JETP Letters, Vol. 79, No. 1, 2004, pp. 53–56. Translated from Pis'ma v Zhurnal Éksperimental'noĭ i Teoreticheskoĭ Fiziki, Vol. 79, No. 1, 2004, pp. 59–62.
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Quantum Magnetostriction Oscillations in a Two-Dimensional Antiferromagnet with Spin–Phonon Interaction in a Magnetic Field

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Received December 8, 2003

The ground state of a two-dimensional antiferromagnet with $S = 1/2$ interacting with acoustic phonons in a magnetic field was studied by the quantum Monte Carlo method in the nonadiabatic approximation. Oscillations of the amplitude of the root-mean-square displacement of ions and the average phonon occupation number in a magnetic field were found. Local maxima were revealed in the distribution functions of site magnetic moments and ion displacements. The saturation magnetization was calculated as a function of the spin–phonon coupling constant. *© 2004 MAIK "Nauka/Interperiodica".*

PACS numbers: 75.10.Jm; 75.30.Cr; 75.80.+q

Phase separation in manganites and the formation of strips in undoped cuprate superconductors are bright effects in condensed state physics. Such effects associated with strip structures are also observed in the spin system with four-spin interaction on a square lattice [1]. The model with four-spin interaction is a particular case of a more general model of spin interaction with acoustic phonons.

Additional incommensurable maxima in the magnetic and nuclear structural factors were calculated for a ferromagnet with spin–phonon interaction on a square lattice [2]. Several maxima were also found in the density of states of bound spin–phonon quasiparticles. Under the action of an external magnetic field, the bound state of spins and phonons decays, resulting in an increase in the average number of phonons. This communication is devoted to the determination of the behavior of the amplitude of the root-mean-square displacement of ions in a magnetic field and the saturation magnetization, which has the constant value $m_s = 1$ for systems with spin–phonon interaction within the adiabatic approximation [3, 4].

Consider the ground state of a quasi-two-dimensional magnet with the interplane exchange interaction that is several orders of magnitude smaller than the intraplane exchange interaction. Therefore, the consideration will be restricted to the spin interaction between the nearest neighbors and with the acoustic modes of in-plane lattice vibrations. The Hamiltonian for a bound spin–phonon system in the harmonic approximation takes the form

$$\begin{aligned} H = & \sum_{i,j}[J + \alpha(u_{i,j} - u_{i+1,j})] \\ & \times [S^z_{i,j}S^z_{i+1,j} + (S^+_{i,j}S^-_{i+1,j} + S^-_{i,j}S^+_{i+1,j})/2] + H_i S^z_i \\ & + [J + \alpha(u_{i,j} - u_{i,j+1})] \\ & \times [S^z_{i,j}S^z_{i,j+1} + (S^+_{i,j}S^-_{i,j+1} + S^-_{i,j}S^+_{i,j+1})/2] + M\dot{u}^2_{i,j}/2 \\ & + K(u_{i,j} - u_{i+1,j})^2/2 + K(u_{i,j} - u_{i,j+1})^2/2, \end{aligned} \quad (1)$$

where $S^{z,\pm}$ are the components of the spin operator $S = 1/2$ on a lattice site, $u_{i,j}$ is the ion displacement along the lattice translation vectors, M is the ion mass, and K is the elastic lattice constant; $J > 0$. Using the canonical transformation

$$\hat{u}_{\mathbf{r}} = \frac{1}{\sqrt{N}}\sum_{\mathbf{q}}\sqrt{\frac{\hbar}{2M\Omega(\mathbf{q})}}(b_{\mathbf{q}} + b^+_{-\mathbf{q}})\exp(i\mathbf{qr}), \quad (2)$$

the variables $u_{i,j}$ will be converted to the phonon creation and annihilation operators b^+ and b with the momenta $q_\beta = 2\pi n/L$, $n = 1, 2, \ldots, L$; $\beta = x, y$; and the lattice constant $a = 1$. The transformed Hamiltonian has the form

