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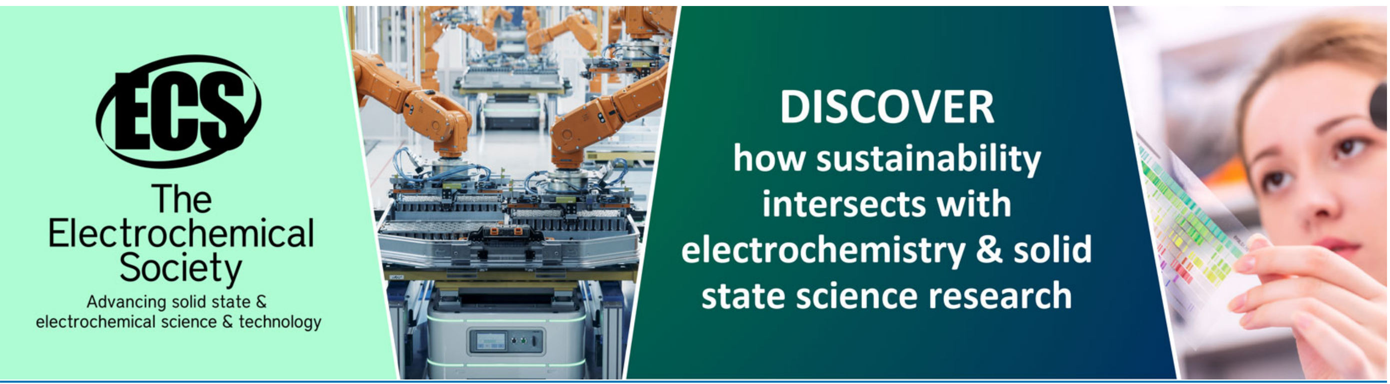

Metamagnetic transitions and CMR from the coexistence and competition of CDW, SDW and FM

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Abstract. We present the results of a generalized mean-field theory of all the conventional electron-hole condensates CDW,SDW and FM taken on the same footing using an eight dimensional spinor formalism. We study in detail the influence of temperature, particle-hole symmetry and external magnetic fields on the interplay of these three order parameters. We show that particle-hole asymmetry implies the presence of either one or else all three order parameters. Considering all order parameters on the same footing we reveal novel phenomena in the presence of a magnetic field like field-induced density waves, single and double first order transitions to itinerant metamagnetism as well as negative colossal magnetoresistance. We argue that the coexistence of CDW, SDW and FM is a quite generic phenomenon that may be involved in a number of open problems of great interest like for example the CMR phenomenon in manganites [4], the metamagnetic transitions in bilayer ruthenites and in heavy fermion systems etc.

A thorough study of singlet and triplet electron-hole condensates, namely Charge/Spin Density Waves (CDW/SDW)[1, 2, 3], has been done over the years mostly in the context of quasi 1D topologies[3]. It is our aim to present a 2D study of CDW/SDWs and itinerant ferromagnetism IFM on the same footing within a mean-field multicomponent framework. Such a system exhibits a rich variety of phenomena. It has already been demonstrated to show negative Colossal Magnetoresistance from the competition of comparable CDWs and SDWs and IFM in the presence of particle-hole asymmetry[4], A field Induced Density Wave transition is also reported along with a spin-flop transition arising from the interplay of CDW+SDW and the Pauli term[5]. There is another very interesting field induced phenomenon on which we focus here: the multistep Itinerant Metamagnetic transitions that exhibit remarkable similarities with experimental findings.

Metamagnetism has been defined empirically as a superlinear rise in the magnetisation over a narrow range of applied magnetic field. An itinerant metamagnetic transition alone is not symmetry breaking because of the background strong magnetic field. Quite surprisingly, distinct multistep metamagnetic first order transitions have been reported over the last few years in a number of materials (for example $Sr_3Ru_2O_7$, and URu_2Si_2)[6, 7, 8, 9]. These transitions are always accompanied by the formation of unidentified phases in the vicinity of the metamagnetic step (for example the Reentrant Hidden Order in the case of URu_2Si_2). Moreover, in all these metamagnetic transitions, as the temperature rises, the 1st order transitions relax to a crossover regime (see for example Fig.3 in[7]). We show here, that within our approach, such double-step metamagnetic transitions accompanied by a reentrant density wave formation are produced self-consistently under quite generic conditions.

