An extended Falicov-Kimball model on a triangular lattice

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Abstract – The combined effect of frustration and correlation in electrons is a matter of considerable interest lately. In this context a Falicov-Kimball model on a triangular lattice with two localized states, relevant for certain correlated systems, is considered. Making use of the local symmetries of the model, our numerical study reveals a number of orbital ordered ground states, tuned by the small changes in parameters while quantum fluctuations between the localized and extended states produce homogeneous mixed valence. The inversion symmetry of the Hamiltonian is broken by most of these ordered states leading to orbitally driven ferroelectricity. We demonstrate that there is no spontaneous symmetry breaking when the ground state is inhomogeneous. The study could be relevant for frustrated systems like GdI₂, NaTiO₂ (in its low-temperature C²/m phase) where two Mott localized states couple to a conduction band.

Geometric frustration in correlated systems brings about a variety of phenomena and is presently a major area of interest in the condensed-matter community. Systems having two-dimensional (2D) layered structure with triangular lattice (for example, transition metal dichalcogenides [1,2], cobaltates [3], GdI₂ [4] and its doped variant [5,6], NaTiO₂ [7–9], NaVO₂ [10] etc.) are known to come up with a host of cooperative phenomena like valence and metal insulator transitions, charge, orbital and magnetic order, unconventional superconductivity, excitonic instability [1] and possible non-Fermi liquid states [4]. These systems pose a challenge to theoretical understanding as the underlying geometric frustration of the triangular lattice, coupled with strong dynamic fluctuations, gives rise to a large degeneracy at low temperatures and competing ground states close by in energy. A consequence of this is a fairly complex phase diagram [5] and the presence of soft local modes strongly coupled to the itinerant electrons [4].

We motivate the model by looking at two systems, GdI₂ and NaTiO₂. Each layer of Gd ions in GdI₂ forms a 2D triangular lattice. They are well separated from each other by intervening layers of large iodine ions and do not interact significantly with each other. From recent LSDA band structure calculations [5] it is known that three nearly degenerate, spin-polarized d-orbitals (d<sub>xy</sub>, d<sub>x²-y²</sub> and d<sub>z²</sub>) cross the Fermi level. Calculations involving dynamical local correlations [4] show that these three nearly degenerate d-orbitals further break down to two doubly degenerate (d<sub>x²-y²</sub> and d<sub>z²</sub>) localized levels below and one extended (d<sub>xy</sub>) level across the Fermi level. From experimental studies [6], it is observed that the ground state is insulating and is likely to be orbitally ordered in a three-sublattice fashion at half-filling (each orbital occupying one sublattice), while a small doping away from half-filling leads to phase segregation. An effective Falicov-Kimball model of spinless fermions with two (degenerate) localized bands and one itinerant band is proposed recently for this system [4]. It would, therefore, be interesting to look for such orbitally ordered states in this context.

The corresponding Hamiltonian, then, is

\[ H = - \sum_{\langle ij \rangle} (t_{ij} + \mu \delta_{ij}) d_i^\dagger d_j + E_f \sum_{i,\alpha=1,2} (f_{i\alpha}^\dagger f_{i\alpha}) + U \sum_{i,\alpha=1,2} (f_{i\alpha}^\dagger f_{i\alpha} d_i^\dagger d_i) + U_f \sum_i (f_{i1}^\dagger f_{i1} f_{i2}^\dagger f_{i2}). \]  

(1)

The first term in eq. (1) is the kinetic energy of d-electrons on a triangular lattice (only nearest-neighbor hopping is considered), while the second term represents the degenerate energy levels \( E_f \) of the \( f_1 \) and \( f_2 \) electrons.
The third term is the on-site Coulomb repulsion between $d$- and $f$-electrons. The last one is the local repulsion between the $f$-electrons. In addition, there is a mixing term between $d$- and $f$-electrons $Vd_i^+f_{i\alpha} + \text{h.c.}$ This term has profound effects on the physics of the model and we keep $V = 0$ in the beginning and take it up later.

