

Dimerization and Entanglement in Spin-Orbital Chains

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Spin-orbital coupling: The study of orbital degeneracy in transition metal oxides is motivated, e.g., by the large variety of spin-charge-orbital ordered phases, the possible control of the orbital degree of freedom at interfaces and heterostructures, the switching from orbital ordered to metallic phases in applied magnetic fields, and the colossal magnetoresistance. The rather complex interplay of orbital and spin degrees of freedom can be formulated in terms of spin-orbital exchange models, which are derived from more general multi-band Hubbard models. A particularly challenging system that stimulated a number of studies is the one-dimensional (1D) spin-orbital model with free coupling parameters x and y :

$$\mathcal{H} = J \sum_{j=1} \left(\vec{S}_j \cdot \vec{S}_{j+1} + x \right) \left(\vec{T}_j \cdot \vec{T}_{j+1} + y \right), \quad (1)$$

where \vec{S}_j and \vec{T}_j represent the spin and orbital pseudospin degrees of freedom (here we consider $S = 1$ and $T = \frac{1}{2}$). On the one hand, this model already contains the full complexity of the interplay of the different degrees of freedom, orbital (T) and spin (S). It also allows one to attack the problem with special tools particularly designed for 1D models. On the other hand, this model reflects to a certain extent generic aspects of the physics of orbital degenerate Mott insulators in three dimension, namely for phases with quasi-1D correlations. An example is the C -AF phase in cubic vanadates, YVO_3 or LaVO_3 , that reveals strong orbital fluctuations accompanied by ferromagnetic (FM) spin order along the c cubic axis. In the case of vanadates, $J > 0$ and \vec{S}_j (\vec{T}_j) represent $S = 1$ spin (t_{2g} orbital) degrees of freedom, respectively. While the Hamiltonian of these compounds is more complex, Eq. (1) captures nevertheless certain essential features, as for example the amazing orbital-Peierls instability towards a phase with alternating orbital singlets coupled to modulated FM exchange (stronger and weaker) spin-couplings along the c axis.

Dimerized spin-orbital chains: Figure 1 shows (a) the phase diagram and (b) the order parameters of the spin-orbital chain (1). The most remarkable feature is the reentrant behavior of the dimerization and the absence of dimerization at zero temperature. In our study the quartic coupling terms, $(\vec{S}_j \cdot \vec{S}_{j+1})(\vec{T}_j \cdot \vec{T}_{j+1})$, are treated by a mean-field decoupling of the spin- and orbital degrees of freedom. The temperature dependence of spin correlations is analyzed by a modified spin wave theory and the XY part of the orbital interaction is treated by Jordan-Wigner theory [1].

