Response functions of gapped spin systems in high magnetic field

Alexei K. KOLEZHUK\textsuperscript{1,2} and Hans-Jürgen MIKESKA\textsuperscript{2}

\textsuperscript{1} Institute of Magnetism, National Academy of Sciences and Ministry of Education, 36(B) Vernadskii avenue, 03142 Kiev, Ukraine
\textsuperscript{2} Institut für Theoretische Physik, Universität Hannover, Appelstraße 2, 30167 Hannover, Germany

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We study the dynamical structure factor of gapped one-dimensional spin systems in the critical phase in high magnetic field. It is shown that the presence of a “condensate” in the ground state in the high-field phase leads to interesting signatures in the response functions.

\section{Introduction}

Recently, there has been an increasing interest in the physics of gapped one-dimensional spin systems subject to an external magnetic field which is strong enough to close the gap and bring the system into a new critical phase with finite magnetization and gapless excitations.\textsuperscript{1-13} The low-energy physics of the critical phase is usually described by the Luttinger liquid,\textsuperscript{9,14} in some cases the problem can be directly mapped to the effective $S=1/2$ chain.\textsuperscript{7,8,10,15} Such a description is equivalent to neglecting certain degrees of freedom (e.g., two of the three rung-triplets in case of the strongly coupled spin ladder\textsuperscript{7,8,10}). Those neglected states, however, form excitation branches which contribute to the response functions at higher energies, and this contribution is generally much easier to see experimentally than the highly dispersed low-energy continuum of the particle-hole (“spinon”) excitations coming from the Luttinger liquid itself. At present, at least in two quasi-one-dimensional materials, Ni(C\textsubscript{2}H\textsubscript{8}N\textsubscript{2})\textsubscript{2}Ni(CN)\textsubscript{4} (known as NENC)\textsuperscript{6} and Ni(C\textsubscript{2}H\textsubscript{8}N\textsubscript{2})\textsubscript{2}NO\textsubscript{2}(ClO\textsubscript{4}) (abbreviated NDMAP)\textsuperscript{5,16} those high-energy branches were found to exhibit interesting behavior in electron spin resonance (ESR) experiments, with changes in the slope of the ESR lines as functions of the field. Quite recently, inelastic neutron scattering (INS) experiments on NDMAP,\textsuperscript{17} and on TlCuCl\textsubscript{3},\textsuperscript{18} featuring a similar behavior, were reported.

Motivated by those observations, we have studied the ESR response in the high-field phase of a large-$D$ $S=1$ chain.\textsuperscript{20} It was shown that presence of the Fermi sea leads to renormalization of the energies of higher-lying excitations, which may result in nontrivial dependence of the excitation energy on the magnetic field.

In the present paper we extend our previous work for the general case of arbitrary transferred momentum $q$ (the ESR case corresponds to $q=0$) and study the contributions of the high-energy excitations to the dynamical structure factor $S(q,\omega)$ in the hardcore boson approximation. We use the $S=1$ Affleck-Kennedy-Lieb-Tasaki\textsuperscript{19} (AKLT) chain and strongly coupled $S=1/2$ ladder as specific examples,
but the general idea behind the calculation is in fact quite universal and applies to any gapped one-dimensional system in the high-field critical phase. We show that characteristic signatures in the response persist for nonzero $q$ as well, and can therefore be observed in INS experiments.

§2. Model examples and hardcore boson approximation

In Ref. 20) we have used the hardcore boson approximation as an effective model to study the response of the large-$D S = 1$ chain. In this section, we show that the same type of approximation can be used essentially for any gapped 1D system.