NaTiO$_2$ is another system where the above model could be useful to study the orbital order. It also has a layered structure with alternating NaO and TiO slabs and shows a transition [7] at around 250 K to a monoclinic phase most likely to be orbitally ordered [8,10]. The Ti$^{3+}$ ions with one electron in the $d$-orbital are arranged on a triangular lattice and are octahedrally coordinated to oxygen ions. In the low-temperature monoclinic phase the TiO$_6$ octahedron gets distorted, leading to a splitting in the triply degenerate $t_{2g}$-orbitals of Ti 3$d$, with one conduction and two localized bands. Orbital order due to electronic correlations has been predicted in this system [8–12].

While the presence of a lone $d$-electron in the $t_{2g}$-orbitals in Ti immediately suggests a role for strong spin fluctuations, the overwhelming experimental and theoretical results appear to indicate that the large entropy is eventually relieved at low temperature via ordering of the orbitals. The absence of magnetic LRO, very small susceptibility below 250 K, lack of Curie-Weiss behavior in any region of temperature and the apparent Pauli paramagnetic behavior above and below the transition point towards a spin degree which is completely quenched at low temperature [7]. In addition, the loss of entropy much in excess of Rh2 at the transition is a clear indication that orbitals are predominantly involved in the ordering process. While the transition is probably affected by the spin fluctuations (evidenced by the drop in susceptibility), the exact role of spin degrees in selecting the ground-state order is not yet established [9,10,12]. Lowest-order energies presuming FM and AFM configurations are almost identical [8], suggesting that an orbitally driven Peierls state quenches the spin to a possible singlet state [9]. Such correlations in the 3$d$-band would further localize the two bands and the effective model above could well describe the low-energy dynamics of this system. Clearly the low-temperature physics is dominated by the orbital degrees and strong correlations therein [12] and the above model is one of the simplest ones, consistent with the electronic structure of NaTiO$_2$ at low temperature, for the emergence of orbital order. Although the notion of spins dictating orbital order is not borne out in both experiments and theory, how the spin gets quenched when added to this model is an interesting question [13].

The Hamiltonian conserves local $f$-electron occupation numbers $n_{f,i\alpha} = f_{i\alpha}^\dagger f_{i\alpha}$ owing to the local $U(1)$ gauge invariance in the absence of $f$-$d$ mixing. Therefore, $[\hat{n}_{f,i\alpha}, H] = 0$ and $\omega_{i\alpha} = f_{i\alpha}^\dagger f_{i\alpha}$ are good quantum numbers taking values only 0 or 1. The local conservation also implies that the Hamiltonian may be written as

$$H = \sum_{<ij>} h_{ij}(\omega)d_i^\dagger d_j + E_f \sum_{i,\alpha} \omega_{i,\alpha} + U_f \sum_i \omega_{i1}\omega_{i2},$$  \hspace{1cm} (2)

where $h_{ij}(\omega) = -t_{ij} + (U \sum_{\alpha} \omega_{i,\alpha} - \mu)\delta_{ij}$.

With only one localized level this model reduces to the usual FKM [14] studied in great detail [15–18] for a long time, primarily on bipartite lattices. We set the scale of energy as the nearest-neighbor hopping $t = 1$. The eigenvalue spectrum of this Hamiltonian, is easily obtained by numerical diagonalization on a finite-size triangular lattice with periodic boundary condition. In order to

Fig. 1: (Colour on-line) $f$-electron configurations are shown at each site for (a) $n_{f_1} = n_{f_2} = 1/8$, (b) $n_{f_1} = n_{f_2} = 1/4$ and (c) $n_{f_1} = n_{f_2} = 1/3$. Black and green circles correspond to sites occupied by $f_1$ and $f_2$ electrons, respectively and open circles correspond to sites with no $f$-electron occupancy.
calculate the average values of physical quantities, the classical Monte Carlo method using Metropolis algorithm can then be employed by “annealing” over a subset of configurations of the “classical” variables [18] \( \{ \omega_{i, \alpha} \} \). This approach is known to give reliable results for the FKM, even on a triangular lattice with macroscopic degeneracies. The details of the method is reported elsewhere [19].

