Correlation Functions in the XXO Heisenberg Chain and their Relations with Spectral Shapes

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Abstract

The spectral shape of one dimensional systems (describing for instance the behaviour of Frenkel excitons) is approached through the exactly solvable model of XXO Heisenberg quantum spin chain in a transverse magnetic field. Some results for finite size chains concerning 2N-point correlators are presented in details. In particular the finite lattice, finite temperature 2-point correlators are explicitely worked out. Moreover, results in closed form are given for 2N-point correlators in the most general situation (finite lattice and thermodynamic limit, finite temperature, finite space and/or time separations). Their relations with frequency moments of the spectral shape are pointed out and the connection with moment expansion through continued fraction representation is given.

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1 Introduction

As far as physical applications are concerned, exactly solvable models are rather few. The development in this area is also rather slow on a time scale usual for condensed matter physics (see, *e.g.*, [1, 2]). However the obtained results can be considered as milestones because they give certainties about the simmetry properties of the models and give insights about approaching general systems using the exact models as the unperturbed ones. Condensed matter physics represents a good training for this activity. As a matter of fact many real systems can be well described by exactly solvable model Hamiltonians and solid state physicists can almost always construct such systems in real life, testing experimentally the theoretical predictions. For instance, this is the case of the Frenkel excitons of one-dimensional systems as studied in Dicke superradiance [3, 4, 5] for coherent emission of two-level atoms or in non-linear lattice vibrations for biopolymers [6, 7] or molecular crystals [8]. By using the well know field-theory approach as developed in Ref. [9] for electron-hole interaction in semiconductors, the relevant features of the afore-mentioned systems can be described by the following one-dimensional Hamiltonian [10, 11]:

$$H_e = \sum_{m=1}^{M} \left[\omega_0 \sigma_z^{(m)} - J \sigma_x^{(m)} \sigma_x^{(m+1)} - J \sigma_y^{(m)} \sigma_y^{(m+1)} 2 - J_z \sigma_z^{(m)} \sigma_z^{(m+1)} \right] \qquad (1)$$

Here ω_0 is the excitation energy of the individual molecule (or atom), J is the interaction which causes the propagation of Frenkel excitons. The last term $\sim J_z$ takes into account the interaction between excitations. Since $\sigma_i^{(m)}$ are Pauli matrices satisfying

$$\left[\sigma_p^{(m)}, \sigma_q^{(n)} \right] = 2i \delta_{mn} \epsilon_{pqr} \sigma_r^{(m)} , \qquad p, q, s = x, y, z \; ; \qquad (2)$$

it is easily recognized that we are involved with the so called XXZ model of spin $\frac{1}{2}$ in a constant external field $h = \omega_0$. The first term in eq. (1) can be considered as a c-number when the number of excitons is very large [11], leading to the XXZ model with no external field. This model also represents some interesting one-dimensional antiferromagnets which have been recently probed by neutron scattering experiments [12]. Instead, when the exciton interaction can be neglected [9], the emission spectra can be calculated from the temperature and time dependent correlation functions of the

XXO Heisenberg chain in a transverse field. This possibility was devised in Ref. [11], using our previous results [13, 14]. However, some results for finite size chains, presented in detail in [14] were not referred properly. It should be pointed out that all results could be obtained from our previous calculations of matrix elements for XXO Heisenberg chain[14]. In this paper we present explicit calculations of the relevant correlation functions related to the emission spectra, giving also the explicit expressions for $2N$-point correlators in closed form; in particular, a recipe is given for calculating the first moments, in order to evaluate eventually the spectral shape by a continued fraction expansion.

2 The XXO Heisenberg Chain

The Hamiltonian of the XXO Heisenberg chain, which is an isotropic case of the Lieb, Schultz and Mattis XY model [15], describing the nearest neighbour interaction of spins $\frac{1}{2}$ situated at the sites of the one-dimensional periodical lattice in a constant transverse magnetic field h, is

$$H(h) = -\sum_{m=1}^{M} \left[\sigma_x^{(m)}\sigma_x^{(m+1)} + \sigma_y^{(m)}\sigma_y^{(m+1)} + h\sigma_z^{(m)}\right] + Mh \tag{3}$$

(the constant is chosen so that $H \mid 0\rangle = 0$, where $\mid 0\rangle \equiv \otimes_{m=1}^{M} |\uparrow\rangle_m$, $\langle 0 \mid 0\rangle = 1$ is the ferromagnetic state (all spins up)). The total number M of sites is supposed to be even.

