Available online at www.sciencedirect.com
SCIENCE DIRECT
PHYSICS LETTERS A
Physics Letters A 333 (2004) 446–449
www.elsevier.com/locate/pla

Two-dimensional quantum spin liquid with $S = 1/2$ spins interacting with acoustic phonons

S.S. Aplesnin

L.V. Kirenskii Institute of Physics, Siberian Branch of the Russian Academy of Sciences, Krasnoyarsk 660036, Russia

Received 15 March 2004; accepted 19 October 2004

Available online 11 November 2004

Communicated by J. Flouquet

Abstract

The spin density of states of a two-dimensional antiferromagnet in magnetic field having spins-1/2 and interacting with acoustic phonons is investigated in the nonadiabatic approximation using the quantum Monte Carlo method. It is found the gap energy Δ in the single particle spin excitations spectrum closes at magnetic field $\Delta \simeq H_c$, $W_{\mathrm{ph}} < W_s$ and $\Delta \simeq (1/2)H_c$, $W_{\mathrm{ph}} > W_s$, where W_{ph} and W_s are the bandwidths of phonon and spin excitations in antiferromagnet.

PACS: 75.10.Jm; 75.30.Ds; 67.20.+k

Keywords: Spin-phonon interactions; Spin-liquid; Spinon excitations

Spin liquid phase have attracted a lot of interest because they display both fractional excitations and topological order. While fractionalization could play an important role in some theories of high-temperature superconductors [1], the topological properties of these liquid states have been proposed as possible devices to implement quantum bits for quantum computations [2]. The concept of fractional quantum excitations (spinons) is now well established both theoretically [3] and experimentally [4] in the spin $S = 1/2$ 1D Heisenberg antiferromagnetic chain and identified with quantum domain walls. Anderson [5] suggested that a 2D fractional quantum spin liquid may be described as a "resonating valence bond" (RVB) state with pairs of excited $S = 1/2$ spinons separating via rearangement of these bonds.

For the spin-1/2 model on the square lattice RVB theory gives an energy of a singlet state within 0.1% of ordered state [6] and gapless fractional excitations. A frustrating interactions may induce fractional phases in 2D. The competition between the nearest J_1 and next-nearest exchange J_2 on the square lattice leads to pairing spins-1/2 into singlets at short distances

E-mail address: apl@iph.krasn.ru (S.S. Aplesnin).

0375-9601/$ – see front matter
doi:10.1016/j.physleta.2004.10.064

to overcome frustration in Heisenberg antiferromagnets. Similar situation has been observed in magnetic system with the spin-Peierls order when spins interacted with the optical phonon mode. In this case the ground-state can be described by one ordered configuration of singlets with gapped magnons $\Delta S = 1$. RVB state and the excitations of pairs of $S = 1/2$ spinons have been observed in the triangular antiferromagnet Cs_2CuCl_4 with the partially released frustration [7]. A gapped dimer liquid phase with the topological degeneracy and the deconfined fractional excitations have been studied in the kagome lattice [8]. A high degree of the frustration can be derived from Hamiltonian with spin-phonon coupling. Moreover the model with multiple spins interaction is a particular case of a more general model of spins interaction with the acoustic phonons. Such systems are nonlinear and may have breather or skyrmion like excitation.

In this Letter we will show that the interaction of $S = 1/2$ spins with the acoustic phonons on a square lattice gives rise to the excitations with different mass depending upon the strength of the phonon frequency. At high phonon frequency the magnetic excitations would have mass more light as compared to magnetic excitations at low phonon frequency. For that we carry out simulations of the density of states of a single particle spin excitations in magnetic field. The interaction between the spin and the elastic subsystems leads to nonlinear interactions not only between spins, but also between phonons. For this reason, a correct solution should be carried out taking into account the nonadiabatic interaction between spins and phonons; this can be done using the quantum Monte Carlo method based on the continuous-time algorithm.