For the systems discussed above, the number of electrons in the d-band is one at every site in the undoped limit. Therefore, in the following calculations, we restrict ourselves to the case, \( N_f + N_d = N \), where \( N_f \), \( N_d \) and \( N \) are the total number of f-electrons, d-electrons and the number of sites in the lattice, respectively (we have used \( N = 144 \) in all the calculations and checked a few results with larger \( N \)). In addition, \( N_f1 = N_f2 = N_f/2 \), as the two f-levels are degenerate.

In fig. 1 we show the ground-state configurations for different \( U \) and \( U_f \) at various f-electron concentrations. Each row shows the progression of states from disorder to order and finally order again as a function of \( U \) and \( U_f \) for different \( n_f \) values. Figure 1(a) presents the case for \( n_f1 = n_f2 = 1/8 \). In the absence of any interaction between the two localized f-electron states \( (U_f = 0) \), no particular order is observed even on increasing the value of \( U \). In fact, a finite \( U \) favors double occupancies of f-electrons, leaving a larger part of the lattice for d-electron motion. Therefore, with increasing \( U \) there is an increasing tendency of phase separation in real space between localized and itinerant electrons. Keeping \( U \) small (for example, \( U = 1 \)) and making \( U_f \) finite begins to remove the local double occupancies of f-electrons, reduces the overall kinetic energy of d-electrons and leads to an ordered stripe-like pattern of the two localized electrons \( (f_1 \) and \( f_2) \). This stripe pattern appears at a higher \( U_f \) when \( U \) is raised. A transition from a state of disordered doubly occupied sites to a stripe-like ordered pattern as a function of \( U_f \) at fixed \( U \) is shown in fig. 1. This is a discontinuous transition appearing at a critical value of \( U_f \) (which increases with \( U \)) and the ordered phase remains stable up to high values of \( U_f \). Note that on raising \( U_f \), the double occupancy is removed very quickly (see later) and the ground state is fairly insensitive to a rise in \( U_f \) further. Similar trends are seen for other fillings too \((e.g., \ n_f1 = n_f2 = 1/4 \) and \( n_f1 = n_f2 = 1/3 \), shown in fig. 1(b) and (c), respectively), albeit with different real space patterns of the f-electrons: for \( n_f1 = n_f2 = 1/4 \) it is a bi-stripe orbital order, whereas for \( n_f1 = n_f2 = 1/3 \) it is a three-sublattice structure involving \( f_1 \), \( f_2 \) and empty (no f-electron) sites decorating the vertices of each triangle.

The traditional FKM has been studied earlier on a triangular lattice [15]. In the large-\( U \) limit, an FKM can be mapped onto an AFM Ising model in a “magnetic field” (where the “spin” \( s_{i, \alpha} = 2\omega_{i, \alpha} - 1 \) is \( \pm 1 \)) and the ground state remains frustrated on a triangular lattice, manifested by degeneracies at low temperature and competing states separated by phase segregation [19,20].

Crystalline charge/orbital orders of various periodicities have been observed in square [15,18] lattice at commensurate and rational fillings, while there are only few such examples in triangular lattices [17,19,20]. Phase segregation is the most usual outcome in much of the phase space in both square and triangular lattice.

There is a local symmetry in the Hamiltonian involving interchange between the two species of f-electrons. However, the conservation of \( n_{f1, \alpha} \) restricts the occupation \( \omega_{i, \alpha} = 0, 1 \) and there is no quantum-mechanical mixing in the Hamiltonian between the two species for \( V = 0 \). Exact solutions in FKM on a triangular lattice show charge/orbital crystals in the ground state [15,17,18] at specific commensurate fillings. This is clearly seen, to order \( 1/V^2 \), in the Ising AFM \( H_{eff} = \frac{J^2}{U^2} \sum_{<ij>, \alpha} s_{i, \alpha} s_{j, \alpha} + \frac{1}{U} \sum_{\alpha \neq \beta} s_{i, \alpha} s_{i, \beta} + \frac{1}{2} (\mu + Ef) \sum_{\alpha} s_{i, \alpha} \). As shown [17] in the original FKM, the degeneracies in the resulting charge-ordered ground state of the effective Hamiltonian are lifted at higher order in \( 1/V \). Such lifting of degeneracies is quite common where the system relieves its large entropy via an ordered ground state\(^1\) [15–17].

