DYNAMIC PROPERTIES OF SPIN–$\frac{1}{2}$ XY CHAINS

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We have considered a numerical scheme for the calculation of the equilibrium properties of spin–$\frac{1}{2}$ XY chains. Within its frames it is necessary to solve in the last resort only the $2N\times 2N$ eigenvalue and eigenvector problem but not the $2^N\times 2^N$ one as for an arbitrary system consisting of N spins $\frac{1}{2}$. To illustrate the approach we have presented some new results. Namely, the xx dynamic structure factor for the Ising model in transverse field, the density of states for the isotropic chain with random intersite couplings and transverse fields that linearly depend on the surrounding couplings, and the zz dynamic structure factor for the Ising model in the random transverse field. The results obtained are hoped to be useful for an interpretation of observable data for one–dimensional spin–$\frac{1}{2}$ XY substances.

Key words: one–dimensional systems, quantum spin chains, XY models, Ising model in transverse field, random systems, computer simulations, density of states, thermodynamics, magnetization, spin correlations, dynamic structure factor.

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Statistical mechanics of the one–dimensional spin–$\frac{1}{2}$ XY models has a history going back more than three decades to the pioneering paper by Lieb, Schultz and Mattis [1] in which it was noted that such systems are as a matter of fact the non–interacting spinless fermions and therefore, a lot of statistical mechanics calculations can be performed exactly. Although many papers concerning thermodynamics, spin correlations and their dynamics have appeared since that time, several problems still call for efforts. One of them regards the study of spin dynamics: in contrast to the time–dependent correlation function between z–components of two spins [2], the xx time–dependent correlation function has been derived exactly only in some limiting cases ($T=0$, the critical value of transverse field, $T=\infty$) [3–9]. Some recent attempts to calculate this correlation function are presented in Refs. [10–14]. New difficulties arose when the one–dimensional spin–$\frac{1}{2}$ XY models were started to be discussed in random versions. The analytical results obtained here are not so impressive as for the perfect case and they are restricted to a special types of disorder [15–20] or renormalization–group analysis [21]. A discovery of the quasi–one–dimensional spin–$\frac{1}{2}$ systems ($Cs(H_{1-X}D_X)_2PO_4$, $PbH_{1-X}D_XPO_4$, $PrCl_3$, $CsCuCl_3$, $CsCu_{1-X}Mn_XCl_3$, J–aggregates etc.) gave rise to additional interest in such calculations since a lot of data obtained in the dynamic experiments for such materials are available. Some approximate studies of dynamic properties were inspired by the corresponding measurements [22–27], however, such estimations contain uncontrolled mistakes. Additional interest in such calculations was caused by the very recent studies of quantum phase transitions in disordered systems [21, 28–30].

Since there are notorious difficulties in the analytical study of some properties of the spin–$\frac{1}{2}$ XY chains it is natural to try to obtain the desired results numerically. Few earlier attempts [31, 32] faced the $2^N\times 2^N$ eigenvalue and eigenvector problem that restricted the computations to $N\sim 10$. However, a peculiarity of spin–$\frac{1}{2}$ XY chains provides an evident possibility to compute all equilibrium quantities facing in the last resort only the $2N\times 2N$ eigenvalue and eigenvector problem [33–35]. This fact allows to consider rather long chains ($N\sim 100--10000$) and therefore to study reliably the dynamics of spin correlations or the influence of disorder on observable properties. In this paper we shall briefly explain such a numerical approach for the calculation of the equilibrium properties of the spin–$\frac{1}{2}$ XY chains. Besides we shall demonstrate how the approach works computing for this purpose the xx dynamic structure factor of the transverse Ising model and some thermodynamic and dynamic properties of several random XY models.

