# Spin-Peierls transition in an anisotropic two-dimensional *XY* model

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(Received 12 November 1999; revised manuscript received 16 January 2001; published 14 June 2001)

The two-dimensional Jordan-Wigner transformation is used to investigate the zero-temperature spin-Peierls transition for an anisotropic two-dimensional $XY$ model in the adiabatic limit. The phase diagram between the dimerized ($D$) state and uniform ($U$) state is shown in the parameter space of dimensionless interchain coupling $h$ $(=J_\perp/J)$ and spin-lattice coupling $\eta$. It is found that the spin-lattice coupling $\eta$ must exceed some critical value $\eta_c$ in order to reach the $D$ phase for any finite $h$. The dependence of $\eta_c$ on $h$ is given by $-1/\ln h$ for $h\to 0$ and the transition between the $U$ and $D$ phases is of first order for at least $h>10^{-3}$.

DOI: 10.1103/PhysRevB.64.012414 PACS number(s): 75.10.Jm, 75.50.Ee

The fact that the $S=\frac{1}{2}$ Heisenberg spin chain is unstable towards dimerization when coupled to an elastic lattice is known as the spin-Peierls (SP) transition.[1] This occurs because dimerization opens a gap in the spin excitation spectrum and lowers the total magnetic energy by a greater amount than the increase in elastic energy due to lattice deformation. Such a transition was first suggested by analogy with the conventional Peierls transition in linear conducting chains and later observed in several organic compounds such as N-methyl-N-ethyl-morpholinium-ditetracyanoquinodimethanide [MEM-$(TCNQ)_2$].[2] It has attracted renewed attention since the discovery of the inorganic compound $CuGeO_3$ in 1993.[3]

In the adiabatic limit, it is well understood for the exact one-dimensional (1D) $XY$ or Heisenberg model that the dimerized ($D$) state, relative to the uniform ($U$) one, is always stable for arbitrarily weak spin-lattice coupling in the ground state.[1] In the presence of some extra mechanisms these two states may compete, leading to an interesting phase diagram. Up to now there are several mechanisms that were found to destroy the $D$ phase, for example, small Ising anisotropy.[4] Another mechanism is quantum lattice fluctuation, which was intensely studied recently.[5,6] Beyond adiabatic approximation it was found that the spin-phonon coupling must be larger than some nonzero critical value for the SP instability to occur.[5,6] The interchain exchange coupling is also a possible mechanism.[7–9] This mechanism is often not negligible for real SP materials, especially for the material $CuGeO_3$ where a relatively large interchain coupling, about $J_\perp/J=0.1$ ($J$ represents the intrachain exchange), was found experimentally.[10] Theoretically the importance of the interchain coupling was also stressed by many authors in descriptions of $CuGeO_3$.[11–13] Therefore it is necessary to study the SP transition for a general *quasi*-1D system with the inclusion of interchain coupling. This should be discussed by answering a central problem of how the interchain coupling modifies the dimerized ground state of the exact 1D case.

In this work we propose to study the above problem through a two-dimensional (2D) $XY$ model with anisotropic intrachain and interchain coupling and leave the generalization to the case of the corresponding Heisenberg model for later study. The reason is twofold: (i) the problem is simplified, especially the 1D limit, which can be exactly solved and (ii) the $XY$ model is believed to contain the essential elements for the spin-Peierls transition.[5] We point out that a similar problem based on the Heisenberg model was studied previously by some authors.[7,8] However, they all treated the interchain coupling within the so-called chain mean-field theory and actually still studied a 1D system. Usually the effect of interchain coupling is underestimated in this way. Here, the two-dimensional (2D) Jordan-Wigner (JW) transformation[14–17,9] is adopted so that the intrachain and interchain exchanges may be treated on an equal footing from the beginning.