In the harmonic approximation, the Hamiltonian for a coupled spin-phonon system has the form

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

Here $S^{z,\pm}$ are a spin operator components associated with the site (i, j), $J > 0$ is the usual antiferromagnetic exchange integral, α 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 elastic rigidity constant of the lattice. Using the quantum representation for phonon operators b, b^+, the Hamiltonian maps to:

$$\begin{aligned}H = \sum_{i,j} & \big(J_{i,j} \mathbf{S}_i \mathbf{S}_j + H_i S^z_i\big) \\ & + \sum_{q_x,q_y} \sum_{n,m} \alpha \sqrt{\frac{\hbar}{2M\Omega(\mathbf{q})}} \exp(i\mathbf{qr}) \\ & \times \big(b_{\mathbf{q}} + b^+_{-\mathbf{q}}\big)\big[\big(1 - \cos q_x - i \sin q_x\big)\mathbf{S}_{n,m}\mathbf{S}_{n+1,m} \\ & + (1 - \cos q_y - i \sin q_y)\mathbf{S}_{n,m}\mathbf{S}_{n,m+1}\big] \\ & + \sum_{\mathbf{q}} \hbar\Omega(\mathbf{q}) b^+_{\mathbf{q}} b_{\mathbf{q}},\ \Omega(\mathbf{q}) \\ = {} & \omega_0\sqrt{2 - \cos(q_x) - \cos(q_y)}, \quad \omega_0 = \sqrt{\frac{2K}{M}}. \qquad (2)\end{aligned}$$

Spin-phonon coupling parameter α, the excitation energy ω and temperature are normalized on the exchange J, $\hbar = 1$, $M = 1$. The temperature used in calculation is $\beta = J/T = 10$. 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 [9] based on the expansion of the statistical evolution operator $e^{-H/T}$ in powers of J and α 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%.

The spectral density of magnetic and phonon excitations can be determined from the corresponding time correlation functions calculated in the imaginary time for $\tau > 0$. We define the spin correlator in the form

$$\begin{aligned}&\big\langle S^-(\tau)S^+(0)\big\rangle \\ &\quad = \sum_\nu \big|\langle\nu|S^+|GS\rangle\big|^2 \exp\big[-(E_\nu - E_0)\tau\big], \qquad (3)\end{aligned}$$

where $|\nu\rangle$ is the complete set of eigenstates of Hamiltonian H_0, $H_0|\nu\rangle = E_\nu|\nu\rangle$, $H_0|GS\rangle = E_0|GS\rangle$. Let us redefine the spin correlator (3) as

$$\left\langle S^-(\tau)S^+(0)\right\rangle = \int_0^\infty d\omega\, \rho_s(\omega)\exp\left[-(\omega\tau)\right],$$
$$\rho_s(\omega) = \sum_\nu \delta(\omega - \Omega_\nu)\left|\langle\nu|S^+|GS\rangle\right|^2,$$
$$\Omega_\nu = E_\nu - E_0, \tag{4}$$

where $\rho_s(\omega)$ defines the spectral density of magnetic excitations. In fact, the Monte Carlo method is used for calculating the time correlator on a finite interval $0 < \tau < \tau_0$. In order to reproduce the spectral density in a wide range of energies, we must solve the integral equation (4). For this purpose, we use the stochastic procedure optimizing the deviation [10]

$$D = \int_0^{\tau_0} \left|G(\tau) - G_t(\tau)\right| G^{-1}(\tau)\, d\tau \tag{5}$$

of the computed correlator $G(\tau)$ from the true correlator $G_t(\tau)$ with the spectral density $\rho_t(\omega)$.

Let us consider two cases when the dispersion curves for magnons and phonons intersect, which is observed at $\omega_0/J < 2$, and additional singularities are formed in the density of states of these quasiparticles and the opposite case at $\omega_0/J > 2$. The firth case is similar to the spin-Peierls interaction. The figures follow two typical cases when $\omega_0/J = 1$ and $\omega_0/J = 6$. Under the action of the magnetic system the ions displacements distribute nonuniform under lattice. The structural factor of lattice fluctuations becomes spatially anisotropic. There are two types of fluctuations: ladder-type containing two nearest chains for $\omega_0/J = 1$ and quasi-one-dimensional chains for $\omega_0/J = 6$, separated by distance $r \simeq 7 - 10$.