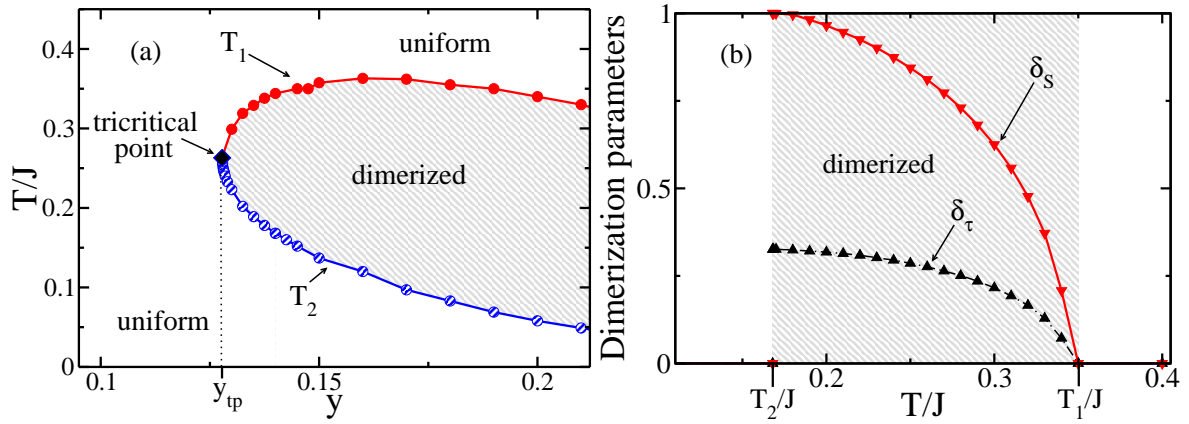


Figure 1: (a) Phase diagram of spin-orbital chain (1) for $x = 1$ as function of temperature T and coupling constant y reflecting a spin-orbital dimerized phase at finite T , and (b) reentrant behavior of the dimerization of the spin-orbital chain calculated in a mean-field theory for $x = 1$, $y = 0.14$ and positive $J > 0$. The dimerization parameters δ_S (δ_τ) acting on the spin (orbital) degrees of freedom, respectively, are finite only in an intermediate temperature range determined by temperatures T_1 and T_2 . It is important to note that the dimerization in the spin sector is induced by the dimerization in the orbital sector and vice versa and does not require a coupling to the lattice as in the Peierls effect.

Peierls dimerization of ferromagnetic Heisenberg chains: For the understanding of the reentrant behavior in Fig. 1(b) it is useful to consider the FM ($J < 0$) spin-Peierls problem. The Hamiltonian can be written as

$$H = J \sum_{j=1}^N \{1 + (-1)^j \delta\} \vec{S}_j \cdot \vec{S}_{j+1} + E_{el}, \quad (2)$$

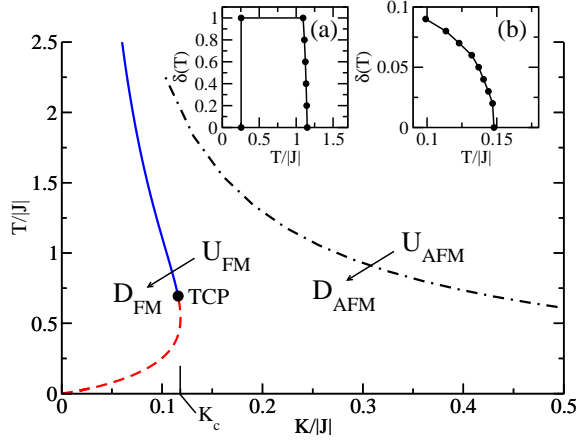


Figure 2: Comparison of phase diagrams of FM ($J < 0$) and AFM ($J > 0$) spin-1/2 Heisenberg chains in the plane determined by temperature and elastic force constant K [2]. The well-known AFM spin-Peierls transition, from the undimerized (U_{AFM}) to the dimerized (D_{AFM}) phase, occurs for any coupling strength (dash-dotted line). In contrast, the FM chain behaves differently and dimerizes (D_{FM} phase) only for sufficiently weak force constants $K < K_c \simeq 0.12|J|$. Moreover, the FM case shows reentrant behavior and dimerization at zero temperature is ruled out. The tricritical point (TCP) separates first and second order behavior. Insets show the order parameter $\delta(T)$ for: (a) the FM chain at $K/|J| = 0.1$, and (b) the AFM chain for $K/J = 2$.

where δ is the dimensionless dimerization (order) parameter and $E_{el} = \frac{1}{2}NK\delta^2$ is the elastic energy determined by the force constant K . The FM case with $J < 0$ is very distinct from the well-known antiferromagnetic (AFM) spin-Peierls chain ($J > 0$) as seen from the phase diagrams in Figure 2, which summarizes our results obtained by transfer-matrix renormalization group (TMRG) calculations for both cases [2,3]. In the AFM case the dimerization occurs always, i.e., for any value $K/J > 0$, whereas in the FM case we find the reentrant behavior as for the spin-orbital chain. Moreover, we observe the FM dimerized phase D_{FM} only for sufficiently small force constants $K/|J|$.

The AFM chain dimerizes because the alternation of the AFM correlations leads to a lowering of magnetic energy, which overcompensates the increase of elastic energy E_{el} . In the FM ground state, however, there are no quantum fluctuations and the FM correlations are saturated. Thus alternation of spin correlations is ruled out. At finite temperature, however, thermal fluctuations weaken these correlations and at the same time allow for the dimerization when the coupling to the lattice is not too strong.