2.1. Strongly coupled ladder

A two-leg $S = \frac{1}{2}$ ladder with the rung coupling $J_R$ much larger than the leg coupling $J_L$ in a strong magnetic field $H$ can be mapped to an effective $S = \frac{1}{2}$ XXZ chain by keeping only two states on each rung, a singlet $|s\rangle$ and a triplet $|t_+\rangle$, and identifying them with the effective spin-$\frac{1}{2}$ states.\(^7\),\(^8\),\(^10\) Alternatively, one may describe the triplets $|t_+\rangle$ as hardcore bosons. The resulting $S = \frac{1}{2}$ chain model

$$\hat{H}_{S=1/2} = \sum_n J_L \left\{ \hat{S}_{x,n} \hat{S}_{x,n+1} + \hat{S}_{y,n} \hat{S}_{y,n+1} + \Delta \hat{S}_{z,n} \hat{S}_{z,n+1} \right\} + \left( J_R - \frac{1}{2} J_L - H \right) \hat{S}_{z,n}$$

(2.1)

has the anisotropy $\Delta = 1/2$ of the easy-plane type and is in turn effectively described by the Luttinger liquid model. If the field is only slightly larger than the critical field $H_c$, the density of triplets is low and the Luttinger parameter $K$ tends to its non-interacting value 1. Thus, in the vicinity of $H_c$ the interaction between the bosons is irrelevant, and only the hardcore constraint is essential.

Now, if one wants to include the neglected $|t_-\rangle$ and $|t_0\rangle$ states, one can consider them as additional species of hardcore bosons. Neglecting all interactions between the bosons with the exception of the hardcore constraint, one arrives at the effective model of the type

$$\hat{H}_{\text{eff}} = \sum_{n \mu} \varepsilon_{\mu} b_{n,\mu}^\dagger b_{n,\mu} + t \left( b_{n,\mu}^\dagger b_{n+1,\mu} + \text{h.c.} \right)$$

(2.2)

where $\mu = +1$, 0 and $-1$ numbers three boson species (triplet components with $S^z = \mu$), $t = J_L$ is the hopping amplitude which is equal for all types of particles, $\varepsilon_{\mu} = \varepsilon_{\mu}^{(0)} - \mu H$, and the zero-field energies are given by $\varepsilon_{\mu}^{(0)} = J_R$. This model is, of course, highly simplified, but nevertheless it captures the main physics which is hidden in the hardcore constraint.

The connection between physical spin operators and bosonic operators for the ladder is given by the formulas $S_n^{(\alpha)} = \pm (1/2)(t^\dagger_\alpha + t_\alpha) - i \varepsilon_{\alpha \beta \gamma} t^\dagger_\beta t_\gamma$, where $\alpha, \beta, \gamma \in (x, y, z)$ and the operators $t$ are connected to $b$ in a standard way, $b_{\pm 1} = \mp 2^{-1/2}(t_x \pm it_y)$, $b_0 = t_z$.

2.2. AKLT chain

Mapping of the $S = 1$ chain to the effective hardcore boson model is somewhat more complicated, but still possible. Consider $S = 1$ AKLT chain in external
magnetic field $H$ described by the Hamiltonian

$$\hat{H} = \sum_n \left\{ S_n S_{n+1} + \frac{1}{3}(S_n S_{n+1})^2 - H S_n^z \right\}, \quad (2.3)$$

where $S_n$ denotes the spin-1 operator at the $n$-th site. The zero-field gap of the AKLT model is known to be $\Delta \simeq 0.70^{21}$, and we are interested in the high-field regime $H > H_c \equiv \Delta$, when the gap closes.

The ground state for $H < H_c$ is exactly known and can be compactly represented in the matrix product (MP) form $^{22,23}$

$$\Psi_0 = \text{tr}\{g_1 g_2 \ldots g_N\}, \quad g_n = (1/\sqrt{3})(\sigma^+|\sigma\rangle_n + \sigma^-|\sigma\rangle_n - \sigma^0|0\rangle_n), \quad (2.4)$$

where $\sigma^\mu$ are the Pauli matrices in the spherical basis and $|\mu\rangle_n$ are the spin-1 states at the $n$-th site, $\mu = 0, \pm 1$.