We shall consider N spins one–half arranged in a row with the following Hamiltonian

$$H=\sum_{j=1}^{N}\Omega_j s_j^z+\sum_{j=1}^{N-1}\sum_{\alpha,\beta=x,y}J_j^{\alpha\beta}s_j^\alpha s_{j+1}^\beta, \qquad (1)$$

where Ω_j is the transverse field at the site j and $J_j^{\alpha\beta}$ is the interaction between α and β spin components at the sites j and $j+1$. Introducing instead of the spin raising and lowering operators via the Jordan–Wigner transformation the Fermi operators c_j^+, c_j one finds that the Hamiltonian (1) is a bilinear fermion form that can be put into diagonal form by linear transformation

$$\eta_k^+=\sum_{j=1}^{N}\left(h_{kj}^*c_j+g_{kj}^*c_j^+\right).$$

Similarly to [1] it can be shown that if

$$(\mathbf{g}_k,\mathbf{h}_k)\left(\begin{array}{cc}\mathbf{A} & \mathbf{B}\\ -\mathbf{B}^* & -\mathbf{A}^*\end{array}\right)=\Lambda_k(\mathbf{g}_k,\mathbf{h}_k) \qquad (2)$$

with

$$\mathbf{g}_k\equiv(g_{k1},...,g_{kN}),$$
$$\mathbf{h}_k\equiv(h_{k1},...,h_{kN}),$$
$$A_{ij}\equiv\Omega_i\delta_{ij}+J_i^{+-}\delta_{j,i+1}+J_{i-1}^{-+}\delta_{j,i-1},$$
$$B_{ij}\equiv J_i^{++}\delta_{j,i+1}-J_{i-1}^{++}\delta_{j,i-1}$$

and

$$J_j^{+-}\equiv\frac{1}{4}[J_j^{xx}+J_j^{yy}+\mathrm{i}(J_j^{xy}-J_j^{yx})]=J_j^{-+*},$$
$$J_j^{++}\equiv\frac{1}{4}[J_j^{xx}-J_j^{yy}-\mathrm{i}(J_j^{xy}+J_j^{yx})]$$

the Hamiltonian transforms into

$$H=\sum_{k=1}^{N}\Lambda_k\left(\eta_k^+\eta_k-\frac{1}{2}\right).$$

Evidently, the knowledge of Λ_ks or their distribution

$$\rho(E)\equiv\frac{1}{N}\sum_{k=1}^{N}\delta(E-\Lambda_k)$$

yields thermodynamics of the spin system (1). For the calculation of spin correlation functions it is convenient to introduce the auxiliary operators

$$\varphi_j^+\equiv c_j^++c_j=\sum_{p=1}^{N}\left(\Phi_{pj}\eta_p^++\Phi_{pj}^*\eta_p\right)$$

and

$$\varphi_j^-\equiv c_j^+-c_j=\sum_{p=1}^{N}\left(\Psi_{pj}\eta_p^+-\Psi_{pj}^*\eta_p\right),$$

where

$$\Phi_{pj}\equiv g_{pj}+h_{pj},$$
$$\Psi_{pj}\equiv g_{pj}-h_{pj}.$$

Since

$$s_j^x=\frac{1}{2}\varphi_1^+\varphi_1^-\dots\varphi_{j-1}^+\varphi_{j-1}^-\varphi_j^+,$$
$$s_j^y=\frac{1}{2\mathrm{i}}\varphi_1^+\varphi_1^-\dots\varphi_{j-1}^+\varphi_{j-1}^-\varphi_j^-$$

and

$$s_j^z=-\frac{1}{2}\varphi_j^+\varphi_j^-,$$

the calculation of thermodynamic average of a product of spin operators reduces to exploiting the Wick–Bloch–de Dominicis theorem with the result that is in fact the Pfaffian of corresponding antisymmetric matrix constructed from the elementary contractions

