bands and the spin structure factor were obtained for the finite lattice up to 12 sites.

In the present paper, we propose an effective continuum theory to study the hole doping in spin-1 chain. The spin-1 chain is modeled by the free Boson model proposed by Ian Affleck et al [8, 10] which is essentially derived from the large N expansion of the $NL\sigma$ model. The effective interaction between the holes and the magnons are derived, based upon the following considerations. Recall the static hole limit, the effective interaction only contains the scattering process and the holes act as the scatter of the magnons. Then the effective Hamiltonian for the static hole doped in spin-1 chain can be even easily interpreted in the first quantization picture. The result shows that there are one or two (depends on the ineraction strength) impurity states with total spin equals 1/2 or 3/2 respectively in
the Haldane gap which are actually the bound states of a hole and a spin-1 magnon. This result is in good agreement with the numerical results. We may then draw an intuition to the moving holes. When the hole moves, the effective interaction should contain two main terms, one describes the scattering process of the hole and the magnon which has the same origin with that of the static hole case, the other describes the emission and absorption process of magnons.

We show in this paper that the first term results in a bound state of one hole and one magnon with the bound energy strongly depending on the total spin of the hole and magnon. Therefore, we will find that if we only consider the scattering process, the result is very similar to the static hole case. The only difference is that each impurity state in the static hole case will extend to a corresponding energy band if the hole can hop. The effect of the emission and absorption term will result in a hybridization of single hole state and the bound state of one hole and one magnon with total spin 1/2. This term plays a crucial role for small $t$, because the energy level of the bound state and that of the single hole state is very close in small $t$ limit and is quite large in large $t$ limit. Then we obtain three branches of excitation, the bound state of one hole and one magnon with total spin 3/2, the “one particle like” state with total spin 1/2 and the “two particle” like state with total spin 1/2. The “one particle like” state approaches to the single hole state in large $t$ limit and the “two particle like” state approaches to the bound state of one hole and one magnon with total spin 1/2. The dispersion of these three branches of excitations are obtained in the whole range of the hopping amplitude $t$. The band minimum of the “two particle like” state is found to be located at $\pi$ for $t > t_c$ and will be move toward $\pi/2$ when $t < t_c$. The value of $t_c$ is found to be near $0.21 \Delta_H$ in our calculation. In fact this can be understood as a result of the above mentioned hybridization effect in the small $t$ case. These results are consistent with the results for VBS model obtained by K. Penc and H. Shiba.

The spin structure factor is also obtained and the result is quite different for large $t$ case and small $t$ case. For large $t$ case the hole contribution to the spin structure factor is mainly contributed from the interband transition (from “two particle like” state to “one particle
like” states) and the spectral weight within the Haldane gap is centered at the minimum energy cost between the two bands, which is consistent with the calculation of Dagotta et al. But for small t case the contribution is mainly from intra band transition(from “two particle like” state to “two particle like” state within the same branch of dispersion), so there exists a diffusion like broad bump in the Haldane gap. The difference of the spin structure factor in the above mentioned two limit is quite interesting and has never been mentioned in the previous works.

The rest of the paper is organized as follows: The effective continuum Hamiltonian is derived in Sec. II, whereas dispersion of the bound states is calculated in Sec. III, and the spin structure factor is calculated in Sec. IV. Finally, we make a few concluding remarks in Sec. VI.

II. The Derivation of The Effective Hamiltonian

In this paper, we assume that the holes can hop within the oxygen sublattice, which is shown in Fig.1.

Then we can begin with the following total Hamiltonian

\[ H_{\text{total}} = H_{\text{ch}} + H_h + H_{J'} + H_{J_1} + H_{J_2} \]

\( H_{\text{ch}} \) is the rotationally invariant spin Hamiltonian for Antiferromagnetic spin-1 chain.

\[ H_{\text{ch}} = J \sum_i \vec{S}_i \cdot \vec{S}_{i+1} \] (1a)

and \( H_h \) is the hopping term of holes

\[ H_h = -t \sum_n f_{n+1/2,\sigma}^+ f_{n+3/2,\sigma} + H.C. \] (1b)

\( H_{J'} \) and \( H_{J_1} \) represent the destroying of super exchange process and a Kondo like interaction of spins and holes respectively,

\[ H_{J'} = -J' \sum_{\sigma,n} \vec{S}_n \cdot \vec{S}_{n+1}^+ f_{n+1/2,\sigma}^+ f_{n+1/2,\sigma} \] (1c)
\[ H_{J_1} = J_1 \sum_{n,\alpha,\beta} \vec{\sigma}_{n,\alpha,\beta} \cdot (\vec{S}_n + \vec{S}_{n+1}) f_{\alpha,n+1/2}^+ f_{\beta,n+1/2} \]  
\[(1d)\]

And \( H_{J_2} \) describes the hole hop to another site with its spin flipped by interacting with the spins of the chain.

\[ H_{J_2} = J_2 \sum_{n,\alpha,\beta} \vec{\sigma}_{n,\alpha,\beta} \cdot \vec{S}_n f_{\alpha,n}^+ f_{\beta,n}^+ + H.C. \]  
\[(1e)\]

It is known that \( H_{ch} \) can be mapped to the non-linear \( \sigma \) model by using the path integral in the spin coherent state representation. The antiferromagnetic order parameter is represented by a three dimensional vector field \( \vec{\phi} \), obeying a constraint as \( |\vec{\phi}|^2 = 1 \). The uniform magnetisation is represented by \( \vec{l} \),

\[ \vec{l} = \left( \frac{1}{v} \right) \vec{\phi} \times \frac{\partial \vec{\phi}}{\partial t} \]  
\[(2a)\]

And the spin operator at site \( i \) can be written as,

\[ \vec{S}_i \approx s(-1)^i \vec{\phi} + \vec{l}, \]  
\[(2b)\]

Then the spin-1 Heisenberg Haltonian can be mapped into an effective continuum field theory with the Hamiltonian density as:

\[ \mathcal{H}_{ch} = \frac{v^2}{2} \vec{\Pi}^2 + \frac{v}{2} \left( \frac{\partial \vec{\phi}}{\partial x} \right)^2 \]  
\[(2c)\]

with the constraint \( |\vec{\phi}|^2 = 1 \).