Entanglement of spin-orbital excitations and von Neumann entropy spectra: In general, spin-orbital systems contain entangled states. Here we investigate entanglement in the 1D spin-orbital model (1) for $S = \frac{1}{2}$. In general, a many-body quantum system can be subdivided into A and B parts and the entanglement entropy is then given by the von Neumann entropy (vNE), $\mathcal{S}_{vN} = -\text{Tr}_A\{\rho_A \log_2 \rho_A\}$, where $\rho_A = \text{Tr}_B\{\rho\}$ is the reduced density matrix of the subspace A and ρ is the full density matrix. In the case of the 1D spin-orbital model (1) we associate subsystem A with spin and B with orbital degrees of freedom. Results for the vNE, \mathcal{S}_{vN} , are shown in Figure 3. It vanishes for ground states which can be factorized into the spin and orbital part, i.e., $|\psi\rangle = |\psi_S\rangle \otimes |\psi_T\rangle$. In the case of the 1D spin-orbital model (1) with $J < 0$ this applies to the ground states of phases I, II and IV where at least one component is a fully polarized (FM or ferro-orbital) state.

Then a natural question arises: What does this imply for the excited states? If we start from a ground state with disentangled spin- and orbital-degrees of freedom, for instance from the phase I, are the spin-orbital excitations entangled or not? To investigate the degree of entanglement of spin-orbital excited states, we introduce the vNE

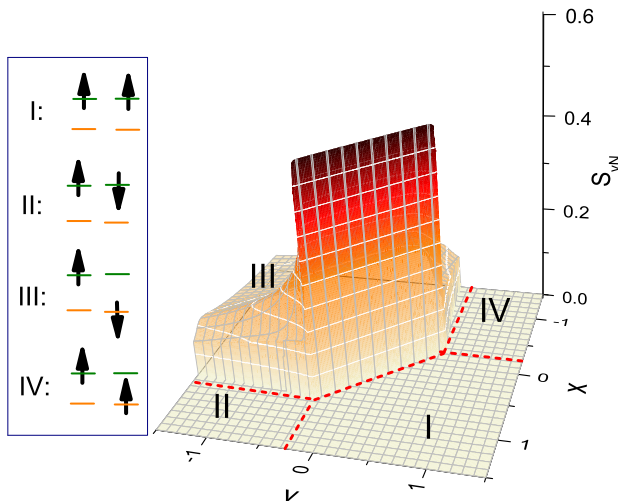


Figure 3: Spin-orbital entanglement entropy \mathcal{S}_{vN} in the ground state of the 1D spin-orbital chain (1) for $J < 0$ as function of x and y . The phase boundaries indicated by dashed lines have been determined by calculating the fidelity susceptibility [4]. The two-site spin-orbital configurations (see box) indicate the prevailing correlations in phases I-IV, respectively. The only spin-orbital entangled ground states with AFM spin and alternating orbital correlations are found in phase III.

