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LETTER TO THE EDITOR

Spin-Peierls dimerization and frustration in two-dimensional antiferromagnets

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Abstract. We have investigated the stability of the antiferromagnetic order in the ground state of the two-dimensional Heisenberg model against a lattice dimerization produced by the electron–lattice interaction. Unlike the one-dimensional case, we found that a critical coupling is required to form a dimerized state via a first-order phase transition. We have also considered the combined effects of frustrating second-neighbour interactions and lattice dimerization in destroying the Néel order. Our approach is based on the Schwinger representation of spin operators, and is in excellent quantitative agreement with exact numerical results on finite lattices.

The discovery of superconductivity in copper oxide compounds has brought a new surge of interest in the two-dimensional (2D) Hubbard model. There have been several proposals to explain the high superconducting temperatures in terms of this model [1], with [2–4] or without [5] novel pairing mechanisms. In some of these proposals [3, 4] the lattice dimerization due to the electron-phonon (e–ph) interaction plays some role, which motivated recent studies of the Peierls instability at half filling [6, 7]. In this work we reinvestigate the problem of lattice dimerization in the strong repulsion (large-U) limit of the half-filled Hubbard model. In this limit, for lattice distortions treated in the adiabatic approximation we are led to consider the spin-Peierls Hamiltonian,

$$H = \frac{1}{2}\sum_{i,j} J_{ij} S_i \cdot S_j + \frac{K}{2}\sum_i u_i^2.$$

The exchange coupling $J_{ij} = 4t_{ij}^2/U$, with $t_{ij} = t - \alpha u_{ij}$. Here α is the e–ph coupling, t is the Hubbard hopping integral, and $u_{ij} = \mid u_i - u_j \mid$ is the change in distance between nearest-neighbour sites i and j after dimerization. We have called K the lattice elastic constant and, according to the adiabatic approximation, we treat the displacements u_i as classical parameters. In this way, the influence of the dimerization phonon mode is reduced to a change in the effective hopping integral.

Without the e–ph coupling, on a square lattice the ground state of (1) displays long-range Néel order. In the presence of lattice distortions, the gain in magnetic energy in the first term of (1) favours dimerization, while the cost in elastic energy (the second term) opposes it. Competition of these two effects eventually leads, for a large enough e–ph coupling, to the destruction of the Néel order and the establishment of a permanent lattice distortion. The displacement patterns considered in this work correspond to dimerizations produced by either a $(\pi, 0)$ or a (π, π) phonon. Other possibilities have been discussed in [7], but

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the differences in energy with these two patterns are negligible, and require consideration of displacements along both lattice directions. In agreement with the results of [7], we found that distortions following the $(\pi, 0)$–phonon pattern lead to a larger energy gain (except for the eight-site lattice, where the two patterns are degenerate). Consequently, we will consider displacements given by $u_i = \pm(u/2)(1, 0)$, where the $\pm$ signs correspond to the two sublattices moving in opposite directions. For $u/a \ll 1$ (a is the lattice constant) the transversal coupling is practically unaffected, $J_T \simeq 4t^2/U \equiv J$, while in the longitudinal direction one has $J_L = 4(t \pm \alpha u)^2/U$. Then, by introducing [6] the adimensional displacement $x = u\alpha/t$ and coupling $\lambda = 32\alpha^2/KU$, the Hamiltonian (1) is reduced to

$$\frac{H}{J} = \frac{1}{2}\sum_{n,n',\alpha\alpha'} \tilde{J}_{\alpha,\alpha'}(n-n')S_{n\alpha}\cdot S_{n'\alpha'} + \frac{Nx^2}{\lambda}.$$

We defined $\tilde{J}_{ij} = J_{ij}/J = (1 \pm x\eta_{ij})^2$, where η_{ij} is equal to unity for i, j nearest neighbours in the longitudinal direction, and is zero otherwise. Furthermore, in order to treat dimerized states we locate sites by lattice vectors n and basis vectors r_α that describe the unit cell of the distorted lattice.