By taking the large \( N \) (the number of the components for \( \vec{\phi} \) field) limit, and further introduce a mass term as the Lagrange multiplier to relax the constraint on the field \( \vec{\phi} \) into an averaged one, we follow the free Boson model or Ginsburg-Landau model proposed by I. Affleck et al \[8-10\], in which an additional \( \vec{\phi}^4 \) term is added for keeping the stability. We then have

\[ \mathcal{H}_{ch} = \frac{v}{2} \vec{\Pi}^2 + \frac{v}{2} \left( \frac{\partial \vec{\phi}}{\partial x} \right)^2 + \frac{1}{2v} \Delta_H^2 \vec{\phi}^2 + \lambda |\vec{\phi}|^4 \]  
\[(3)\]

where \( \vec{\Pi}(x) \) is the canonic momentum conjugated to the field \( \vec{\phi}(x) \) satisfying \([\phi(x)_\alpha, \Pi(x')_\beta] = \delta_{\alpha,\beta} \delta(x - x') \). The three parameters \( v, \Delta_H \) and \( \lambda \) are chosen phenomenologically to fit the
experiment or the numerical result. In our present study we omit the $\phi^4$ term as for a preliminary discussion. We can then diagonalize the $H_{ch}$ by Fourier transformation, and obtain three branches of free magnons, which describe the triplet excitations upon the singlet ground state.

$$H_{ch} = \frac{v}{2} \sum_k \Pi(-k) \cdot \Pi(k) + \left[ \frac{v^2 k^2}{2} + \frac{\Delta H^2}{2v} \right] \phi(-k) \cdot \phi(k)$$

$$= \sum_{k,r} E_k (a_{k,r} a_{k,r}^+ + \frac{1}{2})$$

(4)

In equation(4) $a_{k,r}$ and $a_{k,r}^+$ are the annihilation and creation operators of the magnons satisfying

$$[a_{k,r}, a_{k',r'}^+] = \delta_{rr'} \delta_{kk'}$$

with $r = x, y, z$, $E(k) = \sqrt{v^2 k^2 + \Delta_H^2}$ and:

$$\phi(k) = \sqrt{\frac{v}{2E_k}} \left( \bar{a}_k + \bar{a}_{-k}^+ \right)$$

(5a)

$$\bar{\Pi}(k) = i \frac{E_k}{2v} \left( \bar{a}_k - \bar{a}_{-k}^+ \right)$$

(5b)

Now we have expressed the Hamiltonian for the Heisenberg chain in terms of the three branches of gapful magnons, we have In the continuum limit,

$$(S_i + S_{i+1}) \approx 2\bar{l}(x_i) + \frac{\partial \phi}{\partial x} |_{x=x_i}$$

(6)

For the perfect spin-1 chain, the field $\bar{l}(x)$ is always one order smaller than the field $\phi(x)$ and is of the same order as that of $\frac{\partial \phi(x)}{\partial x}$ which reflects the short range anti-ferromagnetic correlation in low temperature. But if doped with an spin-1/2 holes, as we will show later, the hole will induce a localized mode of magnon which has an extension only of several lattice near the hole. So in the doped case near the site of the hole, the field $\bar{l}(x)$ could be of the same order with field $\phi(x)$, and could be one order larger than $\frac{\partial \phi(x)}{\partial x}$. Therefore, we can omit $\frac{\partial \phi(x)}{\partial x}$ in (6) and only keep the first term. Then the interaction term $H_J'$, $H_J_1$ and $H_J_2$ can be written as,
\[ H' = \sum_i \left[ (\vec{S}_i + \hat{S}_{i+1})^2 - 4 \right] f_{i+1/2,\sigma}^+ f_{i+1/2,\sigma} \approx -2J' \sum_i \left[ \bar{l}(x_i)^2 - 4 \right] f_{i+1/2,\sigma}^+ f_{i+1/2,\sigma} \]  

(7a)

\[ H_J = 2J_1 \sum_i \left[ \bar{l}(x_i) + \frac{\partial \tilde{\phi}}{\partial x} \right] \cdot \vec{\sigma} f_{i+1/2,\alpha}^+ f_{i+1/2,\beta} \approx 2J_1 \sum_i \bar{l}(x_i) \cdot \vec{\sigma} f_{i+1/2,\alpha}^+ f_{i+1/2,\beta} \]  

(7b)

\[ H_J = J_2 \sum_i \left[ \bar{l}(x_i) \right] \cdot \vec{\sigma} f_{i+1/2,\alpha}^+ f_{i-1/2,\beta} \]  

(7c)

We can now express the field \( \bar{l}(x_i) \), \( \bar{l}(x_i)^2 \) and \( \tilde{\phi}(x_i) \) in terms of the magnon creation and annihilation operators. We leave the detail derivation in appendix A. After discarding the multi-magnon processes, the Hamiltonian reads,

\[ H_{ch} = \sum_{k,\mu} E_k (a_{k,\mu}^+ a_{k,\mu} + \frac{1}{2}) \]  

in which \( \mu = -1, 0, 1 \) and

\[ a^+_\pm(k) = \mp \frac{1}{\sqrt{2}} \left[ a_x(k)^+ \pm ia_y(k) \right] \]  

(9a)

\[ a^+_0(k) = a^+_{z}(k) \]  

(9b)

\[ H_{J'} = -4 \sum_{i,q,k,k',\mu,\sigma} \gamma'(k',q) J' a_{\mu,k'\sigma}^+ a_{\mu,k'\sigma} f_{\sigma,k}^+ f_{\sigma,k} \]  

(10)

\[ H_{J_1} = \sum_{\mu,\nu,k,k',\sigma,\alpha,\beta} \gamma_1(k',q) J_1 \vec{S}_{\mu\nu} \cdot \vec{\sigma} a_{\mu,k'\sigma}^+ a_{\nu,k'\sigma} f_{\alpha,k}^+ f_{\beta,k} \]  

(11)

as well as

\[ H_{J_2} = \sum_{\mu,\nu,k,k',\sigma,\alpha,\beta} \gamma_1(k',q) J_2 \cos(k) \vec{S}_{\mu\nu} \cdot \vec{\sigma} a_{\mu,k'\sigma}^+ a_{\nu,k'\sigma} f_{\alpha,k}^+ f_{\beta,k} \]  

\[ + \sum_{\mu,\nu,k,k',\sigma,\alpha,\beta} 2J_2 \sin(k) \sqrt{\frac{\sqrt{3}}{\Delta_H}} D_{\mu,\alpha,\beta} a_{\mu,\alpha/2,\beta}^+ (-q) f_{\alpha,k}^+ (k + q - \pi) f_{\beta,k} + H.C. \]  

(12)

in which \( D_{\mu,\alpha,\beta} = \langle \mu | \alpha | 1/2,\beta \rangle \) is the transformation matrix between the \((J^2, J_z)\) representation and that of \((S_z, \sigma_z)\).