Excitations of the AKLT model are well approximated by the triplet solitons (domain walls in the hidden string order), $^{21}$ which can be also cast into the form of a matrix product. $^{24}$ A soliton which sits at the $n$-th site and has $S^z = \mu$ is well approximated by the MP state

$$|\mu, n\rangle = \text{tr}\{g_1 g_2 \ldots g_{n-1} (g_n \sigma^\mu) g_{n+1} \ldots g_N\} \quad (2.5)$$

Soliton states $|\mu, n\rangle$ with different $n$ are not orthogonal. However, one can introduce the equivalent set of states

$$|\mu, n\rangle = 2^{-3/2} \left\{ 3|\mu, n-1\rangle + |\mu, n\rangle \right\} \quad (2.6)$$

which have the orthogonality property $\langle \mu, n|\mu', n'\rangle = \delta_{\mu\mu'}\delta_{nn'}$. The state (2.6) can be represented in the same MP form (2.5) with $(g_n \sigma^\mu)$ replaced by the matrices $f^\mu$,

$$f^+ = \sqrt{2/3} |+\rangle - \frac{1}{\sqrt{6}}(\sigma^+|0\rangle - \sigma^0|+\rangle), \quad f^0 = \sqrt{2/3} |0\rangle - \frac{1}{\sqrt{6}}(\sigma^+|\sigma\rangle - \sigma^{-1}|+\rangle),$$

$$f^- = \sqrt{2/3} |\sigma\rangle + 1/\sqrt{6}(\sigma^0|0\rangle - \sigma^0|\sigma\rangle), \quad (2.7)$$

where the site index $n$ has been omitted for the sake of clarity.

One can extend this construction to many-particle states by replacing more than one of $g$'s in (2.4) by $f$'s, however one cannot of course get the true full Fock space in this way, because we have four possible matrices $(g, f^\mu)$ for every site, while the original $S = 1$ problem has only three states per site. The price one has to pay is deviations from orthonormality for states with two or more particles close to each other. For example, one may observe that states $|+, n; +, n'\rangle$, describing two solitons with $S^z = +1$, remain orthogonal, but their norm depends on the distance between the solitons, $\langle +, n; +, n'|+, n; +, n'\rangle = 1 + (5/12)(-1/3)^{|n-n'|}$. The deviations vanish with increasing the distance between the solitons. Therefore the approximate description in terms of multisoliton states becomes worse as the density of solitons increases, which means it is useful only in the vicinity of the critical field.

Restricting our Hilbert space to the states of the MP form (2.4) with some number of $g$ matrices replaced with $f^+$ ones, one can identify the presence of the
AKLT matrix $g$ and the $S^z = +1$ soliton matrix $f^\dagger$ at the certain site with the effective spin-down and spin-up states, respectively. The resulting effective $S = \frac{1}{2}$ chain is described by the following Hamiltonian

$$
\hat{H}_{S=1/2} = \sum_n J_{\text{eff}} \left\{ \hat{S}_n^x \hat{S}_{n+1}^x + \hat{S}_n^y \hat{S}_{n+1}^y \right\} + \sum_n \sum_{m>0} V_m \hat{S}_n^z \hat{S}_{n+m}^z + \sum_n (\varepsilon_0 + \sum_m V_m - H) \hat{S}_n^z
$$

(2.8)

where $J_{\text{eff}} = 10/9$, $\varepsilon_0 = 50/27$, and $V_m$ are very small, $V_1 = -0.017$, $V_2 = -0.047$, $V_3 = 0.013$, $V_4 = -0.0046$, etc.

Thus, if one neglects the small interaction $V_m$, then in the vicinity of $H_c$ the AKLT chain is effectively described by the XY model, i.e. by noninteracting hardcore bosons.

Again, as in the case of the ladder, one can include the neglected degrees of freedom in the hard-core approximation, arriving at the model of the form (2.2) with $\varepsilon^{(0)}_\mu = \varepsilon_0$ and $t = J_{\text{eff}}/2$.