In adiabatic approximation, we begin with the following anisotropic 2D $XY$ model on a square lattice:

$$H=J\sum_{i,j}(1+\alpha u_{i,j})(S^x_{i,j}\cdot S^x_{i+1,j}+S^y_{i,j}\cdot S^y_{i+1,j})$$
$$+J_\perp\sum_{i,j}(S^x_{i,j}\cdot S^x_{i,j+1}+S^y_{i,j}\cdot S^y_{i,j+1})+\frac{K}{2}\sum_{i,j}u^2_{i,j}, \quad (1)$$

where $S^{x/y}_{i,j}$ represents the $x/y$ component of the spin-$\frac{1}{2}$ operator at site $\vec{r}_{i,j}=i\vec{x}+j\vec{y}$ ($\vec{x}$, $\vec{y}$ are unit vectors along the $x$ and $y$ axis, respectively), $J(J_\perp)$ is the intra(inter)chain exchange coupling along the $x(y)$ axis, $\alpha$ represents the spin-lattice coupling constant, and $K$ is the intrachain elastic constant. Here the lattice displacement is assumed as $u_{i,j}=(-1)^{i+j}u$, i.e., corresponding to a wave vector $(\pi,\pi)$, which was found to be the case in $CuGeO_3$ by neutron-diffraction measurements.[18] In the following we take $J$ as the unit of energy and use several dimensionless parameters: the dimerization parameter $\delta=\alpha u$, the interchain coupling $h=J_\perp/J$, and the spin-lattice coupling $\eta=\alpha^2 J/K$. The total number of lattice sites is $N$.

The spin operators may be represented as fermions by use of the 2D JW transformation, which has the advantage that all spin commutation relations, as well as the so-called spin on-site exclusion principle are automatically preserved.[15] This method has been proven well for application to real materials.[15,9] For concreteness, the following formulas are adopted,[16,17]

$$S^-_{i,j}=c_{i,j}\exp\{i\phi_{i,j}\},\quad S^+_{i,j}=\exp\{-i\phi_{i,j}\}c^\dagger_{i,j},$$
$$S^z_{i,j}=c^\dagger_{i,j}c_{i,j}-1/2 \quad (2)$$

 

with

$$\phi_{i,j}=\pi\left[\sum_{l=0}^{i-1}\sum_{m=0}^{\infty}n_{l,m}+\sum_{m=0}^{j-1}n_{i,m}\right],$$

where $c_{i,j}^{\dagger}(c_{i,j})$ is the creation (annihilation) operator for a spinless electron at $\vec{r}_{i,j}$ and $n_{i,j}=c_{i,j}^{\dagger}c_{i,j}$ is the particle number operator. The original Hamiltonian can then be transformed into

$$H=\sum_{i,j}\ [1+(-1)^{i+j}\delta](e^{i\psi_{i,j}}c_{i,j}^{\dagger}c_{i+1,j}+\text{H.c.})/2$$

$$+h\sum_{i,j}\ (c_{i,j}^{\dagger}c_{i,j+1}+\text{H.c.})/2+N\delta^2/2\eta, \tag{3}$$

where the phase factor $e^{i\psi_{i,j}}=e^{i(\phi_{i+1,j}-\phi_{i,j})}$ describes an effective gauge field acting on spinless fermions. Note that the Hamiltonian (3) is exact and it may recover to the corresponding one derived from the 1D JW transformation when $h=0$. When going on one has to treat the phase factor approximately. Following previous works, we select a configuration (see Fig. 1 in Refs. 14, 15, and 17) where the phase factor $e^{i\psi_{i,j}}$ has alternative values $e^{i\pi}$ and 1, i.e., it varies with $(-1)^{i+j}$ (note that this coincides with the above dimerization pattern). This configuration ensures that each elementary plaquette encloses a net flux of $\pi$.[14,15] Then the Hamiltonian can be rewritten as follows in terms of fermion operators $e$ and $f$ corresponding to the two sublattices $A$ and $B$ respectively (constants irrelevant to $\delta$ are ignored),

$$H=\frac{1}{2}\sum_{\vec{r}_{i,j}\in A}\ [-(1-\delta)(f_{i-1,j}^{\dagger}e_{i,j}+\text{H.c.})$$

$$+(1+\delta)(e_{i,j}^{\dagger}f_{i+1,j}+\text{H.c.})+h(f_{i,j-1}^{\dagger}e_{i,j}$$

$$+e_{i,j}^{\dagger}f_{i,j+1}+\text{H.c.})]+N\delta^2/2\eta. \tag{4}$$

In the following we want to study the SP transition at $T=0$ based on the above Hamiltonian. Depending on the optimal value $\delta^*$, which minimizes the ground-state energy, the system may be in $D$ phase ($\delta^*\neq 0$) or $U$ phase ($\delta^*=0$) in the parameter space of interchain coupling $h$ and spin-lattice coupling $\eta$.

