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JORDAN–WIGNER FERMIONS AND THE SPIN $1/2$ ANISOTROPIC *XY* MODEL ON A SQUARE LATTICE*

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Using the two-dimensional Jordan–Wigner fermionization we calculate the thermodynamic quantities of the (spatially anisotropic) square-lattice spin $1/2$ anisotropic XY (XZ) model. We compare the results of different approaches for the ground-state and thermodynamic properties of the model.

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Two-dimensional (2D) quantum spin models have been extensively studied during last years mainly because it is believed that they may be of use for describing the magnetic properties of CuO_2 layers in the high-temperature superconductors [1]. There exist a number of analytical approaches for a study of the thermodynamic properties of 2D quantum spin models, *e.g.*, the conventional spin-wave analysis, the Green function technique, the approach based on the 2D Jordan–Wigner fermionization as well as the coupled cluster method, the correlated basis function method *etc.* In what follows we consider the spin $1/2$ anisotropic XY model on a spatially anisotropic square lattice within the framework of the scheme based on the 2D Jordan–Wigner fermionization and compare the results derived for the ground-state and thermodynamic quantities with the exact ones (1D limit, square-lattice

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Ising model) and the predictions of other approximate theories. The performed calculations yield an impression about the region of validity of some approaches usually applied for a study of thermodynamics of 2D quantum spin models.

We start from a model of $N\to\infty$ spins $1/2$ on a spatially anisotropic square lattice governed by the anisotropic XY Hamiltonian

$$H = \sum_{i=0}^{\infty}\sum_{j=0}^{\infty}\Big(J\Big((1+\gamma)s_{i,j}^x s_{i+1,j}^x+(1-\gamma)s_{i,j}^y s_{i+1,j}^y\Big) + J_{\perp}\Big((1+\gamma)s_{i,j}^x s_{i,j+1}^x+(1-\gamma)s_{i,j}^y s_{i,j+1}^y\Big)\Big). \qquad (1)$$

Here J and $J_{\perp}=RJ$ are the exchange interactions between the neighbouring sites in a row and a column, respectively (for concreteness we assume both to be positive), and the parameter γ controls the anisotropy of the exchange interaction. Making use of the 2D Jordan–Wigner fermionization and adopting a mean-field treatment of the phase factors which appear after the fermionization [2, 3] we perform consequently the Fourier and Bogolyubov transformations to arrive at the following Hamiltonian of noninteracting spinless fermions which represent the initial spin model (1)

$$H = {\sum_{\boldsymbol{k}}}' \sum_{\alpha=1}^{2} \Lambda_{\alpha}(\boldsymbol{k})\left(\eta_{\boldsymbol{k},\alpha}^{+}\eta_{\boldsymbol{k},\alpha}-\tfrac{1}{2}\right), \qquad (2)$$

$$\Lambda_1(\boldsymbol{k}) = \sqrt{\left(J_{\perp}\cos k_y+\gamma J\cos k_x\right)^2+\left(J\sin k_x+\gamma J_{\perp}\sin k_y\right)^2}\,,$$

$$\Lambda_2(\boldsymbol{k}) = \sqrt{\left(J_{\perp}\cos k_y-\gamma J\cos k_x\right)^2+\left(J\sin k_x-\gamma J_{\perp}\sin k_y\right)^2}\,,$$

(the prime denotes that $\boldsymbol{k}$ in the thermodynamic limit varies in the region $-\pi\le k_x\le\pi$, $-\pi+|k_x|\le k_y\le\pi-|k_x|$). The Helmholtz free energy per site

$$f=-\frac{1}{2\beta}\int_{-\pi}^{\pi}\frac{dk_x}{2\pi}\int_{-\pi}^{\pi}\frac{dk_y}{2\pi}\left(\ln\left(2\cosh\frac{\beta\Lambda_1(\boldsymbol{k})}{2}\right)+\ln\left(2\cosh\frac{\beta\Lambda_2(\boldsymbol{k})}{2}\right)\right), \qquad (3)$$

