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# Influence of spin–phonon coupling on the magnetic moment in 2D spin-1/2 antiferromagnet

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**Abstract**

The ground state of two-dimensional Heisenberg spin-1/2 antiferromagnet (AF) with the spin–phonon coupling is studied by the quantum Monte Carlo method. The magnetic moment per site, mean-square vibration of ion, phase diagram of AF long range order—quantum spin liquid are simulated. The spin–phonon coupling is estimated for $R_2CuO_4$, R = Gd, Eu.


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The two-dimensional (2D) quantum spin Heisenberg antiferromagnet (AF) has attracted a great deal of attention in connection with the properties of materials with high-temperature superconductivity. The parent compounds $R_2CuO_4$, R = Nd, Gd, Eu reveal low value of magnetic moment on site $\sigma \simeq 0.4$ [1] with fairly high Neel temperature $T_N \sim 250$–$280$ K. These materials have the $T'$ tetragonal structure and strong lattice fluctuations. The reflexes of X-ray measurements show spread ellipsoidal patch which are interpreted as a strong vibrations of oxygen ions [2]. The mean-square vibrations of $Cu^{2+}$ in plane CuO in $Eu_2CuO_4$ are decreased with increasing temperature and exhibit minimum at $T \sim 160$ K [3]. The interaction between magnetic and elastic subsystem is taken into account by spin–phonon coupling $(\alpha)$. Using perturbation theory up to fourth order in $\alpha$ in the antiadiabatic regime authors [4] have been derived effective spin Hamiltonian with long range interactions consisted of four- and six-spin coupling $(S_i \cdot S_j) \times (S_k \cdot S_l) \cdots (S_m \cdot S_n)$. The additional four-spin coupling $(K)$ and next-nearest-neighbor $(J_2)$ antiferromagnetic interaction result in spin nematic state [5] and quantum spin liquid (QSL) at $K/J_1 = 2$ [6]. A frustration caused by the competition between nearest-neighbor $(J_1)$ and $J_2$—interaction breakdowns long-range order and also forms the quantum spin liquid in the parameter range $J_2/J_1 \simeq 0.2$–$0.4$ [7]. The larger values $K$, $J_2$ imply the larger spin–phonon coupling. It means the interaction between spin and phonon subsystems needs to consider nonadiabatic limit. Using the unitary transformation and the second-order of expansion in terms of small parameter the sublattice magnetization, phase diagram AF-QSL [8], spin–spin corre-

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lation functions [9] have been calculated in the AF on a square lattice. These values may be essentially changed if the higher order terms of expansion will take into account.

In this Letter we consider interaction of spins $S = 1/2$ with acoustic phonons by quantum Monte Carlo method. Monte Carlo approaches restricted to finite lattice but without any adiabatic approximation and the truncation of the infinite phonon Hilbert space. The method [10] is based on a path-integral representation for discrete system in which we work directly in the Euclidean time continuum. All the configuration update procedures contain no small parameters.

We consider a model Hamiltonian of an spin–phonon system:

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

Here $S^{z,\pm}$ are a spin operator components associated with the site $(i, j)$, $J > 0$ is the usual antiferromagnetic exchange integral, $\alpha$ is the spin–phonon coupling constant, $u_{i,j}$ is the displacement in the $x$-, $y$-direction, $M$ is the mass of the ion and $K$ is the spring constant. Using the quantum representation for phonon operators $b$, $b^+$, the Hamiltonian maps to:

$$\begin{aligned} H = &\sum_{i,j} J_{i,j} \mathbf{S}_i \mathbf{S}_j \\ &+ \sum_{q_x,q_y} \sum_{n,m} \alpha \sqrt{\frac{\hbar}{M\Omega(\mathbf{q})}} \big[\sin(q_x n + q_y m + \pi/4) \\ &- i \sin(q_x n + q_y m - \pi/4)\big] \\ &\times \big(b_{\mathbf{q}} + b^+_{-\mathbf{q}}\big) \\ &\times \big[\sin q_x \mathbf{S}_{n,m} \mathbf{S}_{n+1,m} + \sin q_y \mathbf{S}_{n,m} \mathbf{S}_{n,m+1}\big] \\ &+ \sum_{\mathbf{q}} \hbar\Omega(\mathbf{q}) b^+_{\mathbf{q}} b_{\mathbf{q}}, \end{aligned}$$