$$H = \sum_{i,j}(J_{i,j}\mathbf{S}_i\mathbf{S}_j + H_i S^z_i)$$

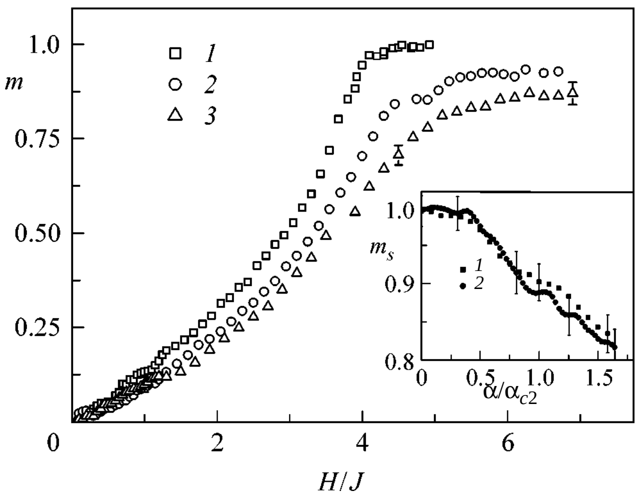

Fig. 1. Field dependence of the magnetization in an AFM and in a spin liquid for $\omega_0 = J$ and α/α_{c2} = (*1*) 0, (*2*) 1, and (*3*) 1.5. The inset displays the dependence of the saturation magnetization on the normalized spin–phonon coupling constant for ω_0/J = (*1*) 1 and (*2*) 6.

$$+\sum_{q_x, q_y}\sum_{n, m}\alpha\sqrt{\frac{\hbar}{2M\Omega(\mathbf{q})}}\exp(i\mathbf{qr})(b_{\mathbf{q}} + b^{+}_{-\mathbf{q}})$$

$$\times[(1-\cos q_x - i\sin q_x)\mathbf{S}_{n,m}\mathbf{S}_{n+1,m} \quad (3)$$

$$+(1-\cos q_y - i\sin q_y)\mathbf{S}_{n,m}\mathbf{S}_{n,m+1}] + \sum_{\mathbf{q}}\hbar\Omega(\mathbf{q})b^{+}_{\mathbf{q}}b_{\mathbf{q}},$$

$$\Omega(\mathbf{q}) = \omega_0\sqrt{2-\cos(q_x)-\cos(q_y)}; \quad \omega_0 = \sqrt{\frac{2K}{M}}.$$

The calculations involve the spin–phonon coupling constant α normalized to the exchange interaction and the distance *r* normalized to the lattice constant. As the computational method, a quantum Monte Carlo method was selected. The method combined the worldline algorithm and the continuous time algorithm [5] on a plane with the size $N = 32 \times 32$ with periodic boundary conditions at the temperature $\beta = J/T = 10$. The computational method was described in detail in [2].

The root-mean-square displacement of an ion is determined as

$$\langle u^2\rangle = \frac{\hbar}{2MN}\sum_q\frac{2n_q+1}{\Omega(q)}.$$

In the ground state of a harmonic oscillator with $\alpha \longrightarrow 0$, the number of phonons equals zero. Therefore, it is important to calculate the variation of zero-point vibrations due to the action of the magnetic system on the elastic subsystem; that is, $\langle U_n^2\rangle = \langle u^2(\alpha)\rangle - \langle u^2(\alpha = 0)\rangle$. Below, the normalized value

$$\langle U^2\rangle = \sum_r\langle U_n^2(r)\rangle/\frac{\hbar}{2NM\omega_0}$$

will be used.

