Supplemental Material to the article

" Thermodynamics of the Symmetric Spin-orbital Model: One- and Two-dimensional Cases"

1. Expressions for Green's functions

Spin-spin and spin-pseudospin retarded Green's functions are.

$$G_{\mathbf{q}} = \left\langle S^z_{\mathbf{q}} \mid S^z_{-\mathbf{q}} \right\rangle_\omega , \tag{S1}$$

$$R_{\mathbf{q}} = \left\langle T^z_{\mathbf{q}} \mid S^z_{-\mathbf{q}} \right\rangle_\omega . \tag{S2}$$

Obviously $\left\langle T^z_{\mathbf{q}} \mid T^z_{-\mathbf{q}} \right\rangle_\omega = \left\langle S^z_{\mathbf{q}} \mid S^z_{-\mathbf{q}} \right\rangle_\omega$, because we consider symmetric case $I = J$.

Self-consistent spherically symmetric approach leads to the following expressions for $G_{\mathbf{q}}$ $R_{\mathbf{q}}$:

$$G_q = \frac{F_{\rm ac}(\mathbf{q})}{\omega^2 - \omega^2_{\rm ac}(\mathbf{q})} + \frac{F_{\rm opt}(\mathbf{q})}{\omega^2 - \omega^2_{\rm opt}(\mathbf{q})}, \tag{S3}$$

$$R_{\mathbf{q}} = \frac{F_{\rm ac}(\mathbf{q})}{\omega^2 - \omega^2_{\rm ac}(\mathbf{q})} - \frac{F_{\rm opt}(\mathbf{q})}{\omega^2 - \omega^2_{\rm opt}(\mathbf{q})}. \tag{S4}$$

2D case. The numerators for acoustic and optical branches are

$$F_{\rm ac} = \frac{F_1 + F_2}{2},\ F_{\rm opt} = \frac{F_1 - F_2}{2}, \tag{S5}$$

$$F_1 = -8Jc_g(1-\gamma_{\mathbf{q}}) - Mm_0,\ F_2 = Mm_0, \tag{S6}$$

and the excitations spectra

$$\omega^2_{\rm ac}(\mathbf{q}) = W_1 + W_2,\ \omega^2_{\rm opt}(\mathbf{q}) = W_1 - W_2, \tag{S7}$$

$$\begin{aligned} W_1 &= 2J^2(1-\gamma_{\mathbf{q}})\Big\{1 + 4\big[\widetilde{c}_{2g} + 2\widetilde{c}_d - \widetilde{c}_g(1+4\gamma_{\mathbf{q}})\big]\Big\} + \\ &\quad + 4JM(2\widetilde{m}_g - \widetilde{m}_g\gamma_{\mathbf{q}} - \widetilde{m}_0\gamma_{\mathbf{q}}) + \frac{1}{8}M^2, \end{aligned} \tag{S8}$$

$$W_2 = -4JM\left[\widetilde{c}_g(1-\gamma_{\mathbf{q}}) + \widetilde{m}_g - \widetilde{m}_0\gamma_{\mathbf{q}}\right] - \frac{1}{8}M^2, \tag{S9}$$

here $c_r = \langle \widehat{S}^z_{\mathbf{i}} \widehat{S}^z_{\mathbf{i+r}} \rangle$, $\quad r = g, d, 2g$ are spin-spin correlation functions, respectively for first (side of the square) $c_g \equiv c_1$, second (diagonal) $c_d \equiv c_2$ and third (doubled side) $c_{2g} \equiv c_3$ nearest neighbors, $\widetilde{c}_r = \alpha_r c_r$ are correlation functions with vertex corrections. The lattice sum for square case $\gamma_{\mathbf{q}} = \frac{1}{4}\sum_{\mathbf{g}} e^{i\mathbf{qg}} = \frac{1}{2}(\cos(q_x) + \cos(q_y))$.

Hereinbefore on-site m_0 and intersite $m_g \equiv m_1$ spin-pseudospin correlation functions are

$$m_0 = \langle S^z_{\mathbf{i}} T^z_{\mathbf{i}} \rangle, \quad m_g = \langle S^z_{\mathbf{i}} T^z_{\mathbf{i+g}} \rangle, \tag{S10}$$

and for the intersubsystem vertex corrections $\widetilde{m}_0 = \alpha^0_{ST} m_0$, $\widetilde{m}_g = \alpha^g_{ST} m_g$ we adopted the approximation $\alpha^0_{ST} = \alpha^g_{ST} = 1$. For simplicity we use the notation $M = 8Km_0$.

Note, that the following relations for the symmetrical points $\mathbf{\Gamma} = (0,0)$ and $\mathbf{Q} = (\pi,\pi)$ in the Brillouin zone are always fulfilled

$$\omega_{\rm opt}(\mathbf{\Gamma}) \geq \omega_{\rm ac}(\mathbf{\Gamma}) = 0, \quad \omega_{\rm ac}(\mathbf{Q}) \geq \omega_{\rm opt}(\mathbf{Q}) \geq 0. \tag{S11}$$

1D case.

