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DRF-G/Service de Physique/DSPE (ER CNRS 216), Centre d'Etudes Nucléaires de Grenoble, 85 X-38041 Grenoble Cedex, France

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Abstract. — We propose a second quantization formalism for the soliton modes in the $s = 1/2$ Ising-like antiferromagnetic chain. We give the exact expressions, within the one-soliton approximation, for the dynamical structure factors in presence of a magnetic field, either parallel or perpendicular to the chain. We show that the field gives rise to a splitting of the soliton modes. We also derive the spin correlation function relative to the antiferromagnetic mode for finite and infinite chains.

1. Introduction.
Antiferromagnetic Ising-like chains are known to offer good examples of soliton excitations. As shown first by Villain, an exact derivation for the fluctuations induced by the solitons can be obtained in the case of quantum spins $s = 1/2$ [1]. For classical spins different derivations have been proposed, which all refer to the sine-Gordon model. Recently, Haldane has established that, in this case, additional internal modes are expected to occur in the solitons [2]. Moreover, the nature of these internal modes should depend on whether the spin value is integer or half integer. In the same line, Affleck has related these predictions to the dyon concept which is used in particle physics. It was also suggested that the application of an external magnetic field in the spin direction might offer a « useful way of disentangling the dyon levels » [3].

In the present work, we consider explicitly the case of quantum spin chains in an external magnetic field which is applied either parallel or perpendicular to the spins. The second quantization approach that we propose provides a clear understanding of the effects of such a field on the solitons. Rather different behaviours are actually observed depending on the field direction. In the following, the dynamical structure factors $S^\alpha(q, \omega) (\alpha = x, y, z)$ associated with the solitons are calculated within the one-soliton approximation in the full Brillouin zone ($-\pi < q \leq \pi$). Concerning the antiferromagnetic mode near $q = \pi$, resulting from the soliton-induced spin flippings in the magnetic sublattices, new statistical arguments are given, which reinforce the phenomenological description proposed by Maki [4].

2. Second quantization.
The starting point is the following Hamiltonian:

$$H = \sum_n \left[2 J s_n^x s_{n+1}^x + 2 \epsilon J (s_n^y s_{n+1}^y + s_n^y s_{n+1}^y) + H_1 s_n^z + H_\perp s_n^z \right]$$

with $\epsilon, H_1/J$ and $H_\perp/J \ll 1$. The first term where $J$ is the exchange coupling describes the Ising energy. It is responsible for the antiferromagnetic ground state with the spins aligned along the z direction (which here coincides with the chain axis). Following Villain [1], we consider chains with an odd number of
spins and cyclic conditions. This situation forces the presence of an odd number of alternance defects or topological solitons in the chains. The diagonalization of the Hamiltonian in equation (1) has been performed by Shiba and Adachi [5] in order to calculate the dynamical susceptibility at $q = 0$. Our second quantization approach allows an extension of this work to any value of $q$.

Let $|p\rangle$ ($p$ half integer) be the state with one soliton between sites $p - 1/2$ and $p + 1/2$. In the subspace with one soliton, the matrix elements of the spin operators are:

$$
\langle p | s^\alpha_n | p' \rangle = \frac{1}{2} \left( \delta_{p,n+1/2} \delta_{p',n-1/2} + \delta_{p,n-1/2} \delta_{p',n+1/2} \right),
$$

$$
\langle p | s^\alpha_n | p' \rangle = \frac{1}{2} i (-)^{n-p} \left( \delta_{p,n+1/2} \delta_{p',n-1/2} - \delta_{p,n-1/2} \delta_{p',n+1/2} \right),
$$

$$
\langle p | s^\alpha_n | p' \rangle = \frac{1}{2} (-)^{n-p} \left( n-p \right) \delta_{pp'}.
$$

(2)

The phase convention chosen in equation (2) is such that the soliton is positive (extra spin up) for $p - 1/2$ odd and negative (extra spin down) for $p - 1/2$ even (see Fig. 1). We now introduce $c_p^+$ and $c_p^-$ the creation and annihilation operators for a soliton at the position $p$ and their Fourier transforms given by:

$$
c_k = \frac{1}{\sqrt{N}} \sum_p e^{-ipk} c_p^- (-\pi < k \leq \pi).
$$

The spin operators are expressed as:

$$
S^\alpha_q = \frac{1}{\sqrt{N}} \sum_p e^{-iqp} \langle p | s^\alpha_n | p' \rangle c^+_{p'} c_p^-.
$$

and using equation (2), evaluated to be:

$$
S^+_{q} = \frac{1}{\sqrt{N}} \sum_k \cos \left( k + \frac{1}{2} q \right) c_k^+ c_{k+q},
$$

$$
S^-_{q} = -\frac{1}{\sqrt{N}} \sum_k \cos \left( k + \frac{1}{2} q \right) c_k^- c_{k+q},
$$

$$
S^x_{q} = \frac{i}{\sqrt{N}} \sum_k \frac{1}{2} \cos \left( k + \frac{1}{2} q \right) c_k c_{k+q}.
$$