In this paper, we choose the amplitude of the Haldane gap \( \Delta_H \) as the unit of energy, so we have \( \Delta_H = 1 \). We choose the value of \( v \) by fitting the correlation length at zero
temperature, which is believed to be closed to 7 \cite{18}. So we have \( \xi = \frac{v}{\Delta} = 7 \), then we have \( v = 7 \). The two vertex functions \( \gamma_1(k, q) \) and \( \gamma'(k, q) \) are derived in appendix A. It is quite difficult for us to treat this \( k, q \) dependent vertex function analytically. So as a low energy effective theory, we simply replace the two \( k, q \) dependent vertex function by two \( k, q \) independent phenomenological parameters \( \lambda_1 \) and \( \lambda' \) respectively, whose value can be fixed by fitting our approach to the existing numerical results for the static hole problem.

In the static limit \( t = J_2 = 0 \), the effective Hamiltonian is quite simple especially in the continuum limit,

\[
H = \int dx \sum_\mu a_\mu^+(x)(1 - \frac{1}{m_b} \frac{\partial^2}{\partial x^2})a_\mu(x) - 4\lambda'J'\sum_\gamma a_\gamma^+(0)a_\gamma(0) + \sum_\gamma \sum_\mu 2\lambda_1 J_1 \vec{S}_\gamma \cdot \vec{s}_\text{imp} a_\gamma^+(0)a_\mu(0)
\]

in which

\[
a_\mu(x) = \frac{1}{\sqrt{N}} \int_{-\infty}^{\infty} dk a_\mu(k) e^{-ikx}
\]

To study the low energy excitation inside the Haldane gap, we need only consider the one magnon state. And this will lead to the following schrodinger equation in first quantized picture.

\[
\left[ -\frac{1}{2m_b} \frac{\partial^2}{\partial x^2} + 2\lambda_1 J_1 \vec{s}_\text{imp} \cdot \vec{S}\delta(x) - 4\lambda_2 J'\delta(x) + \Delta_H \right] \psi(x) = E\psi(x) \tag{15}
\]

The magnon wave function \( \psi(x) \) has six components corresponding to six eigen states of \( s^z_\text{imp} \) and \( S^z \). We can easily solve the above schrodinger equation by first diagnolizing Hamiltonian in spin space. We have

\[
\left[ -\frac{1}{2m_b} \frac{\partial^2}{\partial x^2} + 2J_1 \lambda_1 e_j \delta(x) - 4\lambda_2 J'\delta(x) + \Delta_H \right] \psi_j(x) = E\psi_j(x) \tag{16}
\]

in which \( j \) is the total spin of the impurity and the magnon, and \( e_j = j(j+1)/2 - (S^2 + s^2_\text{imp})/2 \), so

\[
e_{1/2} = -\Delta_H \quad e_{3/2} = 1/2\Delta_H \tag{17}
\]
The Eq.(14) describes a particle with mass \( m_b \) bounded by a \( \delta \) potential which can be solved easily. The corresponding eigenvalues and eigen functions are:

\[
E_{1/2} = \Delta_H - 2m_b(\lambda_1 J_1 + 2\lambda_2 J')^2 \quad \psi_{1/2}(x) = \frac{1}{\sqrt{L}} \exp^{-|x|/L} \quad \text{with} \quad L = \frac{1}{2m_b(\lambda_1 J_1 + 2\lambda_2 J')}
\]

(18a)

\[
E_{3/2} = \Delta - 2m_b(-0.5\lambda_1 J_1 + 2\lambda_2 J')^2 \quad \psi_{3/2}(x) = \frac{1}{\sqrt{L}} \exp^{-|x|/L} \quad \text{with} \quad L = \frac{1}{m_b(-\lambda_1 J_1 + 4\lambda_2 J')}
\]

(18b)

Eq.(18.b) is only meaningful for case of \( \lambda_1 J_1 < 4\lambda_2 J' \) If \( \lambda_1 J_1 > 4\lambda_2 J' \) the effective potential for the state with total spin 3/2 is repulsive which can be easily verified from eq.(16). Therefore there is no bound state with total spin 3/2 in this case. When \( \lambda_1 J_1 < 4\lambda_2 J' \) there always exist two bound state where one has two-fold degeneracy and the other has four-fold degeneracy. We can compare our results with the corresponding numerical results. Firstly we choose \( J' = J = 2.5\Delta_H \) which corresponds to the case that the super exchange interaction got destroyed entirely. If we have further \( J_1 = 0 \), the problem becomes precisely equivalent to an open chain. The numerical studies show that the ground state of the open spin-1 chain is four-fold [20,21]. In the simple approach engaged in this paper, it gives a nice description of these four-fold states. If we simply choose \( \lambda_2 = 1.01 \) the energy cost to create one localized magnon near the chain edge is 0 determined by (18.b), then the degenerated ground state will be zero magnon state as well as three-fold states with one localized magnon near the edge, which is altogether four-fold. The edge states described by (18.b) extend to 5 lattice which is also consistent with the numerical result. For finite \( J_1 \), equation (18.a) leads to \( E_{1/2} \approx -0.4\lambda J_1, E_{3/2} \approx 0.2\lambda J_1 \) in small \( J_1 \) limit while the numerical study predicts that \( E_{1/2} \approx -J_1, E_{3/2} \approx 0.5J_1 \). We then choose \( \lambda_1 = 2.5 \) to fit the numerical results. Fig.2 shows the \(-E_{1/2}\) as the function of \( J_1 \) in a full range of \( J_1 \). Compared with the results obtained by Ian Affleck et al [14], we find that our simple treatment fits quite well with the numerical results especially in weak coupling regime.
III. The Dispersion of the Bound State of Magnon and Hole

