arXiv:0907.2740v1 [cond-mat.str-el] 16 Jul 2009

Green functions and correlation functions of a solvable $S = 1$ quantum Ising spin model with dimerization

Zhi-Hua Yang[1], Li-Ping Yang[2], Hai-Na Wu[3], Jianhui Dai[1], and Tao Xiang[4,2]
[1] *Zhejiang Institute of Modern Physics, Zhejiang University, Hangzhou 310027, China*
[2] *Institute of Theoretical Physics, Chinese Academy of Science, P.O. Box 2735, Beijing 100080, China*
[3] *College of Science, Northeastern University, Shengyang 110006, China*
[4] *Institute of Physics, Chinese Academy of Sciences, P.O. Box 603, Beijing 100080, China*
(Dated: June 12, 2013)

This is a supplementary material of our recent paper[1], where a class of exactly solvable $S = 1$ quantum Ising spin models were studied based on the hole decomposition scheme. Here we provide some details for the Green functions, the spin-spin correlation functions, as well as the spin susceptibility in the presence of dimerization.

I. INTRODUCTION

In Ref.[1] we have studied a class of the $S = 1$ spin chains with the nearest neighbor Ising coupling and both transverse and longitude single-ion anisotropy by a combinational use of a hole decomposition scheme and a recursive method. These models include the first example of the dimerized $S = 1$ quantum spin chain where all the eigen states can be solved exactly. In this supplementary material we present some detailed derivations for the physical quantities of the $S = 1$ dimerized chain. All the notations are the same as in Ref.[1]. In Sec. II, we discuss the Green functions of the uniform or dimerized chains, respectively. In Sec. III, we study the longitudinal spin-spin correlation function at zero- or finite-temperatures. In Sec. V and VI we list some detailed formulae for the segmented M-matrices and the partition functions.

II. GREEN FUNCTIONS

A. Green functions of the uniform spin segments

The original $S = 1$ quantum Ising model is mapped onto a large family of the segmented $S = 1/2$ transverse Ising models classified by the total number of holes[2, 3]. These segmented $S = 1/2$ models are then solved by introducing the Bogoliubov fermionic quasi-particle operators $\eta_k^\dagger$ and η_k as defined in Eq. (14) in Ref. [1]. Inversely, we have

$$c_j^\dagger = \sum_k \frac{\Phi_{kj} + \Psi_{kj}}{2}\eta_k^\dagger + \frac{\Phi_{kj}^* - \Psi_{kj}^*}{2}\eta_k,$$
$$c_j = \sum_k \frac{\Phi_{kj}^* + \Psi_{kj}^*}{2}\eta_k + \frac{\Phi_{kj} - \Psi_{kj}}{2}\eta_k^\dagger.$$

The Green function, or the two-point correlation function, is defined by

$$G_{jq} \equiv \langle F_j^{(-)} F_q^{(+)} \rangle, \tag{1}$$

where $F_j^{(\pm)} \equiv c_j^\dagger \pm c_j$.

For the uniform system, the wavefunctions Φ_{kj} and Ψ_{kj} can be taken as real, we have

$$F_j^{(-)} = \sum_k \Psi_{kj}(\eta_k^\dagger - \eta_k) \ ,$$
$$F_j^{(+)} = \sum_k \Phi_{kj}(\eta_k^\dagger - \eta_k) \ . \tag{2}$$

