Ternally activated Peierls dimerization in ferromagnetic spin chains

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We demonstrate that a Peierls dimerization can occur in ferromagnetic spin chains activated by thermal fluctuations. The dimer order parameter and entanglement measures are studied as functions of the modulation of the magnetic exchange interaction and temperature, using a spin–wave theory and the density–matrix renormalization group. We discuss the case where a periodic modulation is caused by spin–phonon coupling and the case where electronic states effectively induce such a modulation. The importance of the latter for a number of transition metal oxides is highlighted.

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Structural instabilities of electronic systems can occur due to the coupling of electronic and lattice degrees of freedom (phonons). They are particularly important for quasi one–dimensional (1D) systems where the gain in electronic energy due to a lattice distortion often out–weighs the cost in elastic energy. A well known example is the Peierls instability [1] of the 1D free electron system towards a static lattice distortion determined by the Fermi momentum. For a commensurate distortion, an excitation gap is opened turning a metallic system into a band insulator. This Peierls metal–insulator transition is parameterized by δ ∈ [0, 1]. The elastic energy $E_{el}$ contains the elastic constant $K$. Both parameters $K$, δ can be related to the spin–phonon interaction strength. Note that writing the Hamiltonian as a sum of a magnetic and an elastic part as in Eq. (1) corresponds to the random–phase approximation (RPA) by Cross and Fisher [2]. Although the model (1) is strictly 1D, the static, mean–field (MF) treatment of the three–dimensional phonons allows for a finite temperature phase transition if δ(T) is treated as a thermodynamical degree of freedom determined by minimizing the free energy.

$E_{mag} = \frac{N}{2} \sum_{j=1}^{N} \left\{ S_j \cdot S_{j+1} + J S_j \cdot S_{j+1} \right\}$

and $E_{el} = N K \delta^2 /2$. Here J is the exchange constant, $S_j$ is a spin S operator at site j, and N is the number of sites.

Quite recently, another type of Peierls instability for spin chains has been found which is not driven by spin–phonon coupling but rather by a coupling of the spins with electronic degrees of freedom (orbitals). Here a ferromagnetic (FM) spin chain shows a periodic modulation (dimerization) of the magnetic exchange in a certain finite temperature region while the ground state is the uniform fully polarized FM state [3]. In [4], it has been argued that this mechanism is responsible for the remarkable electronic properties of YVO3 in the finite temperature C–type AFM phase. Clearly, the lattice will react to a modulation of the magnetic exchange, however, spin–phonon coupling is not the driving force in this case and any lattice distortion is only a secondary effect.

In this Letter we want to establish general mechanisms which can drive a Peierls dimerization in FM spin chains. To highlight the differences between AFM and FM chains we will first consider a coupling to lattice degrees of freedom. The phonons are often treated adiabatically which is justified if the phonon frequency is smaller than the Peierls gap. In the adiabatic approximation the Hamiltonian can be written as $H = H_{mag} + E_{el}$ with

$H_{mag} = J \sum_{j=1}^{N} \{ 1 + (-1)^j \delta \} S_j \cdot S_{j+1}$

and $E_{el} = N K \delta^2 /2$. Here J is the exchange constant, $S_j$ is a spin S operator at site j, and N is the number of sites.

Let us start with the case where $S_j \cdot S_{j+2} \rightarrow S_j^z S_{j+1}^z + S_j^y S_{j+1}^y = (S_j^z S_{j+1}^z + S_j^y S_{j+1}^y)/2$, i.e., we replace the SU(2)–symmetric spin exchange by an XX–type of interaction. In this case the sign of J does not matter and the system becomes equivalent to a free spinless fermion model by Jordan–Wigner transformation. The Hamiltonian is then easily diagonalized by Fourier transformation and in the ground state for small δ one finds a gain in magnetic energy $E_{mag} \sim \delta^2 \ln \delta$. This outweighs the cost in elastic energy $E_{el} \sim \delta^2$ and constitutes the Peierls instability for lattice fermions [10]. For the isotropic antiferromagnet ($J > 0$, SU(2)–symmetric exchange), field theoretical arguments show that $E_{mag} \sim -\delta^{4/3}$ [9]. Again this outweighs the cost in elastic energy leading to a SP transition and the opening of a spin gap, $\Delta \sim \delta^{2/3}$.

Contrary to the two cases discussed above there is no gain in magnetic energy in the ground state for FM coupling, $J < 0$. For $\delta \in [0, 1]$ the ground state is always the fully polarized FM state. We will show in the following that thermal fluctuations can, however, activate a Peierls dimerization. We will use the density–matrix renormal-
The order parameter for the FM chain with \( K < K_c \neq 2 \) (the lines are guides to the eye).
The two-qubit reduced density matrix \( \tilde{\rho} \) we will concentrate on the case of linearly driven dimerization for systems with orbital degrees of freedom. This mechanism is particularly important for transition metal oxides with perovskite structure where the valence electrons are situated in the t_{2g} orbitals. Because t_{2g} orbitals are not bond oriented the electron–phonon coupling is weak so that we might ignore lattice degrees of freedom to first approximation. With appropriately rescaled parameters, the physics discussed below is almost independent of the spin value 3. For definiteness, we will consider in the following the case of an effective spin 1/2 appropriate for systems with a 3d^2 valence electron configuration, as for example, YVO₃, and a twofold orbital degeneracy described by an orbital pseudospin \( \tau = 1/2 \). A 1D Hamiltonian reflecting the spin–orbital physics for such a system is given by

