Dynamics of $zz$ spin correlations
in the square–lattice spin–$\frac{1}{2}$ isotropic $XY$ model

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Using the Jordan–Wigner fermionization in two dimensions we obtain the $zz$ wave
vector– and frequency–dependent structure factor for the spin–$\frac{1}{2}$ isotropic $XY$ model on
a spatially anisotropic square lattice. We use the obtained results to discuss a role of the
interchain interaction for the dynamic properties of quasi–one–dimensional systems.

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Dynamic properties of the two–dimensional quantum spin models have attracted much attention for
the last years mainly due to the discovery of high–temperature superconductivity of the layered copper
oxides$^1$. At present, many compounds are known to be good realizations of the square–lattice quantum
spin model and the experimental investigations of their dynamic properties$^2$ require corresponding theo-
retical studies. In most cases the isotropic Heisenberg Hamiltonian is used to appropriately model the
spin degrees of freedom. However, some generic features of the square–lattice quantum spin systems can
be illustrated within the context of the spin–$\frac{1}{2}$ isotropic $XY$ model, which is far more amenable to a
Theoretical analysis. Moreover, a study of the latter model can be viewed as a first step for examining the more complicated case of the square–lattice spin–$\frac{1}{2}$ Heisenberg model.

The aim of this study is to examine the dynamic properties of the spin–$\frac{1}{2}$ isotropic XY model on a square lattice. Many theoretical and numerical investigations concerning the thermodynamic properties of this model have been performed until now\(^4\). Less progress has been made in the studies of its dynamic properties. To examine the dynamic properties of the model we use the two–dimensional Jordan–Wigner fermionization\(^4–7\) (for a brief review see Ref. 8) thus extending the approach which was previously applied mainly to the study of thermodynamics (see also several recent papers\(^9\) on calculation of the magnetization curves of some two–dimensional spin systems). More specifically, we calculate the two–site time–dependent correlation functions of $z$ spin components and the corresponding dynamic structure factor $S_{zz}(\mathbf{k}, \omega)$ for the spin–$\frac{1}{2}$ isotropic XY model on a spatially anisotropic square lattice. To trace a one–dimensional to two–dimensional crossover, we compare the results obtained with the corresponding ones for the spin–$\frac{1}{2}$ isotropic XY chain thus demonstrating the role of the interchain interaction for the dynamic properties of quasi–one–dimensional spin–$\frac{1}{2}$ isotropic XY systems. The recent study of the static properties of the square–lattice spin–$\frac{1}{2}$ isotropic XY model\(^10\) suggests that the approach based on the two–dimensional Jordan–Wigner fermionization works well as long as the interchain interaction is small and it gives qualitatively correct results for larger values of the interchain interaction.

We consider a spin model consisting of $N \rightarrow \infty$ spins $\frac{1}{2}$ on a spatially anisotropic square lattice governed by the isotropic XY Hamiltonian

$$H = \frac{1}{2} \sum_{i=0}^{\infty} \sum_{j=0}^{\infty} \left( J \left(s_{i,j}^+ s_{i+1,j}^- + s_{i,j}^- s_{i,j+1}^+ \right) + J_\perp \left(s_{i,j}^+ s_{i,j+1}^- + s_{i,j}^- s_{i,j+1}^+ \right) \right).$$

(1)

Here $J \geq 0$ and $J_\perp \geq 0$ are the exchange interactions between the neighbouring sites in a row and in a column, respectively. We are interested in the two–site time–dependent spin correlation functions $\langle s_{n,m}^z(t) s_{n+p,m+q}^z \rangle$ (the angular brackets denote the canonical thermodynamic average with the Hamiltonian (1)) and the $zz$ dynamic structure factor

$$S_{zz}(\mathbf{k}, \omega) = \sum_{p=0}^{\infty} \sum_{q=0}^{\infty} e^{ik_x p + k_y q} \int_{-\infty}^{\infty} dt e^{i\omega t} \left( \langle s_{n,m}^z(t) s_{n+p,m+q}^z \rangle - \langle s_{n,m}^z \rangle \langle s_{n+p,m+q}^z \rangle \right).$$

(2)

To calculate these quantities we use the two–dimensional Jordan–Wigner transformation\(^5\) reformulating
the problem in fermionic language. First we introduce the annihilation and creation operators of (spinless) fermion \( d_{i,j} = e^{-i\alpha_{i,j}}s_{i,j}^-, \alpha_{i,j} = \sum_{f=0}^{\infty} \sum_{g=0}^{\infty} B_{i,j:f,g} d_{f,g}^+ d_{i,j} \), \( B_{i,j:f,g} = \text{Im} \ln (f - i + (g - j)) \).