The Green function can be then expressed as

$$G_{jq}(\beta) = -\sum_k \Psi_{kj}\Phi_{kq} \tanh[\beta\Lambda(k)/2] \ .$$

Note that $\tanh[\beta\Lambda(k)/2] \to 1$ at the ground state ($\beta \to \infty$), so we have

$$G_{jq}(\beta \to \infty) = -\sum_k \Psi_{kj}\Phi_{kq} \ .$$

We denote the wavefunctions for the chain with periodic boundary condition (cyclic) and open boundary condition (free ends) by (Φ^c, Ψ^c) and (Φ^f, Ψ^f), respectively. Then we have

$$\Phi_{kj}^c = \begin{cases} \sqrt{2/l}\sin jk \ , & k > 0, \\ \sqrt{2/l}\cos jk \ , & k \le 0, \end{cases}$$
$$\Psi_{kj}^c = -\frac{D}{\Lambda(k)}\left[(1 + \lambda\cos k)\Phi_{kj}^c + \lambda \sin k \Phi_{-kj}^c\right], \tag{3}$$

where l is the length of the segment. The Green function is

$$G_r^c = L_r + \lambda L_{r+1}, \tag{4}$$

where $r \equiv |j - q|$ and L_r was defined in Refs. [4, 5]

$$L_r = \frac{1}{\pi}\int_0^\pi dk \frac{1}{\sqrt{1 + \lambda^2 + 2\lambda\cos k}}\cos kr.$$

Similarly,

$$\Phi_{kj}^f = A_k \sin(j - q + 1)k,$$
$$\Psi_{kj}^f = A_k\delta_k \sin jk, \tag{5}$$

where

$$A_k = \frac{1}{2}\left[2l+1-\frac{\sin(2l+1)k}{\sin k}\right]^{-1/2}. \quad (6)$$

Consequently, we have

$$G^f_{jq} = -\sum_k A_k^2 \delta_k \sin jk \sin(j-q+1)k. \quad (7)$$

At the finite temperatures, we need to add the factor $\tanh[\beta\Lambda(k)/2]$ to Eqs.(4) and (7).

B. Green functions of the dimerized segments

In the presence of dimerization, the wavefunctions Φ_{kj} and Ψ_{kj} are complex in general. So we now have,

$$\begin{aligned} F^{(-)}_j &= \sum_k \Psi_{kj}\eta^\dagger_k - \Psi^*_{kj}\eta_k, \\ F^{(+)}_j &= \sum_k \Phi_{kj}\eta^\dagger_k + \Phi^*_{kj}\eta_k. \end{aligned} \quad (8)$$

Then, the Green function is expressed by

$$G_{jq} = \sum_k (\Psi_{kj}\Phi^*_{kq} + \Psi^*_{kj}\Phi_{kq})\langle\eta^\dagger_k\eta_k\rangle - \sum_k \Psi_{kj}\Phi^*_{kq}. \quad (9)$$

Where, $\langle\eta^\dagger_k\eta_k\rangle = [\exp(\Lambda_k/(k_BT)) + 1]^{-1}$, satisfying Fermi-Dirac statistics. At the zero temperature, the Green function can be written as

$$G_{jq} = D_j Y[j,q] + 2J_j Y[j+1,q], \quad (10)$$

where

$$\begin{aligned} Y[j,q] &= -\sum_k \frac{e^{i(j-q)k}}{\Lambda(k)}[1+(-1)^{j+q}\gamma^*\gamma \\ &\quad + (-1)^j\gamma + (-1)^q\gamma^*]. \end{aligned} \quad (11)$$

The dimerization parameter γ is defined by

$$\gamma = \frac{1-\tau}{1+\tau} \quad (12)$$

with τ being determined by Eqs. (19) in Ref. [1].

Generally, τ has two solutions, corresponding to the upper/lower signs of $\pm$ respectively in Eqs. (19) in Ref. [1]. In order to numerically calculate the Green function, we need to express $Y[j,q]$-function in terms of real variables. We introduce $p_{1,2}$, $q_{1,2}$ to express complex γ as follows.