Eigenvectors $\mid \Psi_N(\{p\})\rangle$, $\{p\} \equiv \{p_1, ..., p_N\}$ of the Hamiltonian are well known and can be regarded as the states containing N ($N = 0, 1, ..., M$) quasiparticles with quasimomenta p_a and energies $\varepsilon(p_a)$

$$\varepsilon(p) = -4\cos p + 2h \, , \tag{4}$$

over the state $\mid 0\rangle$ (corresponding to $N = 0$):

$$H \mid \Psi_N(\{p\})\rangle = (\sum_{a=1}^{N} \varepsilon(p_a)) \mid \Psi_N(\{p\})\rangle \, . \tag{5}$$

The quasimomenta $-\pi < 0 \leq \pi$ parametrizing quasiparticles are all different and "quantized" due to periodical boundary condition, $e^{iMp_a} =$

$(-1)^{N+1}$, so that the permitted values are given as

$$p_a = \frac{2\pi}{M} n_a \ , \qquad \begin{array}{llll} n_a = -\frac{M}{2} + j \ , & j = 1, 2, ..., M & \text{for } N \text{ odd,} \\ n_a = -\frac{M+1}{2} + j \ , & j = 1, 2, ..., M & \text{for } N \text{ even,} \end{array} \tag{6}$$

and are different for N even or odd.

The explicit form of these eigenvectors is (as usual, $\sigma_{\pm}^{(m)} \equiv \frac{1}{2}[\sigma_x^{(m)} \pm i\sigma_y^{(m)}]$)

$$\mid \Psi_N(\{p\})\rangle = \frac{1}{\sqrt{M^N N!}} \sum_{m_1,...,m_N}^{M} \chi_N(\{m\} \mid \{p\})\, \sigma_-^{(m_1)} ... \sigma_-^{(m_N)} \mid 0\rangle \ , \tag{7}$$

where the eigenfunction χ_N is proportional to the "Slater determinant",

$$\chi_N(\{m\} \mid \{p\}) = \frac{1}{\sqrt{N!}} \left[\prod_{1\le a<b\le N} \epsilon(m_b - m_a) \right] \cdot \sum_Q (-1)^{[Q]} \exp\left[i \sum_{a=1}^{N} m_a p_{Q_a} \right] \ , \tag{8}$$

$\epsilon(m)$ being the sign-function, defined as

$$\epsilon(m) = 1, \ \ m > 0; \qquad \epsilon(m) = 0, \ \ m = 0; \qquad \epsilon(m) = -1, \ \ m < 0. \tag{9}$$

All the quasimomenta entering a given $\mid \Psi_N\rangle$ should be different, otherwise the eigenfunction vanishes identically.

There are 2^M different eigenstates, and to avoid the multiple counting of states due to the antisymmetry of the state vector under permutation of p's, we suppose that $p_a < p_b$, if $a < b$. The eigenstates are orthogonal for different sets of quasimomenta, and the normalization is

$$\langle \Psi_N(\{p\}) \mid \Psi_N(\{p\})\rangle = 1 \ . \tag{10}$$

3 Temperature dependent correlation functions on the finite lattice

We consider, following reference [13, 14], the temperature correlation functions on the finite lattice. These are, *e.g.*

(i) the generating function of σ_z-σ_z correlators,

$$g_0^{(M)}(\alpha, m, h, T) \equiv \langle \exp[\alpha Q(m)]\rangle_T^{(M)} \ , \tag{11}$$

where $Q(m) \equiv \frac{1}{2}\sum_{n=1}^{m}(1+\sigma_z^{(n)})$ is the operator of the number of quasiparticles in the first m sites of the lattice;

(ii) the temperature and time dependent correlators

$$g_+^{(M)}(m,t,T) \equiv \langle \sigma_+^{(n_2)}(t_2)\sigma_-^{(n_1)}(t_1)\rangle_T^{(M)}\ , \qquad (12)$$

$$g_-^{(M)}(m,t,T) \equiv \langle \sigma_-^{(n_2)}(t_2)\sigma_+^{(n_1)}(t_1)\rangle_T^{(M)}\ , \qquad (13)$$

where $m \equiv n_2 - n_1$; $t \equiv t_2 - t_1$ (due to the obvious symmetries, it is sufficient to consider the case $m \geq 0$, $t \geq 0$, $h \geq 0$). The Heisenberg operators are defined as $\sigma_\pm^{(m)}(t) = \exp[iHt]\sigma_\pm^{(m)}\exp[-iHt]$.