We adopt the mean–field treatment of the phase factors which appear in the initial Hamiltonian (1) after fermionization (for details see Refs. 5, 8). This is the only approximation made. Then we perform the Fourier transformation and the Bogolyubov transformation to arrive at the Hamiltonian of noninteracting fermions. Next, we rewrite the correlation function \( \langle \sigma_{n,m}(t)\sigma_{n+p,m+q}^\dagger \rangle \) in fermionic language and use the Wick–Bloch–de Dominicis theorem to calculate it. Finally, we insert the derived result into (2) and get the \( zz \) dynamic structure factor

\[
S_{zz}(k,\omega) = \pi \int_{-\pi}^{\pi} \frac{dk_{1y}}{2\pi} \int_{-\pi}^{\pi} \frac{dk_{1x}}{2\pi} \left( \cos^2 \frac{\gamma_{k_1+k} - \gamma_{k_1}}{2} (n_{k_1} (1 - n_{k_1+k}) \delta (\omega + \Lambda_{k_1} - \Lambda_{k_1+k})) + (1 - n_{k_1}) n_{k_1+k} \delta (\omega - \Lambda_{k_1} + \Lambda_{k_1+k})) \right.
\]

\[
+ \sin^2 \frac{\gamma_{k_1+k} - \gamma_{k_1}}{2} (n_{k_1} n_{k_1+k} \delta (\omega + \Lambda_{k_1} + \Lambda_{k_1+k})) + (1 - n_{k_1}) (1 - n_{k_1+k}) \delta (\omega - \Lambda_{k_1} - \Lambda_{k_1+k})).
\]

(3)

Here \( \Lambda_k = \sqrt{J_2 \sin^2 k_x + J_1^2 \cos^2 k_y} \geq 0 \) is the fermion energy, \( \cos \frac{\gamma_k}{2} = \sqrt{\frac{1}{2} + \frac{J_1 \cos k_y}{2\Lambda_k}}, \sin \frac{\gamma_k}{2} = \text{sgn} (J \sin k_x) \sqrt{\frac{1}{2} - \frac{J_1 \cos k_y}{2\Lambda_k}}, \) and \( n_k = \frac{1}{\cosh^2 k + 1} \) is the Fermi factor. In Figs. 1 – 3 we present \( S_{zz}(k,\omega) \) for the square–lattice spin \( \frac{1}{2} \) isotropic XY model as it follows from Eq. (3) (to integrate over \( k_{1y} \) we use the relation \( \delta (\varphi(x)) = \sum_j \delta (x - a_j) |\varphi'(a_j)|^{-1} \), \( a_j \) are the roots of equation \( \varphi(x) = 0 \), and then we do the integral over \( k_{1y} \) numerically). Let us discuss the dynamic properties of the considered spin model (1) concentrating in particular on the appearance of one–dimensional behaviour at low and high temperatures as \( \frac{1}{\beta} \) decreases.

It is useful to start the analysis of dynamic properties by reminding what is long known for the one–dimensional case. From the exact calculation for spin–\( \frac{1}{2} \) isotropic XY chain\(^{11} \) we know that \( S_{zz}(k,\omega) \) at zero temperature \( \beta = \infty \) is governed by a two–fermion excitation continuum with lower and upper boundaries \( J |\sin k| \) and \( 2J |\sin \frac{k}{2}| \), respectively. The spectral weight is finite at the lower boundary. The lower boundary touches the line \( \omega = 0 \) at \( k = 0 \), \( 2\pi \) and \( k = \pi \) (gapless modes). The spectral weight increases towards the upper boundary where \( S_{zz}(k,\omega) \) diverges. With the increasing temperature, the
lower boundary gets smeared out and finally disappears, whereas the upper boundary remains unchanged.