$$\gamma_1 = p_1 + iq_1, \quad \gamma_2 = p_2 + iq_2, \quad (13)$$

$p_{1,2}$ and $q_{1,2}$ are the real and imaginary parts of $\gamma_{1,2}$, respectively,

$$\begin{aligned} p_{1,2} &= \frac{b_1^2+b_2^2+4b_1b_2\cos 2k-(\zeta_1\mp\zeta_2)^2}{[(b_1+b_2)\cos k-\zeta_1\pm\zeta_2]^2+(b_2-b_1)^2\sin^2 k}, \\ q_{1,2} &= \frac{-2(b_2-b_1)\sin k\,[(b_1+b_2)\cos k+\zeta_1\mp\zeta_2]}{[(b_1+b_2)\cos k-\zeta_1\pm\zeta_2]^2+(b_2-b_1)^2\sin^2 k}, \end{aligned}$$

where the subscript 1 corresponds to the upper case, the subscript 2 corresponds to the lower case. $\zeta_{1,2}$ are given by

$$\begin{aligned} \zeta_1 &= (a_2-a_1)/2, \\ \zeta_2 &= \Gamma^2\sqrt{1-P+Q\cos 2k}\,. \end{aligned}$$

where a_1, a_2, P, Q and Γ are defined in Ref.[1].

For convenience, we divide k-region $[-\pi,\pi)$ into two subregions: (I) for $[-\pi/2,\pi/2)$ and (II) for $[-\pi,-\pi/2)\cup[\pi/2,\pi)$, respectively. Thus G_{jq} can be expressed by

$$G_{jq} = G^{(I)}_{jq} + G^{(II)}_{jq}. \quad (14)$$

In Region (I), because of the symmetry between k and $-k$, the Green function can be reduced in $(0,\pi/2)$,

$$\begin{aligned} G^{(I)}_{jq} = -\sum_{(0,\pi/2)} \frac{2}{\Lambda_{-1}(k)}\{&D_j[1+(-1)^{j+q}(p_1^2+q_1^2) \\ &+(-1)^j p_1+(-1)^q p_1]\cos(j-q)k \\ &+2J_j[1+(-1)^{j+q+1}(p_1^2+q_1^2) \\ &+(-1)^{j+1}p_1+(-1)^q p_1]\cos(j-q+1)k\}\,. \end{aligned} \quad (15)$$

A similar Green function can be obtained for Region (II). The function $Y[j,q]$ can be rewritten as

$$\begin{aligned} Y[j,q] = -\sum_{(0,\pi/2)} &\frac{2}{\Lambda_{-1}(k)}[1+(-1)^{j+q}(p_1^2+q_1^2) \\ &+(-1)^j p_1+(-1)^q p_1]\cos(j-q)k \\ -\sum_{(\pi/2,\pi)} &\frac{2}{\Lambda_{-2}(k)}[1+(-1)^{j+q}(p_2^2+q_2^2) \\ &+(-1)^j p_2+(-1)^q p_2]\cos(j-q)k. \end{aligned} \quad (16)$$

So it is convenient to express the total Green function Eq. (10) in terms of $Y[j,q]$. In the dimerization case, there are four such Green functions associated with the four different parity combinations of the segments.

III. CORRELATION FUNCTIONS

A. Zero temperature

In this subsection, we discuss the spin-spin correlations at zero temperature. In Ref. [1] we show that the ground state has no hole if $D_z > -\Delta_h(0)$, otherwise, it has holes once $D_z \le -\Delta_h(0)$. In the latter case, the holes break the original chain into segments. We note that only the intra-segment spin-spin correlations are non-zero.

For $D_z > -\Delta_h(0)$, the spin-spin correlation function of S^z is defined by $C^z_{mn} = \langle\Psi_0|S^z_m S^z_n|\Psi_0\rangle$, where $|\Psi_0\rangle$ is the normalized ground state of the Hamiltonian. By use of the Jordan-Wigner transformation, one has

$$C^z_{mn} = \langle\Psi_0|F^{(-)}_m F^{(+)}_{m+1} F^{(-)}_{m+1}\cdots F^{(-)}_{n-1}F^{(+)}_n|\Psi_0\rangle. \quad (17)$$