In order to treat all order parameters on the same footing we adopt an eight component spinor space formalism defined by the following spinor which has been also used in the study of antiferromagnetic superconductors[10, 11, 12]:

$$\zeta_{\boldsymbol{k}}^{\dagger} = (c_{\boldsymbol{k}\uparrow}^{\dagger}, c_{\boldsymbol{k}\downarrow}^{\dagger}, c_{-\boldsymbol{k}\uparrow}, c_{-\boldsymbol{k}\downarrow}, c_{\boldsymbol{k}+\boldsymbol{Q}\uparrow}^{\dagger}, c_{\boldsymbol{k}+\boldsymbol{Q}\downarrow}^{\dagger}, c_{-\boldsymbol{k}-\boldsymbol{Q}\uparrow}, c_{-\boldsymbol{k}-\boldsymbol{Q}\downarrow}) \tag{1}$$

using nambu notation we may write our mean-field Hamiltonian in the compact form $\mathcal{H} = \sum_{\boldsymbol{k}} \zeta_{\boldsymbol{k}}^{\dagger} \hat{E}_{\boldsymbol{k}} \zeta_{\boldsymbol{k}}$, where:

$$\hat{E}_{\boldsymbol{k}} = \gamma_{\boldsymbol{k}} \hat{\tau}_3 \hat{\rho}_3 + \delta_{\boldsymbol{k}} \hat{\rho}_3 - W \hat{\tau}_1 \hat{\rho}_3 - M_z \hat{\tau}_1 \hat{\rho}_3 \hat{\sigma}_3 - (F_z + \mu_B H)\, \hat{\rho}_3 \hat{\sigma}_3 \tag{2}$$

in the presence of a Zeeman field ($\mu_B H$) and $\hat{\tau}_i, \hat{\rho}_j, \hat{\sigma}_k \quad i,j,k = 0,1,2,3$ are Pauli matrices whose Kronecker products form a convenient basis to work with.

Starting from the third term on the rhs of eq. 2 we identify the Order Parameters (OPs) that we include in our study: W is the Charge Density Wave (CDW) gap, M_z, F_z are the Spin Density Wave and itinerant ferromagnetic components respectively, polarized along the z-axis. The above orders along with the order parameter (OP) for the spin dependent pomeranchuk instability, $A_{\boldsymbol{k}}^z$, form a closed group in the sense that no other OP may be induced from the ones already considered here. A more complete study including the implications the $A_{\boldsymbol{k}}^z$ term may arise is to be addressed in a separate work. A discussion about such emerging patterns of coexisting phases can be found in [13].

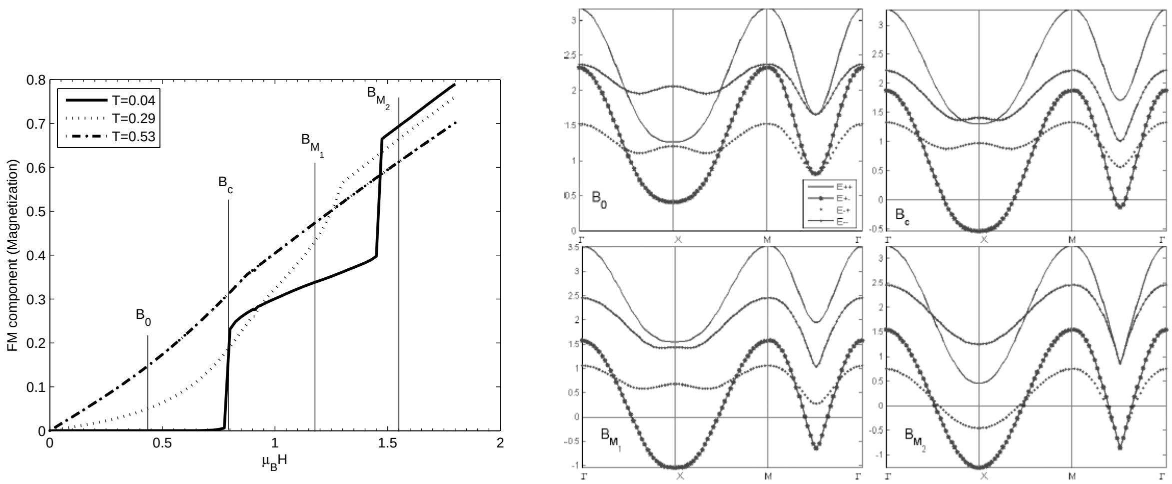

Figure 1. a) Magnetization versus the applied magnetic field for different temperatures. At the lowest-T regime (full line) two metamagnetic steps are evident, whereas for higher temperatures (dotted, dot-dashed) the steps are relaxed. b) Quasiparticle energy spectrum along high symmetry lines of the 1st Brillouin zone of the square lattice when the external magnetic field takes the values:B_0,B_c,B_{M_1} and B_{M_2} noted in the previous figure with vertical lines. Note that because of the presence of three order parameters, our one band tight binding dispersion splits into four branches each-one noted with a different line. We observe that the emergence of the metamagnetic step coincides with the crossing of the Fermi level by a new quasiparticle branch accounting for the related anomalies observed by quantum oscillations measurements.