\[
H_{S\tau} = J \sum_j (S_j \cdot S_{j+1} + 1) \left( \tau_j \cdot \tau_{j+1} + \frac{1}{4} - \gamma_H \right),
\]

where \( J > 0 \) is the superexchange and \( \gamma_H \) is proportional to the Hund’s coupling and promotes FM spin correlations. Using a MF decoupling, which is reasonable for FM spin correlations \( |J| \), we write \( H_{S\tau} \approx H_S + H_{\tau} \), where \( H_S \) (\( H_{\tau} \)) is the Hamiltonian for the spin (orbital) sector, respectively. If we allow for a dimerization in both sectors then \( H_{S(\tau)} \) is — up to a constant — given by Eq. \( \mathbf{1} \) with \( J -> J_\tau S_{\tau(j)} \), \( \delta -> \delta_{S(\tau)} \), and \( S \) representing the spins \( S = 1 \) or the orbital pseudospins \( \tau = 1/2 \), respectively. The effective superexchange constants are given by \( J_\tau = \Delta_{\tau (\tau)}^{-} / 2 + 1/4 - \gamma_H \) and \( J_\tau = \Delta_{\tau (\tau)}^{+} / 2 + 1 \), with \( \Delta_{\tau (\tau)}^{\pm} \) defined analogously to \( \Delta_{SS}^{\pm} \). Strong quantum fluctuations for pseudospin 1/2 and \( \gamma_H > 0 \) will favor AFM coupled orbitals, \( J_\tau > 0 \), and FM coupled
FIG. 4: (color online) Phase diagram and dimerization parameters $\delta_S$, $\delta_\tau$ for the spin–orbital model $[5]$ with $\gamma_H = 0.1$ in MF decoupling. The dashed lines denote the phase boundaries between the uniform (U) and dimerized (D) phases.

spins, $J_S < 0$. The dimerizations are then given by $\delta_S = \Delta/\tau/(2J_S)$ and $\delta_\tau = \Delta_{SS}/(2J_\tau)$. This means that the exchange constants and the dimerizations for each sector are determined by the nearest-neighbor correlations in the other sector and therefore have to be calculated self-consistently. We can simplify this procedure by noting that $\Delta_{SS(\tau)}$ show only a weak dependence on dimerization and temperature for low temperatures. We therefore fix $J_{S(\tau)}$ by using the values for $\Delta_{SS(\tau)}$ obtained for an undimerized chain at zero temperature. This leads to $J_\tau = 2$ and $J_S = 1/2 - \ln 2 - \gamma_H$ $[2]$. Now the dimerizations $\delta_{S(\tau)}$ can be easily determined self-consistently. The results for $\gamma_H = 0.1$ — which is a realistic value for cubic vanadates — are shown in Fig. 4. For $0.10 \lesssim T/J \lesssim 0.49$ the self-consistent MF decoupling leads to nonzero values for $\delta_{S(\tau)}$. The evolution of the dimerization parameters in this temperature regime has a dome-shaped form with a maximum at $\sim 0.25$. Agreement with Fig. 4 shows that the dimerization in the AFM orbital chain is much larger than the dimerization in the FM spin chain, and at $T/J = 0.2$ we have $\delta_S \approx 0.86$ which is already close to perfect dimerization (Fig. 3). This underlines that the thermally activated dimerization in the FM chain is the driving force behind the finite temperature dimerized phase for the spin–orbital chain. The phase transitions at finite temperature between a uniform and a dimerized phase are a consequence of the MF decoupling. Such phase transitions will not occur for the strictly 1D model $[5]$. Nevertheless, numerical calculations for this model $[8]$ show that a dimerization is the leading instability at temperatures which support the dimerized phase in the MF decoupling solution.

Summarizing, we have shown that a dimerization can occur in FM spin chains but has to be activated by thermal fluctuations. The gain in magnetic energy at finite temperatures can be related to an increased entanglement entropy on the weak bonds. For a FM chain with spin–phonon coupling we have derived the phase diagrams as a function of temperature $T$ and the effective elastic constant $K$ for spin values $S = 1/2$ and $S = 1$. Thermodynamic properties of the dimerized FM chain can be calculated analytically with good accuracy for temperatures $T \lesssim |J|S$ by a MSWT. Remarkably, this approach works for all dimerizations $\delta \in [0, 1]$ if quartic terms are taken into account appropriately. For a system of coupled FM spin-1 and AFM orbital pseudospin-1/2 degrees of freedom we found, using a mean–field decoupling, a finite temperature dimerized phase. This shows that a dimerization is a universal instability of FM chains at finite temperatures, and may be triggered by the coupling to purely electronic degrees of freedom. This latter mechanism seems to be relevant for many transition metal oxides with (nearly) degenerate orbital states.

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