$$\langle\varphi_j^+(t)\varphi_m^+\rangle=\sum_{p=1}^{N}\left[\frac{\Phi_{pj}\Phi_{pm}^*}{\mathcal{F}(\Lambda_p)}+\frac{\Phi_{pj}^*\Phi_{pm}}{\mathcal{F}(-\Lambda_p)}\right],$$
$$\langle\varphi_j^+(t)\varphi_m^-\rangle=\sum_{p=1}^{N}\left[-\frac{\Phi_{pj}\Psi_{pm}^*}{\mathcal{F}(\Lambda_p)}+\frac{\Phi_{pj}^*\Psi_{pm}}{\mathcal{F}(-\Lambda_p)}\right],$$
$$\langle\varphi_j^-(t)\varphi_m^+\rangle=\sum_{p=1}^{N}\left[\frac{\Psi_{pj}\Phi_{pm}^*}{\mathcal{F}(\Lambda_p)}-\frac{\Psi_{pj}^*\Phi_{pm}}{\mathcal{F}(-\Lambda_p)}\right],$$
$$\langle\varphi_j^-(t)\varphi_m^-\rangle=-\sum_{p=1}^{N}\left[\frac{\Psi_{pj}\Psi_{pm}^*}{\mathcal{F}(\Lambda_p)}+\frac{\Psi_{pj}^*\Psi_{pm}}{\mathcal{F}(-\Lambda_p)}\right]$$

with

$$\mathcal{F}(x)\equiv\left(1+\mathrm{e}^{\beta x}\right)\mathrm{e}^{-\mathrm{i}xt}.$$

Thus, the solution of the $2N\times 2N$ eigenvalue and eigenvector problem (2) completely determines thermodynamics, spin correlations and their dynamics for model (1).

In what follows we have collected several new results obtained within the frames of the described approach. We shall start from the xx dynamic structure factor

$$S_{xx}(\kappa,\omega)\equiv\sum_{n=1}^{N}\mathrm{e}^{\mathrm{i}\kappa n}\int_{-\infty}^{\infty}\mathrm{d}t\mathrm{e}^{-\varepsilon|t|}\mathrm{e}^{\mathrm{i}\omega t}\langle s_j^x(t)s_{j+n}^x\rangle$$

for the uniform transverse Ising chain putting in (1)

$$\Omega_j=\Omega=0.2,$$
$$J_j^{xx}=J=-1,$$
$$J_j^{xy}=J_j^{yx}=J_j^{yy}=0.$$

At first we solved the eigenvalue and eigenvector problem (2) for $N=280$ obtaining in result Λ_k, Φ_{kj}, Ψ_{kj}. Then for several values of temperature we calculated the required elementary contractions and computed the relevant Pfaffian

$$\langle s_{32}^x(t)s_{32+n}^x\rangle = \frac{1}{4}\langle\varphi_1^+(t)\varphi_1^-(t)\dots\varphi_{31}^+(t)\varphi_{31}^-(t)\varphi_{32}^+(t)\varphi_1^+\varphi_1^-\dots\varphi_{32+n-1}^+\varphi_{32+n-1}^-\varphi_{32+n}^+\rangle$$

$$= \mathrm{Pf}\begin{pmatrix} 0 & \langle\varphi_1^+\varphi_1^-\rangle & \langle\varphi_1^+\varphi_2^+\rangle & \cdots & \langle\varphi_1^+(t)\varphi_{32+n}^+\rangle \\ -\langle\varphi_1^+\varphi_1^-\rangle & 0 & \langle\varphi_1^-\varphi_2^+\rangle & \cdots & \langle\varphi_1^-(t)\varphi_{32+n}^+\rangle \\ \vdots & \vdots & \vdots & \dots & \vdots \\ -\langle\varphi_1^+(t)\varphi_{32+n}^+\rangle & -\langle\varphi_1^-(t)\varphi_{32+n}^+\rangle & -\langle\varphi_2^+(t)\varphi_{32+n}^+\rangle & \cdots & 0 \end{pmatrix}.$$

