Disentangling Canted Phases and Phase Separation Regions with Spin Waves in Doped Manganites

J. M. Román *CSIC, Madrid.*

J. Soto *Univ. de Barcelona.*

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The system: Doped manganites present a rich phase structure at zero temperature: antiferromagnetic, canted and ferromagnetic phases, together with phase separation regions.

The problem: Upon increasing the doping the system goes from an AF-insulator to a F-conductor. It is not clear if in its way passes through a canted phase or a phase separation region (F-AF).

A solution: The interaction of the spin waves with the charge carriers lead to a doping dependence of the dispersion relation of the spin waves. This may allow to experimentally differentiate canted phases from phase separation regions in doped manganites.

Doped Manganites

The manganites are a generic group of alloys which present a rich magnetic structure in their ground state, from antiferromagnetism to ferromagnetism going through canted phases (i.e., a non-collinear arrange of the magnetic moments with $0 < \theta < \pi$) or phase separation regions [1, 2, 3, 4, 5].

General Formula:

$$La_{1-x}A_xMnO_3 \qquad \begin{array}{l} A = Ca^{2+},\ Sr^{2+},\ Ba^{2+} \\ (0 \leq x \leq 1) \\ La^{3+},\ Mn^{3+},\ or\ Mn^{4+} \end{array}$$

Each substitution $La^{3+} \to A^{2+}$ corresponds in the manganese atom to $Mn^{3+} \to Mn^{4+}$.

Electronic Structure:

$$3d \text{ (5-fold)} \longrightarrow \begin{cases} t_{2g} & \text{(3-fold)} \\ e_g & \text{(2-fold)} \end{cases}$$

Magnetic Structure:

$$LaMnO_3 \text{ and } AMnO_3 \longrightarrow \text{Ground State: AF-insulator.}$$

$$La_{1-x}A_xMnO_3 \ \ (0.2 \leq x \leq 0.4) \longrightarrow \text{Ground State: F-conductor.}$$

Continuum Double Exchange Model

Double Exchange Model by Zener [2] suggested a relation between the electronic and magnetic properties through the exchange of electrons among the Mn^{3+} and Mn^{4+} ions.

Low energy and momentum properties of the system can be studied from a continuum model, Continuum Double Exchange Model, where the fields representing the excitations are slowly varying in space and time:

- Background Magnetizations are generated by the magnetic moments in the t_{2g}-band: $\mathbf{M}_1(x)$ and $\mathbf{M}_2(x)$.
- Charge Carriers correspond to the holes generated in the e_g-band as the doping increases: $\psi_1(x)$ and $\psi_2(x)$, which interact locally (Hund coupling) with the corresponding magnetization.

$$\begin{aligned}
\mathcal{L}(x) \;=\; & \psi_1^\dagger(x)\left[(1+i\epsilon)i\partial_0 + \frac{\partial_i^2}{2m} + \mu + J_H\frac{\boldsymbol{\sigma}}{2}\mathbf{M}_1(x)\right]\psi_1(x) \\
& + \psi_2^\dagger(x)\left[(1+i\epsilon)i\partial_0 + \frac{\partial_i^2}{2m} + \mu + J_H\frac{\boldsymbol{\sigma}}{2}\mathbf{M}_2(x)\right]\psi_2(x) \\
& + t\left(\psi_1^\dagger(x)\psi_2(x) + \psi_2^\dagger(x)\psi_1(x)\right) - J_{AF}\mathbf{M}_1(x)\mathbf{M}_2(x).
\end{aligned}$$

$2m \sim \dfrac{z}{a^2 t}$, $\qquad$ (a - lattice spacing, $z = 6$ - coordination number)

Effective Potential: Phase Diagram

The integration of the fermionic fields in the path-integral yields an effective potential for doped manganites ($t \ll J_H$) in terms of $y = \cos(\theta/2)$ (θ is the angle between $\mathbf{M}_1$ and $\mathbf{M}_2$) in doped manganites.

$$V_{eff} = V_0 \left[(2y^2 - 1) - A \left((y_0 + y)^{5/2} \theta(y_0 + y) + (y_0 - y)^{5/2} \theta(y_0 - y) \right) \right]$$

$$V_0 = J_{AF} M^2 \qquad\qquad A = \frac{z^{3/2}}{15\pi^2} \frac{t}{(J_{AF} a^3 M^2)}$$

$$\text{Chemical potential} \sim y_0 \longrightarrow \text{Doping: } x = -\frac{a^3}{t} \frac{\partial V_{eff}}{\partial y_0}$$

Upon minimization with respect to y the following phases arise:

Antiferromagnetic: $y = 0$, AFI, $AFC2$

Canted: $0 < y < 1$, $CC1$, $CC2$

Ferromagnetic: $y = 1$, $FC1$

- For typical values of the coupling constants $A \sim 1 - 2$.
- In this range either, canted phases or phase separation regions can arise from the phase diagram shown in fig. 1.