The temperature mean value of a given operator $\mathcal{O}$ is defined as usual,

$$\langle \mathcal{O}\rangle = \frac{1}{Z}\mathrm{Tr}\left[e^{-\beta H}\mathcal{O}\right] = \frac{1}{Z}\sum_{N=0}^{M}\sum_{p_1<\ldots<p_N} e^{-\beta\sum_{a=1}^{N}\varepsilon(p_a)}\langle \Psi_N(\{p\}) \mid \mathcal{O} \mid \Psi_N(\{p\})\rangle\ , \qquad (14)$$

where

$$Z \equiv \mathrm{Tr}\left[e^{-\beta H}\right] = 1 + \sum_{N=1}^{M}\sum_{p_1<\ldots<p_N} e^{-\beta\sum_{a=1}^{N}\varepsilon(p_a)} \qquad (15)$$

is the partition function and $\beta \equiv \frac{1}{T}$ is the inverse temperature.

All the diagonal matrix elements entering the sums (14) for correlators (11)-(13) were calculated explicitly in paper [14]; the answer were given there as determinants of $N \times N$ matrices. Non-diagonal matrix elements can be calculated in exactly the same way. In the thermodynamic limit, the correlators turned out to be the Fredholm determinants [13, 14]. In papers [16, 17] these Fredholm determinant representations were used to derive integrable differential equations for correlators and construct explicitly the large time and distance asymptotics.

Here we give the representations for the temperature correlators also on the finite lattice, as determinants of $M \times M$ matrices. These representations are the immediate and straightforward consequences of the expressions for the diagonal matrix elements on the finite lattice obtained in paper [14]. It should be mentioned that the expressions for these matrix elements were used also in paper [11] to investigate correlator (13) (though paper [14] was not cited). The answer for this correlator given there does not however coincide with the one given below.

As was mentioned, the derivation of representation on the finite lattice is quite simple ($cfr.$ [11]) after the matrix elements are computed [14], and can be explained on the example of the partition function (15). If the M possible values of the quasimomenta had been the same for N even and odd, the right hand side of (15) would have been equal to $\det_{_M}(I_{_M} + A)$, where $I_{_M}$ is the $M \times M$ unit matrix and A is the diagonal $M \times M$ matrix with matrix elements

$$A_{ab} = \delta_{ab} \exp[-\beta\varepsilon(p_a)] \; ; \qquad a, b = 1...., M. \tag{16}$$

It is easy to take into account the difference in the permitted values for N even and odd, just representing

$$Z = \frac{1}{2}(Z_1 + Z_2) + \frac{1}{2}(Z_3 - Z_4) \tag{17}$$

with

$$Z_{1,2} = \det{}_M(I_M \pm A); \qquad\qquad Z_{3,4} = \det{}_M(I_M \pm \bar{A}) \tag{18}$$

and (6) should be taken into account in definition of matrices A and $\bar{A}$:

$$A_{ab} = \delta_{ab} \exp[-\beta\varepsilon(p_a)], \qquad p_a = \frac{2\pi}{M}(-\frac{M+1}{2} + a); \qquad a, b = 1, ..., M; \tag{19}$$

$$\bar{A}_{ab} = \delta_{ab} \exp[-\beta\varepsilon(p_a)], \qquad p_a = \frac{2\pi}{M}(-\frac{M}{2} + a); \qquad a, b = 1, ..., M. \tag{20}$$

The first term in the right hand side of (17) gives thus the contribution of the states with even N, and the second term corresponds to odd N. It is easily seen that quantities Z_i can be represented as

$$Z_1 = \det{}_{_M}[A\Theta_F^{-1}] \; , \qquad Z_2 = \det{}_{_M}[A\Theta_B^{-1}] \; , \qquad Z_3 = \det{}_{_M}[\bar{A}\bar{\Theta}_F^{-1}] \; , \qquad Z_4 = \det{}_{_M}[\bar{A}\bar{\Theta}_B^{-1}] \; , \tag{21}$$

where $M \times M$ diagonal matrices $\Theta_F = (I + A)^{-1}A$ and $\Theta_B = (I - A)^{-1}A$ are introduced,

$$(\Theta_F)_{ab} = \vartheta_F(p_a) \, \delta_{ab} \; ; \qquad (\Theta_B)_{ab} = \vartheta_B(p_a) \, \delta_{ab} \; , \tag{22}$$

and "Fermi" and "Bose" weights $\vartheta_{F,B}$ are

$$\vartheta_{F,B}(p) = \frac{1}{\exp[\beta\varepsilon(p_a)] \pm 1} \; . \tag{23}$$

The difference between Θ and $\bar{\Theta}$ is just as the one between A and $\bar{A}$. All the mean values entering representation (14) for the correlators were obtained in