At last we performed the integration over the time up to $t = 1600$ with $\varepsilon = 0.001$ and took into account in the sum over n up to 100 neighbours. The obtained dependences $S_{xx}(\kappa,\omega)$ vs. ω for different κ at low temperature and $S_{xx}(0,\omega)$ vs. ω for few temperatures are depicted in Fig. 1. As can be seen from Fig. 1 $S_{xx}(\kappa,\omega)$ exhibits two peaks. At $\beta = 5$ and $\kappa = 0$ one finds a high peak at $\omega_1 = 0.00$ and a low and broad one at $\omega_2 = 0.76$. As κ increases the height of the first peak decreases and it shifts towards high frequencies ($\omega_1 \approx 0.11$ at $\kappa = \frac{\pi}{4}$, $\omega_1 \approx 0.25$ at $\kappa = \frac{\pi}{2}$, $\omega_1 \approx 0.34$ at $\kappa = \frac{3\pi}{4}$, $\omega_1 \approx 0.38$ at $\kappa = \pi$), whereas the width of the second peak decreases, its height increases and it moves towards high frequencies ($\omega_2 \approx 0.80$ at $\kappa = \frac{\pi}{4}$, $\omega_2 \approx 0.88$ at $\kappa = \frac{\pi}{2}$, $\omega_2 \approx 0.96$ at $\kappa = \frac{3\pi}{4}$, $\omega_2 \approx 1.01$ at $\kappa = \pi$). As the temperature increases $S_{xx}(0,\omega)$ qualitatively remains the same: the heights of both peaks decrease and the high–frequency peak shifts slightly towards high frequencies ($\omega_2 \approx 0.76$ at $\beta = 5$, $\omega_2 \approx 0.77$ at $\beta = 4$, $\omega_2 \approx 0.81$ at $\beta = 3$, $\omega_2 \approx 0.86$ at $\beta = 2$, $\omega_2 \approx 0.91$ at $\beta = 1$, $\omega_2 \approx 0.95$ at $\beta = 0.1$, $\omega_2 \approx 0.96$ at $\beta = 0.001$). The discussed case of a small transverse field may be of interest for understanding the dielectric measurement and neutron scattering data for quasi–one–dimensional hydrogen–bonded ferroelectrics. However, detailed comparison with experimental results demands the introduction of weak interchain interactions (see [24, 26]) which requires a separate study.

Next example regards thermodynamics of the isotropic XY chain determined by (1) with

$$J_j^{xx} = J_j^{yy} = J_j,$$
$$J_j^{xy} = J_j^{yx} = 0$$

with the random intersite couplings given, for example, by the Lorentzian probability distribution density

$$p(\dots,J_j,\dots) = \prod_{j=1}^{N}\frac{1}{\pi}\frac{\Gamma}{(J_j-J_0)^2+\Gamma^2}$$

and the transverse fields that depend linearly on the surrounding couplings

$$\Omega_j - \Omega_0 = \frac{a}{2}(J_{j-1}+J_j-2J_0), \qquad |\, a\,|\geq 1.$$

In Ref. [20] the random–averaged density of states $\overline{\rho(E)}$ was calculated that yielded thermodynamics of the model. In particular, it was shown that the introduced randomness may cause the appearance of non–zero averaged transverse magnetization

$$\overline{m_z} = -\frac{1}{2}\int_{-\infty}^{\infty}\mathrm{d}E\overline{\rho(E)}\tanh\frac{\beta E}{2}$$

at zero averaged transverse field $\Omega_0 = 0$. This is conditioned by the fact that $\overline{\rho(E)}$ is not symmetric with respect to the change $E-\Omega_0 \to -(E-\Omega_0)$ and at $T = 0$

$$-2\overline{m_z} = \int_{-\infty}^{0}\mathrm{d}E\overline{\rho(E)} - \int_{0}^{\infty}\mathrm{d}E\overline{\rho(E)} \neq 0.$$

We considered the described model for $N = 15000$ with $J_0 = 1$ for $a = \pm 1.01$ with the Lorentzian and Gaussian random couplings; the probability distribution for the latter case reads

$$p(\dots,J_j,\dots) = \prod_{j=1}^{N}\frac{1}{\sqrt{2\pi}\sigma}\exp\left[-\frac{(J_j-J_0)^2}{2\sigma^2}\right].$$