$$\Omega(\mathbf{q}) = \omega_0 \sqrt{2 - \cos(q_x) - \cos(q_y)},$$

$$\omega_0 = \sqrt{\frac{2K}{M}}. \tag{2}$$

Spin–phonon coupling parameter $\alpha$ and temperature are normalized on the exchange $J$, $\hbar = 1$, $M = 1$. The temperature used in calculation is $\beta = J/T = 50$. The elastic subsystem is described by phonons with the number of occupation $n_{\text{ph}} = 0, 1, 2 \ldots$ and magnetic subsystem is in the $S^z$ representation. The continuous time world-line Monte Carlo approach based on the expansion of the statistical evolution operator $e^{-H/T}$ in powers of $J$ and $\alpha$ is applied. The world-line configuration of spins and phonons are updated through the space–time motions of the creation and annihilation operators. The periodic boundary conditions are applied on $L \cdot L$, $L = 32$ square lattices. 4000 Monte Carlo steps (MCS) per site are spent to reach equilibrium and another 8000 MCS are used for the averaging. The root mean square errors of the computed quantities lie in the range 0.1% to 0.6%.

Magnetic moment per site is evaluated by summing over imaginary-time and over lattice

$$\sigma = \left\langle \frac{1}{N} \sum_{i,j} (-1)^{i+j} \int_0^\beta S^z_{i,j}(\tau)\, d\tau \right\rangle,$$

where bracket $\langle \cdots \rangle$ denotes the thermal averages. Mean-square vibration of ion $\langle u^2 \rangle$ is simulated by

$$\langle u^2 \rangle = \frac{\hbar}{2MN} \sum_q \frac{2n_q + 1}{\Omega(q)}. \tag{3}$$

More important is to determine the relative change $\langle U^2 \rangle = \langle u^2(\alpha) \rangle - \langle u^2(\alpha = 0) \rangle$.

The values of $\sigma(\alpha)$ and $\langle U^2(\alpha) \rangle$ are simulated for set of acoustic frequency $\omega_0/J = 1, 2, 4, 6, 8, 10$ vs. spin–phonon coupling. The normalized value $\sigma(\alpha)/\sigma(0)$ and $\langle U^2(\alpha) \rangle$ reveal universal dependence on $\alpha/\alpha_c$ for case $\omega_0 < 2J$ and $\omega_0 > 2J$, as shown in Figs. 1 and 2. This difference may be due to appearing additional peculiarities in the density state of spin and phonon excitations if the branches of the corresponding excitations are intersected. The magnetic moment per site fits well to a straight line $\sigma/\sigma(0) = 1.14 - 1.3\alpha/\alpha_c$, $\omega_0 < 2J$ and $\sigma/\sigma(0) = 1.12 - 0.96\alpha/\alpha_c$, $\omega_0 > 2J$ in the parameters range $0.15 < \alpha/\alpha_c < 0.7$ and disappears sharp at the critical spin–phonon coupling $\alpha = \alpha_c$. Mean square vibrations of ions exhibit anisotropy, as illustrated in Fig. 2,

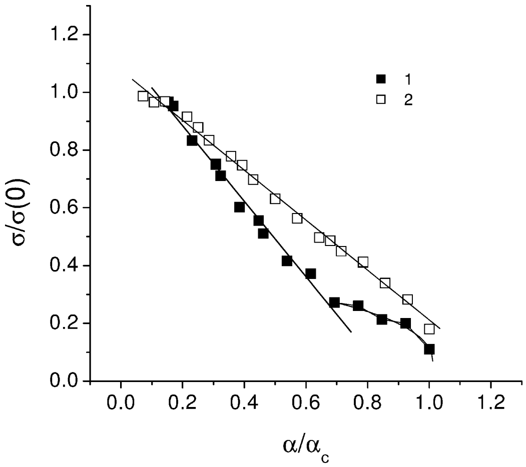


Fig. 1. The magnetic moment per site as a function of the spin–phonon coupling for $\omega_0 = J$ (1), $\omega_0 = 6J$ (2).

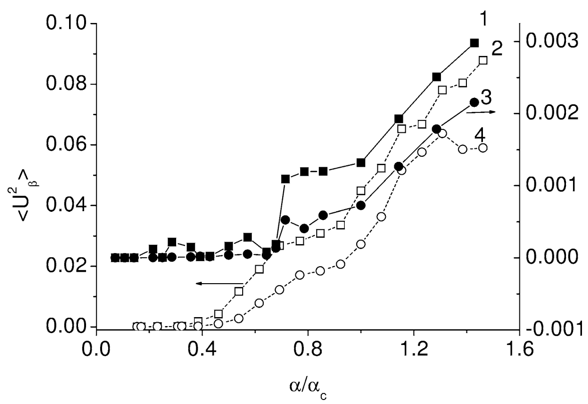


Fig. 2. Mean-square vibration $\langle U^2 \rangle$ vs. spin–phonon coupling at $\omega_0 = J$ (2,4), $\omega_0 = 6J$ (1, 3) along [10] (1, 2, $\beta = x$), [01] (3, 4, $\beta = y$) directions.