(3)

Similarly, the Hamiltonian can be rewritten as:

$$
\mathcal{H} = \sum_k \left( J + 2 eJ \cos 2k + H_\perp \cos k \right) \times c_k^+ c_k + \frac{i}{2} H_1 \left( c_k^+ c_{k+\pi} + c_k c_{k-\pi} \right).
$$

(4)

The corresponding eigenvalues are obtained by diagonalization in the $|k\rangle$, $|k-\pi\rangle$ subspace [5]:

$$
E_{\pm}(k) = J + 2 eJ \cos 2k \pm \sqrt{\left( H_\perp \cos k \right)^2 + \left( \frac{1}{2} H_1 \right)^2}. \quad (5)
$$

With no magnetic field, the $|k\rangle$ and $|k-\pi\rangle$ states are degenerate and the Brillouin zone can be reduced to $-\frac{1}{2} \pi < k < \frac{1}{2} \pi$. The effect of a magnetic field is seen to lift this degeneracy. As a result, one obtains a splitting of the soliton energy in two branches as shown in figure 2.

![Fig. 1. — Antiferromagnetic ground state (a), positive soliton (b) and negative soliton (c).](image)

![Fig. 2. — Band-structure of the one-soliton excitations without magnetic field (a), and with a magnetic field parallel (b) and perpendicular (c) to the chain.](image)

3. Parallel field.

For a field parallel to the chain axis ($H_\parallel = 0$), the Hamiltonian (Eq. (4)) becomes:

$$
\mathcal{H} = \sum_{k\sigma} E_{k\sigma} c_{k\sigma}^+ c_{k\sigma}, \quad (6)
$$

where

$$
E_{k\sigma} = J + 2 eJ \cos 2k + \frac{1}{2} \sigma H_1 \quad (7)
$$

$$
c_{k\sigma} = \frac{1}{2} \left( c_k + i \sigma c_{k-\pi} \right) \quad (8)
$$

with $\sigma = \pm 1$ and $-\frac{1}{2} \pi < k < \frac{1}{2} \pi$. The $\sigma = +1$ ($\sigma = -1$) states correspond to a combination of
positive (negative) solitons as shown by the following decomposition:

\[ c_{k+} = \frac{1}{2\sqrt{N}} \sum_\sigma (\exp(-ipk + i\sigma(\pm k - \nu)) c_p \]
\[ = \frac{1}{\sqrt{N}} \sum_\sigma \exp(-ipk) c_p \]
\[ c_{k-} = \frac{1}{2\sqrt{N}} \sum_\sigma (\exp(-ipk - i\sigma(k - \nu)) c_p \]
\[ = \frac{1}{\sqrt{N}} \sum_\sigma \exp(-ipk) c_p \]

Thus, one obtains for \( H_{\parallel} \), a simple Zeeman splitting favoring the negative solitons in the \(|k-\rangle\) states with respect to the positive solitons in the \(|k+\rangle\) states. Moreover, the energy splitting is independent of the wave vector \( k \) (Fig. 2b).

Using equations (3) and (8), the spins operators are now given by:

\[ S_q^z = \frac{\sigma}{2\sqrt{N}} \sum_\sigma \exp(\sigma q) c_{k+q} \]
\[ S_q^+ = \frac{1}{2\sqrt{N}} \sum_\sigma \exp(k + \frac{1}{2} q) c_{k+q} c_{k+q} \]
\[ S_q^- = \frac{1}{2\sqrt{N}} \sum_\sigma \exp(k - \frac{1}{2} q) c_{k-} c_{k+q} \]

and the spin correlation functions can be expressed as:

\[ S_\parallel(q,0) = \langle S_\parallel(q) S_\parallel(q,0) \rangle = \frac{1}{4N} \sum_\sigma \exp\left(-\frac{1}{2} q^2 \right) \sum_\nu \exp(\nu q) \exp(\nu q) \exp(i(E_{k+} - E_{k+})t) \]
\[ S_\perp(q,0) = \langle S_\perp(q) S_\parallel(q,0) \rangle = \frac{1}{4N} \sum_\sigma \exp\left(-\frac{1}{2} q^2 \right) \sum_\nu \exp(\nu q) \exp(i(E_{k+} - E_{k+})t) \]

where \( \tilde{\xi}_{k\nu} \) defines the thermal population of the \(|k\rangle\) state. It can be expressed as \( \tilde{\xi}_{k\nu} = n_s \frac{e^{-\beta \left(2\epsilon_1 \cos 2k + \frac{1}{2}\sigma H_1 \right)} \exp(\nu q)}{Z_1} \)