For $\alpha > \alpha_c$, a gap is observed in the single particle spin excitations spectrum. The dependence of the gap energy on the magnitude of the spin-phonon coupling together with the approximating power function

$$\Delta/J \simeq \left[(\alpha - \alpha_{c1})/\alpha_{c2}\right]^{0.50(8)}, \qquad \omega_0 = J \tag{6}$$

is depicted in Fig. 1. For $\alpha > \alpha_{c2}$ the long-range magnetic order disappears and a quantum spin liquid is formed [11]. Magnetic field suppress the quantum spin fluctuations. The typical densities of spin excitations

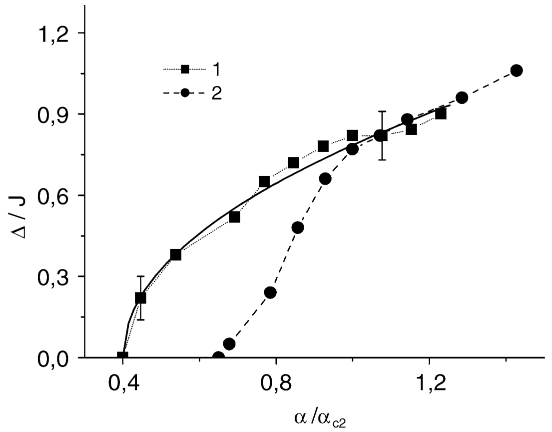

Fig. 1. The gap energy Δ/J in the single particle spin excitation spectrum as a function of spin-phonon interaction parameter for $\omega_0/J = 1$ (1), 6 (2). The fitting function $\Delta/J \simeq [(\alpha - \alpha_{c1})/\alpha_{c2}]^{0.5}$ is plotted by solid line.

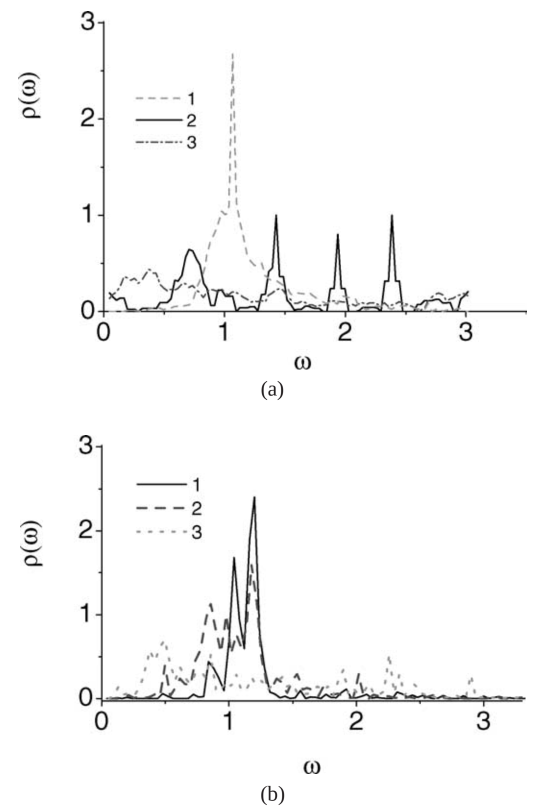

Fig. 2. The density of states of single particle spin excitations for $\omega_0/J = 1$, $\alpha/\alpha_{c2} = 1.2$, $H = 0.6$ (1), 1.0 (2) 1.5 (3) (a) $\omega_0/J = 6$, $\alpha/\alpha_{c2} = 1.0$, $H = 0.3$ (1), 0.9 (2), 1.5 (3) (b).