In the following we will use the Schwinger representation of spin operators: $S_{n\alpha} = \frac{1}{2}a^\dagger_{n\alpha}\cdot\sigma\cdot a_{n\alpha}$, where σ are the Pauli matrices and the bosonic spinors $a_{n\alpha} = (a_{n\alpha,\uparrow}, a_{n\alpha,\downarrow})$ are constrained to $a^\dagger_{n\alpha}\cdot a_{n\alpha} = 2S$. Then, by defining the spin singlets $\hat{B}^\dagger_{nn'\alpha\alpha'} = \frac{1}{2}\sum_\sigma a^\dagger_{\sigma n\alpha}a_{\sigma n'\alpha'}$, $\hat{A}_{nn'\alpha\alpha'} = \frac{1}{2}\sum_\sigma \sigma a_{\sigma n\alpha}a_{-\sigma n'\alpha'}$, we perform a rotational invariant decomposition of (2) in terms of the order parameters $B_{\alpha\alpha'}(n-n') = \langle\hat{B}^\dagger_{nn'\alpha\alpha'}\rangle$ and $A_{\alpha\alpha'}(n-n') = \langle\hat{A}^\dagger_{nn'\alpha\alpha'}\rangle$ [8]. Bogoliubov diagonalization of the resulting Hamiltonian allows us to obtain the ground-state energy, which is a function of the order parameters and the Lagrange multipliers λ_α that impose the boson number restriction (on average). Minimization with respect to these quantities produces self-consistency equations that are solved numerically. The ground-state energy of the full Hamiltonian (2) is finally obtained by adding the contribution of the elastic energy due to the lattice distortion, and minimizing with respect to x. We repeat this procedure for the different distortion patterns considered. As mentioned before, we found that the pattern associated with a $(\pi, 0)$ phonon is energetically preferred to that corresponding to a (π, π) phonon.

We have checked the reliability of our approach by comparing its predictions with exact results on finite lattices. Following [6], we note that the ground-state energy *per site* can be written as

$$E = E_0 + (a_2 + 1/\lambda)x^2 + f(x)$$

where E_0 is the energy of the undistorted lattice, and $f(x) = a_4x^4 + a_6x^6 + \ldots$. In figure 1 we show the function $f(x)$ for a eight-site lattice calculated as described above, and the exact one obtained by numerical diagonalization [6]. There is an excellent agreement between the two curves. In particular, numerically one finds $a_2 \simeq -0.792$, while the present approach gives $a_2 = -0.750$. Our results predict that a critical e–ph coupling $\lambda_c \simeq 1.175$ is required to dimerize the lattice, with the incipient antiferromagnetic order in this finite lattice being stable for weaker couplings. For $\lambda \geqslant \lambda_c$ there is a finite distortion $x \geqslant x_c \simeq 0.6$, which suggests that the transition to the dimerized state would be of first order. Note that a necessary condition for a second-order transition is $a_4 > 0$ in the expansion of $f(x)$. The exact treatment in [6] and our approximation produce both negative values for a_4. In our

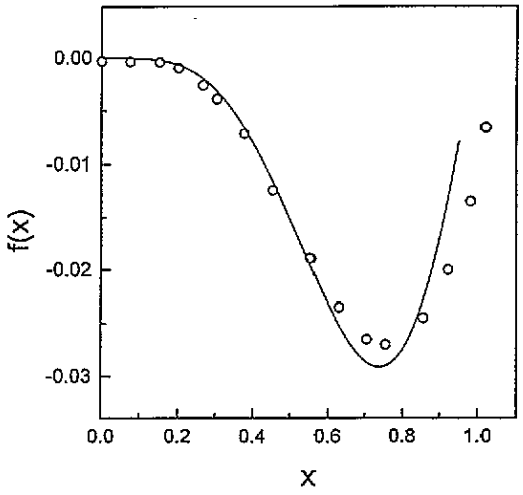

Figure 1. The function $f(x)$, defined in (3) of the main text, for the eight-site lattice. The full line is the prediction of the present work; open points are exact results from [6].