In the last equation, \( I_0(\nu) \) is the zero-order modified Bessel function. The dynamical structure factors \( S(q,\omega) \) are obtained by Fourier transformation of equation (10). After an integration over \( k \), one gets:

\[ S_\parallel(q,\omega) = \frac{1}{2\sqrt{\Omega_q}} \sum_\sigma \exp(\nu q) \exp(i(E_{k+} - E_{k+})t) \]
\[ S_\perp(q,\omega) = \frac{1}{2\sqrt{\Omega_q}} \sum_\sigma \exp(\nu q) \exp(i(E_{k+} - E_{k+})t) \]

where \( \gamma^z = \beta \left(\Omega_q^2 + \omega^2\right)^{1/2} \) and \( \gamma^z = \beta \left(\Omega_q^2 + \omega + H_1\right)^{1/2} \) for \( kT \gg H_1, \epsilon J \), the two energy branches are uniformly occupied and the thermal factors are simplified in \( A(q) = A(q) = n_s(1 - n_s) \) and \( B(q) = 0 \). At lower temperature, \( n_s \) can be neglected compared to 1 and for \( H_1 = 0 \), one recovers the results previously given by Villain for the \( z \)-component [1] and by Nagler et al. for the transverse spin component [6]. Finally, at very low temperature (\( kT < H_1, \epsilon J \)), only the lower states of the lower band are occupied: \( \tilde{\xi}_{k\nu} = n_s \delta_{k\nu} \) and \( A(q) = A(q) = n_s(1 - n_s) \) are replaced by \( \delta \)-functions which can be easily derived from equations (10).

All the dynamical structure factors in equation (11) exhibit a square root divergence. This corresponds to the nesting condition characteristic of one-dimensional bands. It is also worth noting that \( S(q,\omega) \) is unaffected by the external magnetic
field. This is expected as this function corresponds to transitions inside each energy band of figure 2b. On the opposite, for the transverse spin fluctuations which describe transitions from one band to the other, the position of the divergence is shifted by the interband splitting: 

\[ \Omega^a_q = \pm (\Omega_q \pm \varepsilon H_1) \] 

with \( \varepsilon = \pm 1 \). This results in a doubling of the soliton modes, as shown in figure 3 where we have drawn the function:

\[ S^a_i(q, \omega) = S^a_f(q, \omega) = \frac{1}{4} \left( S^a_i(q, \omega) + S^a_f(q, \omega) \right) \]

for \( H = 0 \) (Fig. 3a) and \( H = \varepsilon J \) (Fig. 3b). One notices that, at \( q = 0 \) and \( q = \pi \) (i.e. for \( \Omega_q = 0 \)), the spreaded distribution of frequencies merges into δ-functions. In particular the ESR mode \( S^a_i(q = 0, \omega) \) (\( \alpha = x \) or \( y \)), which corresponds to vertical transitions between the two subbands in figure 2b is peaked at the conventional Larmor frequency:

\[ \omega = \pm H_1. \]

4. Perpendicular field.

In perpendicular field \( (H_1 = 0) \), the Hamiltonian (Eq. (4) can be diagonalized in the initial \( |k> \) basis:

\[ \mathcal{K} = \sum_k c_k^* c_k \]

\[ E_k = J + 2 \varepsilon J \cos 2 k + H_{1\perp} \cos k \]

with \( -\pi < k < \pi \). Again, two distinct energy branches are obtained in the reduced Brillouin zone as shown in figure 2c. The states in the upper branch correspond to \( |k| > \frac{1}{2} \pi \) in equation (13); they can be viewed as triplet states (positive combination of adjacent positive and negative solitons), while the lower branch \( (|k| < \frac{1}{2} \pi \) in equation (13)) can be considered as singlet states. Using equation (3), the correlation functions are expressed as:

\[ S^λ_λ(q, t) = \frac{1}{N} \sum_k \cos^2 \left( k + \frac{1}{2} q \right) \sum_k \tilde{n}_k(1 - \tilde{n}_{k+q}) \exp[i(E_k - E_{k+q}) t] \]

\[ S^λ_\perp(q, t) = \frac{1}{N} \sum_k \cos^2 \left( k + \frac{1}{2} q \right) \sum_k \tilde{n}_k(1 - \tilde{n}_{k+q}) \exp[i(E_k - E_{k+q}) t] \]

\[ S^\perp_\perp(q, t) = \frac{1}{4 N} \sum_k \tilde{n}_k(1 - \tilde{n}_{k+q}) \sum_k \tilde{n}_k(1 - \tilde{n}_{k+q}) \exp[i(E_k - E_{k+q}) t] \]

with \( \tilde{n}_k = n_s P_k / Z_\perp, \ Z_\perp = 1/N \sum_k P_k \) and:

\[ P_k = \exp[-\beta(2 \varepsilon J \cos 2 k + H_{1\perp} \cos k)]. \]

Exact calculations of the dynamical structure factors can also be performed (see Appendix). However, their expressions are too complicated to allow a simple formulation. As an example, the function \( S^λ_\perp(q, \omega) \) has been calculated; it is shown in figure 4c for \( H_{1\perp} = \varepsilon J \). A doubling of the soliton mode is also observed, which, however differs drastically from the case of parallel field. The position of the square root singularities can be expressed (see Appendix) as a function of the scattering wave vector \( q \) as:

\[ \Omega^a_q = \pm \frac{1}{8} \Omega_q [3 h^a_q + \eta (h^a_q + 8)^{1/2}] \]

\[ \times [8 - 2 h^a_q + 2 \eta h^a_q (h^a_q + 8)^{1/2}]^{1/2} \]

(15)

For \( h^a_q = 1 \), four singularities are obtained which correspond to \( \eta = \pm 1 \) in equation (15); however, for \( h^a_q > 1 \), there are only two singularities obtained for \( \eta = +1 \). This remarkable result is displayed in figure 4 where the dispersion relation of the singularities of \( S^λ_\perp(q, \omega) \) and \( S^\perp_\perp(q, \omega) \) are shown for different values of \( H_{1\perp}/\varepsilon J \). The twice degenerated singularity line for \( H_{1\perp} = 0 \) is splitted into two distinct lines for \( H_{1\perp} > 0 \). While a gap with frequency \( \omega = \pm 2 H_{1\perp} \) is open at \( q = 0 \) for one line, the second line is now restricted to the interval comprised between \( q = 2 \sin^{-1}(H_{1\perp}/8 \varepsilon J) \) and \( q = \pi \). With \( H_{1\perp} \) increasing, this second line is reduced to a...
Fig. 4. — Dispersion relation of the singularities of $S_1^z(q, \omega)$ and $S_2^z(q, \omega)$ for different values of the perpendicular field : $H_{\perp} = 0$ (full line), $H_{\perp} = 2 \varepsilon J$ (dotted line), $H_{\perp} = 4 \varepsilon J$ (dotted-broken line) and $H_{\perp} = 8 \varepsilon J$ (broken line). The singularity lines for $S_1^z(q, \omega)$ are obtained by changing $q$ in $\pi - q$.

smaller and smaller zone near $q = \pi$, where it condensates for $H_{\perp} = 8 \varepsilon J$. For larger field, only the first singularity line remains present. A similar behaviour is observed for the function $S_1^z(q, \omega)$ by changing $q$ in $\pi - q$. For this function, the gap occurs at $q = \pi$ and the condensation point at $q = 0$. Finally, one notices that, contrary to the parallel field case, the ESR modes $S_1^z(q = 0, \omega)$ and $S_1^z(q = 0, \omega)$ consist of a continuum of resonance frequencies and present square-root divergences at the somewhat unusual values : $\omega = \pm 2 H_{\perp}$, which actually correspond to the nesting condition for vertical transitions in figure 2c.