The described picture agrees with what we see from the greyscale plots of $S_{zz}(k_x, 0, \omega)$ for $J_\perp = 0.1$ (Figs. 1a and 2a), i.e., for a system of almost noninteracting chains for momentum transfer along the chain direction. (The gap seen in Fig. 2a arises due to a finite interchain interaction: as $J_\perp \to 0$ it shrinks and disappears.) For momentum transfer perpendicularly to the chain direction, the dynamic structure factor for a system of almost noninteracting chains disappears (Figs. 1b and 2b).

Let us pass to the two–dimensional case (the rest of the plots in Figs. 1, 2). Similar to the one–dimensional case $S_{zz}(k, \omega)$ within the framework of our approach is conditioned by two–fermion excitations and hence it exhibits nonzero values only within the restricted region having a sharp high–frequency cutoff (evidently, $S_{zz}(k, \omega)$ (3) equals to zero if the frequency $\omega$ exceeds $2\sqrt{J^2 + J_\perp^2}$). Contrary to the one–dimensional case, for which $S_{zz}(k, \omega)$ is almost structureless within the excitation continuum (apart from the upper boundary singularities), $S_{zz}(k, \omega)$ exhibits several washed–out excitation branches (modes).

Consider at first zero temperature. As it follows from Eq. (3), the $\delta$–function $\delta(\omega - \Lambda_{k_1} - \Lambda_{k_1+k})$ admits the spectral weight at $k, \omega$ due to the two fermions with $k_1 = \left(-\frac{k_x}{2}, \frac{\pi}{2} - \frac{k_y}{2}\right)$ and $k_1 + k = \left(\frac{k_x}{2}, \frac{\pi}{2} + \frac{k_y}{2}\right)$ with the energy of the pair

$$\omega^{(1)}_k = 2\sqrt{J^2 \sin^2 \frac{k_x}{2} + J_\perp^2 \sin^2 \frac{k_y}{2}}. \quad (4)$$

This excitation is known as the spin wave$^3$. Note, that since the derivative of the argument of $\delta$–function with respect to $k_{1x}$ tends to zero (except for $k_x = 0$, $2\pi$ if $k_y = 0$, $2\pi$ and vice versa) the peaks of $S_{zz}(k, \omega)$ along the line $\omega^{(1)}_k$ (4) are expected. They are nicely visible in Figs. 1, 2.

It is easy to note that the branch which almost everywhere in the regions $(k_x, 0, \omega)$ and $(0, k_y, \omega)$ forms the upper boundary (see Figs. 1, 2) is given by

$$\omega^{(2)}_{k_x,0} = 2\sqrt{J^2 \sin^2 \frac{k_x}{2} + J_\perp^2}, \quad \omega^{(2)}_{0,k_y} = 2\sqrt{J^2 + J_\perp^2 \sin^2 \frac{k_y}{2}}. \quad (5)$$

$S_{zz}(k, \omega)$ arises along the lines $\omega^{(2)}_{k_x,0}$ and $\omega^{(2)}_{0,k_y}$ (5) when it is conditioned by the two fermions with $(-\frac{k_x}{2}, 0)$, $(\frac{k_x}{2}, 0)$ and $\left(\frac{\pi}{2}, \frac{\pi}{2} - \frac{k_y}{2}\right)$, $\left(\frac{\pi}{2}, \frac{\pi}{2} + \frac{k_y}{2}\right)$, respectively. There are other high–frequency excitations in Figs. 1, 2, conditioned by two fermions with $k_1 = (0, 0)$ and $k_1 + k$ ($k_y = 0$) or with $k_1 = (\frac{\pi}{2}, \frac{\pi}{2})$ and $k_1 + k$ ($k_x = 0$), i.e.,
\[ \omega_{k_x,0}^{(3)} = J_{\perp} + \sqrt{J^2 \sin^2 k_x + J_{\perp}^2}, \quad \omega_{0,k_y}^{(3)} = J + \sqrt{J^2 + J_{\perp}^2 \sin^2 k_y}. \] (6)

It is interesting to note, that the derivative of the argument of \( \delta (\omega - \Lambda_{k_1} - \Lambda_{k_1+k}) \) with respect to \( k_{1x} \) tends to zero at \( k_x = \frac{\pi}{2}, \frac{3\pi}{2} \) \((k_y = 0)\) or at \( k_y = \frac{\pi}{2}, \frac{3\pi}{2} \) \((k_x = 0)\) that manifests itself as the increase of spectral weight in these regions clearly seen in some plots in Figs. 1, 2.