In this section we consider the bound state constituted by one magnon and one hole. In the present paper, we assume that the local super exchange is destroyed entirely, so we choose $J' = J$, $\lambda_1 = 2.5$, $\lambda' = 1.01$, $J_1 = J_2 = 0.2\Delta_H$, and $m_0 = 1/49$. We will consider this problem in two limiting cases, one is the large $t$ limit and the other is small $t$ limit. We can reorganize the total Hamiltonian as $H = H_h + H_{ch} + H_1 + H_2$, in which $H_h$ and $H_{ch}$ are the free Hamiltonian for holes and spins respectively as shown in (1b) and (4) and $H_1$ and $H_2$ are two kinds of interaction representing the scattering process and the magnon emission and absorption process respectively.

$$H_1 = \sum_{\mu,k,k',q,\alpha,\beta} [2\lambda_1 J_1 + 2\lambda_1 J_2 \cos(k)] \vec{S}_{\mu \nu} \cdot \vec{\sigma}_{\alpha,\beta} a_{\mu, k'}^+ a_{\nu, k'} f_{\alpha, k-q}^+ f_{\beta, k}$$

$$H_2 = \sum_{\mu,k,k',q,\alpha,\beta} g(k) D_{\mu \alpha, \frac{1}{2} \beta} a_{\mu}^+ (-q) f_{\alpha}^+(k + q - \pi) f_{\beta}^+(k) + H.C.$$  \hspace{1cm} (20)

in which $g(k) = 2J_2 \sin(k) \sqrt{\frac{v}{\Delta H}} \sqrt{\frac{\pi}{2}}$.

a. The large $t$ limit

In large $t$ limit, the holes are mainly distributed near $P = 0$, so we can treat the bare hole dispersion in continuum approximation. We have $E_h(P) = -2t(\cos P - 1) \approx \frac{t^2}{2m_f}$, in which $m_f = \frac{1}{2t}$.

In order to study the dispersion relation of the bound state, we should consider the two-particle Green’s function with total spin $j(j=1/2$ or 3/2$)$ and its $z$-component $m$ which is defined as the following.

$$\Gamma_{jm}(x, t) = -i \sum_{\alpha'\mu'\alpha\mu} <jm|\alpha'\mu'> <Ta_{\mu'}(x, t)f_{\alpha'}(x, t)|a_{\mu}^+(0, 0)f_{\alpha}^+(0, 0)> <\alpha\mu|jm>$$  \hspace{1cm} (21)

The above two-particle Green’s function can be obtained by using Feynman diagram expansion. One may easily verify that the magnon emission and absorption term only act on the total spin-1/2 state and can’t affect the state with total spin 3/2. So the spin-3/2 state only feels the scattering term as shown in Fig.3, which leads to,
\[ \Gamma_{\frac{3}{2}}(P, i\nu) = \pi_0(P, i\nu) + \tilde{\pi}_0(P, i\nu) \Gamma_{\frac{3}{2}}(P, i\nu) \quad (22) \]

So we have
\[ \Gamma_{\frac{3}{2}}(P, i\nu) = \frac{\pi_0(P, i\nu)}{1 - \tilde{\pi}_0(P, i\nu)} \]
\[ \tilde{\pi}_0(P, i\nu) = \int_{-\pi}^{\pi} dq V_{\frac{3}{2}}(P - q) \frac{1 + n_B\left(\frac{q^2}{2m_b} + 1\right) - n_F\left(\frac{(P-q)^2}{2m_f}\right)}{i\nu - \frac{(P-q)^2}{2m_f} - \frac{q^2}{2m_b} - \Delta_H} \quad (23) \]

and
\[ \pi_0(P, i\nu) = \int dq \frac{1 + n_B\left(\frac{q^2}{2m_b} + 1\right) - n_F\left(\frac{(P-q)^2}{2m_f}\right)}{i\nu - \frac{(P-q)^2}{2m_f} - \frac{q^2}{2m_b} - \Delta_H} \quad (24) \]

in which \( V_{\frac{3}{2}}(k) = \lambda_1 [J_1 + J_2 \cos(k)] - 4\lambda_2 J' \) and P is the total momentum for the hole-magnon system.

In above equations \( n_B \) and \( n_F \) are the Boson and Fermi distribution function respectively. But in our present study if we consider only the dilute limit of the hole doping, so we can assume that the temperature satisfy \( T_F \ll T \ll \Delta_H \), in which \( T_F \) is the Fermi temperature of the holes. Then we can replace the Fermi-Dirac distribution function \( n_F(E) \) by its classic limit which is the Boltzman distribution function. In equation(26), we can further ignore the \( n_B \) and \( n_F \) in dilute doping and low temperature case. Then we have
\[ \tilde{\pi}_0(P, \omega + i0^+) \approx \int dq \frac{V_{\frac{3}{2}}(P - q)}{\omega + i0^+ - \frac{(P-q)^2}{2m_f} - \frac{q^2}{2m_b} - \Delta_H} = \int_{-\pi}^{\pi} dq' \frac{V_{\frac{3}{2}}[(1 - \frac{m_b}{M})P - q']}{\omega + i0^+ - \frac{P^2}{2M} - \frac{q'^2}{2\mu} - \Delta_H} \quad (25) \]

in which \( q' = q - \frac{m_b}{M}P \) and \( \frac{1}{\mu} = \frac{1}{m_f} + \frac{1}{m_b} \). We may expand the function \( V_{\frac{3}{2}} \) with respect to \( q' \) and only keep the leading order, because the main contribution to the integration comes from \( q' < \sqrt{2m_b(\Delta_H + \frac{P^2}{2M} - \omega)} \), which is quite small in the \( \omega \) regime in which we are interested. So we have
\[ Re\tilde{\pi}_0(P, \omega + i0^+) \approx -\frac{1}{2} V_{\frac{3}{2}}[(1 - \frac{m_b}{M})P]\sqrt{\frac{2\mu}{\Delta_H - \omega + \frac{P^2}{2M}}} \quad (26) \]

and
\[ \text{Re} \pi_0(P, \omega) = -\frac{1}{2} \sqrt{\frac{2\mu}{\Delta_H - \omega + \frac{P^2}{2M}}} \]  

(27)

for \( \omega < \Delta_H \).