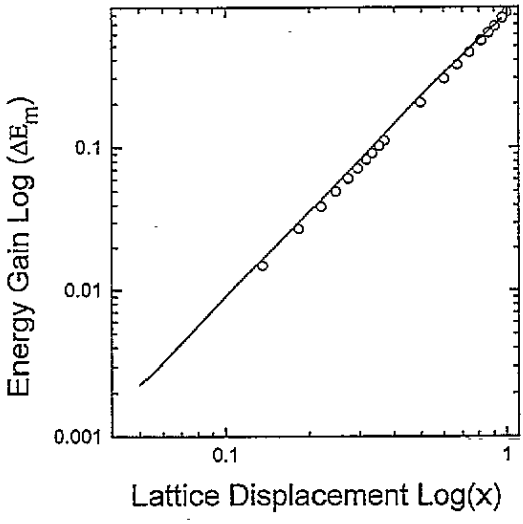

Figure 2. The magnetic energy gain ΔE_M as a function of the lattice distortion x. The full line is the prediction of the present work; open points are Monte Carlo results from [7].

case we obtained $a_4 \simeq -0.059$ (performing numerical derivatives of the energy to the given accuracy requires solving the consistency equations to $O(10^{-16})$). The corresponding value is not quoted in [6]. As a further check, in figure 2 we compare the magnetic energy gain ΔE_M with the Monte Carlo results of [7]. The agreement is again quite good.

After validating our approximation by comparison with exact results on finite lattices, we turn to the consideration of the thermodynamic limit. To approach this limit we have solved the numerical problem on a 40×40 lattice, which produces a negligible error in the relevant quantities. In this case we found $\lambda_c \simeq 1.08$, with a critical displacement $x_c \simeq 0.48$.

The coefficients in the expansion of $f(x)$ are $a_1 2 \simeq -0.91$ and $a_4 \simeq -0.02$, which indicates again a first-order transition for the infinite lattice. We stress that this is at variance with the results of standard spin-wave theory, which predicts a second-order transition. It agrees, however, with the conclusions of numerical studies on finite lattices [6,7]. In figure 3 we plot the infinite-lattice ground-state energy *per site* as a function of x, for several values of the e–ph coupling.

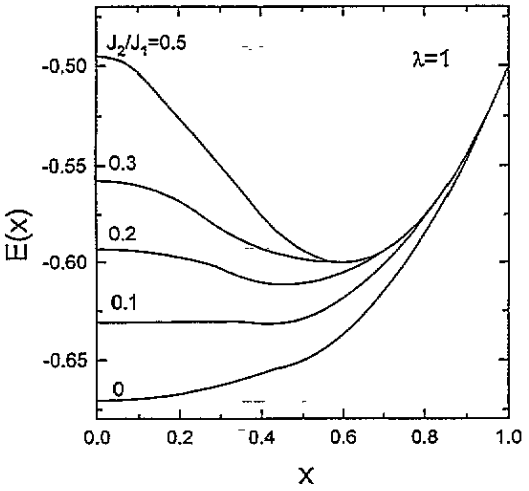

Figure 3. The ground-state energy *per site* $E(x)$ as a function of the lattice distortion x, for $J_2 = 0$ and different values of λ. Inset, the function $f(x)$ defined in (3) of the main text.

We have also considered the effects of including a second neighbour spin interaction J_2. Partially this is motivated by the suggestion that next-nearest-neighbour interactions model to some extent the effects of holes in the low-doping regime of the Cu–O_2 planes [9]. In particular, even without considering the e–ph coupling, in the region near $J-2/J-1=0.5$ the system is believed to have a dimer phase [10] produced by the strong frustration. We have previously studied this rigid-lattice J_1–J_2 model [11], and in the following we will discuss the effects of including the e–ph interaction.

Under the assumption that the interaction between second neighbours i, k is originated by the hole movement [9], the coupling $J_{ik} \simeq 4t_{ij}t_{jk}\delta/U$. Here t_{ij} and t_{jk} are the hopping integrals between nearest neighbours in the longitudinal and transverse directions respectively. This result is obtained for dopings $\delta = 1 - n \simeq 0$. As before, we considered $t_{ij} = t \pm \alpha u$ and $t_{jk} \simeq t$, so that $J_{ik} = J_2(1 \pm x\eta_{ij})$ with $J_2 = J\delta$. On the other hand, the hole movement also affects the nearest-neighbour exchange, producing an effective coupling $J_1 \simeq J[1 - (5 + U/t)\delta]$ (for simplicity we will disregard momentarily the third-neighbour coupling $J_3 \simeq J_2/2$ [9].) We have solved the consistency equations with J_2/J_1 as a new parameter. In figure 4 we show the energy of the infinite lattice as a function of the reduced displacement x, for $\lambda = 1$ and several values of J_2/J_1. In figure 5 we plot λ_c and x_c as functions of J_2/J_1. As expected, the critical values decrease with the frustration level. The dashed lines are quadratic (for λ_c) and linear (for x_c) extrapolations into the region where the Néel order becomes metastable [11]. There, the solution corresponding to this order becomes increasingly harder to find, since the consistency-equation iterations