The results of computations for one random realization are presented in Fig. 2. The displayed results are in complete agreement with the ones derived analytically for the Lorentzian disorder. However, the developed numerical procedure allows to study an arbitrary disorder. The performed calculations have indicated the appearance of $\overline{m_z} \neq 0$ for $\Omega_0 = 0$ at low temperature for the correlated disorder. This can be clearly demonstrated by the results of the calculation of a number of negative and positive eigenvalues Λ_k (2) $\mathcal{N}_-$ and $\mathcal{N}_+$, since at $T = 0$

$$-2\overline{m_z} = \frac{\mathcal{N}_- - \mathcal{N}_+}{N}.$$

Putting $a = 1.01$ for a certain Gaussian random realization with $\sigma = 0.25(1)$ that yields

$$\frac{1}{N}\sum_{j=1}^{N} J_j = 0.999757(0.999027)$$

we found $\mathcal{N}_- = 7192(6024)$ and $\mathcal{N}_+ = 7808(8976)$. Another Gaussian random realization with $\sigma = 0.25(1)$ that yields

$$\frac{1}{N}\sum_{j=1}^{N} J_j = 1.000118(1.000473)$$

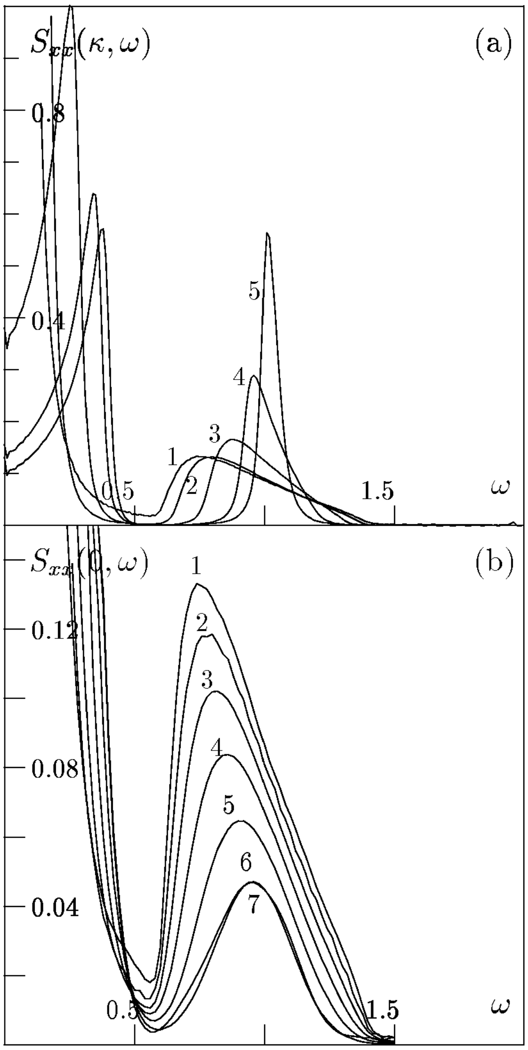

Fig. 1. The dynamic structure factor for the Ising chain in transverse field. (a) $S_{xx}(\kappa,\omega)$ vs. ω at $\beta = 5$ for $\kappa = 0, \frac{\pi}{4}, \frac{\pi}{2}, \frac{3\pi}{4}, \pi$ (curves $1, \dots, 5$, respectively) and (b) $S_{xx}(0,\omega)$ vs. ω for $\beta = 5, 4, 3, 2, 1, 0.1, 0.001$ (curves $1, \dots, 7$, respectively).