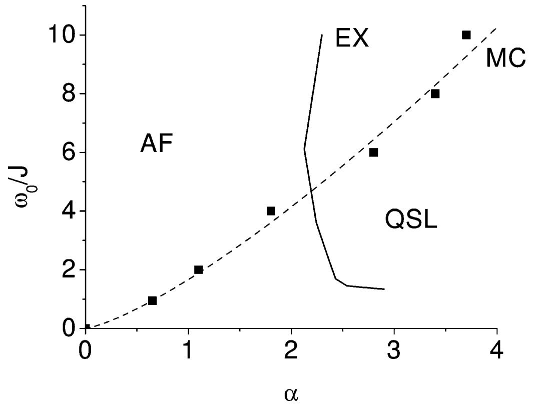


Fig. 3. The phase boundary AF-QSL calculated by MC and the expansion in terms of small parameter (EX) [8].

as result of dynamical lattice dimerization favored to decreasing magnetic energy.

Models of a static dimerized exchange are widely used to describe the spin-Peierls materials. Consideration of various kinds of exchange dimerization $\delta = J_{i,i+1} - J_{i,i-1}$ in square lattice [11] shows existence of the critical value $\delta_c \sim 0.5$. For $\delta < \delta_c$ the energy gain is achieved by exchange dimerization along of one direction lattice so-called $(\pi, 0)$ mode condensation and $(\pi, \pi)$ mode condensation for $\delta > \delta_c$. Long range AF order becomes unstable at the critical value $\delta_c \sim 0.75$ simulated by quantum Monte Carlo [12] in terms of Heisenberg model with exchange dimerization along of one direction lattice. The exchange dimerization is $\delta \sim \alpha u$ and shows nonlinear dependence on the ion displacement $u$. Interaction between elastic and magnetic systems causes elastic tensions that induce local exchange dimerization. Staggered magnetization is decreased and disappeared at $\delta > \delta_c$. Ions displacement anisotropy corresponds to symmetry lowering of lattice and qualitatively agrees with results obtained for static lattice dimerization [11].

Phase diagram of AF long range order—quantum spin liquid in plane the upper bound of acoustic phonon frequency—spin–phonon coupling is presented in Fig. 3. The phase boundary AF-QSL is well approximated by the power function $\omega_0 = 1.65(3)\alpha_c^{1.31(4)}$. For comparison the boundary computed by unitary transform up to the second-order of $\alpha$ (all higher order terms are omitted) [8] is shown in Fig. 3. When bandwidths of the spin-wave and phonon spectrum become comparable in magnitude the contribution of all higher order terms of expansion are important.

Low magnetic moment on site $\sigma = 0.4(1)$ in $Gd_2CuO_4$ and $Eu_2CuO_4$ [1], established from neutron scattering and electronic spin resonans on $Gd^{+3}$ ion in $Eu_2CuO_4$, $\sigma = 0.35(4)$ [13] seem results from spin–phonon coupling. This confirms the anomaly of acoustic phonon excitation along $\Gamma X$ direction in parent compound $Nd_2CuO_4$ [14], strong vibrations of oxygen ion in CuO plane in $Gd_2CuO_4$ [2] and small decreasing mean square vibration of $Cu^{+2}$ in plane CuO in $Eu_2CuO_4$ [3] with temperature rise. Typical upper bound of acoustic frequency is $\omega_0 \simeq 4 \times 10^{12}$ Hz

[14], antiferromagnetic exchange $J \simeq 0.1$ eV and parameters of spin–phonon coupling in $Gd_2CuO_4$ and $Eu_2CuO_4$ determined from $\sigma(\alpha)$ are $\alpha \sim 0.06$, $\sim 0.07$.

So, summarizing, the dependence of magnetic moment per site in two-dimensional antiferromagnet as a function of spin–phonon coupling is determined. Parameters of spin–phonon coupling in $Gd_2CuO_4$ and $Eu_2CuO_4$ are found. The calculated phase diagram AF-QSL allows to estimate the validity of using small expansion parameter for calculation of sublattice magnetization.

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