The bound energy for the bound state of one hole and one magnon with total spin-3/2 is determined by the pole of \( \Gamma_{3/2}(P, \omega) \), which is \( 1 - \text{Re} \tilde{\pi}_0(P, \omega) = 0 \). We then have

\[ E_{3/2}(P) = 1 - \frac{1}{2} \mu V_{3/2} \left[ (1 - \frac{m_b}{M})P \right]^2 + \frac{P^2}{2M} \]  

(28)

The situation of the bound state with total spin-1/2 is not as simple as the case of total spin-3/2, because the interaction term \( H_{J_2} \) will mix the two particle state and the one particle state, which is illustrated in Fig.3. Therefore we should take into consideration the contribution from both the two terms. Following the diagrammatic rule shown in Fig.(4b), we then have

\[
\Gamma(P, i\nu) = \Gamma_0(P, i\nu) + \Gamma_1(P, i\nu)G(P + \pi, i\nu)\Gamma_1(P, i\nu) + \\
\Gamma_1(P, i\nu)G(P + \pi, i\nu)\Gamma_2(P, i\nu)G(P + \pi, i\nu)\Gamma_1(P, i\nu) + \ldots \]  

(29)

where

\[
\Gamma_0(P, i\nu) = \frac{\pi_0(P, i\nu)}{1 - V_{1/2} \left[ (1 - \frac{m_b}{M})P \right] \pi_0(P, i\nu)} \]  

(30)

\[
\Gamma_1(P, i\nu) = \frac{g(P, \frac{m_b}{M}P)\pi_0(P, i\nu)}{1 - V_{1/2} \left[ (1 - \frac{m_b}{M})P \right] \pi_0(P, i\nu)} \]  

(31)

and

\[
\Gamma_2(P, i\nu) = g(P, \frac{m_b}{M}P)^2\pi_0(P, i\nu) + \frac{g(P, \frac{m_b}{M}P)^2\pi_0^2(P, i\nu)V_{1/2} \left[ (1 - \frac{m_b}{M})P \right] \pi_0(P, i\nu)}{1 - V_{1/2} \left[ (1 - \frac{m_b}{M})P \right] \pi_0(P, i\nu)} \]  

(32)

in which \( V_{1/2}(k) = 2\lambda_1 [J_1 + J_2\cos(k)] - 4\lambda J' \). To derive the above equation, the same approximation is done as (26). Then we have

\[
\Gamma(P, \omega) = \frac{\Gamma_0(P, \omega)}{1 - g^2(P, \frac{m_b}{M}P)G(P + \pi, \omega)\Gamma_0(P, \omega)} \]  

(33)
in which

\[ G(P + \pi, \omega) = \frac{1}{\omega - 4t + P^2/2m_f} \]  

is the Green’s function near \( \pi \). Then we can obtain the energy of the bound state with total spin-1/2 by solving the equation:

\[ 1 - g^2(P, m_bP)G(P + \pi, \omega)\Gamma_0(P, \omega) = 0 \]  

The result is

\[ E_{\frac{1}{2}}(P) = \Delta_H - \frac{1}{2}\mu V^2_{\frac{1}{2}} + \frac{P^2}{2M^*} \]  

with the renormalized effective mass

\[ \frac{1}{M^*} = \frac{1}{M} - \frac{3J^2_2(1 - \frac{mb}{2m_f})^2\xi\mu V^2_{\frac{1}{2}} - \Delta + \frac{2}{m_f}\mu^2 V^2_{\frac{1}{2}}} + 4\mu\lambda_1 J_2 [\lambda_1 (J_1 + J_2) + 2J'\lambda'] \]  

in which \( m_f = \frac{1}{2}t \). We find that if \( t \) is smaller than a critical value \( t_c \), the effective mass will change sign which means the band minimum may move away from the \( P = 0 \) state and will be located at a point between 0 and \( \pi \). From the above expression, the \( t_c \) is determined by the condition \( \frac{1}{M^*} = 0 \). And the result is \( t_c = 0.21\Delta_H \).

For the case of \( t >> t_c \), the magnon emission and absorption processes are no longer important and can be ignored, so the number of the magnons is conserved. Then the essential physics can be viewed more clearly as a two-body problem in the first quantization picture.

We can write again a Schrödinger equation for the hole-magnon system.

\[ \left[ -\frac{1}{2m_b}\frac{\partial^2}{\partial x_b^2} - \frac{1}{2m_f}\frac{\partial^2}{\partial x_f^2} + J\vec{s}_{\text{imp}} \cdot \vec{S}\delta(x_b - x_f) - 4\lambda_2 J'\delta(x_b - x_f) + 1 \right] \psi(x_b, x_f) = E\psi(x_b, x_f) \]  

in which \( m_f = \frac{1}{2}t \) and \( \vec{J} = 2\lambda_1 (J_1 + J_2) \). The above Hamiltonian describes a two body problem with an attractive interaction between them. We can divide the Hamiltonian into two parts, one describe the motion of center of mass and the other describe the relative motion.
\[ H_c = -\frac{1}{2M} \frac{\partial^2}{\partial x^2} \]  

\[ H_r = -\frac{1}{2\mu} \frac{\partial^2}{\partial x^2} + \vec{J}_\text{imp} \cdot \vec{\delta}(x) - 4\lambda_2 J' \delta(x) + 1 \]  

with \( \mu = \frac{m_f m_b}{m_f + m_b} \), \( M = m_b + m_f \), \( x = x_f - x_b \) and \( \bar{x} = \frac{m_b x_b + m_f x_f}{M} \). Equation (23a) describes a free propagation of a composite particle constituted by a hole and a magnon with total mass \( M \), and equation (23b) describes a particle in an attractive potential which is solved in (19a) and (19b). So the situation in large \( t \) limit is quite clear. One magnon and one hole form a bound state with the bound energy \( 1 - 2\mu(-0.5\lambda_1 J_1 + 2\lambda_2 J')^2 \) for \( S_{\text{total}} = 3/2 \) state or a bound energy \( 1 - 2\mu(\lambda_1 J_1 + 2\lambda_2 J')^2 \) for \( S_{\text{total}} = 1/2 \) state. These results are consistent with and further confirm the results obtained by using Feynman diagram techniques in the case of \( t >> t_c \).