The Hamiltonian (4) may be exactly diagonalized. The electronic spectrum is written as $\varepsilon_{\mathbf{k}}=\pm\sqrt{(\delta\cos k_x+h\cos k_y)^2+\sin^2 k_x}$ within the (reduced) Brillouin zone: $-\pi<k_x\pm k_y\leqslant\pi$, and the ground-state energy is simply given by $E_{\mathrm{GS}}=-\Sigma_{\mathbf{k}}|\varepsilon_{\mathbf{k}}|+N\delta^2/2\eta$. Before continuing we add a comment here on the above-used JW transformation. In the definition of $\phi_{i,j}$ in Eq. (2) the summation is selected over the lattice sites along the direction perpendicular to the chains so that the phase factor appears in the intrachain hopping term as shown in Eq. (3). One may also think to do the summation along the chain direction, i.e., redefine $\phi_{i,j}=\pi[\Sigma_{m=0}^{j-1}\Sigma_{l=0}^{\infty}n_{l,m}+\Sigma_{l=0}^{i-1}n_{l,j}]$, and then the phase factor will appear in the interchain (rather than intrachain) hopping term. With the similar treatment for this phase factor as done above one may obtain an alternative spectrum

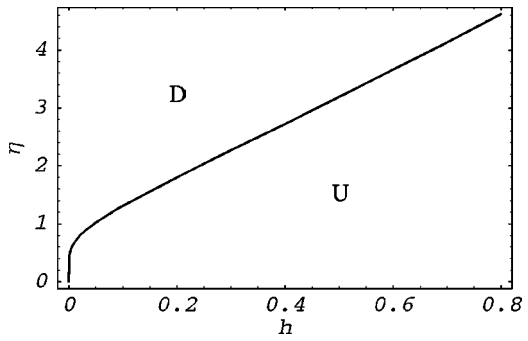


FIG. 1. The $D/U$ phase diagram for the anisotropic 2D $XY$ model in the parameter space of interchain coupling $h$ and spin-lattice coupling $\eta$.

$\pm\sqrt{(\delta\sin k_x+h\sin k_y)^2+\cos^2 k_x}$. However, the ground-state energy $E_{\mathrm{GS}}$ (i.e., the summation over the Brillouin zone) is not changed by the new spectrum, nor all the subsequent results derived from it. A similar discussion was given in Ref. 16. Then we go on to search for the value $\delta^*$, which may be obtained from the condition $\partial E_{\mathrm{GS}}/\partial\delta=0$, yielding the following equation:

$$\delta=\frac{\eta}{2\pi^2}\int_0^{\pi}dk_x\int_{k_x-\pi}^{\pi-k_x}dk_y\frac{(\delta\cos k_x+h\cos k_y)\cos k_x}{\sqrt{(\delta\cos k_x+h\cos k_y)^2+\sin^2 k_x}}. \tag{5}$$

It is interesting to notice that Eq. (5) will reduce to the corresponding rigorous equation for the exact 1D case[19] if we set $h=0$, which means

$$1=\frac{\eta}{\pi}\int_0^{\pi/2}dk_x\frac{\sin^2 k_x}{\sqrt{\delta^2\sin^2 k_x+\cos^2 k_x}}. \tag{6}$$

Equation (6) always has a single nonzero solution for $\delta$ as long as $\eta>0$,[20] which predicts a dimerized ground state. For $h\neq 0$, Eq. (5) may give one or two nonzero solutions $\delta_i$ ($i=1,2$) except for the trivial solution $\delta=0$. We need to consider the sign of $\partial^2 E_{\mathrm{GS}}^{XY}/\partial\delta^2|_{\delta=\delta_i}$, as well as compare the energies between at $\delta=\delta_i$ and at end points $\delta=0,1$ to obtain the actual $\delta^*$. Without details, we give the results shown in Figs. 1 and 2. Figure 1 gives the $D/U$ phase diagram in the parameter space $(h,\eta)$. As expected, the interchain coupling tends to suppress the $D$ phase. As long as the interchain

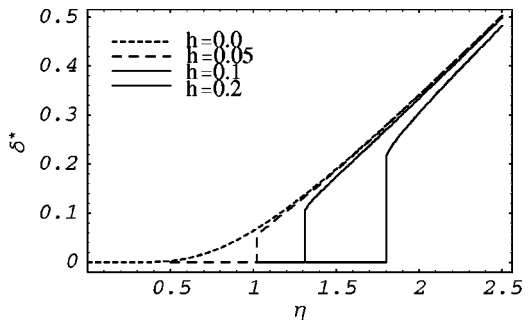


FIG. 2. The order parameter $\delta^*$ as a function of $\eta$ for $h=0$, 0.05, 0.1, and 0.2.