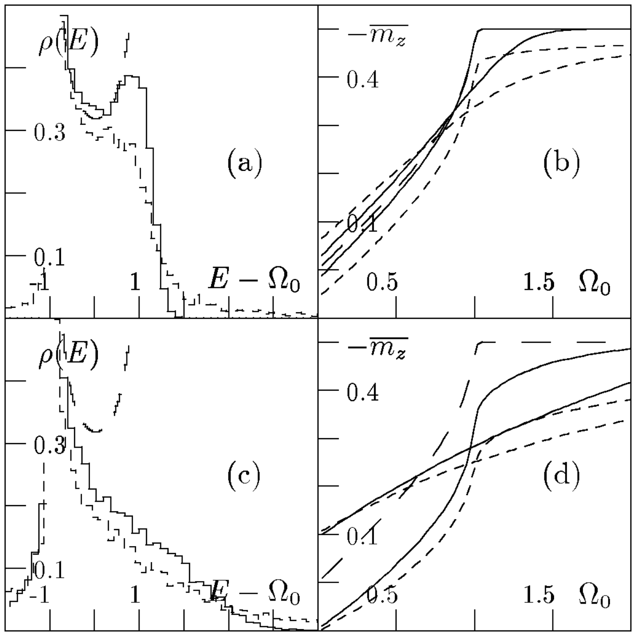

Fig. 2. The density of states and transverse magnetization for the isotropic XY chain with random couplings and transverse fields that depend linearly on the surrounding couplings. $\rho(E)$ vs. $E - \Omega_0$ (a,c) and $-\overline{m_z}$ vs. Ω_0 at $\beta = 100$ (b,d) for the Lorentzian (short dashed lines) and Gaussian (solid lines) disorder with $\Gamma = \sigma = 0.25$ (a,b) and $\Gamma = \sigma = 1$ (c,d); the results for non–random case $\Gamma = \sigma = 0$ are depicted by long dashed lines.

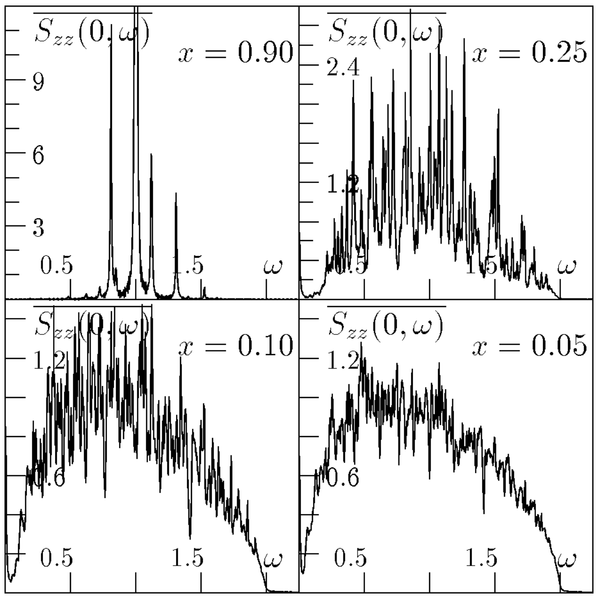

Fig. 3. The frequency dependence of the averaged dynamic structure factor $\overline{S_{zz}(0,\omega)}$ for the Ising chain in random transverse field at $\beta = 5$.

gave $\mathcal{N}_- = 7187(6073)$ and $\mathcal{N}_+ = 7813(8927)$. These results definitely point out the appearance of "spontaneous magnetization" due to disorder.

We end up with the calculation of the zz dynamic structure factor

$$S_{zz}(\kappa,\omega) \equiv \sum_{n=1}^{N} \mathrm{e}^{\mathrm{i}\kappa n} \int_{-\infty}^{\infty} \mathrm{d}t \mathrm{e}^{-\varepsilon|t|} \mathrm{e}^{\mathrm{i}\omega t} \times \left(\langle s_j^z(t) s_{j+n}^z \rangle - \langle s_j^z \rangle \langle s_{j+n}^z \rangle \right)$$

for the Ising chain that follows from (1) if

$$J_j^{xx} = J = 1,$$
$$J_j^{xy} = J_j^{yx} = J_j^{yy} = 0$$

in the random transverse field defined by the probability distribution density

$$p(\ldots,\Omega_j,\ldots) = \prod_{j=1}^{N} \left[x\delta(\Omega_j) + (1-x)\delta(\Omega_j - 0.5) \right],$$
$$0 \le x \le 1.$$