$$F_{\rm ac} = \frac{F_1 + F_2}{2},\ F_{\rm opt} = \frac{F_1 - F_2}{2}, \tag{S12}$$

$$F_1 = -4Jc_g(1-\gamma_{\mathbf{q}}) - Mm_0,\ F_2 = Mm_0 \tag{S13}$$

$$W_1 = J^2(1-\gamma_{\mathbf{q}})\Big\{1+4\big[\widetilde{c}_{2g}-\widetilde{c}_g(1+2\gamma_{\mathbf{q}})\big]\Big\}+ \\ +2JM\,(2\widetilde{m}_g-\widetilde{m}_o\gamma_{\mathbf{q}}-\widetilde{m}_g\gamma_{\mathbf{q}})+\frac{1}{8}M^2, \tag{S14}$$

$$W_2 = -2JM\,[\widetilde{c}_g(1-\gamma_{\mathbf{q}})+\widetilde{m}_g-\widetilde{m}_0\gamma_{\mathbf{q}}]-\frac{1}{8}M^2, \tag{S15}$$

now $M = 4Km_0$, $\gamma_{\mathbf{q}}$ is one-dimensional, other notations are the same as for 2D case.

2. Three Figures from [1]. In Figures S1, S3 almost invisible nonzero values of m_0 and m_1 just before the transition ($T \gtrsim T_c$ for Fig. S1 and $K \gtrsim K_c$ for Fig. S3) show the accuracy of the self-consistent calculations.

References

[1] M. Y. Kagan, K. I. Kugel, A. V. Mikheyenkov, and A. F. Barabanov, JETP Lett. **100**, 187 (2014).

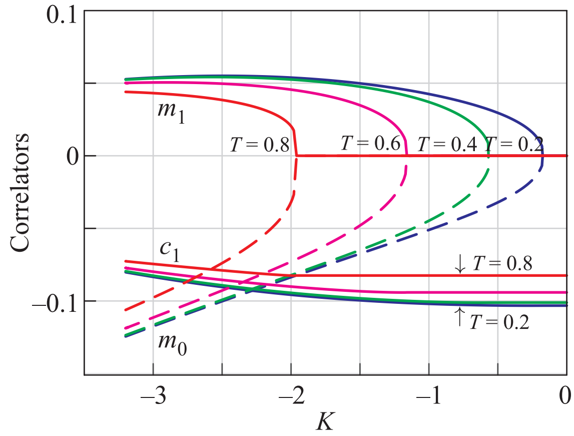

Fig. S1. (Color online) 2D lattice. Spin-spin and spin-pseudospin correlation functions versus the intersubsystem exchange parameter K for different temperatures. Spin-spin nearest neighbor correlator c_1 – lower solid lines, on-site spin-pseudospin correlators m_0 – upper solid, nearest neighbor spin-pseudospin correlators m_1 – dotted. Different colors correspond to different temperatures. For m_0 and m_1 curves the temperatures are marked on the zero y-axis. For c_1 lines the boundary values of T are indicated (from [1])

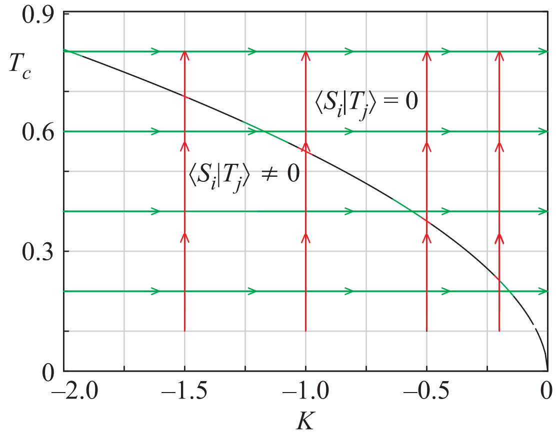

Fig. S2. (Color online) 2D lattice. Regions corresponding to zero and nonzero spin-pseudospin correlations. The phase boundary is well fitted by the $T_c = 0.55|K|^{0.55}$ curve (from [1]). Lines with arrows show the paths, along which the results for 2D case are presented (Figs. 1, 2 in Supllemenraty, Figs. 1, 2 in the main text)

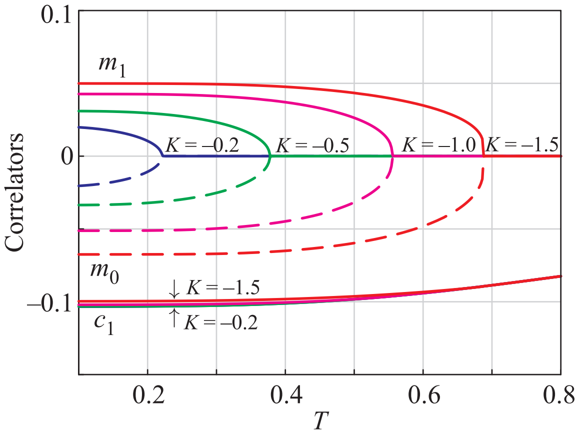

Fig. S3. (Color online) 2D lattice. T-dependence of the correlation functions at several fixed K values. As in Fig. 1, spin-spin nearest neighbor correlator c_1 – lower solid lines, on-site spin-pseudospin correlators m_0 – upper solid, nearest neighbor spin-pseudospin correlators m_1 – dotted. Different colors correspond to different K-values. For m_0 and m_1 curves K-values are marked on the zero y-axis. For c_1 lines the boundary K-values are indicated. The curves $|m_0|(T)$ and $m_g(T)$ are well fitted by power law $m \sim (T_c - T)^\alpha$ with the exponent $\alpha \sim 0.3 \div 0.5$ nearly independent of K (from [1])