[14] under the form $\langle\mathcal{O}\rangle_N \sim \det_{_N}[\mathcal{M}_N]$, where the $N \times N$ matrix $\mathcal{M}_N$ (in general case nondiagonal) possesses matrix elements

$$(\mathcal{M}_N)_{ij} = \mathcal{M}(p_i, p_j)\ ; \qquad i, j = 1, ..., N; \tag{24}$$

one can then build trivially from it the two $M \times M$ matrices $\mathcal{M}$ and $\bar{\mathcal{M}}$. It is then obvious from (14) that

$$\begin{aligned}\langle\mathcal{O}\rangle_{_T}^{(M)} &= \frac{1}{Z}\left[\frac{1}{2}(\mathrm{det}_M[I+A\mathcal{M}]+\mathrm{det}_M[I-A\mathcal{M}])+\frac{1}{2}(\mathrm{det}_M[I+\bar{A}\bar{\mathcal{M}}]-\mathrm{det}_M[I-\bar{A}\bar{\mathcal{M}}])\right] = \\ &= \frac{1}{2Z}(Z_1\mathrm{det}_M[I+\Theta_F(\mathcal{M}-I)]+Z_2\mathrm{det}_M[I-\Theta_B(\mathcal{M}-I)]+ \\ &\qquad +Z_3\mathrm{det}_M[I+\bar{\Theta}_F(\bar{\mathcal{M}}-I)]-Z_4\mathrm{det}_M[I-\bar{\Theta}_B(\bar{\mathcal{M}}-I)])\ .\end{aligned} \tag{25}$$

Taking the expression for the corresponding matrices $\mathcal{M}$ from paper [14], one obtains the temperature correlators on the finite lattice. For $g_0^{(M)}(\alpha, m, h, T)$ (see (11)),

$$\begin{aligned}\langle\exp[\alpha Q(m)]\rangle_{_N} &= \det_{_N}[\mathcal{M}(m)]\ ; \\ [\mathcal{M}(m)]_{i,j} &= \delta_{ij}(1+\gamma\frac{m}{M})+(1-\delta_{ij})\frac{\gamma}{M}\frac{\sin\frac{m}{2}(p_i-p_j)}{\sin\frac{1}{2}(p_i-p_j)}\ ,\end{aligned} \tag{26}$$

(here $\gamma \equiv e^\alpha - 1$), and one gets

$$\begin{aligned}g_0^{(M)}(\alpha, m, h, T) &= \frac{1}{2Z}\,(Z_1\mathrm{det}_M[I+\Theta_F N]+Z_2\mathrm{det}_M[I-\Theta_B N]+ \\ &\qquad +Z_3\mathrm{det}_M[I+\bar{\Theta}_F\bar{N}]-Z_4\mathrm{det}_M[I-\bar{\Theta}_B\bar{N}])\ ,\end{aligned} \tag{27}$$

where N is the $M \times M$ matrix defined as

$$N_{ab} = \delta_{ab}\frac{\gamma m}{M} + (1-\delta_{ab})\frac{\gamma}{M}\frac{\sin\frac{m}{2}(p_a-p_b)}{\sin\frac{1}{2}(p_a-p_b)} \tag{28}$$

For the time dependent correlators (12),(13), applying the same procedure, one gets

$$\begin{aligned}g_+^{(M)}(m,t,T) = e^{-2iht}\frac{1}{Z}\Big[\Big(g(m,t)+\frac{\partial}{\partial x}\Big) &\cdot \Big(Z_1\mathrm{det}_{_M}[I+\Theta_F S-x\Theta_F R^{(+)}]+ \\ &\qquad +Z_2\mathrm{det}_{_M}[I-\Theta_B S+x\Theta_B R^{(+)}]\Big) \\ +\Big(\bar{g}(m,t)+\frac{\partial}{\partial x}\Big) &\cdot \Big(Z_3\mathrm{det}_{_M}[I+\bar{\Theta}_F\bar{S}-x\bar{\Theta}_F\bar{R}^{(+)}]- \\ &\qquad -Z_4\mathrm{det}_{_M}[I-\bar{\Theta}_B\bar{S}+x\bar{\Theta}_B\bar{R}^{(+)}]\Big)\Big]\Big|_{x=0}\end{aligned} \tag{29}$$

and

$$g_{-}^{(M)}(m,t,T) = e^{2iht}\frac{1}{Z} \qquad \frac{\partial}{\partial x}\Bigg[Z_1 \mathrm{det}_{_M}[I+\Theta_F S + x\Theta_F R^{(-)}] + Z_2 \mathrm{det}_{_M}[I-\Theta_B S - x\Theta_B R^{(-)}] +$$
$$+Z_3 \mathrm{det}_{_M}[I+\bar{\Theta}_F \bar{S} + x\bar{\Theta}_F \bar{R}^{(-)}] - Z_4 \mathrm{det}_{_M}[I-\bar{\Theta}_B \bar{S} - x\bar{\Theta}_B \bar{R}^{(-)}]\Bigg]_{x=} ($$