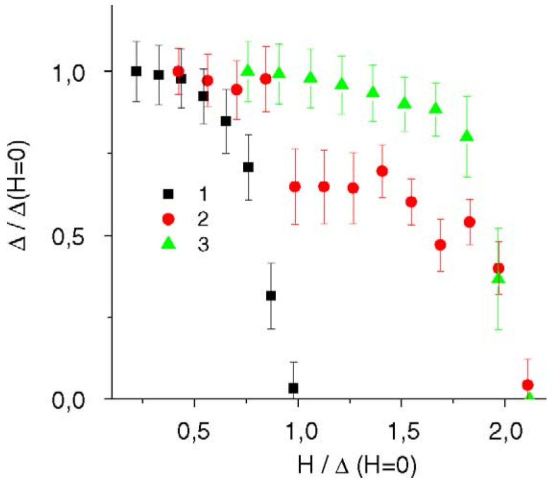

Fig. 3. The gap energy $\varDelta/\varDelta(H=0)$ in the single particle spin excitation spectrum as a function of magnetic field $H/\varDelta(H=0)$ for $\omega_0/J=1$, $\alpha/\alpha_{c2}=1.2$ (1), $\omega_0/J=6$, $\alpha/\alpha_{c2}=1$ (2), 1.8 (3).

calculated in the magnetic field are shown in Fig. 2. The gap closes at the critical field H_c as exhibits in Fig. 3. Gap energy is equal to Zeeman energy for $\omega_0/J=1$, $\varDelta \simeq H_c$. In the spin liquid phase the relation between the gap energy and critical field is different in two times for $\omega_0/J=6$, $\varDelta \simeq (1/2)H_c$. When $\omega_0 < 2J$ the short wavelenth phonons gives rise to ions displacements and to dynamic local lattice dimerization. The excitation spectrum of dimerized lattice is triplet. At $\omega_0/J=6$ an effective interaction between spins realizes via the long wavelenth phonons which beaked down at the critical field H_c. It is possible this state may be interpreted as a classical breather in the kind of domain composed of the rotated spins in the range of angles $(0,\pi/2)$.

Let us summarize the main results. If the bandwidth of phonon excitations is less than the bandwidth of magnon excitations in two-dimensional antiferromagnet $W_{\rm ph} < W_m$ (dispersion curves of magnon and phonon excitations are intersected) the excitation spectrum of quantum spin liquid is the gapped magnon excitations with $\varDelta S^z = 1$. In contrast limit $W_{\rm ph} > W_m$ the mass of low-lying energy excitations in the spin liquid is in two times less as compared to mass of triplet excitations.

References

[1] P.W. Anderson, Science 235 (1987) 1196.
[2] I.B. Ioffe, M.V. Feigel'man, A. Ioselevich, D. Ivanov, M. Troyer, G. Blatter, Nature 415 (2002) 503.
[3] J.C. Talstra, F.D.M. Haldane, Phys. Rev. B 50 (1994) 6889.
[4] D.C. Dender, D. Davidovic, D.H. Reich, C. Broholm, Phys. Rev. B 53 (1996) 2583.
[5] P.W. Anderson, Mater. Res. Bull. 8 (1973) 153.
[6] S. Liang, B. Doucot, P.W. Anderson, Phys. Rev. Lett. 61 (1988) 365.
[7] R. Coldea, D.A. Tennant, A.M. Tsvelik, Z. Tylczynski, Phys. Rev. Lett. 86 (2001) 1335.
[8] G. Misguich, D. Serban, V. Pasquier, Phys. Rev. Lett. 89 (2002) 137202.
[9] N.V. Prokof'ev, B.V. Svistunov, I.S. Tupitsin, JETP 87 (1998) 310.
[10] A.S. Mishchenko, N.V. Prokofev, A. Sakamoto, B.V. Svistunov, Phys. Rev. B 62 (2000) 6713.
[11] S.S. Aplesnin, Phys. Lett. A 313 (2003) 122.