The center of mass moves like a free particle with total mass \( M \). So in the case of large \( t \) limit, the bound state of magnon and hole with total spin 1/2 is energetically favorable against the free hole state. Therefore, the ground state of the system will be the bound pairs of the holes and magnons with total spin 1/2, in another words, every hole will induce a magnon binding with it. Further, these bound pairs can be viewed as a composite Fermions with spin 1/2 which can propagate freely in the spin-1 chain.

**b. The Small \( t \) limit**

In the small \( t \) limit, we should calculate the same diagrams as in large \( t \) limit. Also we can calculate the dressed two particle Green’s function by considering the diagram shown in Fig(4). The difference between the two limiting cases is that we can’t use the long wave length expansion anymore for holes in the small \( t \) case. The \( \pi_0(P, \omega + i0^+) \) in small \( t \) limit can be written as:

\[ \pi_0(P, \omega + i0^+) = \int dq \frac{1}{\omega + i0^+ + (2t \cos(P - q) - 2t) - \frac{q^2}{2m_b} - \Delta_H} \]  

(40)
Since in small $t$ limit we always have $1/m_b \gg t$, the main contribution for the integrand comes from a quite narrow $q$ regime near $q$ equals to zero. So we can expand $\cos(P - q)$ in $q$ near $P$, that is

$$\pi_0(P, \omega + i0^+) = \int dq \frac{1}{\omega + i0^+ + 2t \cos(P) + 2t \sin(P) \cdot q - t \cos(P)q^2 - \frac{q^2}{2m_b} - \Delta_H - 2t}$$

then integrate it using the method described before. Also we can obtain the values of $\pi_1$ and $\pi_2$ using the same method. The dispersion relation of the quasiparticle which is the mixed state of the single hole state and the bound state of one magnon and one hole is determined by searching for the low energy poles of the Green’s function similar to what we have done in the large $t$ limit. Two branches of excitation are obtained with energy $\omega_{\pm}(P)$ as shown in Fig.5 for various value of $t$. Near the poles, the two particle propagator can be written as

$$\Gamma(P, \omega + i0^+) = \frac{z_i(P)}{\omega - \omega_i + i0^+}$$

for $i = +, -$. The result of $z_i(P)$ is shown in Fig.6. From Fig.6 we can find that for $P$ near zero the lower branch is almost two particle like and the higher branch is one particle like, but for $P$ near $\pi$ the lower branch is one particle like and the higher branch is two particle like. Between the above two limit, the one particle state and two particle state are strongly hybridized. So near 0 and $\pi$, the mixing of the one particle state and the two particle state is quite small and the effect of the magnon emission and absorption term is only modifying the effective mass of the bounded states. But for $P$ near $\pi/2$, the one particle state and the two particle state are strongly hybridized, which may split the two energy level remarkably. When $t$ is large this hybridization effect only increases the effective mass. But if $t$ is sufficiently small the energy split caused by $J_2$ term which is of the order $J_2$ could be much large than the kinetic energy of order $t$. Then the band minimum of the lower excitation will no longer stay at $P = 0$ but move towards $\pi/2$. We can find from Fig.5 the critical value of $t$ is $0.21\Delta_H$, which is consistent with the value that we obtained in the large $t$ limit calculation. From equ.(12) we can see that the origin of the magnon emission and
absorption term is the coupling between the mobile holes and the antiferromagnetic field $\tilde{\phi}(x)$. Although the long range antiferromagnetic order is not stable in 1D spin chain, the short range antiferromagnetic fluctuation is still quite strong in low temperature. If the holes can feel such antiferromagnetic fluctuation, the band minimum will move to $\pi/2$. It is rather interesting to note that this feature is quite similar to that of the single hole moving in the 2D antiferromagnetic lattice.

Also, we can calculate the renormalized single particle Green’s function considering the diagrams showing in Fig(4c). And the same quasiparticle poles are obtained. But we provide here a transparent intuitive picture.

Our results for small $t$ limit are very similar with the results obtained by Shiba el al [18] for the VBS model, in which the band minimum is moved towards $\pi/2$ when the hopping term $t$ is smaller than a critical value.

IV. Calculation of the Spin Structure Factor

The spin structure factor can also be calculated in our approach. Since in the doped spin-1 chain both the holes and the spins can contribute to the spin structure factor, so we have

$$S(\pi, \omega) = \frac{1}{2\pi} \int dt e^{i\omega t} \langle \tilde{\phi}(0, t) + \sum_k \sigma_{\alpha\beta} f^+_{\alpha,k+\pi}(t) f_{\beta,k}(t) \rangle \langle \tilde{\phi}(0, 0) + \sum_k \sigma_{\alpha\beta} f^+_{\alpha,k+\pi}(0) f_{\beta,k}(0) \rangle$$

(43)

So the spin structure factor can be divided into three parts, the magnon part $S_m$, the hole part $S_h$ and the mixed part. We can prove that the contribution from the mixed term is zero, because the magnon emission and absorption vertex functions satisfy $g(k, 0) = -g(-k, 0)$. Using the fluctuation-disipative theorem, we have

$$S_m(\pi, \omega) = 3 [Im D_1(0, \omega) - Im D_1(0, -\omega)] [1 + n_b(\omega)]$$

(44)

in which $D_1(0, \omega)$ is the dressed magnon Green’s function with $S_z = 1$. 

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\[
S_h(\pi, \omega) = \text{Im}\chi_h(\pi, \omega)n_b(\omega)
\] (45)

in which \(\chi_h(\pi, \omega)\) is the spin susceptibility of holes.

Firstly the dressed Green’s function of magnons is calculated by considering the self energy diagram in Fig.7(a,b). Fig.7(a) represents the contribution of scattering term and the \(\Lambda_s(P, \omega)\) is the effective scattering potential of the holes and magnons, which can be easily derived from the full two particle Green’s function \(\Gamma_s(P, \omega)\) as \(\Lambda_s(P, \omega) = V_s + V_s\Gamma(P, \omega)V_s\) in which index \(s\) represent two different channels with total spin 1/2 and 3/2. The Fig.7(b) represent the four kinds of contribution from the magnon emission and absorption term which correspond to single particle to single particle, single particle to two particle, two particle to single particle and two particle to two particle transition respectively. And the diagrams considered by us to calculate \(\chi_h(\pi, \omega)\) are shown is Fig.7(c), which is quite similar with Fig.7(b) except that there are no vertex function \(g(k)\).

