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The paper presents a new numerical approach for studying the thermodynamical and dynamical properties of finite spin-$1/2$ XY chains. Special attention is given to examining the influence of disorder on the average transverse dynamical susceptibility of Ising chain in random transverse field.

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The present paper deals with the equilibrium properties of spin-$1/2$ non-uniform anisotropic $XY$ chain in transverse field that is defined by the Hamiltonian

$$H = \sum_{j=1}^{N} \Omega_j s_j^z + \sum_{j=1}^{N-1} (J_{j}^{xx}s_j^xs_{j+1}^x + J_{j}^{yy}s_j^ys_{j+1}^y).$$

(1)

The quantities of main interest are the time-dependent correlation functions $< s_j^\alpha(t)s_{j+n}^\beta >$, $< (...) > = \text{Sp}[e^{-\beta H}(...)]/\text{Sp}e^{-\beta H}$, $s_j^\alpha(t) \equiv e^{iHt}s_j^\alpha e^{-iHt}$ and dynamical susceptibilities $\chi_{\alpha\beta}(\omega) \equiv \sum_n e^{i\omega n} \int_0^\infty dt e^{i(\omega+\epsilon)t} \frac{1}{\beta} < [s_j^\alpha(t), s_{j+n}^\beta] >$.

The system considered in partial cases has well-known ferroelectric interpretation in connection with some quasi-one-dimensional hydrogen-bonded ferroelectric crystals like $Cs(H_{1-x}D_x)_2PO_4$, $PbH_{1-x}D_xPO_4$ etc. Indeed, in such compounds the hydrogen bonds, that play an important role for the ferroelectricity, run along chains, the intrachain interactions are much stronger than the interchain ones, and a suitable model for describing protons behaviour in a chain is spin-$1/2$ Ising model in transverse field, which is contained in (1) ($J_{j}^{yy} = 0$, $J_{j}^{xx}$ is interaction between neighbouring hydrogen bonds along chain and $\Omega_j$ describes proton tunneling motion). The non-uniformity may be caused physically by deuteration of some hydrogen bonds. Under simplest assumption one believes that the substitution $H \rightarrow D$ changes significantly the tunneling probability and practically does not affect the intersite interaction parameters. For this case one should put $J_{j}^{xx} = J$ and suppose that $\Omega_j$ varies randomly from site to site taking value $\Omega$ with probability $1 - x$ and zero value with probability $x$, that is, one should consider random chain (1) with the probability distribution density

$$p(..., \Omega_j, J_{j}^{xx}, J_{j}^{yy}, ...) = \prod_{j=1}^{N} [x\delta(\Omega_j) + (1 - x)\delta(\Omega_j - \Omega)]\delta(J_{j}^{xx} - J)\delta(J_{j}^{yy}).$$

(2)
Statistical mechanics calculations for this model bear strong relevance for paraelectric phase properties of mentioned crystals and have been performed mainly in the limiting cases $x = 1$ and $x = 0$ (see e.g.\textsuperscript{1-3} and references therein). Such studies were encouraged by the fact that the model (1) with the help of Jordan-Wigner transformation can be rewritten as a system of non-interacting fermions and thus a lot of result can be obtained exactly\textsuperscript{4}. Nevertheless, there are serious difficulties in calculation of longitudinal time-dependent correlation function $\langle s_j^x(t)s_{j+n}^x \rangle$ and therefore the dynamical susceptibility $\chi_{xx}(\omega, \omega)$, and the complete solution even for perfect (non-random) case has never been found. The results obtained within different approximate approaches have serious shortcomings.

In our previous papers\textsuperscript{5-7} we suggested a new numerical approach for evaluation of thermodynamical properties and both equal-time and different-time spin correlation functions for the model defined by (1). In the present paper the proposed approach is described in more detail and is applied for examining the influence of disorder on the average transverse dynamical susceptibility of spin-$\frac{1}{2}$ Ising chain in random transverse field (1), (2). Such results, up to the best authors’ knowledge, are obtained for the first time.