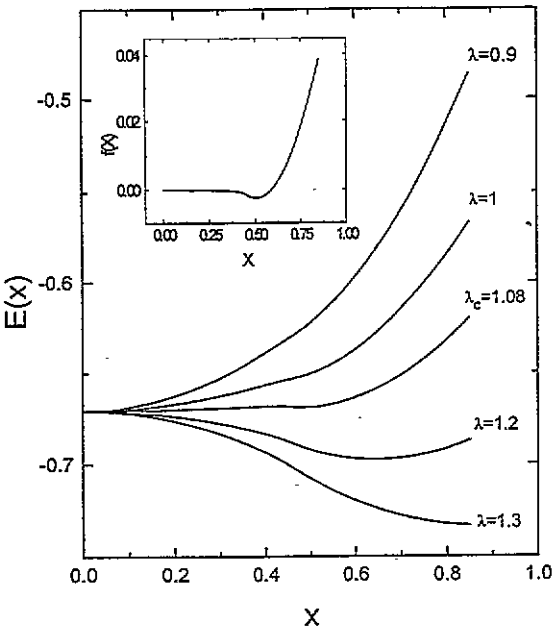

Figure 4. The ground-state energy *per site* $E(x)$ as a function of the lattice distortion x for $\lambda = 1$ and different values of the ratio J_2/J_1.

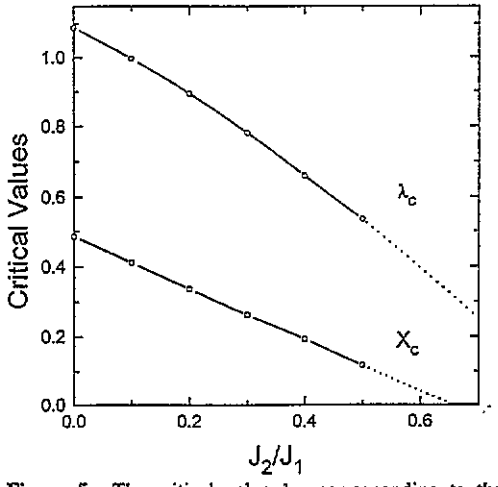

Figure 5. The critical value λ_c, corresponding to the minimum electron–phonon coupling required to dimerize the lattice, as a function of J_2/J_1. The value x_c is the lattice displacement produced by λ_c at the first-order dimerization transition. Dashed lines are extrapolations as described in the main text.

lead to other more stable solutions. For x_c the extrapolation indicates that it vanishes near $J_2/J_1 \simeq 0.63$, the point at which the Néel order of the undistorted lattice is melted by the

frustration [11]. At this point the scenario is similar to the one-dimensional case, where the transition is second-order and the lattice becomes highly susceptible to dimerization. Then, in the neighbourhood of this point Hirsch's [4] ideas concerning the connection between superconductivity and a 'bond charge-density-wave' state could apply. However, the extrapolation for λ_c shows that, unlike the one-dimensional case, here a finite e–ph is required to distort the lattice.

To conclude, let us discuss the application of the above results to the Cu–O_2 planes in La_2CuO_4, keeping always in mind the limitations of our approach. In a previous work [8] we studied the J_1–J_2–J_3 model on the special line $J_2 = 2J_3$, a situation that corresponds to next-nearest-neighbour interactions generated by the hole movement [9]. We found that in this case the Néel order disappears at $J_2/J_1 = \delta_c/[1 - (5 + U/t)\delta_c] \simeq 0.38$, which for $U/t = 5$–10 gives $\delta_c = 0.079$–0.057, that is, in the observed range. On the other hand, Zhang and Prelovsek have estimated [6] and reduced e–ph coupling of the Cu and O ions to be $\lambda_{CuO} \simeq 2.1$–2.6. The e–ph coupling for Cu–Cu ions is related to a second-order hopping process (via O ions), and is then expected to be appreciably less than this value. However, in view of the decrease of λ_c shown in figure 5, it seems likely that near the point where the antiferromagnetic order is destroyed by doping the lattice becomes highly susceptible to dimerization.

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