Slightest non-zero mixing \( V \), would also, for example, remove this degeneracy in favour of the ordered state (by \( \sim V^4 p^2 (E_F U)/U_f \), where \( \rho(E_F) \) is the d-electron density of states at the Fermi level). This is the right ground state on a triangular lattice at this filling in the small but finite \( V \) limit and as we will show below (shown in square lattice by Czycholl [21]), the ground states obtained in the two limits, \( V = 0 \) and very small but finite \( V \), could be adiabatically continued to each other.

One of the most interesting consequences of the various orbital orders seen in fig. 1 is that many of them break the inversion symmetry of the Hamiltonian. This will induce spontaneous displacements of the ions and the resulting lattice distortion will lead to ferroelectricity with a spontaneous finite polarisation. This is due to a specific realization of the unconventional orbital order that breaks inversion symmetry. It is driven by electronic correlation, a very different route from the conventional ones to ferroelectricity.

In fig. 2 we present the d-electron densities at each site. It is interesting to observe how the competition among different interaction energies (such as kinetic energy of the d-electrons, on-site correlation energies between d- and f-electrons as well as between two localized f-electrons) affect the transport of the system. The d-electron density plots at each site (presented in fig. 2 for \( n_{f1} = n_{f2} = 1/3 \)) clearly show the appearance of metallic and insulating and re-entrant metallic phases by tuning the parameters \( U \) and \( U_f \). From figs. 2(b) and (c) we see that on increasing \( U \) to a high value, keeping \( U_f \) fixed, the system goes from a stripe-like

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\(^1\)Approaching the ground state numerically from a finite temperature one arrives at an ordered state in statistically overwhelming majority of trials, thereby quenching the entropy.
ordered configuration to a phase-separated state. This transition is accompanied as well by an insulator-to-metal transition as we discuss below. Again by keeping $U$ fixed and increasing $U_f$, the ordered structure reappears and the system becomes insulating (figs. 2(c), (d)). By tuning the interaction parameters $U$ and $U_f$ one can switch between these metallic and insulating states. Note that in some cases there are also sites substantially occupied by electrons of all three types ($f_1$, $f_2$ and $d$). The number of sites doubly occupied by localized $f$-electrons predominantly plays a crucial role in determining the critical $U$ for the metal-insulator transitions discussed above. We show the dependence of this double occupancy ($do$) on the interaction parameters $U$ and $U_f$ for $n_{f_1} = n_{f_2} = 1/8$ in fig. 3. The double occupancy $do$ is extremely sensitive to $U_f$, dropping off to zero rapidly for $U_f$ as small as 0.25 for various value of $U$ and $n_{f,α}$. It increases with $U$ as expected and saturates quite rapidly thereafter. These features are quite general and are observed at other fillings of $n_{f,α}$ too.

In order to investigate the electronic properties of these ordered phases further we have calculated the gap\(^2\) in the spectrum for each of these phases. Figure 4(a) shows the gap as a function of $U_f$ for a series of $U$ values, for the filling 1/8. The disorder-to-order transition is indeed accompanied by a metal-to-insulator transition (MIT), the disordered phase has no gap at the Fermi energy, whereas the ordered states are insulating with a finite gap. In addition, the gap appears at a critical $U_f$ and remains constant beyond (independent of $U_f$ as long as $U$ is fixed). The discontinuous nature of the transition is clearly visible in fig. 4. On increasing $U$ the same feature is observed, though the critical $U_f$ for MIT increases. As $U_f$ is the correlation energy between two localized $f$-electrons and $U$ is the same between localized and itinerant electrons, there is a competition between these two interactions and therefore the critical $U_f$ depends strongly on $U$. In fig. 4(a) we show the energy gap as a function of $U_f$ at fixed values of $U$ for $n_{f_1} = n_{f_2} = 1/8$.