Here matrix elements of $M\times M$ matrices $S = S(m,t)$, $R^{(+)} = R^{(+)}(m,t)$ and $R^{(-)} = R^{(-)}(m,t)$ are

$$\begin{aligned}
S_{ab} &= \delta_{ab}\left[d(m,t,p_a)\exp\left[-imp_a - 4it\cos p_a\right] - 1\right] + \\
&\quad + (1-\delta_{ab})\,\frac{e_+(m,t,p_a)e_-(m,t,p_b) - e_-(m,t,p_a)e_+(m,t,p_b)}{M\tan\frac{1}{2}(p_a - p_b)} - \\
&\quad - \frac{1}{M}g(m,t)e_-(m,t,p_a)e_-(m,t,p_b)\,; \\
R^{(+)}_{ab} &= \frac{1}{M}e_+(m,t,p_a)e_+(m,t,p_b)\,; \\
R^{(-)}_{ab} &= \frac{1}{M}e_-(m,t,p_a)e_-(m,t,p_b)\,. \qquad (31)
\end{aligned}$$

Functions $e_{\pm}$ are defined as

$$\begin{aligned}
e_-(m,t,p_a) &\equiv \exp\left[-\frac{im}{2}p_a - 2it\cos p_a\right]\,, \\
e_+(m,t,p_a) &\equiv e_-(m,t,p_a)e(m,t,p_a)\,, \qquad (32)
\end{aligned}$$

and functions g, e, d are given as the sums:

$$g(m,t) \equiv \frac{1}{M}\sum_q \exp\left[imq + 4it\cos q\right]\,, \qquad (33)$$

$$e(m,t,p_a) \equiv \frac{1}{M}\sum_q \frac{\exp\left[imq + 4it\cos q\right]}{\tan\frac{1}{2}(q-p_a)}\,, \qquad (34)$$

$$d(m,t,p_a) \equiv \frac{1}{M^2}\sum_q \frac{\exp\left[imq + 4it\cos q\right]}{\sin^2\frac{1}{2}(q-p_a)}\,, \qquad (35)$$

where $p_a = \frac{2\pi}{M}(-\frac{M+1}{2} + a)$, $a = 1,...,M$ ("even sector", see (6)). The sums over q's in the definition of functions g, e, d, are taken over all "odd" q's.

Matrix elements of $M\times M$ matrices $\bar{S} = \bar{S}(m,t)$, $\bar{R}^{(+)} = \bar{R}^{(+)}(m,t)$ and $\bar{R}^{(-)} = \bar{R}^{(-)}(m,t)$ have analogous expression in terms of $\bar{g}$, $\bar{e}$, $\bar{d}$, with

$p_a = \frac{2\pi}{M}(-\frac{M}{2} + a)$, $a = 1, ..., M$ ("odd sector", see (6)). Now the sums over q's in the definition of functions $\bar{g}$, $\bar{e}$, $\bar{d}$ are taken over all "even" q's.

The thermodynamic limit of all the previous formulas is quite obvious as soon as we recognize that for a given operator $\mathcal{O}$ (see eq. (25)), when we send M to ∞, the distinction between the two sets of possible quasimomenta ("even" and "odd") disappears, and $Z_3 \longrightarrow Z_1$, $Z_4 \longrightarrow Z_2$ and $\bar{\mathcal{M}} \longrightarrow \mathcal{M}$; in this limit only one determinant survives, which is just the Fredholm determinant of the corresponding linear operator. This is, of course, in complete correspondence with the general theorem for the Bethe Ansatz solvable models [18, 19]. It was, in fact, how the Fredholm determinant representations in [13, 14] were obtained.

4 $2\bar{N}$-point Correlation Functions

We want now to present some new results for $2\bar{N}$-point correlators of operators σ_+, σ_-.

As shown in [14], correlators can be expressed (on the finite lattice and at zero temperature) as determinants of some matrices. In this case correlators are nothing else but diagonal elements of the corresponding operators. But it is easy to repeat the steps performed in [14] to compute non diagonal elements of the previous operators, similarly to the case of the impenetrable bosons [2, 20]. This in turn allows to compute multi-point correlation functions of the kind:

$$\langle \sigma_+(n_{2\bar{N}}, t_{2\bar{N}})\sigma_-(n_{2\bar{N}-1}, t_{2\bar{N}-1})...\sigma_+(n_2, t_2)\sigma_-(n_1, t_1)\rangle_N \tag{36}$$