yields the thermodynamic properties of the spin model (1). In Fig. 1 we plot the ground-state energy per site of the spin model (1), (2) (dotted curves) in comparison with the exact results if $R=0$ (1D XY model) or $\gamma=1$ (square-lattice Ising model) and the spin-wave theory result for $\gamma=0$, $R=1$ (spatially isotropic square-lattice isotropic XY model). Eq. (3) contains the exact result in 1D limit (Fig. 1(b)), however, deviates noticeably from the exact result for $\gamma = 1$ (compare the curves 3 in Fig. 1(a)). For $\gamma = 0$, $R = 1$ Eq. (3) yields the result which differs from the spin-wave theory prediction denoted by the full circles. (The outcomes of different numerical approaches (see [4]) lie within the full circles.) From the exact calculation for $\gamma = 1$ [5] we know that the temperature dependence of the specific heat exhibits a logarithmic singularity. Obviously, the Jordan–Wigner fermions (2), (3) cannot reproduce this peculiarity inherent in the spin model.

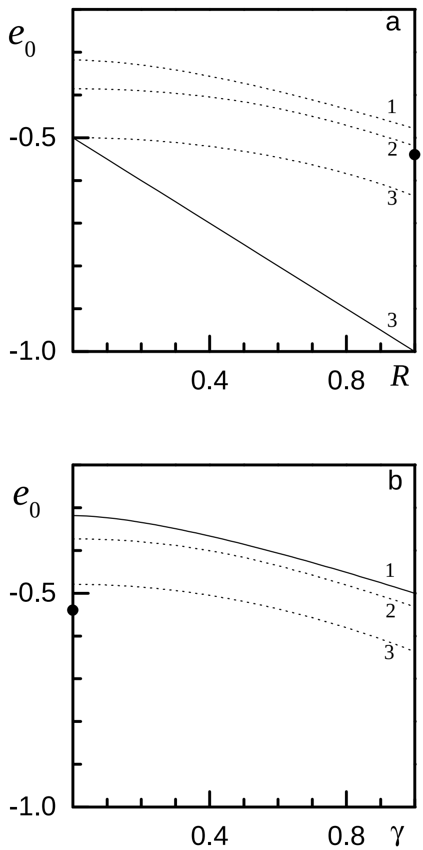

Fig. 1. The ground-state energy per site for the square-lattice spin $^1/_2$ anisotropic XY model (1) e_0 *versus* R (a) ($1 - \gamma = 0$, $2 - \gamma = 0.5$, $3 - \gamma = 1$) and e_0 *versus* γ; (b) ($1 - R = 0$, $2 - R = 0.5$, $3 - R = 1$); exact results (solid curves) and the approximate results obtained on the basis of (2) (dotted curves); the full circles correspond to the spin-wave result for $\gamma = 0$, $R = 1$.

It is worth to remind here that the conventional spin-wave theory was originally thought to be unsatisfactory for quantum XY models [6]. However, the authors of the paper [7] showed that considering the XZ rather than the XY Hamiltonian one gets within the spin-wave theory satisfactory results of the same quality as for the Heisenberg Hamiltonian. Following this idea we perform the rotation of the spin axes $s^x \to -s^z$, $s^y \to s^x$, $s^z \to -s^y$ and consider instead of (1) the following Hamiltonian

$$H = \sum_{i=0}^{\infty}\sum_{j=0}^{\infty}\Big(J\Big((1-\gamma)s^x_{i,j}s^x_{i+1,j} + (1+\gamma)s^z_{i,j}s^z_{i+1,j}\Big) + J_{\perp}\Big((1-\gamma)s^x_{i,j}s^x_{i,j+1} + (1+\gamma)s^z_{i,j}s^z_{i,j+1}\Big)\Big). \quad (4)$$

Proceeding further with (4) in the described above manner and assuming (for concreteness) antiferromagnetic long-range order while decoupling the quartic fermionic terms [8] we get instead of (2) the following Hamiltonian

$$H = {\sum_{\boldsymbol{k}}}' \sum_{\alpha=1}^{2} \Lambda_{\alpha}(\boldsymbol{k})\left(\eta^+_{\boldsymbol{k},\alpha}\eta_{\boldsymbol{k},\alpha} - \frac{1}{2}\right) + N(1+\gamma)(J+J_{\perp})\,m^2, \quad (5)$$