We have decomposed the energy of the unperturbed system into periodic and antiperiodic terms in respect with the density wave nesting wavevector $\boldsymbol{Q}$: $\xi_{\boldsymbol{k}} = \gamma_{\boldsymbol{k}} + \delta_{\boldsymbol{k}}$, with $\gamma_{\boldsymbol{k}+\boldsymbol{Q}} = -\gamma_{\boldsymbol{k}}$

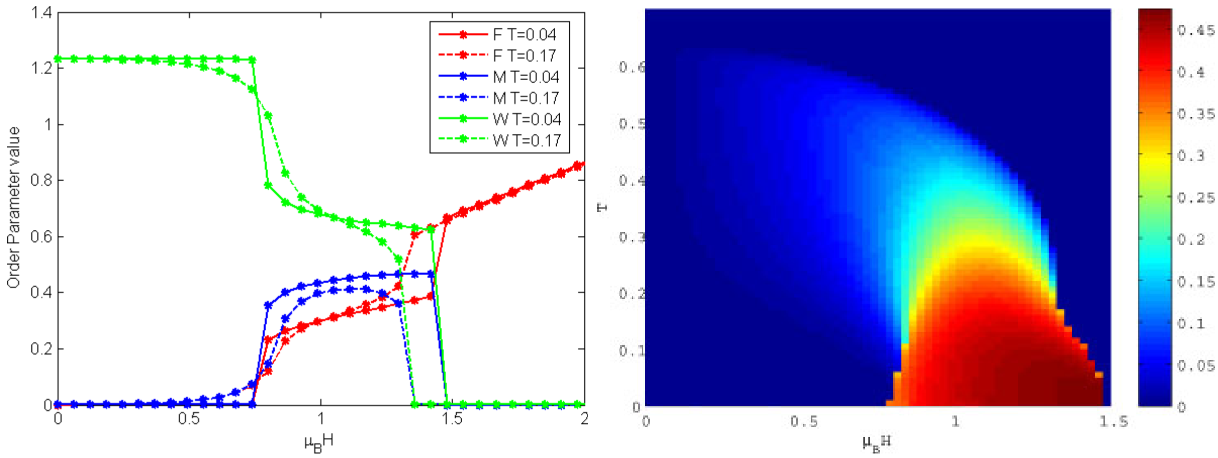

Figure 2. a) The field dependence of the three order parameters at the lowest temperature regime (full lines) and a finite temperature regime (dashed lines). The field induces simultaneously a SDW (blue) and a FM (red) component while weakening the CDW (green). As temperature is rised, critical points of 1st order transitions move towards each other, narrowing the metamagnetic step. b) Filed and temperature dependence of the SDW order parameter. In the low-T regime it builts up in a first order transition at the 1st metamagnetic step (dark blue - red interface) and dissappears at the second metamagnetic step (red - dark blue interface) in a first order transition as well. The end of the dark blue - red interfaces corresponds to a critical end-point. Note that in the low field regime a very weak SDW component exists up to very high temperatures compared to its magnitude (the temperatures at which the CDW develops). This is a weak induced SDW order because of particle-hole asymmetry that may be a missing piece to the puzzle of multiple hidden orders observed in URu_2Si_2[9] and elsewhere.

and $\delta_{\boldsymbol{k}+\boldsymbol{Q}} = \delta_{\boldsymbol{k}}$. A tetragonal system is considered here where transformations with respect to $\boldsymbol{Q} = (\pi, \pi)$ are fundamental. For calculations, a simple tight-binding band is assumed where $\gamma_{\boldsymbol{k}} = -t(\cos k_x + \cos k_y)$ and $\delta_{\boldsymbol{k}} = -t' \cos k_x \cos k_y$. For $\delta_{\boldsymbol{k}} = 0$ the system is particle-hole symmetric and perfectly nested at the wavevector $\mathbf{Q}$. When $\delta_{\boldsymbol{k}} \neq 0$ the system is considered doped and deviates from perfect nesting.