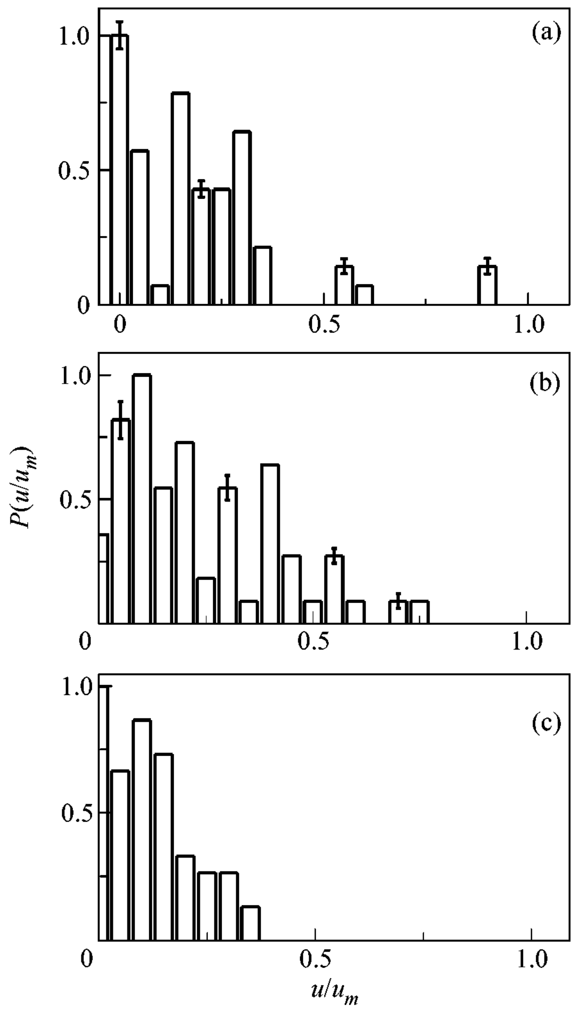

Fig. 2. Distribution functions of site ion displacements normalized to the maximum displacement u_m at $H = 0$ for $\omega_0 = J$, $\alpha/\alpha_{c2} = 1$, and H/J = (a) 0.5, (b) 2, and (c) 5.

In this work, two characteristic cases of the interaction of the spin and elastic subsystems are considered. These are the case when the threshold of the band of magnon excitations W_{tm} exceeds the threshold of the band of phonon excitations W_{tph}, which corresponds to the crossing of the dispersion curves of magnons and phonons, for example, at $\omega_0/J = 1$, and the opposite case when $W_{tph} > W_{tm}$ for $\omega_0/J = 6$. Typical dependences of the magnetization on the external magnetic field are presented in Fig. 1 for the magnetically ordered state and the magnetically disordered singlet state. The critical field of magnetic saturation for an antiferromagnet

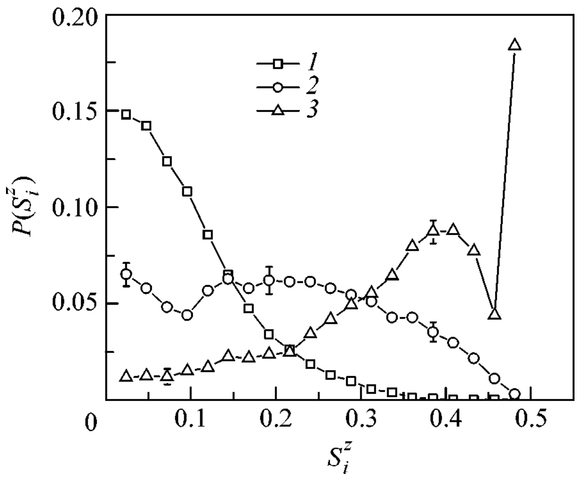

Fig. 3. Distribution functions of site magnetic moments for $\omega_0 = J$, $\alpha/\alpha_{c2} = 1$, and H/J = (*1*) 0.5, (*2*) 3, and (*3*) 5.

(AFM) is in good agreement with the known result $H_c = 2zSJ$. If the spin–phonon coupling parameter exceeds the critical value α_{c1}, at which the isotropy of spin–spin correlation functions becomes broken [2], the saturation field increases and the saturation magnetization m_s decreases. The corresponding values of m_s determined in the range of fields $H_c < H < 2H_c$ are displayed in the inset in Fig. 1. Here, the spin–phonon coupling parameters are normalized to the critical value α_{c2}, at which the long order disappears and a quantum spin liquid is formed. In the region of low fields, the magnetization grows linearly with increasing field even in the spin liquid state but with a smaller slope of $m(H)$. This dependence qualitatively differs from the dependence of the magnetization in the spin liquid with dimer ordering, for which $m(H) \longrightarrow 0$ at $H < \Delta$, where Δ is the energy gap in the spectrum of triplet excitations [6].