$$\Lambda_{1,2}(\boldsymbol{k}) = 2\sqrt{\mathcal{A}^2+\mathcal{B}^2+\mathcal{C}^2+\mathcal{D}^2+\mathcal{M}^2 \pm 2\sqrt{2\mathcal{ABCD}+\mathcal{A}^2\mathcal{D}^2+\mathcal{B}^2\mathcal{C}^2+\mathcal{M}^2(\mathcal{B}^2+\mathcal{D}^2)}},$$

$$\begin{aligned}
\mathcal{A} &= \frac{1-\gamma}{4}J_{\perp}\cos k_y,\\
\mathcal{B} &= \frac{1-\gamma}{4}J_{\perp}\sin k_y,\\
\mathcal{C} &= \frac{1-\gamma}{4}J\sin k_x,\\
\mathcal{D} &= \frac{1-\gamma}{4}J\cos k_x,\\
\mathcal{M} &= (1+\gamma)(J+J_{\perp})\,m,
\end{aligned}$$

where m is determined self-consistently by minimizing the Helmholtz free energy per site

$$2(1+\gamma)(J+J_{\perp})\,m = \frac{1}{4}\int_{-\pi}^{\pi}\int_{-\pi}^{\pi}\frac{d\boldsymbol{k}}{(2\pi)^2}\left(\frac{\partial\Lambda_1(\boldsymbol{k})}{\partial m}\tanh\frac{\beta\Lambda_1(\boldsymbol{k})}{2} + \frac{\partial\Lambda_2(\boldsymbol{k})}{\partial m}\tanh\frac{\beta\Lambda_2(\boldsymbol{k})}{2}\right). \quad (6)$$

In Fig. 2 we plot the ground-state energy of the spin model (4) – (6) (dashed curves). The results based on Eqs. (5), (6) for $\gamma = 1$ reproduce the exact result for square-lattice Ising model (curve 3 in Fig. 2(a)) as well as the spin-wave theory prediction for $\gamma = 0$, $R = 1$. However, the result based on Eqs. (5), (6) for $R = 0$ does not coincide with the exact one in 1D limit (curve 1 in Fig. 2(b)).

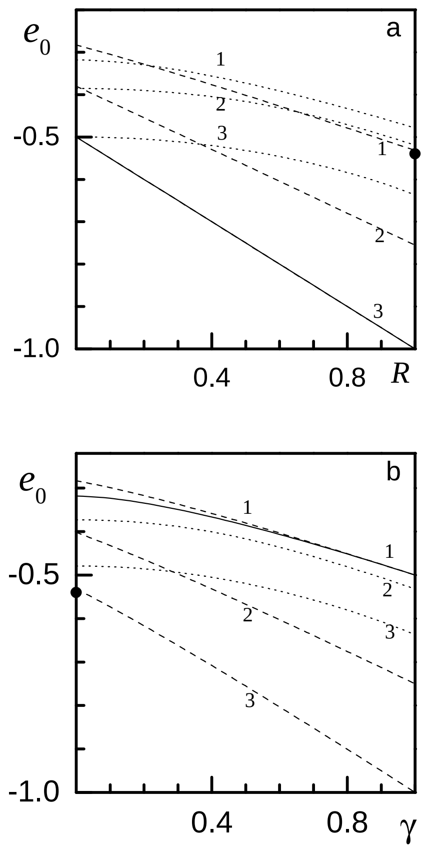

Fig. 2. The same as in Fig. 1 for the XZ Hamiltonian (4); the approximate results obtained on the basis of (5), (6) are shown by dashed curves.

To summarize, we have calculated the thermodynamic quantities for the spin $^1/_2$ anisotropic XY (XZ) model on a spatially anisotropic square lattice using the 2D Jordan–Wigner fermionization. To reveal a quality of the results obtained within the framework of this approach we have compared them with the exact results available in 1D limit and extremely anisotropic exchange interaction limit (Ising interaction). We have found that although there is an agreement with the spin-wave theory and other approximate approaches a disagreement with the exact results may be noticeable. Thus, the question about the quality of the results based on the 2D Jordan–Wigner fermionization (as well as, *e.g.*, of the spin-wave theory results) remains still open and requires further studies. Moreover, for arbitrary values of anisotropy parameter γ ($\gamma \neq 1$) for $R \neq 0$ a comparison with the exact diagonalization data and results of other numerical approaches is desirable.

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