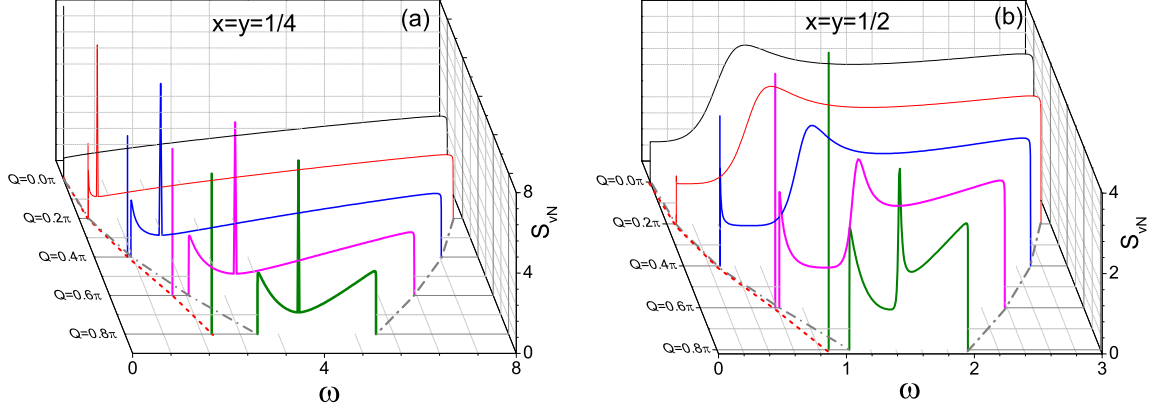


Figure 4: The von Neumann entropy spectral function $S_{vN}(Q, \omega)$ displays the entanglement of the lowest spin-orbital excitations in phase I [4], i.e., in a phase where the ground state itself is disentangled and spin and orbital degrees of freedom can be factorized! $S_{vN}(Q, \omega)$ is calculated for a 1D spin-orbital chain (1) of 400 sites, for: (a) $x = y = 1/4$ and (b) $x = y = 1/2$. The spectra show a continuum of spin-orbital excitations (between dashed-dotted lines); in addition one finds: (i) a bound state below the continuum (dashed line), and (ii) a sharp spin-orbital resonance inside the continuum in the highly symmetric 1D SU(4) model ($x = y = 1/4$). In contrast, in case (b) one recognizes a damping of the spin-orbital resonance, while the bound state below the continuum survives but is closer to the continuum.

spectral function in the Lehmann representation [4],

$$S_{vN}(Q, \omega) = - \sum_n \text{Tr} \{ \rho_s^{(\mu)} \log_2 \rho_s^{(\mu)} \} \delta \{ \omega - \omega_n(Q) \}, \quad (3)$$

where $(\mu) = (Q, \omega_n)$ denote momentum and excitation energy, and $\rho_s^{(\mu)} = \text{Tr}_o |\Psi_n(Q)\rangle \langle \Psi_n(Q)|$ is the spin density matrix obtained by tracing out the orbital degrees of freedom.

Figure 4 gives two examples ($x = y = 1/4$ and $x = y = 1/2$) of the von Neumann spectral function (3) for phase I of the 1D spin-orbital chain (1), i.e., for the ground state with coexisting FM spin and ferro-orbital correlations. We focus here on the elementary excitations in the Hilbert space with one spin and one orbital flip, respectively. The spectra are characterized by three distinct types of excitations: (i) the spin-orbital continuum with energies,

$$\Omega(Q, q) = \omega_s \left(\frac{Q}{2} - q \right) + \omega_t \left(\frac{Q}{2} + q \right), \quad (4)$$

where $\omega_s(Q) = (\frac{1}{4} + y)(1 - \cos Q)$ and $\omega_t(Q) = (\frac{1}{4} + x)(1 - \cos Q)$ are the elementary spin- and orbital-excitations (i.e., spin waves and orbitons) at momentum Q ; (ii) the spin-orbital excitonic bound state (BS) with energy $\omega_{BS}(Q)$, and (iii) a spin-orbital resonance $\omega_{SOR}(Q)$ which is degenerate with $\omega_s(Q)$ and $\omega_t(Q)$ at the SU(4) point $x = y = 1/4$, Figure 4(a). Interestingly, all excitations have finite entanglement entropy and in general spin-orbital bound states are strongly entangled states. In particular, the SOR at $x = y = 1/4$ is maximally entangled, $S_{vN} = \log_2 L$ where L is the length of the system. From this we may conclude that a system, which is disentangled at $T = 0$, will become entangled at finite temperatures.

The entanglement spectral function $S_{vN}(Q, \omega)$ has a similar form as any other dynamical spin- or charge-correlation function. There is, however, an important difference — as there is no direct probe for the von Neumann entropy of a state, the spin-orbital entanglement spectra can be calculated but cannot be measured directly. On the other hand, we have shown [4] that the intensity distribution of certain resonant inelastic x-ray scattering (RIXS) spectra of spin-orbital excitations in fact probe qualitatively spin-orbital entanglement.

References:

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