The connection between the physical spin operators and the bosonic operators for the AKLT chain is more complicated than in case of ladder. The reason for that is the fact that the actions of $S^\mu$ on the AKLT state are most naturally expressed in terms of the states $|\mu, n\rangle$ which are in turn non-locally expressed through the orthogonalized states $|\mu, n\rangle$. For example, the action of a physical spin operator $S^\mu_n$ on the vacuum state $|v\rangle$ (with no bosons) is given by

$$
S^\mu_n |v\rangle = (2c_\mu/3) \left( b^\dagger_{n,\mu} + 4 \sum_{m=1}^{\infty} (-1/3)^m b^\dagger_{n+m,\mu} \right) |v\rangle,
$$

(2.9)

where $c_0 = 1/\sqrt{2}$ and $c_{\pm 1} = \mp 1$.

§3. Dynamical structure factor in the hardcore approximation

Thus, we are led to the problem of calculating the response functions of the hard-core model (2.2). The dynamical structure factor (DSF) $S^{\alpha\alpha}(q, \omega)$ in the spectral representation has the form

$$
S^{\alpha\alpha}(q, \omega) = \frac{1}{Z} \sum_i e^{-E_i/T} |\langle f | S^{\alpha}(q) | i \rangle|^2 \delta(\omega - E_f + E_i), \quad Z = \sum_n e^{-E_n/T},
$$

(3.1)

where $S^{\alpha}(q)$ is the Fourier-transformed total spin operator. The DSF is related to the dynamical susceptibility $\chi(q, \omega)$ through the fluctuation-dissipation theorem,

$$
S^{\alpha\alpha}(q, \omega) = \frac{1}{\pi} \frac{1}{1 - e^{-\omega/T}} \Im \chi^{\alpha\alpha}(q, \omega).
$$

(3.2)

The spin operator is generally a sum of linear and bilinear terms in bosonic operators, which correspond to different physical processes. The ground state at $H > H_c$ contains a “condensate” (Fermi sea) of $b_{+1}$ bosons, and at low temperature the most important excitations are of the particle-hole type. We will thus take into account only those processes which involve states with at most one $b_{0,-1}$ particle:

(A) creation/annihilation of a low-energy $b_{+1}$ boson,
(B) creation/annihilation of one high-energy \((b_{-1} \text{ or } b_0)\) particle, and
(C) transformation of a \(b_{+1}\) particle into \(b_0\) one.

The processes of the type (A) can be considered completely within the model of effective \(S = \frac{1}{2}\) XY chain, in this case there is no need to take into account the high-energy states. For example, for the transversal DSF \(S_{\perp}^x = S_{xx}^x + S_{yy}^y\), for \(q = \pi + k\) close to the antiferromagnetic wave number \(\pi\) one can use the known results\(^{13},26,27\) for the dynamical susceptibility \(\chi_{xx}^x(q, \omega) = \chi_{yy}^y(q, \omega)\) which yields

\[
\chi_{xx}^x(\pi + k, \omega) = A_x(H) \frac{\Gamma^2(3/4)\Gamma^{1/2}}{4(\pi T)^{3/2}} \frac{\Gamma \left( \frac{1}{8} - i \frac{\omega + i k}{4\pi T} \right) \Gamma \left( \frac{1}{8} - i \frac{\omega - i k}{4\pi T} \right)}{\Gamma \left( \frac{7}{8} - i \frac{\omega + i k}{4\pi T} \right) \Gamma \left( \frac{7}{8} - i \frac{\omega - i k}{4\pi T} \right)}. \tag{3.3}
\]

Here \(A_x(H)\) is the non-universal amplitude which is known numerically\(^{12}\), and \(v\) is the Fermi velocity. A similar expression is available for the longitudinal susceptibility\(^{13}\) for the longitudinal DSF of the XY chain in case of zero temperature a closed exact expression is available as well\(^{28}\), and for \(T \neq 0\) the exact longitudinal DSF can be calculated numerically.\(^{29}\) Applying (3.2), one obtains in this way the contribution \(I_A(q, \omega)\) of the (A) processes into the dynamic structure factor. This contribution describes a low-energy “spinon” continuum.

The processes of (B) and (C) type, however, cannot be analyzed in the language of \(S = \frac{1}{2}\) chain and require going back to the hardcore boson problem.

3.1. (B)-type transitions

Let us consider first the zero temperature case to understand the main features.