coupling $h>0$, the spin-lattice coupling $\eta$ must exceed some critical value $\eta_c$ to reach the $D$ phase and the value $\eta_c$ increases monotonically with $h$. Careful analysis shows that the critical value $\eta_c$ has the functional form $-1/\ln h$ in the region $h\rightarrow 0$, which increases starting from zero much faster than any power law. Moreover, we have found that the transition from the $U$ to $D$ phase with increasing $\eta$ is of first order for at least $h>10^{-3}$.[21] As shown in Fig. 2 we may see how the order parameter $\delta^*$ jumps from zero to finite value with an increase of $\eta$ for several $h$ values. Although the transition is of second order at the point $h=0$ as can be proven from Eq. (6), we speculate that it becomes of first order as long as $h>0$.

It is also interesting to notice that the excitation spectrum may be gapless even for finite dimerization in the presence of the interchain coupling. From $\varepsilon_{\mathbf{k}}$, it is easy to find that a gap is not fully opened at the Fermi surface until the dimerization $\delta$ reaches the same value as the interchain coupling $h$. Qualitatively this gives the physical reason for the conditional SP transition when $h>0$ as shown by Fig. 1: The incomplete opening of the gap by the dimerization is unfavorable to an adequate reduction for the electronic energy so that the gain from it is not always enough to overcome the increase of the elastic energy. Here it deserves to be mentioned that the same property of the excitation spectrum is also present for another dimerized state with the pattern corresponding to a wave vector $(\pi,0)$, i.e., $u_{i,j}=(-1)^i u$, see Ref. 22. Thus it is reasonable to predict that the similar conditional SP transition will occur if this different dimerization pattern is considered.

We emphasize that the above results were obtained under the 2D JW transformation, where the interchain and intrachain exchanges were treated on the same level although the phase factor was approximately averaged. One may expect that the effect of interchain coupling, i.e., favoring the existence of the $U$ state, could be adequately considered in this treatment. Actually, this point has been reflected in Fig. 1 prominently by the relationship between $\eta_c$ and $h$ in the region $h\rightarrow 0$: $\eta_c\sim -1/\ln h$. Even an infinitesimal interchain coupling may induce a rapid increase of $\eta_c$ away from zero, i.e., the $U$ state is largely stabilized once the interchain coupling is switched on.

As mentioned before, a natural extension is to consider the case of the Heisenberg model. In this case the $U$ state should imply $z$-axis (and rotationally invariant) antiferromagnetic long-range order (LRO).[23] But we believe that the above qualitative results for the $XY$ model, especially the rapid increasing property for $\eta_c$ away from zero, is not changed by the extra Ising terms except that the $U$ phase in Fig. 1 is replaced by the more-precisely-called Néel phase (i.e., a uniform state with antiferromagnetic LRO).[7,8] More work is necessary for justification.

Before closing we note that recently there are intensive studies on the material $CuGeO_3$, which show surprising phenomena under doping,[24] and theoretically it has been understood that the interchain coupling plays a key role for these phenomena.[25,26] For their better understanding our phase diagram given here (for the pure system), which addresses the effect of the interchain coupling, will be helpful. Furthermore it is of great interest to extend this work to study the phase diagram for a doped quasi-1D SP system. In addition, we also notice that the nonadiabatic effect as referred to before is important for really modeling $CuGeO_3$,[5,6,8,27] so inclusion of dynamic phonons beyond this work is another interesting topic for future investigation.

In conclusion, based on the 2D JW transformation we have studied the ground state $D/U$ phase diagram for an anisotropic 2D $XY$ model in the adiabatic limit. It is found that the spin-lattice coupling $\eta$ must exceed some critical value $\eta_c$ in order to reach the $D$ phase for any finite $h$. The value $\eta_c$ has the dependence $-1/\ln h$ on $h$ in the region $h\rightarrow 0$ and the transition between the $U$ and $D$ phases is of first order for at least $h>10^{-3}$.

One of the authors (Q. Y.) would like to thank P. Thalmeier, T. Yamamoto, and M. Azzouz for helpful discussions and the support of the Visitor Program of MPI-PKS, Dresden. This work was also partly supported by the Chinese National Science Foundation.

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