It is straightforward to show that $\langle\Psi_0|F_j^{(\pm)}F_q^{(\pm)}|\Psi_0\rangle = \pm\delta_{jq}$. By further utilizing the Wick Theorem, we find that

$$C^z_{mn} = \begin{vmatrix} G_{m,m+1} & G_{m,m+2} & \cdots & G_{m,n} \\ G_{m+1,m+1} & G_{m+1,m+2} & \cdots & G_{m+1,n} \\ \vdots & \vdots & \ddots & \vdots \\ G_{n-1,m+1} & G_{n-1,m+2} & \cdots & G_{n-1,n} \end{vmatrix}, \quad (18)$$

for $n > m$, where, $G_{jq} = \langle\Psi_0|F_j^{(-)}F_q^{(+)}|\Psi_0\rangle = -\langle\Psi_0|F_j^{(+)}F_q^{(-)}|\Psi_0\rangle$.

The general expression of G_{jq} is derived in Sec. II A for the uniform chain and in Sec. II B for the dimerized chain respectively. In general, one has

$$G_{jq} = D_j Y[j,q] + 2J_j Y[j+1,q], \quad (19)$$

where $Y[j,q]$ is given by Eq. (16). For a uniform system, $Y[j,q] = Y[q,j] = \frac{1}{D}L_{j-q}$.

B. Finite temperatures

At finite temperatures, the contribution from $p \neq 0$-sector should be taken into account. A recursion formula similar to Eq. (36) in Ref. [1] can be derived for the correlation function as following

$$\sum_{m,n}^{L} C^z_{mn}(\beta) = \frac{1}{Z(L)}\sum_{p=0}^{L}\sum_{l=0}^{L-p}\sum_{m,n}^{l}\alpha^p(p+1)\rho^z_{mn} z(l)Z^{(p-1)}(L-p-l). \quad (20)$$

Where, ρ^z_{mn} is the correlation function of individual segments. It has a similar form with that in Eq. (18), but now G_{jq} should be replaced by $G_{jq}(\beta)$.

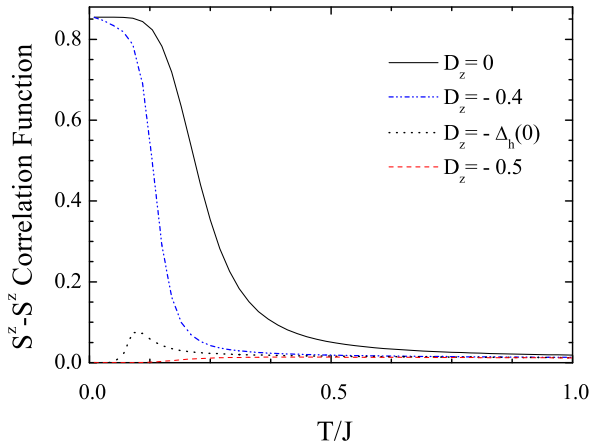

FIG. 1: Temperature dependence of the spin-spin correlation function in a uniform spin chain with $\lambda = 1.5$.

In Fig. 1, we plotted the temperature dependence of the spin-spin correlation function per site, $\sum_{m,n}^{L} C^z_{mn}(\beta)/L$. We find that when $D_z \leq -\Delta_h(0)$, the correlation function approaches to zero in the limit $T \to 0$. This indicates that the ground state is in the hole condensation phase. On the other hand, when $D_z > -\Delta_h(0)$, the correlation function approaches to a finite value (about 0.85 for the two cases shown in the figure) in the zero temperature limit.