5. Antiferromagnetic mode.

The one-soliton approximation becomes insufficient to describe the fluctuations in the $z$ direction near the antiferromagnetic point $q = \pi$, as evidenced by the divergent $1/\cos^2 \frac{1}{2} q$ factor in equations (10) and (14). To go beyond this approximation, we calculate the fluctuations resulting from the flipping induced by the solitons, considered as independent random events. The $z$-component of the spin at site $n$ is fixed by two conditions : i) the parity of $n$ and ii) the total number of solitons on the left hand side of the site $n$. The corresponding correlation function can be written as:

$$S^z(n, t) = \langle s^z_n(t) s^z_0(0) \rangle = \frac{1}{4} (-)^n e^{i \pi \Delta N(n, t)}.$$ (17)

In this equation, we have used $(-)^N = e^{i \pi N}$ and we have defined $\Delta N(n, t) = N(n, t) - N(0, 0)$, where $N(n, t)$ is the operator which describes the number of solitons present at time $t$ between the left end of the chain and the site $n$. This number is the result of a random process, which accounts for the presence or the absence of solitons in a given $|k\rangle$ state. At any time, $\Delta N$ can be considered as the sum of two terms $\Delta N = \Delta N_+ + \Delta N_-$, corresponding to solitons which give positive (+1) and negative (-1) contributions. In equation (17), one can actually replace this sum by the difference $\Delta N = N_+ - N_-$, which remains a positive quantity. The correlation function appears therefore to be the characteristic function (or the Fourier transform) $\phi(n, t ; \pi)$ of the probability distribution $\rho(\Delta N)$ for $u = \pi$:

$$S^z(n, t) = \frac{1}{4} (-)^n \phi(n, t ; \pi).$$

In order to evaluate the moments of this distribution, $\Delta N$ is expressed as a function of the creation-annihilation operators:

$$\Delta N = \sum_{p = -\frac{1}{2} N + 1}^{N - \frac{1}{2} N} c^+_p c_p - \sum_{p = -\frac{1}{2} N + 1}^{N - \frac{1}{2} N} c^+_p c_p$$

$$A(k, K) = \left( e^{i \left( \frac{n}{2} + \frac{1}{2} \right) K} - e^{-i \left( \frac{1}{2} N - 1 \right) K} \right)$$

$$\times \frac{e_k - e_{k + K}}{e_k - 1} + e^{\frac{1}{2} K} e^{i n K} \frac{1}{e_k - 1}.$$ (18)

In an infinite system, the second term in the parenthesis occurring in equation (19) can be dropped out since it gives vanishing contribution when integrated over $K$ if $N \to \infty$. As the contributions of the different $|k\rangle$ states are statistically independent, the first two moments of $\rho(\Delta N)$ are given by:

$$M_1(n, t) = \langle \Delta N \rangle = \langle \Delta N_+ \rangle - \langle \Delta N_- \rangle$$

$$M_2(n, t) = \langle \Delta N^2 \rangle - \langle \Delta N \rangle^2 = \langle \Delta N_+^2 \rangle - \langle \Delta N_- \rangle^2$$

$$\times \bar{\bar{n}}_k (1 - \bar{\bar{n}}_{k + K}).$$
Using equation (19), one obtains:

\[ M_1(n, t) = \frac{1}{N} \sum_k n_k |n - v_k t| \]  

\[ M_2(n, t) = \frac{1}{N^2} \sum_{k,k'} n_k (1 - n_{k+k'}) \sin^2 \frac{1}{2} \left[ \frac{1}{2} (E_k - E_{k+k'}) t - nK \right] \sin^2 \frac{1}{2} K \]

\[ \approx \frac{1}{N} \sum_k n_k |n - v_k t| \]

where \( v_K = dE_K/dk \). In the last step of equation (21), we have made the approximations \( 1 - n_{k+K} = 1 \) and \( E_{k+k} - E_k = v_k K \). Otherwise the integration over \( K \) is exact [7]. It appears therefore that the two first moments of the distribution \( p(\Delta N) \) are equal. This result agrees formally with the assumption of a Poisson distribution and justifies in the quantum case, the description first proposed by Krumhansl and Schrieffer [8] for solitons in the classical \( k^4 \) model. Since the characteristic function associated with the Poisson distribution is \( \Phi(u) = \exp[M_1(e^{iu} - 1)] \), we obtain:

\[ S^i(0, t) = \frac{1}{4} \left( - \right)^n \exp \left( - \frac{2}{N} \sum_k n_k |n - v_k t| \right) \]

This expression was first given by Maki [4], but not explicitly demonstrated. It can be viewed as an extension to this quantum case of the effects of an external magnetic field on the soliton excitations in Ising-like quantum spin chains. New specific features have been established for both field parallel and perpendicular to the spins. For parallel field, an additional Zeeman splitting is found. For perpendicular field, one is led to a simultaneous change of both the energy and the velocity of the solitons. The corresponding dynamical structure factors have been calculated in the one-soliton model. It is known that this approximation is quite insufficient to describe realistic spin systems [1, 10, 13]. Interactions between solitons, between solitons and magnons and with impurities are expected to round off the square-root singularities [14]. However, the main feature — the doubling of the soliton modes — established by our formulation would be maintained. The lineshapes displayed in figure 3 have been evaluated for the physical parameters \( J = 100 \, K \), \( T = 25 \, K \) and \( EJ = H = 10 \, K \). The magnetic resonance techniques can provide a check of the Zeeman splitting and of the gaps of the singularity lines expected at \( q = 0, H_{II} \) and \( H_{I} \), respectively [17, 18].