An interesting observation can be gleaned from the energy gaps if we keep $U_f$ fixed (say $U_f = 1$) and vary $U$. For $U = 0$ there is no gap in the spectrum and on increasing $U$, the gap increases almost linearly with $U$ (fig. 4(b)). Above a certain value of $U$ (for $U_f = 1$, at around $U = 3.2$), however, the gap suddenly drops to zero and the system becomes metallic. Therefore, as a function of $U$ and at a fixed $U_f$, there is a metallic phase appearing at large $U$. This seemingly counterintuitive result is understood from the fact that there are two competing processes at hand (coming from $U$ and $U_f$). At $U = 0$ the $d$-electrons are free and the system is metallic. As $U$ increases they avoid sites occupied by $f$-electrons and a gap appears. There is also a tendency towards $f$-$d$ phase segregation as discussed above. A finite value of $U_f$, however, strongly disfavours double occupancy (as in fig. 3) and spreads the $f$-electrons out. Therefore, when, at a higher $U$, double occupancy (with $f_1$ and $f_2$ electrons) is energetically favorable over a joint occupation by $f_{α}$- and $d$-electrons at a site, the metallic state reappears. In fig. 4(c) we show the corresponding phase diagram in the $U$-$U_f$ plane for $n_{f_1} = n_{f_2} = 1/3$.

The presence of the local $U(1)$ gauge symmetry for each of the two localized levels has additional advantages. As the conservation of $f_{αi}^+ f_{αi}$ renders the $d$-electron part diagonalisable (in a “local” potential of the $f$-electrons), the problem then becomes exactly solvable in the infinite-dimensional limit where the $d$-electron self-energy is local [22]. Such a solution has been obtained by Brandt and Mielsch [23] for the original Falicov-Kimball model. A straightforward generalization is possible in the present model as well. The local Green’s function, in the limit of infinite spatial dimension, turns out to be

\[
G(ω_n) = \langle (1 - n_{f_1})(1 - n_{f_2}) \rangle G_0(ω_n) \\
+ \langle n_{f_1}(1-n_{f_2})+n_{f_2}(1-n_{f_1}) \rangle (G^{-1}_0(ω_n)-U)^{-1} \\
+ ⟨n_{f_1}n_{f_2}⟩(G^{-1}_0(ω_n)-2U)^{-1},
\]

(3)
at $U_f$ for different values of $U_f$ (b) as a function of $U_f$ for different $U_f$, at $n_{f_1} = n_{f_2} = 1/8$ and (c) phase diagram showing metallic and insulating regions for $n_{f_1} = n_{f_2} = 1/3$, in the $U-U_f$ plane. The $x$-axis ($U = 0$ line) is trivially metallic.

where $G_0(\omega_n) = (i\omega_n + \mu + \delta(\omega_n))^{-1}$ with $\omega_n = (2n + 1)\pi KT$ the fermionic Matsubara frequency, $\delta(\omega_n)$ is the self-consistent, time-dependent generalized potential. Inserting the Dyson equation $G_{\omega_n}(\omega_n) = G^{-1}(\omega_n) + \Sigma(\omega_n)$ in the above eq. (3), a cubic equation for the self-energy $\Sigma(\omega_n)$ can be written. If one further takes the limit of $U_f \to \infty$, then the last term on the right side in eq. (3) above vanishes and writing $n_f = n_{f_1} + n_{f_2}$, one gets back the Brandt-Mielch solution. Note that the Green’s function appears identical to that of the coherent potential approximation [24] (as also alloy analogy, Hubbard-III), but the difference here is that $\langle n_{f_\alpha} \rangle$ are determined by the Green’s function $G(\omega_n)$ through $n_f = f(E_{f_\alpha})$ and $E_{f_\alpha} = E_{f_\alpha} - KT \sum_{\omega_n} \log(1 - U G_0(\omega_n))$ (here $f(x)$ is the Fermi function $[1 + \exp(x - \mu)/KT]^{-1}$). In this limit, the self-energy is easily obtained in the case where the filling is $\langle n_{f_1} \rangle = \langle n_{f_2} \rangle = \langle n_d \rangle = 1/3$. The choice of Hartree self-energy $\Sigma = U \langle n_f \rangle$ evidently minimizes the ground-state energy. The corresponding configuration is an ordered three-sublattice arrangement of $d$, $f_1$ and $f_2$ electrons (with $d$, $f_1$, $f_2$ electrons occupying A, B, C sublattices), in the limit $U_f \to \infty$ where the two types of $f$-electrons must not occupy the same site. In fact the argument, following Czycholl [21], can be extended (for the ground state at least) to the case where a small hybridization term like $V d_\alpha^\dagger f_{\alpha}$ breaks the local invariance of the $f_{\alpha}$-electron number, though the global $U(1)$ symmetry is still extant. We turn to this situation now.