In the low–temperature limit, because of the Fermi factors, the \( \delta \)-functions \( \delta (\omega - \Lambda_{k_1} + \Lambda_{k_1+k}) \) and \( \delta (\omega + \Lambda_{k_1} - \Lambda_{k_1+k}) \) in Eq. (3) may contribute only if the energy of one of the two fermions equals to zero, i.e., if either \( \Lambda_{k_1} = 0 \) or \( \Lambda_{k_1+k} = 0 \). As a result, we easily derive the lower boundary for the region of nonzero values of \( S_{zz}(k,\omega) \)

\[ \omega_{k}^{(4)} = \sqrt{J^2 \sin^2 k_x + J_{\perp}^2 \sin^2 k_y}. \] (7)

At high temperatures, the Fermi factors do not impose the mentioned restriction. Putting \( k_{1x} = -k_x, \ k_{1y} = \frac{\pi}{2} - k_x \) for \( k_y = 0 \) and \( k_{1x} = k_y, \ k_{1y} = \frac{\pi}{2} - k_y \) for \( k_x = 0 \) we get

\[ \omega_{k_x,0}^{(5)} = \left( \sqrt{J^2 + J_{\perp}^2} - J \right) \left| \sin k_x \right|, \quad \omega_{0,k_y}^{(5)} = \left( \sqrt{J^2 + J_{\perp}^2} - J \right) \left| \sin k_y \right|. \] (8)

The excitation branch \( \omega_{k}^{(5)} \) (8) contains most of the spectral weight at high temperatures (see Fig. 2).

Obviously in our analysis of \( S_{zz}(k,\omega) \) we focus mainly on the consequences presumed by the \( \delta \)-functions involved in (3) omitting the precise examination of a role of the rest of the factors (e.g., of the Fermi factors which controls a redistribution of the spectral weight as temperature increases). On the other hand, the results presented in Figs. 1, 2 (and Fig. 3) reflect all those underlying features of Eq. (3).

In Fig. 3, we show the constant wave vector scans of \( zz \) dynamic structure factor, i.e., the frequency dependence of \( S_{zz}(k,\omega) \) for certain wave vectors (the corresponding sections in Figs. 1, 2 can be easily located). All the discussed properties of \( S_{zz}(k,\omega) \) clearly manifest themselves in the depicted frequency profiles which may be almost symmetric or asymmetric, resemble \( \delta \)-peaks, result from two coalesced peaks or exhibit tails which gradually disappear or are abruptly cut off. We indicate by numbers \( j \) some well pronounced peaks and cusps corresponding to the modes \( \omega_{k}^{(j)} \) (4) – (8).

To summarize, we have presented the first results for \( zz \) dynamic structure factor of the spin–\( \frac{1}{2} \) isotropic \( XY \) model on a spatially anisotropic square lattice derived on the basis of the two–dimensional Jordan–Wigner fermionization. Our study has indicated excitations which govern the \( zz \) dynamic structure factor.
The established modes may manifest themselves as peaks or cusps in frequency profiles of $S_{zz}(k, \omega)$ and may be used for determining the Hamiltonian parameters. (For example, the gap seen in Fig. 2a and Fig. 3e is controlled by $\omega_{k_x,0}^{(3)}$, $\omega_{k_x,0}^{(4)}$, and $\omega_{k_x,0}^{(5)}$, and, in particular, $\omega_{z,0}^{(3)} = \sqrt{J^2 + J_\perp^2 + J_\perp}$, $\omega_{z,0}^{(4)} = J$, and $\omega_{z,0}^{(5)} = \sqrt{J^2 + J_\perp^2 - J_\perp}$.) Thus, the theoretical result observed in our work should prove valuable in understanding the experimentally observable dynamic properties of two-dimensional spin-$\frac{1}{2}$ isotropic XY materials. However, there are, to our knowledge, no experimental results yet available (therefore, no compound specific parameters were considered above) that enable a direct comparison between theory and experiment to be made.