The elastic stresses induced by the spin subsystem have a hierarchical structure. The distribution function of ion displacements depicted in Fig. 2a exhibits several local maxima. In the region of local stresses, spins form singlet states. The existence of states is confirmed by the distribution function of the site magnetic moment $P(S^z \longrightarrow 0) \neq 0$ (Fig. 3) and by the calculation of the four-spin correlation function of parallel spin pairs

$$R(r) = \langle(\sigma_i + \sigma_{i+1})S_i^z S_{i+1}^z \times (\sigma_{i+r} + \sigma_{i+r+1})S_{i+r}^z S_{i+r+1}^z\rangle, \quad (4)$$

$$\sigma_i = \mathrm{sgn}(S_i^z).$$

The minima in the distance dependence of the four-spin correlation function presented in Fig. 4 correspond to the characteristic distance between the square-lattice sites with either zero values of the magnetic moment or an antiparallel arrangement of spins on the sites. Two such distances are observed in a magnetic field $H < H_c$,

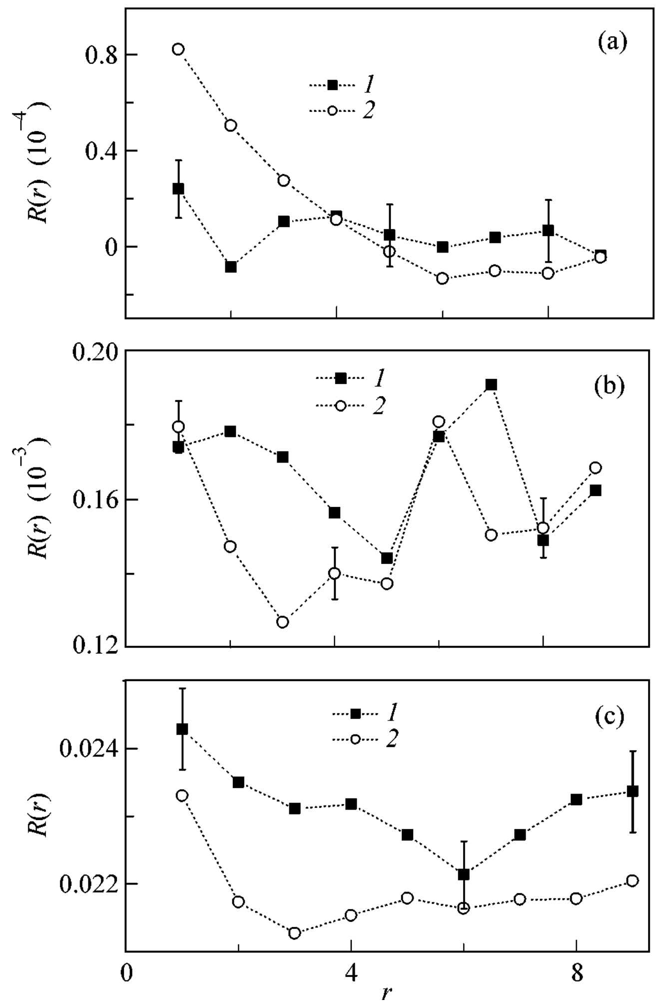

Fig. 4. Four-spin correlation functions for pairs of parallel spins calculated according to Eq. (4) for $\omega_0 = J$, $\alpha/\alpha_{c2} = 1$, and H/J = (a) 0.5, (b) 2, and (c) 5 in the (*1*) [100] and (*2*) [010] directions.

and one minimum in $R(r)$ exists in the saturation field. The wave function of this state can be represented as a linear combination of the singlet and triplet states of dimers $\psi \sim u(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle) - v|\uparrow\uparrow\rangle$, where the coefficients u and v depend on the field and the spin–phonon coupling parameter $u^2 \sim (1 + \delta/J)$, $v^2 \sim (1 - \delta/J)$, and $\delta = \alpha(u_i - u_{i+1})$.