There have been several studies on the FKM on a square lattice over the years with a hybridization term that mixes localized and extended electrons. An important issue in this context was raised by Portengen et al. [25] regarding the spontaneous symmetry breaking (SSB) in such a model. A term $V d_\alpha^\dagger f_{\alpha}$ would induce non-zero excitonic (or ferroelectric [25]) averages like $\langle d_\alpha^\dagger f_{\alpha} \rangle$ as long as $V$ is non-zero. It was shown [25] from a mean-field theory calculation on a square lattice at half-filling that this average tends to a finite value even when $V \to 0$, leading to a spontaneously broken symmetry in the ground state. Although the soft local dynamic fluctuations between $f$- and $d$-electrons in the limit $V \to 0$ cannot be treated properly in the static mean field, we nevertheless undertake a similar mean-field analysis on the triangular lattice following previous work [21,25]. Assuming a homogeneous ground state and excitonic mean fields, we find (fig. 5) that when $U$ is finite, averages of the type $\Delta f_{\alpha} = \langle d_\alpha^\dagger f_{\alpha} \rangle$ do not vanish in the limit $V \to 0$, indicating an SSB similar to the situation on a square lattice [25]. Such a non-zero average would, then, imply a homogeneously mixed valent ground state.

However, the assumption of a homogeneous ground state itself is called into question for the ranges of parameters being studied. It is important to note that there could possibly be other ordered states with lower energy at half-filling and one would therefore need to first ascertain the correct ground state. Czycholl [21] had shown that on the square lattice, this is indeed the case and the right ground state is an ordered two-sublattice charge density state. He also showed that such a ground state does not support SSB and a homogeneous mixed valence. It is not clear a priori whether on a triangular

\textsuperscript{3}The matrix element $V$ in the hybridization term can be chosen as constant without any loss of generality [21], although when the localized and itinerant states have different parities, an appropriate $V(r)$ is required. The results presented here do not change even in such a situation.
lattice, similar considerations would apply. Clearly our mean-field analysis above shows that on a homogeneous ground state, the results of Portengen et al. hold. We, therefore, look for the ground state in the mean-field theory and work out the possibility of an SSB on a triangular lattice.

Following the arguments in the infinite-dimensional limit above, we expect an ordered three-sublattice orbital density state to appear at half-filling when \( n_d = n_f = 1/3 \) even for small finite \( V \). We set up the mean-field calculation to look for an orbitally ordered state and allow for inhomogeneous local order parameters. This involves calculating all the local order parameters in the real space iteratively for self-consistency. We describe the result in fig. 6 where an inhomogeneous mean-field solution with a three-sublattice orbital structure emerges as the lowest energy state. The corresponding orbital density order parameter is shown in the inset of fig. 6. The A sublattice has negligible \( f \)-occupation and a finite \( d \)-electron density, while B (C) sublattice has predominantly \( f_1 \) \( (f_2) \) occupation and a small \( d \)-occupation. Clearly as \( V \) rises, such a state becomes less stable and at a critical \( V \) the orbital order would melt (although mean-field analysis may not be quite valid in that range) due to strong quantum fluctuations. On reducing \( V \), we observe that in the limit of \( V \rightarrow 0 \), the excitonic order parameter (note that \( \Delta f_{\alpha} = \langle d_i^\dagger f_{\alpha} \rangle \) is the same for \( \alpha = 1, 2 \) in the degenerate limit considered) vanishes leading to an absence of SSB in this case. For comparison, we also show the behavior of this order parameter in a homogeneous ground state. In this case the solution supports a non-vanishing expectation value even at \( V \rightarrow 0 \).