IV. SPIN SUSCEPTIBILITY

The spin susceptibility of the $S = 1$ QIM can be also calculated using the recursion formula introduced in the previous section. To do this, one needs to first evaluate the partition functions of each $S = 1/2$ Ising segments in the applied magnetic field ξ, denoted by $z(l_n,\xi)$. The partition function of the original $S = 1$ QIM is then given by $Z(L,\xi) = \sum_{p=0}^{L}\sum_{\{l_n\}}\prod_{n=1}^{p+1} z(l_n,\xi)\alpha^p$. In terms of the segment magnetization $m(l_n,T) = -\frac{1}{\beta}\frac{\partial \ln z(l_n,\xi)}{\partial\xi}$ and the segment susceptibility $\chi(l_n,T) = \frac{\partial m(l_n,T)}{\partial\xi}$, the total susceptibility $\chi(T)$ at zero-magnetic field can be expressed as

$$\chi(T) = \frac{1}{Z(L)}\sum_{p=0}^{L}\sum_{l=0}^{L-p}\alpha^p(p+1) \chi(l,T)z(l)Z^{(p-1)}(L-p-l). \quad (21)$$

Thus the hole decomposition scheme provide an alternative approach to calculate the susceptibility of the $S = 1$ QIM. This approach is efficient provided that the susceptibilities of the corresponding $S = 1/2$ TIM's with varying chain length L are available. We note that the susceptibility of the $S = 1/2$ TIM has already been studied by a number of groups[6, 7, 8]. So in principle these results could be used in the numerical study of the susceptibility of the $S = 1$ QIM.

V. DIAGONALIZATION OF THE M-MATRIX

For a periodic spin chain, the diagonalization of the M-matrix has been discussed in Sec. IV A in Ref. [1]. Here we consider the diagonalization of this $l \times l$ M-matrix for an open spin chain with the length l. The aim here is to solve the following eigen equation

$$M\Phi_k = \Lambda^2(k)\Phi_k \quad (22)$$

in various cases, where $\Phi_k(j)$'s take the form of Eqs. (23) in Ref. [1].

We assume that the two ends of the open chain are located at the sites r_1 and r_2, respectively. r_1 and r_2 can be either odd or even, so there are four kinds of M-matrices. In the following, we will present the results for each cases.

A. $(r_1, r_2) = (odd, even)$

In this case, the matrix M is defined by

$$M = \begin{pmatrix} a_0 & b_1 & 0 & \cdots & 0 & 0 \\ b_1 & a_2 & b_2 & \cdots & 0 & 0 \\ 0 & b_2 & a_1 & \cdots & 0 & 0 \\ \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\ 0 & 0 & 0 & \cdots & a_1 & b_1 \\ 0 & 0 & 0 & \cdots & b_1 & a_2 \end{pmatrix}, \quad (23)$$

where $a_{1,2},\ b_{1,2}$ are defined in the main text and $a_0 = D_1^2$.

The energy spectra can be solved following the approach introduced in Section IV. The result is given by

$$\begin{aligned} \Lambda^2(k) &= \frac{1}{e^{2ik} - t_e e^{-2ik}}[b_1\tau(e^{ik} - t_o e^{-ik}) \\ &\quad + a_2(e^{2ik} - t_e e^{-2ik}) + b_2\tau(e^{3ik} - t_o e^{-3ik})], \end{aligned}$$

The reflection parameters are

$$\begin{aligned} t_o &= e^{2i(l+1)k}, \quad (24) \\ t_e &= \frac{t_o(b_1 e^{ik} + b_2 e^{-ik})}{(b_1 e^{-ik} + b_2 e^{ik})}. \end{aligned}$$

Then, the secular equation is given by

$$\begin{aligned} &[(a_2 - a_1) \pm W]\,[b_1 \sin(l+2)k + b_2 \sin lk] \\ &= \frac{2(a_0 - a_1)(b_1^2 + b_2^2 + 2b_1 b_2 \cos 2k)\sin lk}{b_2}, \quad (25) \end{aligned}$$

where W is defined as in Eq. (20) in Ref. [1].

Other cases can be solved by the same way and the results are listed below.