For the case when not more than one high-energy particle is present, the model (2.2) can be solved exactly.\(^{30}\) One deals essentially with a mobile “impurity” in the hardcore boson system; creation of the impurity leads to the orthogonality catastrophe\(^{31}\) and to the corresponding Fermi-edge type singularity in the response.

In absence of the impurity, the eigenstates have a determinantal form

\[
|\Psi_{k_1\ldots k_N}\rangle = \sum_{x_1 x_2 \ldots x_N} \frac{1}{\sqrt{N!}} \det \{\psi_i(x_j)\}, \tag{3.4}
\]

where \(\psi_i(x) = \frac{1}{\sqrt{L}} e^{i k x}\) are the free plane wave functions, \(N\) is the number of \(b_{+1}\) particles (let us assume it to be even, for definiteness), \(x_j\) denote their positions, and \(L\) is the system length. The absolute value sign above (and throughout the paper) should be understood as a shorthand for having the antisymmetric sign factor attached to the determinant, which ensures symmetry of the wave function under permutations. The allowed values of momenta \(k_i\) are given by

\[
k_i = \pi + (2\pi/L) I_i, \quad i = 1, \ldots, N \tag{3.5}
\]

where the numbers \(I_i\) should be all different and half-integer (integer if \(N\) is odd). The energy of this state is \(E = \sum_{i=1}^{N} (\varepsilon_{+1} + 2t \cos k_i)\), and the total momentum \(P = \sum k_i\) is zero (mod2\(\pi\)) when \(N\) is even. The ground state is defined by the Fermi sea configuration with \(I_i\) running from \(-(N-1)/2\) to \((N-1)/2\), which corresponds to the momenta in the interval \([k_F, 2\pi - k_F]\) with the Fermi momentum defined as

\[
k_F = \pi (1 - N/L) \tag{3.6}
\]
The excited configuration with one “impurity” boson $b_\mu$ having the momentum $\lambda$ can be also represented in the determinantal form

$$
| (\mu, \lambda)_{k'_1 \cdots k'_N} \rangle = \frac{1}{\sqrt{L}} \sum_{x_0} e^{i P' x_0} | x_0 \rangle_{k'_1 \cdots k'_N}, \quad | x_0 \rangle_{k'_1 \cdots k'_N} = \sum_{y_1 \cdots y_N} \frac{1}{\sqrt{N!}} \det \{ \varphi_i(y_j) \}.
$$

(3.7)

Here $x_0$ denotes the coordinate of the impurity, and $y_j = x_j - x_0$ are the coordinates of other particles relative to the impurity. The functions $\varphi_j(y)$ are given by

$$
\varphi_j(y) = A_j \left[ e^{i (k'_j y + \delta_j)} - (\sin \delta_j / \sum_l \sin \delta_l) \sum_l e^{i (k'_l y + \delta_l)} \right],
$$

where the phase shifts $\delta_j$ are in our case of noninteracting hardcore particles independent of $k'_j$ and are all equal to $-\pi/2$, and $A_j$ are the normalization factors. The functions $\varphi_j(y)$ were shown to be in the thermodynamic limit $L \to \infty$ asymptotically equivalent to the free scattering states $\varphi_j(y) \simeq \frac{1}{\sqrt{L}} e^{i (k'_j y + \delta_j)}$. The energy $E'$ and the total momentum $P'$ of the excited state are given by

$$
E = \sum_{j=1}^{N} (\varepsilon_1 + 2t \cos k'_j) + \varepsilon_\mu + 2t \cos \lambda, \quad P' = \sum_{j=1}^{N} k'_j + \lambda.
$$

(3.8)

The allowed wave vectors $k'_j$ and $\lambda$ are given by the same formula (3.5), but since the total number of particles has changed by one, they are different from those of the ground state: if $N$ is even, the numbers $I_j$ in (3.5) are half-integer for the ground state, but integer for the excited state (3.7).

![Fig. 1](image)

(a) The final-state configuration corresponding to (B)-type processes where a new higher-energy boson is added and thus the allowed wave vectors change because the total number of particles is changed by one; (b) schematic view of the “inter-band” transitions of (C) type which do not change the total number of particles.