In order to obtain the equilibrium statistical properties of the system in question (1) one should first perform Jordan-Wigner transformation from operators $s_j^\pm \equiv s_j^x \pm is_j^y$ to Fermi operators $c_1 = s_1^-, c_j = \prod_{n=1}^{j-1}(-2s_n^z)s_j^-$, $j = 2, ..., N$ and then to diagonalize the obtained quadratic form by a canonical transformation $\eta_k = \sum_{j=1}^N (g_{kj}c_j + h_{kj}c_j^+)$ with the outcome $H = \sum_{k=1}^N \Lambda_k(\eta_k^+\eta_k - \frac{1}{2})$. The elementary excitation spectrum $\Lambda_k$ and the coefficients $g_{kn}$ \equiv
(Φ_{kn} + Ψ_{kn})/2, h_{kn} \equiv (Φ_{kn} - Ψ_{kn})/2 are determined from
\[ \Lambda_k Φ_{kn} = \sum_{j=1}^{N} Ψ_{kj}(A + B)_{jn}, \]
\[ \Lambda_k Ψ_{kn} = \sum_{j=1}^{N} Φ_{kj}(A - B)_{jn}, \]

where \( A_{ij} \equiv Ω_i δ_{ij} + J_{xx}^i + J_{yy}^i δ_{j,i+1} + J_{xx}^i + J_{yy}^i δ_{j,i-1}, \) \( B_{ij} \equiv \frac{J_{xx}^i - J_{yy}^i}{4} δ_{j,i+1} - \frac{J_{xx}^i - J_{yy}^i}{4} δ_{j,i-1}. \) Eqs. (3) reduce to standard problems
\[ \Lambda_k^2 Φ_{kn} = \sum_{j=1}^{N} Φ_{kj}[(A - B)(A + B)]_{jn}, \]
\[ \Lambda_k^2 Ψ_{kn} = \sum_{j=1}^{N} Ψ_{kj}[(A + B)(A - B)]_{jn} \]

for \( N \times N \) five diagonal banded matrices \((A \mp B)(A \pm B)\).

Next it is necessary to express the quantities of interest through \( Λ_k, Φ_{kj}, Ψ_{kj} \). Since the partition function \( Z(β, N) = \Pi_{k=1}^{N} 2 \cosh \frac{βΛ_k}{2} \) involves all \( Λ_k^2, \) the knowledge of eigenvalues of matrices \((A \mp B)(A \pm B)\) permits one to obtain the thermodynamical properties of the model in question (1). Reformulating spin operators in terms of operators \( \varphi_j^+ \equiv c_j^+ + c_j = \sum_{m=1}^{N} Φ_{mj}(η_m + η_m) \) and \( \varphi_j^- \equiv c_j^+ - c_j = \sum_{m=1}^{N} Ψ_{mj}(η_m^+ - η_m), \) that is, \( s_j^x = \Pi_{n=1}^{j-1}(\varphi_n^+ \varphi_n^-)\varphi_j^+ / 2, \) \( s_j^y = \Pi_{n=1}^{j-1}(\varphi_n^+ \varphi_n^-)\varphi_j^- / 2i, \) \( s_j^z = -\varphi_j^+ \varphi_j^- / 2, \) noting that the calculation of spin correlation functions reduces to exploiting Wick-Bloch-de Dominicis theorem, and calculating the elementary contractions
\[ < \varphi_j^+(t) \varphi_m^+ > = \sum_{p=1}^{N} Φ_{pj} Φ_{pm} \frac{\cosh(iΛ_p t - \frac{βΛ_p}{2})}{\cosh \frac{βΛ_p}{2}}, \]
\[ < \varphi_j^-(t) \varphi_m^- > = \sum_{p=1}^{N} Φ_{pj} Ψ_{pm} \frac{\sinh(-iΛ_p t + \frac{βΛ_p}{2})}{\cosh \frac{βΛ_p}{2}}, \]
\[ < \varphi_j^-(t) \varphi_m^+ > = -\sum_{p=1}^{N} Ψ_{pj} Φ_{pm} \frac{\sinh(-iΛ_p t + \frac{βΛ_p}{2})}{\cosh \frac{βΛ_p}{2}}, \]
\begin{align}
< \varphi_j^-(t) \varphi_m^- > &= - \sum_{p=1}^{N} \Psi_{pj} \Psi_{pm} \frac{\cosh(i\Lambda_p t - \frac{\beta \Lambda_p^2}{2})}{\cosh \frac{\beta \Lambda_p^2}{2}}, 
\end{align}

one finds that \( \Phi_{kp}, \Psi_{kg} \) for all \( \Lambda_k \) are involved in final expressions for equal-time and different-time spin correlation functions. Further numerical computation may be performed in a following way: first, to solve the eigenvalues and eigenvectors problem for matrix \((A + B)(A - B)\) (4) obtaining in result \( \Lambda_k^2 \) and \( \Psi_{kj} \), and second, having \( \Psi_{kj} \) and \( \Lambda_k = \sqrt{\Lambda_k^2} \), to find \( \Phi_{kj} \) from Eq.(3); thermodynamics and spin correlation functions are expressed via the sought quantities. It should be stressed that here appears only the eigenvalues and eigenvectors problem for \( N \times N \) five diagonal banded matrix that is the remarkable peculiarity of the system under consideration (1). This is a key difference of our approach in comparison with other finite-chain calculations (reported e.g. in\(^8\)) where the numerical diagonalization of the Hamiltonian (1) in the Hilbert space of dimension \( 2^N \) is performed.