The local singlet state decays in the magnetic field through the formation of two antiferromagnetic domain boundaries in which the loss in the Zeeman energy of the triplet with the effective exchange interaction $J - \delta$ is compensated by the gain in the exchange energy of the boundaries $J + \delta$. Estimations of the energy with regard to the exchange energy only for the longitudinal spin components lead to the critical magnetization $m_c = \sqrt{4 + 3\delta - 1.5K(\delta/\alpha)^2}/2\sqrt{(2)}$, above which the local stresses disappear.

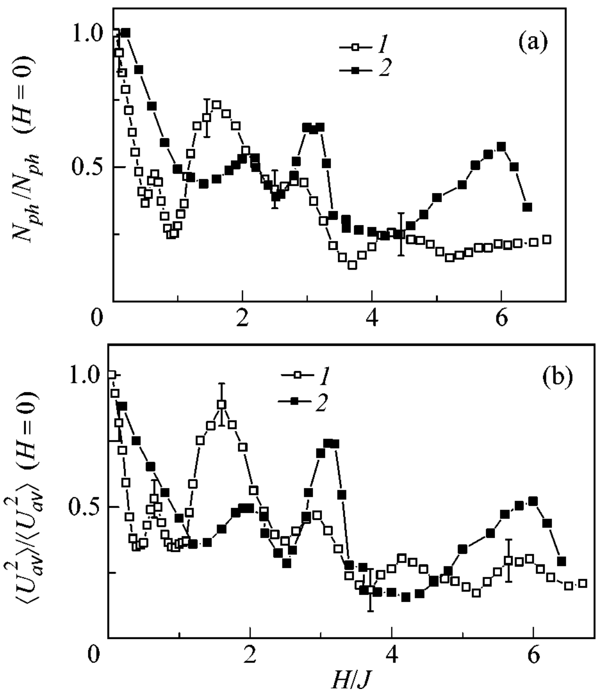

Fig. 5. (a) Average occupation numbers of phonons and (b) amplitudes of root-mean-square ion displacements $\langle U_{av}^2\rangle / \langle U_{av}^2(H = 0)\rangle$ normalized to the maximum zero-field value for (*1*) $\omega_0/J = 1$ and $\alpha/\alpha_{c2} = 1$ and (*2*) $\omega_0/J = 6$ and $\alpha/\alpha_{c2} = 1.35$ calculated as a function of the magnetic field.

The field dependences of the average occupation number of phonons and the root-mean-square displacement of ions are displayed in Fig. 5. The oscillations in the dependences $N_{ph}(H)$ and $\langle U^2(H)\rangle$ are due to the decay of the bound spin–phonon state $\langle S^\alpha \dots S^\beta b^\gamma \dots b^\nu\rangle \longrightarrow \langle S^\alpha \dots S^\beta\rangle\langle b^\gamma \dots b^\nu\rangle$ in the magnetic field corresponding to the effective bond energy. The resulting phonons give rise to new local maxima in the distribution function of ion displacements (Fig. 2b). In the saturation field, the dispersion of the distribution function $P(u_i/u_{max})$ decreases. In this case, it can be approximated by a double-peaked Gaussian function; this can also be done for the distribution function of site magnetic moments $P(S^z)$ depicted in Fig. 3. Thus, in fields $H > H_c$, the nonuniformity of the interrelated spin-density and elastic-stress distributions is retained.

In conclusion, the main results will be emphasized. Interaction between the elastic and magnetic subsystems leads to a disordered single state with a hierarchical structure of ion displacements. The decay of bound spin–phonon particles in magnetic fields induces phonons, which are pinned at domain boundaries. As a result, the field dependence of the amplitude of the root-mean-square displacement has an oscillating shape. In the saturation field, the nonuniformity of the distributions of site magnetic moments and ion displacements is retained, and the saturation magnetization monotonically decreases with increasing spin–phonon coupling constant.

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Translated by A. Bagatur'yants