In conclusion, we have studied an extended Falikov-Kimball model with two localized states on a triangular lattice. Such a model is found to lead to orbitally ordered ground states. Orbital order is reported (or predicted) in frustrated systems like GdI\(_2\) [6], NaTiO\(_2\) where electrons in localized valence bands interact with conduction band electrons. The exact nature of orbital ordering in them, however, is still debated. Furthermore, the disorder-to-order transitions have generally been seen to accompany a metal-insulator transition. Many of these orbitally ordered ground states would induce spontaneous lattice distortions due to the breaking of inversion symmetry and lead to ferroelectricity driven not by the conventional mechanisms, but by electronic correlations instead. We also investigate the possibility of a spontaneously broken symmetry in the form of an excitonic order parameter in this Hamiltonian and resolve that there is no SSB in the ground state on a triangular lattice.

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REFERENCES

[1] CERCCELLIER H. et al., Phys. Rev. Lett., 99 (2007) 146403.
[2] MOROSAN E. et al., Nat. Phys., 2 (2006) 544; QIAN D. et al., Phys. Rev. Lett., 98 (2007) 117007.
[3] QIAN D. et al., Phys. Rev. Lett., 96 (2006) 216405.
[4] TARAPHDER A. et al., Phys. Rev. Lett., 101 (2008) 136410.
[5] MAITRA T. et al., Eur. Phys. J. B, 49 (2006) 433.
[6] SIMON A., private communication.
[7] CLARKE S. J. et al., Chem. Mater., 10 (1998) 372.
[8] PEN H. F. et al., Phys. Rev. Lett., 78 (1997) 1323.
[9] KHOFSKI D. and MIZOKAWA T., Phys. Rev. Lett., 94 (2005) 156402.
[10] MCQUEEN T. M. et al., Phys. Rev. Lett., 101 (2008) 166402.
[11] JACKELI G. and IVANOIV D. A., Phys. Rev. B., 76 (2007) 132407.
[12] EZHOV S. YU. et al., Europhys. Lett., 44 (1998) 491.
[13] NORMAND M. and OLES A., Phys. Rev. B., 78 (2008) 094427, have recently used an orbital-spin coupled model for NaTiO\(_2\) to study this.
[14] FALICOV L. M. and KIMBALL J. C., Phys. Rev. Lett., 22 (1969) 997.
[15] FREERICKS J. K. and ZLATIV C., Rev. Mod. Phys., 75 (2003) 1333; FREERICKS J. K. et al., Phys. Rev. Lett., 88 (2002) 106401.
[16] ZLATIV C. et al., Philos. Mag. B, 81 (2001) 1443.
[17] GRUBER C. et al., J. Stat. Phys., 86 (1997) 57.
[18] KENNEDY T., Rev. Math. Phys., 6 (1994) 901.
[19] YADAV UMESH K. et al., J. Phys.: Condens. Matter, 22 (2010) 295602.
[20] CENKARIKOVA H. and FARKASOVSKY P., Phys. Status Solidi b, 244 (2007) 1900.
[21] CZYCHOLL G., Phys. Rev. B, 59 (1999) 2642.
[22] METZNER W. and VOLLMHARDT D., Phys. Rev. Lett., 62 (1989) 324.
[23] BRANDET U. and MIELSCH M., Z. Phys. B, 75 (1989) 365; 79 (1990) 295.
[24] VELICKY B. et al., Phys. Rev., 175 (1968) 747.
[25] PORTENGEN T. et al., Phys. Rev. B, 54 (1996) 17452.