as

$$\exp[-2ih\sum_{\alpha=1}^{\bar{N}}(t_{2\alpha} - t_{2\alpha-1})] \cdot \prod_{\alpha=1}^{\bar{N}}[g(n_{2\alpha} - n_{2\alpha-1}, t_{2\alpha} - t_{2\alpha-1}) + \frac{\partial}{\partial z_\alpha}] \cdot \det{}_N[K]_{z_\alpha=0} \tag{37}$$

with

$$K_{ab} = K(p_a, p_b) = \sum_{q_{\bar{N}-1}} ... \sum_{q_1} \left[\prod_{\alpha=1}^{\bar{N}} \tilde{K}_\alpha(q_\alpha, q_{\alpha-1})\right], \tag{38}$$

where $q_0 = p_a$, $q_{\bar{N}} = p_b$ and

$$\tilde{K}_\alpha(q_\alpha, q_{\alpha-1}) \quad = \quad \exp[-4it_{2\alpha}\cos q_\alpha - in_{2\alpha}q_\alpha + 4it_{2\alpha-1}\cos q_{\alpha-1} + in_{2\alpha-1}q_{\alpha-1}] \cdot$$

$$\cdot\{\delta_{q_\alpha,q_{\alpha-1}}[d(m_\alpha,\tau_\alpha,q_\alpha)-\frac{1}{M}g(m_\alpha,\tau_\alpha)]+$$
$$+(1-\delta_{q_\alpha,q_{\alpha-1}})[\frac{1}{M}\frac{e(m_\alpha,\tau_\alpha,q_\alpha)-e(m_\alpha,\tau_\alpha,q_{\alpha-1})}{\tan\frac{1}{2}(q_\alpha-q_{\alpha-1})}-\frac{1}{M}g(m_\alpha,\tau_\alpha)]-$$
$$-\frac{z_\alpha}{M}e(m_\alpha,\tau_\alpha,q_\alpha)e(m_\alpha,\tau_\alpha,q_{\alpha-1})\} \qquad (39)$$

with $m_\alpha \equiv n_{2\alpha}-n_{2\alpha_1}$, $\tau_\alpha \equiv t_{2\alpha}-t_{2\alpha-1}$.

Going to the case of finite temperature, the previous formula generalizes in an obvious way to the following

$$\langle\sigma_+(n_{2\bar{N}},t_{2\bar{N}})\sigma_-(n_{2\bar{N}-1},t_{2\bar{N}-1})...\sigma_+(n_2,t_2)\sigma_-(n_1,t_1)\rangle_T^{(M)}= \qquad (40)$$
$$=e^{-2ih\sum_{\alpha=1}^{\bar{N}}\tau_\alpha}\{\prod_{\alpha=1}^{\bar{N}}[g(m_\alpha,\tau_\alpha)+\frac{\partial}{\partial z_\alpha}]\cdot\Big(\frac{Z_1}{Z}\det{}_M[I+\Theta_F K']+\frac{Z_2}{Z}\det{}_M[I-\Theta_B K']\Big)+$$
$$+\prod_{\alpha=1}^{\bar{N}}[\bar{g}(m_\alpha,\tau_\alpha)+\frac{\partial}{\partial z_\alpha}]\cdot\Big(\frac{Z_3}{Z}\det{}_M[I+\bar{\Theta}_F\bar{K}']-\frac{Z_4}{Z}\det{}_M[I-\bar{\Theta}_B\bar{K}']\Big)\}_{z_\alpha=0}$$

where $K'_{p_ap_b}{=}K_{p_ap_b}-\delta_{p_a,p_b}$, $\bar{K}'_{p_ap_b}{=}\bar{K}_{p_ap_b}-\delta_{p_a,p_b}$, are $M\times M$ matrices and $K_{p_ap_b}$ has been defined in equations (38),(39). The difference between barred and unbarred matrices is in the sector ("even" or "odd") to which belong the quasimomenta p_a, p_b, as specified in (19-20).

The thermodynamic limit is performed in straightforward way (see comment at the end of section 2). At zero temperature we obtain

$$\langle\sigma_+(n_{2\bar{N}},t_{2\bar{N}})\sigma_-(n_{2\bar{N}-1},t_{2\bar{N}-1})...\sigma_+(n_2,t_2)\sigma_-(n_1,t_1)\rangle=$$
$$=e^{-2ih\sum_{\alpha=1}^{\bar{N}}\tau_\alpha}\prod_{\alpha=1}^{\bar{N}}[G(m_\alpha,\tau_\alpha)+\frac{\partial}{\partial z_\alpha}]\cdot\det[W]_{z_\alpha=0}\,. \qquad (41)$$