The matrix element $\langle \mu, \lambda | b_\mu^\dagger(q) | \text{g.s.} \rangle$, $b_\mu^\dagger(q) = L^{-1/2} \sum_n b_n^\dagger e^{i q n}$, which determines the contribution to the response from the (B)-type processes, is nonzero only if the selection rules $\lambda = q$, $P' = P + q$ are satisfied, and is proportional to the determinant of the overlap matrix:

$$
\langle (\mu, \lambda)_{k'_1 \cdots k'_N} | b_\mu^\dagger(q) | \text{g.s.} \rangle = \delta_{\lambda q} \delta_{P' - P + q} M_{fi}, \quad M_{fi} = \det \{ \langle \varphi_i | \psi_j \rangle \}
$$

(3.9)
Due to the orthogonality catastrophe (OC), the overlap determinant is generally algebraically vanishing in the thermodynamic limit, $|M_{fi}|^2 \propto L^{-\beta}$. The response is, however, nonzero and even singular because there is a macroscopic number of “shake-up” configurations with nearly the same energy.

The value of the OC exponent $\beta$ is connected to another exponent $\alpha = 1 - \beta$ which determines the character of the singularity in the response,

$$I^B(q, \omega) = \langle b^\dagger_\mu(-q)b^\dagger_\mu(q) \rangle_\omega \propto 1/(\omega - \omega_\mu(q))^\alpha, \quad (3\cdot10)$$

where $\omega_\mu(q)$ is the minimum energy difference between the ground state and the excited configuration.

For $q = \pi$ the lowest energy excited configuration is symmetric against $k = \pi$ and is given by $\lambda = \pi, k'_j = \pi \pm \pi/2, j$, $j = 1, \ldots, N/2$. If $q$ deviates from $\pi$, $\lambda$ must follow $q$, and in order to satisfy the selection rules one has to create an additional particle-hole pair to compensate the unwanted change of momentum (see Fig. 1a). It is easy to see that for $q$ slightly larger than $\pi$ the lowest energy is achieved when $k_2 = 2\pi - k_F$ and $k_1 = 2\pi - k_F - (q - \pi)$; respectively, for $q$ slightly smaller than $\pi$ one has $k_2 = k_F$ and $k_1 = k_F + (\pi - q)$. As $q$ moves further from $\pi$, this configuration does not necessarily have the lowest energy. Indeed, as we have discussed in Ref.~20, there are also other possible configurations with generally large number of umklapp-type of particle-hole pairs, whose energy may be lower, but their contribution to the response can be neglected because the corresponding OC exponent is larger than 1 for this type of configurations.

Thus, the configuration described above (and its “shake-up” perturbations) will give the main contribution to the response for $k_F < q < 2\pi - k_F$. The energy difference $\omega(q)$ with the ground state configuration which determines the position of singularity in (3·10) is given by

$$\omega_\mu(q) = \varepsilon_\mu + 4t \cos k_F - 2t \cos(k_F + |q - \pi|), \quad q \in [k_F, 2\pi - k_F]. \quad (3\cdot11)$$

For $q$ outside the Fermi sea the symmetric configuration with the hole at $k = \pi$ gives the main contribution,~20 and the corresponding energy difference is

$$\omega_\mu(q) = \varepsilon_\mu + 2t \cos q + 2t(1 + \cos k_F), \quad q \notin [k_F, 2\pi - k_F]. \quad (3\cdot12)$$
The OC exponent $\beta$ is in both cases the same and equal to $1/2$, so that the singularity is of the square-root type.