Since in this paper we are only interested in the low energy response within the Haldane gap, we can discard the high energy part during our calculation. When \(t\) is much larger than \(t_c\), the band minimum of the lowest excitation is at zero. Therefore the diagrams in Fig.7(b,c) describe the intra band transition from zero to \(\pi\) which costs the energy \(4t\). In the large \(t\) limit this energy scale is much larger than the Haldane gap, so the intra band transition can be ignored in the large \(t\) limit. Therefore the only important diagram in large \(t\) limit is Fig.7(a), which is the inter band transition from the two particle bound state to the one particle state. According to Fig.7(a) the self energy of the magnon can be written as,

\[
\Sigma(k; \mu, i\omega) = \int dP \sum_{\alpha, m, s, n} G^0(i\nu_n - i\omega, P - k) D^{s,m}_{\mu,\alpha} \Lambda_s(i\nu_n, P)
\] (46)

in which \(\mu\) and \(\alpha\) are the spin index of magnon and hole respectively.

\(\Lambda_s(i\nu_n, P)\) can be expressed by its spectral function as

\[
\Lambda_s(i\nu_n, P) = \frac{\bar{\Lambda}_s}{i\nu_n - \Delta_H - \frac{P^2}{2M} + \frac{1}{2} \mu V_s^2} + \int d\omega' \frac{\rho_c(\omega')c}{\nu_n - \omega'}
\] (47)
in the above expression the first term is contributed by the bound state with $\tilde{\Lambda}_s = \mu V_s^3$ and $\rho_c(\omega')$ and the second term which is nonzero above the Haldane gap is attributed to the scattering state of one magnon and one hole. Since we are only interested in the spin response within the Haldane gap, we can omit the continuous part and only keep the first term in the above equation. Then we have

$$Im \Sigma(\omega, \mu, k) = \int dP \sum_{s, m, a} \tilde{\Lambda}_s D_{s, m, \mu, \alpha} \left[ n_F \left( \frac{(P - k)^2}{2m_f} \right) - n_F \left( \Delta_H - \frac{1}{2} \mu V_s^2 - \frac{P^2}{2M} \right) \right]$$

$$\delta (\omega - \Delta_H + \frac{1}{2} \mu V_s^2 + \frac{P^2}{2m_f} - \frac{P^2}{2M})$$

(48)

The spin response function within the Haldane gap for $t=2$ (large $t$ limit) is shown in fig.8(a), we can see clearly that there is a resonate peak in the Haldane gap. This low energy peak can be attributed to the transition from the bound state of one magnon and one hole with total spin $1/2$ (which is the ground state under the parameters we chosen here) to the free hole state.

The situation of small $t$ limit is quite different with the large $t$ limit. Now the band minimum of the lower state is moved toward $\pi/2$. So unlike the large $t$ limit, the holes dressed with magnons are distributed near $\pi/2$. Therefore the intra band transition described by fig.(7b) and fig.(7c) become very important now, because the momentum transfer $\pi$ costs very small energy for the states near $\pi/2$. While the energy cost for the inter band transition is increased by the virtual magnon emission and absorption process. So in small $t$ limit all of the diagrams in fig.7 must be considered. We have calculated all these diagrams numerically, and the result is shown in fig.(8b) for $t = 0.1 \Delta_H$. The contribution from all these figures are evaluated under the same approximation as the large $t$ limit which keeps only the low energy peak in the spectral function. For example the contribution from the second diagram in fig.7(b) can be written as

$$\Sigma_1(i\omega, \pi) = \int dP \sum_{\nu} \gamma^2(P, i\nu, i\omega) \Lambda_{\frac{1}{2}}(P, i\nu) \Lambda_{\frac{1}{2}}(P + \pi, i\nu + i\omega)$$

(49)
in which

\[
\gamma(P, iv, i\omega) = \int \frac{-1}{2\pi \beta} dk \sum_{i\nu} \frac{1}{i\nu + \epsilon(k) - i\omega + \epsilon(k + \pi)} \cdot \frac{1}{i\nu - \epsilon(k) - \Delta_H - \frac{(P-k)^2}{2m_b}}
\]

\[
= -\int \frac{dk}{2\pi} \left\{ n_F[\epsilon(k)] \cdot \frac{1}{i\omega + \epsilon(k) - \epsilon(k + \pi)} \cdot \frac{1}{i\nu - \epsilon(k) - \Delta_H - \frac{(P-k)^2}{2m_b}}
\right.

\[
+ n_F[\epsilon(k + \pi)] \cdot \frac{1}{\epsilon(k + \pi) - i\omega - \epsilon(k)} \cdot \frac{1}{i\nu + i\omega - \epsilon(k + \pi) - \Delta_H - \frac{(P-k)^2}{2m_b}}
\left.
\right\}
\]

\[
+ \left[ 1 + n_b(\Delta_H + (P-k)^2) \right] \cdot \frac{1}{i\nu - \Delta_H - \frac{(P-k)^2}{2m_b} - \epsilon(k)} \cdot \frac{1}{i\nu + i\omega - \epsilon(k + \pi) - \Delta_H - \frac{(P-k)^2}{2m_b}}
\]

(50)

where \( \epsilon(k) = -2t[\cos(k) - 2] \). The first two terms in the above equation can be ignored if we only consider the low temperature case. Also we use the same approximation that only the low energy peak of \( \lambda(P, iv) \) is considered. Then after the summation of \( iv \) has been done, we have

\[
Im\Sigma_1(\omega, \pi) = \int dP \sum_{mn} \delta(\omega - \omega_m(P + \pi) + \omega_n(P)) \tilde{\lambda}_n(P) \tilde{\lambda}_m(P + \pi)
\]

\[
[n_F(\omega_n(P)) - n_F(\omega_m(P + \pi))] \gamma^2(P, \omega_n(P), \omega)
\]

(51)

in which \( \omega_n(P) \) is the dispersion relation of the two branches obtained in equation(42). The other diagrams in fig.7(b) can be calculated similarly. Finally we calculated the numerical result for the spin response function in small t limit. The result is shown in Fig.8(b). We can see clearly from fig.8 that a diffusion like peak is present at low energy near zero resulted from the intra band transition in small t limit. The energy of the inter band transition is near \( 1.22\Delta_H \) which is out of the range in which we are interested.