It should be stressed that our results for the considered two-dimensional spin model contains the exact ones in the one-dimensional limit (after putting $J_\perp = 0$ or $J = 0$). On the other hand, our approach is approximate because of the mean-field description of the phase factors which arise after fermionization. Such a treatment neglects the complicated interaction between fermions. It would be desirable to estimate the effects of this simplification going beyond the mean-field scheme for the phase factors. A possible test of the results for spin correlation functions is a comparison with the corresponding data of exact diagonalization and other numerical approaches. (Note, however, that the results reported in Refs. 3, 10 refer to the in-plane spin correlation functions but not to the $zz$ spin correlation functions which are different for the isotropic XY model in contrast to the case of the isotropic Heisenberg model.) In the case of the isotropic Heisenberg model the interaction between fermions is present even within the adopted approximate procedure due to the (Ising) interaction of $z$ spin components. The quartic terms in the fermion Hamiltonian are treated after making further approximation\textsuperscript{5}. One of the ways to proceed (the uniform flux solution) yields the same results for both the XY and Heisenberg models and from such a viewpoint our results for the dynamic properties may refer to the square-lattice spin-$\frac{1}{2}$ isotropic Heisenberg model as well. However, as one can conclude from the studies reported in Refs. 5, 6, a more sophisticated treatment of the fermion interaction inherent in the latter spin model (the in-phase flux solution, the Néel flux solution, the in-phase Néel flux solution) would be more appropriate. It seems obvious to extend the present investigation to the study of the square-lattice spin-$\frac{1}{2}$ isotropic Heisenberg model which is used for interpreting the data for corresponding compounds\textsuperscript{2}. It is interesting to note
that the recent neutron scattering studies on Cs$_2$CuCl$_4$ (the minimal model of this two-dimensional compound is the spin-$\frac{1}{2}$ antiferromagnetic Heisenberg model on a triangular lattice)$^{12}$ definitely show a highly dispersive continuum of excited states. The conventional spin–wave theory clearly fails to account for the observed line shapes which do not show single particle poles but rather extended continua. We can also see some similarities at a qualitative level of the frequency profiles plotted in Fig. 3 of the present paper and in Fig. 3 of Ref. 12. However, we should bear in mind that Cs$_2$CuCl$_4$ is a triangular but not a square–lattice two-dimensional system and that the minimal Hamiltonian determining the magnetic order is the isotropic Heisenberg model but not the isotropic $XY$ model. New theoretical work is needed to elaborate the two-dimensional Jordan–Wigner fermionization results for this compound. Another possible application refers to dynamics of spin-$\frac{1}{2}$ ladders. Recently$^{13}$ the dynamic properties of the two-leg spin-$\frac{1}{2}$ ladder have been examined using the one-dimensional Jordan–Wigner fermionization. It seems interesting to compare these results with the corresponding ones which arise within the two-dimensional Jordan–Wigner fermionization approach.

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FIGURE CAPTURES

FIGURE 1. The $zz$ dynamic structure factor (greyscale plots) for the square–lattice spin–$\frac{1}{2}$ isotropic $XY$ model as it follows from Eq. (3) at zero temperature. $J = 1$, $J_\perp = 0.1$ (a, b), $J_\perp = 0.5$ (c, d), $J_\perp = 0.9$ (e, f); $k_y = 0$ (a, c, e), $k_x = 0$ (b, d, f).

FIGURE 2. The same as in Fig. 2 at high temperature $\beta = 0.1$.

FIGURE 3. Frequency dependence of the $zz$ dynamic structure factor (3) for momentum transfer along the chain ($k_x = \frac{\pi}{2}$ (a, e), $k_x = \pi$ (b, f), $k_y = 0$) and for momentum transfer perpendicularly to the chain ($k_x = 0$, $k_y = \frac{\pi}{2}$ (c), $k_y = \pi$ (d)) as the interchain interaction changes ($J = 1$, $J_\perp = 0.1$ (dotted curves), $J_\perp = 0.5$ (dashed curves), $J_\perp = 0.9$ (solid curves)) at zero temperature (a, b, c, d) and high temperature $\beta = 0.1$ (e, f).
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