The quantity $\omega_\mu(q)$, which determines the position of the peak in the response and is normally interpreted as the energy of the corresponding mode with $S^2 = \mu$, has a counter-intuitive dependence on the magnetic field: indeed, since the definition of $k_F$ is $\varepsilon_{+1} + 2t \cos k_F = 0$, it is easy to see that e.g. for $q = \pi$ one has $\omega_\mu(q) = \varepsilon_\mu - \varepsilon_{+1} \propto (1 - \mu)H$ instead of $-\mu H$ as one would expect. The resulting picture of modes which should be seen e.g. in the INS experiment is schematically shown in Fig. 2. This effect may explain the ESR lines with the resonance energy proportional to $2H$, which were observed in the high-field phase of NDMA$_2^{16}$ (such lines would be normally interpreted as “forbidden” transitions with $\Delta S^2 = 2$). In recent INS experiments on the same compound($^{17}$) the change of the slope in the field dependence of the $q = \pi$ gap for the $S^2 = 0$ mode from zero for $H < H_c$ to 1 for $H > H_c$ was observed, which is also consistent with the above picture. One should have in mind, however, that this change of the slope from $-\mu$ to $1 - \mu$ is obtained in the model of noninteracting hardcore bosons, and it will be renormalized by eventually present interactions.

At finite temperatures the edge singularity becomes damped. In the vicinity of the singularity, i.e. for $\omega \to \omega_\mu(q)$, one can deduce qualitatively the behavior of $S^\lambda(q, \omega)$ from the formula derived by Ohtaka and Tanabe($^{32}$) for the edge singularity in the photoemission spectrum in case of the contact core hole potential

$$I^\lambda(q, \omega) = \frac{C(q)(1 - \beta)e^{-\beta\gamma(\beta)}}{4\pi T \Gamma(\beta)} \left( \frac{2\pi T(D + \bar{D})}{DD} \right)^\beta e^{\bar{\omega}/2T} \left| \Gamma \left( \frac{\beta}{2} + i\frac{\bar{\omega}}{2\pi T} \right) \right|^2, \quad (3.13)$$

where $\beta = 1/2$ is the OC exponent, $\bar{\omega} = \omega - \omega_\mu(q)$, $\bar{D} = \varepsilon_{+1} + 2t$ has the sense of the energetic depth of the Fermi sea, $D = \varepsilon_{+1} + 2t$ is the width of the rest of the $b_{+1}$ band, $\gamma(\beta)$ is defined as $\gamma(\beta) = \gamma + \sum_{n=2}^{\infty} \frac{C(2n-1)-1}{n} \beta^{n-1}$, $\gamma$ being the Euler constant and $\zeta(z)$ the Riemann zeta function, and, finally, $C(q)$ is the $q$-dependent factor which takes into account the modification of the overlap determinant $M_{fi}$ in (3.9) due to the presence of “compensating” particle-hole excitations in the final state for $q \in [k_F, 2\pi - k_F]$ (it is identically 1 for $q \notin [k_F, 2\pi - k_F]$):

$$C(q) = F^2(\lambda_1 \lambda_2, \rho_1 \rho_2), \quad F(\lambda_1 \lambda_2, \rho_1 \rho_2) = F(\lambda_1 \rho_1)F(\lambda_2 \rho_2) - F(\lambda_1 \rho_2)F(\lambda_2 \rho_1)$$

$$\lambda_1 = \widetilde{k}_F + \pi - q, \quad \lambda_2 = q, \quad \rho_1 = \widetilde{k}_F, \quad \rho_2 = \pi, \quad (3.14)$$

$$F(\lambda \rho) = \frac{\pi}{L(\lambda - \rho)} \prod_{m=1}^{N[\lambda]} \left( 1 + \frac{1}{2m} \right) \prod_{m=1}^{N[\rho]} \left( 1 - \frac{1}{2m} \right),$$

where $\widetilde{k}_F = k_F$ if $q < \pi$ and $2\pi - k_F$ if $q > \pi$, and $N[x]$ is defined as $N[x] = L[k_F - x]/2\pi$. Here $\lambda$ and $\rho$ denote the discrete momenta of “holes” and “particles”, and for $\rho \to \lambda$ one has $F(\lambda \rho) \to 1$. One can see that for $q \to \pi$, as well as for $q \to k_F$ or $q \to 2\pi - k_F$, the factor $C(q) \to 1$, and it decays very rapidly if $q$ moves away from those points inside the $[k_F, 2\pi - k_F]$ interval.
3.2. Transitions of the (C) type