Here now $\det[W]$ is the Fredholm determinant of linear integral operator W acting on functions $f(q)$ on interval $[-k_F,k_F]$ according to the rule:

$$(Wf)(p)=\frac{1}{2\pi}\int_{-k_F}^{k_F}dq\,W(p,q)f(q) \qquad (42)$$

with kernel $W(p,q)$ given as

$$W(p,q)=\int_{-\pi}^{\pi}\frac{dq_{\bar{N}-1}}{2\pi}...\int_{-\pi}^{\pi}\frac{dq_1}{2\pi}\left(\prod_{\alpha=1}^{\bar{N}}[\delta(q_\alpha-q_{\alpha-1})+\tilde{W}_\alpha(q_\alpha,q_{\alpha-1})]\right)\,,\qquad q_0\equiv q\,,\ q_{\bar{N}}\equiv p\,, \qquad (43)$$

and

$$\tilde{W}_\alpha(q_\alpha, q_{\alpha-1}) = \exp[-4it_{2\alpha}\cos q_\alpha - in_{2\alpha}q_\alpha + 4it_{2\alpha-1}\cos q_{\alpha-1} + in_{2\alpha-1}q_{\alpha-1}] \cdot$$
$$\cdot \left\{ \frac{E(m_\alpha, \tau_\alpha, q_\alpha) - E(m_\alpha, \tau_\alpha, q_{\alpha-1})}{\tan\frac{1}{2}(q_\alpha - q_{\alpha-1})} - G(m_\alpha, \tau_\alpha) - z_\alpha E(m_\alpha, \tau_\alpha, q_\alpha) E(m_\alpha, \tau_\alpha, q_{\alpha-1}) \right\} \quad (44)$$

At finite temperature, in the thermodynamic limit, we get instead:

$$\langle \sigma_+(n_{2\bar{N}}, t_{2\bar{N}}) \sigma_-(n_{2\bar{N}-1}, t_{2\bar{N}-1}) ... \sigma_+(n_2, t_2) \sigma_-(n_1, t_1) \rangle_T =$$
$$= e^{-2ih\sum_{\alpha=1}^{\bar{N}} \tau_\alpha} \prod_{\alpha=1}^{\bar{N}} [G(m_\alpha, \tau_\alpha) + \frac{\partial}{\partial z_\alpha}] \cdot \det[W_T]_{z_\alpha=0} \, . \quad (45)$$

Here now $\det[W_T]$ is the Fredholm determinant of linear integral operator W_T acting on functions $f(q)$ on interval $[-\pi, \pi]$ according to the rule:

$$(W_T f)(p) = \frac{1}{2\pi} \int_{-\pi}^{\pi} dq \, W_T(p, q) f(q) \quad (46)$$

with kernel $W(p, q)$ given as

$$W_T(p, q) = \delta(p - q) + \vartheta(p)[W(p, q) - \delta(p - q)] \quad (47)$$

In previous formulae functions $G(m, t)$ and $E(m, t, q)$ are the thermodynamic limit version of corresponding functions $g(m, t)$, $e(m, t, q)$ defined in (33-34):

$$G(m, t) = \frac{1}{2\pi} \int_{-\pi}^{\pi} dp \, \exp[imp + 4it\cos p] \; ; \quad (48)$$
$$E(m, t, q) = \frac{1}{2\pi} \mathcal{P} \int_{-\pi}^{\pi} dp \, \frac{\exp[imp + 4it\cos p]}{\tan\frac{1}{2}(p - q)} \, . \quad (49)$$

Going to the unit circle in the complex plane through the mapping

$$p \to \mu = e^{ip} \quad (50)$$

it is possible to express the kernel of integral operator $\tilde{W}$ in the form

$$\frac{1}{\mu - \lambda} \sum_j^2 f_j(\mu) \tilde{f}_j(\lambda) \, . \quad (51)$$

Integral operators with kernels like (51) form an infinite dimensional group [21]. This makes it possible to perform explicitly the operator product in (43) representing the kernel of integral operators $W^{(2\bar{N})}$ as

$$W^{(2\bar{N})}(\mu, \lambda) = \delta(\mu - \lambda) + \frac{1}{\mu - \lambda} \sum_j^{2\bar{N}} f_j(\mu) \tilde{f}_j(\lambda) \, . \quad (52)$$

5 Second moment of correlator $g_+(m,t)$ at finite T and h

The spectral density of emission intensity in the case of Frenkel excitons system is given by

$$I_{em}(\omega) = \frac{1}{2\pi}\sum_{i,j}\int_{-\infty}^{+\infty} dt e^{-i\omega t}\langle\sigma_+(i,0)\sigma_-(j,t)\rangle \ . \tag{53}$$