B. $(r_1, r_2) = (odd, odd)$

The reflection parameters $t_{o,e}$ are

$$\begin{aligned} t_e &= e^{2i(l+1)k}, \quad (26) \\ t_o &= \frac{t_e(b_1 e^{-ik} + b_2 e^{ik})}{(b_1 e^{ik} + b_2 e^{-ik})}. \end{aligned}$$

The secular equation is

$$\begin{aligned} &[(a_1 - a_2) \pm W]\,[b_1 \sin(l-1)k + b_2 \sin(l+1)k] \\ &= \frac{2b_2(b_1^2 + b_2^2 + 2b_1 b_2 \cos 2k)\sin(l+1)k}{a_0 - a_1}. \quad (27) \end{aligned}$$

C. $(r_1, r_2) = (even, even)$

The reflection parameters $t_{o,e}$ are

$$\begin{aligned} t_e &= e^{2i(l+1)k}, \quad (28) \\ t_o &= \frac{t_e(b_1 e^{ik} + b_2 e^{-ik})}{(b_1 e^{-ik} + b_2 e^{ik})}. \end{aligned}$$

The secular equation is

$$\begin{aligned} &[(a_2 - a_1) \pm W]\,[b_1 \sin(l+1)k + b_2 \sin(l-1)k] \\ &= \frac{2b_1(b_1^2 + b_2^2 + 2b_1 b_2 \cos 2k)\sin(l+1)k}{a_3 - a_2} \quad (29) \end{aligned}$$

where, $a_3 = D_2$.

D. $(r_1, r_2) = (even, odd)$

The reflection parameters $t_{o,e}$ are

$$\begin{aligned} t_o &= e^{2i(l+1)k}, \quad (30) \\ t_e &= \frac{t_o(b_1 e^{-ik} + b_2 e^{ik})}{(b_1 e^{ik} + b_2 e^{-ik})}. \end{aligned}$$

The secular equation is

$$\begin{aligned} &[(a_1 - a_2) \pm W] \\ &= \frac{2b_1[b_1 \sin(lk) + b_2 \sin(l+2)k]}{a_3 - a_2}. \quad (31) \end{aligned}$$

VI. THE PARTITION FUNCTIONS OF SEGMENTS

The partition function of individual segment of length l and parity (r_1, r_2) (defined in Sec. V) is given by

$$z_{(r_1,r_2)}(l) = \prod_{\substack{k_1 \in (0,\pi/2), \\ k_2 \in (\pi/2,\pi)}} \cosh\left[\frac{\beta\Lambda_1(k_1)}{2}\right] \cosh\left[\frac{\beta\Lambda_2(k_2)}{2}\right], \quad (32)$$

where, $k_{1,2}$ satisfy the corresponding secular equations.

Acknowledgments

This work was supported in part by the National Natural Science Foundation of China, the national program for basic research of China (the 973 program), the PCSIRT (IRT-0754), and SRFDP (No.J20050335118) of Education Ministry of China.

[1] Z.H. Yang, L.P. Yang, H.N. Wu, J. Dai, and T. Xiang, Phys. Rev. B **79**, 214427(2009).
[2] J. Oitmaa and A.M.A. von Brasch, Phys. Rev. B **67**, 172402 (2003).
[3] Z.H. Yang, L.P. Yang, J. Dai, and T. Xiang, Phys. Rev. Lett. **100**, 067203 (2008).
[4] E. Lieb, T. Schultz, and D. Mattis, Ann. Phys. N.Y. **16**, 407 (1961).
[5] P. Pfeuty, Ann. Phys. N.Y. **57**, 79 (1970).
[6] R.J. Elliott, P. Pfeuty and C. Wood, Phys. Rev. Lett. **25**, 443 (1970).
[7] A. A. Ovchinnikov, D. V. Dmitriev, V.Ya. Krivnov, and V. O. Cheranovskii, Phys. Rev. B **68**, 214406 (2003) .
[8] H. C. Fogedby, J. Phys. C. **11**, 2801 (1978).