Our results in large t limit are consistent with the results of Dagoto and et al which have two peaks represent the bound state to single hole state and the intrinsic magnon excitation respectively. In the paper of Dagoto and et al [13], the dynamically spin structure factor in small t limit has not been calculated. So our calculation is the first work which indicate the difference in the dynamically spin structure factor for large t limit and small t limit. We
find that when $t$ is smaller than a critical value, the main contribution to the dynamically spin structure factor will change from the inter band transition to intra band transition.
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In the appendix, we derive the representation of field $\vec{l}(q)$ and $l^2(q)$.

First we have

$$
\vec{l}(q) = \sum_k \vec{\phi}(k + q) \times \vec{\Pi}(-k) = \sum_k \frac{i}{2} \sqrt{\frac{E_k}{E_{k+q}}} (\vec{a}_{k+q} + \vec{a}_{-k-q}^-) \times (\vec{a}_{-k} - \vec{a}_k^+)
$$

$$
= \sum_k \frac{i}{2} \sqrt{\frac{E_k}{E_{k+q}}} (-\vec{a}_{k+q} \times \vec{a}_k^+ + \vec{a}_{-k-q}^- \times \vec{a}_{-k} + \vec{a}_{k+q} \times \vec{a}_{-k} - \vec{a}_{-k-q}^- \times \vec{a}_k^+) 
$$

(52)

It is quite clear that the first two terms describe the scattering process and the last two terms describe the multi-magnon processes which is unimportant when we are only interested in the low energy physics. So the terms describing the multi-magnon processes can be omitted in our present paper. And we have

$$
\vec{l}(q) \approx \sum_k \gamma_1(k, q) \vec{a}_k^+ \times \vec{a}_{k+q}
$$

(53)

in which $\gamma_1(k, q) = i \sqrt{\frac{E_k}{E_{k+q}}}$.

$$
l^2(q) = \sum_k \vec{l}(k + q) \cdot \vec{l}(-k) = \sum_{k, k', k''} \gamma_1(k', k + q) \gamma_1(k'', -k)(\vec{a}_{k'}^+ \times \vec{a}_{k+q}) \cdot (\vec{a}_{k''}^+ \times \vec{a}_{k''-k})
$$

$$
= \sum_{k, k', k''} \gamma_1(k', k + q) \gamma_1(k'', -k)[-2a_{y,k'}^+ a_y k' + k, k'' - k a_{x,k', k''}^+ a_{x, k'' - k} - 2a_{x,k', k''}^+ a_{x, k'' - k} a_{x, k'' - k} - 2a_{z,k'}^+ a_{z, k''} a_{z, k''}]
$$

$$
+ a_{x,k'}^+ a_{x, k''}^+ a_{y, k'' + q a_{y, k'' - k}} + a_{y,k'}^+ a_{y, k''}^+ a_{z, k'' + q a_{z, k'' - k}} + a_{z,k'}^+ a_{z, k''}^+ a_{x, k'' + q a_{x, k'' - k}}
$$

$$
+ a_{y,k'}^+ a_{y, k''}^+ a_{x, k'' + q a_{x, k'' - k}} + a_{x,k'}^+ a_{x, k''}^+ a_{y, k'' + q a_{y, k'' - k}} + a_{z,k'}^+ a_{z, k''}^+ a_{x, k'' + q a_{x, k'' - k}}
$$

$$
- a_{y,k'}^+ a_{y, k''}^+ a_{x, k'' + q a_{x, k'' - k}} - a_{z,k'}^+ a_{z, k''}^+ a_{x, k'' + q a_{x, k'' - k}} - a_{x,k'}^+ a_{x, k''}^+ a_{y, k'' + q a_{y, k'' - k}} - a_{z,k'}^+ a_{z, k''}^+ a_{x, k'' + q a_{x, k'' - k}}
$$

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\[-a_{x, k'}^+ a_{y, k''}^+ a_{y, k' + k + q} a_{x, k'' - k} - a_{y, k'}^+ a_{z, k''}^+ a_{z, k' + k + q} a_{y, k'' - k} - a_{z, k'}^+ a_{x, k''}^+ a_{x, k' + k + q} a_{z, k'' - k}\]

After discarding the multi-magnon terms, we have

\[l^2(q) = \sum_{k', \alpha} 2\gamma'(k', q) a_{\alpha, k'}^+ a_{\alpha, k' + q}\]

(54)

with \(\gamma'(k', q) = \sum_k \gamma_1(k', k + q) \gamma_1(k' + k + q, -k)\).
Figure Caption

Fig.1 The illustration of holes doped antiferromagnetic chain.

Fig.2 The comparison of our result and the numerical result for the lowest excitation in static hole limit. The line represents our result and the squares represent the corresponding numerical result.

Fig.3 The Feynman diagrams used in this paper. (a) The full line represents the hole’s Green Function. (b) The dashed line represents the magnon’s Green function. (c) The scattering vortex contributed by $H_1$. (d) The magnon emission and absorption vortex contributed by $H_1$.

Fig.4 (a) The dressed two-particle Green function with total spin 3/2. (b) The dressed two-particle Green function with total spin 1/2. (c) The dressed hole’s Green function.

Fig.5 From down to up, the up three curves represent the $\omega_+(P)$ for $t=0.22, 0.20, 0.18$ respectively. And from up to down, the lower three curves represent the $\omega_-(P)$ for $t=0.22, 0.20, 0.18$ respectively.

Fig.6 The full and dashed lines represent the spectral weight $z_+(P)$ and $z_-(P)$ respectively.

Fig.7 (a) The magnon self energy caused by the scattering term. (b) The magnon self energy caused by the magnon emission and absorption term. (c) The hole’s contribution to the spin susceptibility.

Fig.8 (a) The spin structure factor in large t limit ($t=2$). (b) The spin structure factor in small t limit ($t=0.1$).
Fig. 1
Fig. 3
Fig. 4
Fig. 5
Fig. 6
Fig. 7
Fig. 8(a)

Fig. 8