The present results have been obtained in the case of quantum spin chains. We may wonder if they can be extrapolated to classical spin chains. The Zeeman splitting obtained for \( H_I \) might be the analog of the dyon levels described by Affleck. It would remain to...
find the classical analog of the soliton doubling for $H_1$. Similar calculations in Ising-like classical spin chains are highly desirable. Finally, the present work which concerns a spin 1/2 system can be a first contribution to the crucial question concerning the different behaviours expected for antiferromagnetic chains with integer and half-integer spins.

Appendix A : dynamical structure factors in perpendicular field.

To get the Fourier transforms of equations (14), one uses the relation:

$$\delta (f(k)) = \sum \frac{\delta (k_i)}{|f'(k_i)|}$$

with $k_i$ being the solutions of $f(k) = 0$. This gives:

$$S_1^x(q, \omega) = \sum_i \cos^2 k_i \tilde{n}_{k_i} \left(1 - \tilde{n}_{k_i} + \frac{1}{2} q\right) \left\{ \frac{1}{8 \epsilon J \sin q \cos 2 k_i + 2 H \sin \frac{1}{2} q \cos k_i} \right\}$$

$$S_1^y(q, \omega) = \sum_i \cos^2 k_i \tilde{n}_{k_i} \left(1 - \tilde{n}_{k_i} + \frac{1}{2} q - \pi\right) \left\{ \frac{1}{8 \epsilon J \sin q \cos 2 k_i - 2 H \cos \frac{1}{2} q \sin k_i} \right\}$$

$$S_1^z(q, \omega) = \sum_i \frac{1}{4 \cos^2 \frac{1}{2} q} \left(1 - \tilde{n}_{k_i} + \frac{1}{2} q - \pi\right) \left\{ \frac{1}{8 \epsilon J \sin q \cos 2 k_i - 2 H \cos \frac{1}{2} q \sin k_i} \right\}$$

(A.1)

where $k_i$ are the solutions of the energy conservation equations:

$$4 \epsilon J \sin q \sin 2 k_i + 2 H \sin \frac{1}{2} q \sin k_i +$$

$$+ \omega = 0 \quad \text{for } S^x$$

(A.2)

$$4 \epsilon J \sin q \sin 2 k_i + 2 H \cos \frac{1}{2} q \cos k_i +$$

$$+ \omega = 0 \quad \text{for } S^y \text{ and } S^z.$$

By changing $k_i$ into $\frac{1}{2} \pi - k_i$ for $S^x$ and taking $u = \cos k_i$, one gets an unique equation:

$$u^4 + u^2(h_q^a - 1) + 2 h_q^a \Omega u + \Omega^2 = 0$$

(A.3)

where $\Omega = \omega / 2 \Omega_q$ and $h_q^a$ are defined by equations (16). It can be solved by standard methods, but only the solutions $|u| \leq 1$ should be retained. As the solutions of this fourth degree equation are quite complicated, we will not give the explicit expressions for the resulting dynamical structure factors; it is, however, easy to have them calculated with a computer by replacing $k_i$ in equation (A.1) with the solutions obtained from equation (A.3).

On the other hand, the singularities are obtained as the poles of equation (A.1) which are given by:

$$v^2 + \frac{1}{2} h_q^a v - \frac{1}{2} = 0$$

(A.4)

with $v = \sin k_i$ (again $k_i$ has been changed into $\frac{1}{2} \pi - k_i$ for $S^x$). Among the two existing solutions:

$$v = \frac{1}{4} (- h_q^a + \eta (h_q^a^2 + 8)^{1/2})$$

with $\eta = \pm 1$, both are valid for $h_q^a \leq 1$, but only that with $\eta = +1$ is correct for $h_q^a > 1$ because of the condition $|v| \leq 1$. The general expression for the singularity frequencies (Eq. (15)) immediately follows using equation (A.2). Moreover, it can be checked by making a development near $\Omega_q^a$ that the singularities are of square root type as in parallel field.

References