Defining as usual the Kubo relaxation function [22] as

$$R_A(t) \equiv \int_0^\beta d\lambda\langle A^+(0)A(t+i\lambda)\rangle \ , \qquad A(t) = \sum_i \sigma_-(i,t) \ , \tag{54}$$

with its Fourier transform given by

$$\tilde{R}_A(\omega) = \frac{1-e^{\beta\omega}}{\omega} I_{em}(\omega) \ , \tag{55}$$

and the normalized Kubo function

$$\Xi_0(\omega) \equiv \frac{\tilde{R}_A(\omega)}{R_A(t=0)} \ , \tag{56}$$

the n^{th}-moment $\langle\omega^n\rangle$ is given by:

$$\langle\omega^n\rangle \equiv \int_{-\infty}^{\infty} d\omega \ \omega^n \Xi_0(\omega) \tag{57}$$

and can be worked out explicitely as

$$\langle\omega^n\rangle = \frac{(-1)^n}{R_A(t=0)} \cdot \langle[[...[[A,H],H]...,H],A^+]\rangle \qquad \text{(n commutators)} \ , \tag{58}$$

where the odd moments vanish because of the even character of $R(t)$ and $\Xi_0(t)$.

The relevance of the moments is due to the fact they are experimentally accessible. Moreover the calculation of $\Xi_0(t)$ and consequently $I(\omega)$ can be performed starting from the short time expansion of $\Xi_0(t)$

$$\Xi_0(t) = 1 - \frac{1}{2}\langle\omega^2\rangle t^2 + \frac{1}{4!}\langle\omega^4\rangle t^4 + ... \tag{59}$$

or better by the continued fraction expansion of its Laplace transform [23, 24, 25]:

$$\Xi_0(z) = \frac{1}{z + \frac{\delta_1}{z + \frac{\delta_2}{\cdots}}} \tag{60}$$

where the δ_n's are related to the frequency moments, *i.e.*

$$\delta_1 = \frac{\langle\omega^2\rangle}{\langle\omega^0\rangle}, \qquad \delta_2 = \frac{\langle\omega^4\rangle}{\langle\omega^2\rangle} - \frac{\langle\omega^2\rangle}{\langle\omega^0\rangle} . \tag{61}$$

In our case we obtain for the second moment of the spectral density of emission intensity

$$\begin{aligned}\langle\omega^2\rangle = \frac{1}{R_A(t=0)} \quad \cdot \quad & [4\langle\sigma_+(m)\sigma_-(m+1)\rangle_T + 4\langle\sigma_-(m)\sigma_+(m+1)\rangle_T + \\ & +2h\langle\sigma_z(m)\rangle_T - 4\langle\sigma_z(m)\sigma_z(m+1)\rangle_T] \ .\end{aligned} \tag{62}$$

The previous expression can be given a very explicit form. Since it involves only first neighbour correlators, the latter are essentially determinant of operators of the form "Identity + 1-dimensional projector" and can be easily reduced to traces. Let us work out in detail $\langle\sigma_+(m)\sigma_-(m+1)\rangle$; using relation(6.23) of Ref. [14], we immediately get (on the finite lattice at zero temperature):

$$\begin{aligned}\langle\sigma_+(m)\sigma_-(m+1)\rangle_N &= \frac{\partial}{\partial z}\mathrm{det}_N[\tilde{s} + zr^+]_{z=0} \\ &= \frac{\partial}{\partial z}\mathrm{det}_N[\delta_{ab} + zf_af_b]_{z=0} \qquad (\text{with } f_a = \frac{1}{\sqrt{M}}e^{-\frac{i}{2}p_a}) \\ &= \mathrm{Tr}[f_af_b] \\ &= \frac{1}{M}\sum_{a=1}^{N} e^{-ip_a}\end{aligned} \tag{63}$$

and in the thermodynamic limit at finite T

$$\langle\sigma_+(m)\sigma_-(m+1)\rangle_T = \langle\sigma_-(m)\sigma_+(m+1)\rangle_T = \frac{1}{2\pi}\int_{-\pi}^{\pi} dq\, \vartheta(q)\cos q\ . \tag{64}$$

Analogously,

$$\langle\sigma_z(m)\sigma_z(m+1)\rangle_T = (\langle\sigma_z\rangle_T)^2 - 4\,|\langle\sigma_+(m)\sigma_-(m+1)\rangle_T|^2\ , \tag{65}$$

$$\langle\sigma_z\rangle_T = 1 - \frac{1}{\pi}\int_{-\pi}^{\pi} dq\, \vartheta(q)\ . \tag{66}$$

Higher moments can be calculated in the same way.

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