The remainder of the paper deals with numerical calculation of transverse dynamical susceptibility \( \chi_{zz}(\omega, \omega) \) for spin-\( \frac{1}{2} \) Ising chain in random transverse field (1), (2). Acting as described above one finds that 4 < \( s_j^z(t)s_{j+n}^z \) > = < \( \varphi_j^+(t)\varphi_j^+(t)\varphi_{j+n}^+\varphi_{j+n}^- \) > = < \( \varphi_j^+(t)\varphi_j^-(t) \) > < \( \varphi_{j+n}^+\varphi_{j+n}^- \) > - < \( \varphi_j^+(t)\varphi_{j+n}^+ \) > < \( \varphi_j^-(t)\varphi_{j+n}^- \) > + < \( \varphi_j^+(t)\varphi_{j+n}^- \) > < \( \varphi_j^-(t)\varphi_{j+n}^+ \) > < \( s_{j+n}^z(t) \) > = < \( s_{j+n}^z(-t)s_j^z \) >. Computing then numerically the elementary contractions (5) involved in the correlation functions < \( s_{100}^z(t)s_{100+n}^z \) >, < \( s_{100+n}^z(-t)s_{100}^z \) > for the random chain of 200 spins with \( J = -2, \Omega = 1 \) at \( \beta = 20 \), performing numerically the integration over \( t \) and summation over \( n \), and averaging over the realization (typically few hundred) we have obtained the results some of which are presented in Fig.1. As the concentration of the sites with transverse field \( \Omega \) increases \( \chi_{zz}(\omega, \omega) \) rebuilds from
the generally known Ising-like type behaviour to the behaviour inherent to
Ising model in transverse field derived for the first time with periodic bound-
ary conditions imposed in\(^9\). Note, that the depicted frequency shapes lose
their symmetry and develop into smooth curves at \(x = 0\). The obtained
susceptibilities exhibit a lot of structure. The detailed structure is induced
by the disordered arrangement of two values of transverse field 0 and \(\Omega = 1\).
Considering at first the case of small concentrations of \(\Omega\) one can find that
each well-defined peak is associated with the susceptibility of certain chain
that is determined by values of transverse field only in the local environment
of spin at site \(j = 100\) (see Figs.2-4). While \(x\) decreases the number of possible
local structures (and thus the number of peaks) increases and the peaks
appear almost at all frequencies. Nevertheless, since the difference in their
magnitudes conditioned by the probability of their appearance is large, even
at rather small \(x\) it is still possible to recognize the peaks corresponding to
some simple local structures. Completely smooth curves appear only in the
limiting case \(x = 0\). It should be added that the similar calculations for
some other types of disorder yield smooth frequency shapes. Finally, one
should remind that the obtained results are exact only for finite chains and
it is necessary to be careful while making extrapolations to \(N = \infty\), but,
apparently, the picture qualitatively will remain the same.

In conclusion it should be underlined, that the suggested method appears
to be of great use in study of dynamical properties and random versions of
spin-\(\frac{1}{2}\) \(XY\) chains and the derived results may be useful for interpretation
of observable data in dynamical experiments on quasi-one-dimensional com-
ounds that can be described in frames of model (1).

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**Figure captions**

Fig.1. Frequency-dependent real and imaginary parts of transverse susceptibility $\chi_{zz}(\alpha, \omega)$ for spin-$\frac{1}{2}$ Ising chain in random transverse field (1), (2) at $\alpha = 0$ for different values of concentration $x$; $\epsilon = 0.01$.

Fig.2. $\chi_{zz}(0, \omega)$ for certain spin-$\frac{1}{2}$ Ising chains. It is determined by values of transverse field in local environment of spin at site $j = 100$ (no transverse fields) and not denoted $\Omega_j$s do not influence it; $\epsilon = 0.01$.

Fig.3. The same as in Fig.2 for one transverse field in local environment of spin at site $j = 100$; $\epsilon = 0.01$.

Fig.4. The same as in Fig.2 for two transverse fields in local environment of spin at site $j = 100$; $\epsilon = 0.01$. 
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