In our notation, all information about the OPs and any measurable quantities can be obtained by having as a starting point the bare Matsubara matrix Green function defined in reciprocal space as:

$$\hat{\mathcal{G}}_0(i\omega_n, \boldsymbol{k}) = \frac{1}{i\omega_n - \hat{E}_{\boldsymbol{k}}} \tag{3}$$

An analytic expression of the quasipartcle poles of the Green function may be found either by direct diagonalization of $\hat{E}_{\boldsymbol{k}}$ or by inversion of $\hat{\mathcal{G}}_0(i\omega_n, \boldsymbol{k})$. A compact form in Pauli matrix notation can be shown to be:

$$\hat{E}_{\pm\pm}(\boldsymbol{k}) = \pm\Big\{\delta_{\boldsymbol{k}} - (F_z + \mu_B H)\,\hat{\sigma}_3 \pm \Big[\gamma_{\boldsymbol{k}}^2 + M_z^2 + W^2 + 2M_z W \hat{\sigma}_3\Big]^{1/2}\Big\} \tag{4}$$

where we have neglected the $A_{\boldsymbol{k}}^z$ term as stated above.

The system of self-consistent gap equations that we get exhibits a qualitatively different structure than usual BCS-like equations. It has the following general form:

$$W_{\mathbf{k}} = \sum_n \sum_{\mathbf{k}'} V_{\mathbf{k}\mathbf{k}'}^{CDW} \Big\{ W_{\mathbf{k}'}\{...\} + \delta_{\mathbf{k}'} M_{\mathbf{k}'} F_{\mathbf{k}'}\{...\} \Big\}$$

$$\begin{aligned} M_{\mathbf{k}} &= \sum_n \sum_{\mathbf{k}'} V^{SDW}_{\mathbf{k}\mathbf{k}'} \Big\{ M_{\mathbf{k}'}\{...\} + \delta_{\mathbf{k}'} W_{\mathbf{k}'} F_{\mathbf{k}'}\{...\} \Big\} \\ F_{\mathbf{k}} &= \sum_n \sum_{\mathbf{k}'} V^{FM}_{\mathbf{k}\mathbf{k}'} \Big\{ F_{\mathbf{k}'}\{...\} + \delta_{\mathbf{k}'} W_{\mathbf{k}'} M_{\mathbf{k}'}\{...\} \Big\} \end{aligned} \tag{5}$$

On the right hand side of each of the gap equations, there are terms which *are not proportional to the gap of the left hand side.* When there is particle-hole asymmetry (i.e. $\delta_{\mathbf{k}} \neq 0$) then if two of the order parameters are non-zero, zero is not a trivial self-consistent solution for the third order parameter which has to be non-zero as well. Therefore, *in the presence of both CDW and SDW orderings, particle-hole asymmetry would imply the presence of a FM component* which corresponds in fact to a generalization of the picture of excitonic FM.

We have solved the above system of coupled self-consistent gap equations numerically with an iterative technique. We have chosen $t = 1$ so that we get a bandwidth of 4. The relevant parameters that we have varied are temperature, external magnetic field and doping which is imposed by t'. We have also explored a large phase space of combinations of the pairing potentials so that we can verify that our qualitative results are quite generic. In this report we present a particle-hole asymmetric scenario where $t'/t = 0.4$, $V^{CDW}/V^{SDW} = 1.2$ and $V^{FM} = V^{SDW} = 2.5t$. Four values of the external field are discerned: B_0, B_c, M_{M_1} and B_{M_2} which correspond to the region before the 1st step-like metamagnetic transition, just after the 1st step, right in the middle of the 1st step and after the 2nd metamagnetic step as shown in Fig.1a. The discussion is embodied to the figure captions to save space.

In conclusion, we present here some of our results on a system of competing and coexisting CDW, SDW and FM within a mean-field approach. We show that this pattern of order parameters is quite generic imposed by particle-hole asymmetry in the presence of a magnetic field. Moreover, an external magnetic field may trigger double-step metamagnetic transitions very similar to those reported in various systems such as $Sr_3Ru_2O_7$ and URu_2Si_2 accompanied by the emergence of new Fermi surface sheets. An extensive study dedicated to those materials will be presented elsewhere where we intent to address also the implications of a spin dependent pomeranchuk instability [14, 15].

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