We computed the correlation functions

$$4\langle s_{100}^z(t) s_{100+n}^z \rangle = \langle \varphi_{100}^+ \varphi_{100}^- \rangle \langle \varphi_{100+n}^+ \varphi_{100+n}^- \rangle - \langle \varphi_{100}^+(t) \varphi_{100+n}^+ \rangle \langle \varphi_{100}^-(t) \varphi_{100+n}^- \rangle + \langle \varphi_{100}^+(t) \varphi_{100+n}^- \rangle \langle \varphi_{100}^-(t) \varphi_{100+n}^+ \rangle$$

for 250 random chains of 200 spins, performed the integration over time t with $\varepsilon = 0.005$ and the summation over neighbours n. The obtained random–averaged zz dynamic structure factor that for $\kappa = 0$ is presented in Fig. 3. The depicted plots demonstrate how the frequency–dependent zz structure factor rebuilds from the Ising type behaviour to the transverse Ising type behaviour as the concentration of sites with transverse field increases from 0 ($x = 1$) to 1 ($x = 0$). The obtained dynamic structure factor exhibits a lot of structure that is induced by the disorder arrangement of two values of transverse field 0 and 0.5. It appears that each well–defined peak for small concentrations of $1-x$ is connected with $S_{zz}(0,\omega)$ for a certain chain determined by the local environment of spin at $j = 100$ (for example, $\ldots 0\mathbf{0}0 \ldots$, $\ldots 0\Omega\mathbf{0}0 \ldots$, $\ldots 0\Omega\mathbf{0} \ldots$, $\ldots 0\Omega\Omega\mathbf{0}0 \ldots$, $\ldots 0\Omega\boldsymbol{\Omega}0 \ldots$, $\ldots 0\Omega\mathbf{0}\Omega \ldots$ etc., the transverse field Ω_{100} is written in bold font, the unwritten Ω_js do not influence $S_{zz}(0,\omega)$). With decreasing x the number of possible local structures in the vicinity of $j = 100$ (and thus a number of peaks) increases and the peaks appear almost at all frequencies. However, the difference in their heights is conditioned by the probability of their appearance that is large. As a result one gets fine structure that transforms into the smooth curve only in the limiting case $x = 0$. The described random model has a simple interpretation in connection with partially deuterated quasi–one–dimensional hydrogen–bonded ferroelectrics. However, a study of relevant there xx spin dynamics is more cumbersome and will be reported separately.

To summarize, we have presented a numerical approach suitable for the calculation of time–dependent correlation functions for non–random and random spin–$\frac{1}{2}$ XY chains. We have illustrated the numerical procedure deriving some new results. It is relevant to mention here the papers [36, 37] devoted to numerical calculations of the xx time–dependent spin correlation functions for the isotropic XY model. The authors used explicit expressions for the elementary contractions (in contrast to our formulae that also fit the random models) and computed determinants of the corresponding antisymmetric matrices that yielded only the square of correlation functions (this causes some difficulties in calculating the dynamic structure factor or susceptibility further as well as in the study of random models). We hope that the numerical analysis of the properties of spin–$\frac{1}{2}$ XY chains will be useful for understanding the results of the corresponding measurements on quasi–one–dimensional hydrogen–bonded ferroelectrics like CsH_2PO_4, $Cs(H_{1-X}D_X)_2PO_4$, $PbHPO_4$, $PbH_{1-X}D_XPO_4$ (neutron scattering, dielectric measurements) and J–aggregates (absorption and emission spectra). However, a comparison of theoretical predictions and experimental data requires further studies.

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