So far we have been considering the (B)-type transitions. The dynamical structure factor for \( H > H_c \) will also have a contribution from (C)-type transitions corresponding to the transformation of \( b_{+1} \) bosons into \( b_0 \) ones. Those processes do not change the total number of particles and thus do not disturb the allowed values of the wave vector, so that there is no orthogonality catastrophe in this case. The action of the total spin operator \( S^- \) is in this case proportional to that of \( R(q) = \frac{1}{\sqrt{L}} \sum_n b_0^\dagger b_{+1} e^{i q n} \). It is easy to see that the action of \( R(q) \) on a state \((3.4)\) characterized by the set of wave numbers \( \{ k_1, \ldots, k_N \} \)

\[
R(q) |\Psi_{k_1 \cdots k_N} \rangle = \sqrt{\frac{N}{L}} \frac{1}{2\pi} \int \frac{dP}{2\pi} \delta_{P+P+q} \delta_{\lambda,k_{m+q}} |\Psi_{k_1 \cdots k_{m-1} k_{m+1} \cdots k_N} \rangle ,
\]

where \( x_0 \) denotes the position of the created \( b_0 \) particle and the rest of notations is as in \((3.7)\). The corresponding matrix element has a very simple form,

\[
\langle \mu, \lambda | R(q) |\Psi_{k_1 \cdots k_{m-1} k_{m+1} \cdots k_N} \rangle = \frac{1}{\sqrt{L}} \left[ e^{-\omega/T} k_F \right] \int dk \left\{ n[\varepsilon_{+1}(k)] - n[\varepsilon_0(k+q)] \right\} \delta(\omega - \varepsilon_0(k+q) + \varepsilon_{+1}(k)),
\]

and the problem of calculating the response is thus equivalent to that for the 1D Fermi gas, with the only difference that we have to take into account the additional change in energy \( \varepsilon_0 - \varepsilon_{+1} \) which takes place in the transition (see Fig. 1b). One can use the well-known formula for the susceptibility \((33)\) to obtain the contribution

\[
I^C(q, \omega) = \langle R(q) | R(-q) \rangle_{\omega} \]

of (C) type processes into the response:

\[
I^C(q, \omega) = \frac{1}{1 - e^{-\omega/T}} \int \frac{dP}{2\pi^2} \delta_{P+P+q} \delta_{\lambda,k_{m+q}} \left\{ n[\varepsilon_{+1}(k)] - n[\varepsilon_0(k+q)] \right\} \delta(\omega - \varepsilon_0(k+q) + \varepsilon_{+1}(k)),
\]

where \( \varepsilon_\mu(k) = \varepsilon_\mu + 2 t \cos k, \) and \( n(\varepsilon) = (e^{\varepsilon/T} + 1)^{-1} \) is the Fermi distribution function. This contribution contains a square-root singularity, which survives even for finite temperature and is located at

\[
\omega = \varepsilon_0 - \varepsilon_{+1} + 2 t \sqrt{2(1 - \cos q)}. \tag{3.18}
\]

It is interesting to note that though \( I^C(q, \omega) \) generally does not contain any quasiparticle contribution, there is an exception: it transforms into a \( \delta \)-function as \( q \to 0 \).

§4. Summary

The dynamical structure factor \( S(q, \omega) \) of a gapped one-dimensional spin system in the high-field critical phase is studied in the hardcore boson approximation. It is shown that the presence of a “condensate” (Fermi sea) of \( S^z = +1 \) triplets in the ground state in the high-field phase leads to interesting peculiarities in the contributions to \( S(q, \omega) \) from the high-energy excitations (uncondensed triplet components with \( S^z = 0, -1 \)). The energy of high-energy triplets gets renormalized because of the presence of the Fermi sea, which leads to a substantial change in the magnetic...
field dependence of the triplet energies, typically from $-HS^z$ to $H(1-S^z)$. Extending our previous study, we show that such peculiarities in the response persist for any $q$, and can therefore be observed in INS experiments.

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