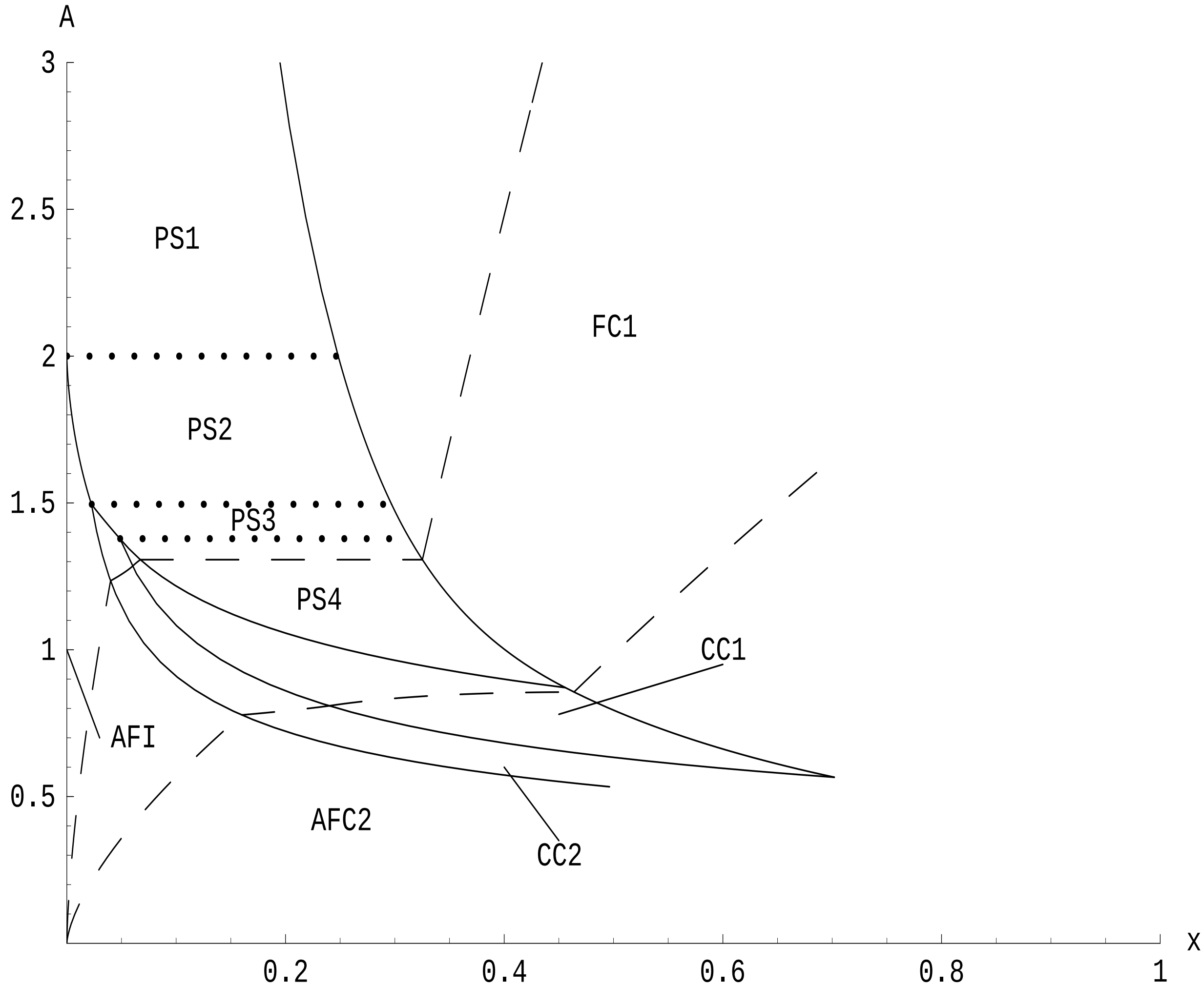

Figure 1: Phase diagram in the (x, A) plane.
AFI: Antiferromagnetic Insulator ($x = 0$)
AFC2: Antiferromagnetic Conductor (2-bands)
CC2: Canted Conductor (2-bands)
CC1: Canted Conductor (1-band)
FC1: Ferromagnetic Conductor (1-band)
PSi: Phase Separation regions ($i = 1, 2, 3, 4$)

Effective Lagrangian for Spin Waves

In magnetically ordered systems the spontaneous symmetry breaking of the $SU(2)$ group and the crystallographic group allows to write an effective lagrangian for the lowest lying excitation: spin waves [6].

$$\left.\begin{array}{c}\text{charge carriers}\\ +\\ \text{background magnetization}\end{array}\right\} \longrightarrow \left\{\begin{array}{c}\text{doping dependence}\\ \text{of the}\\ \text{dispersion relation}\end{array}\right.$$

Canted Spin Waves: $(0 < \theta < \pi)$

$$\begin{aligned}\mathcal{L}(x) \;=\;& \pi^- i\partial_t \pi^+ - \frac{1}{2m'}\partial_i\pi^-\partial_i\pi^+ && \longleftarrow \quad \text{One branch}\\ &+\frac{1}{2}\partial_t\pi^3\partial_t\pi^3 - \frac{v^2}{2}\partial_i\pi^3\partial_i\pi^3 && \longleftarrow \quad \text{One branch}\end{aligned}$$

$$\begin{aligned}\frac{1}{2m'} \;\sim\;& \frac{1}{(2M+x)y}\sqrt{2-4y^2+\frac{5A}{2}\left(\frac{6\pi^2 x}{z^{3/2}}\right)}\\ &\times\sqrt{\frac{5A}{2}\left(\frac{6\pi^2 x}{z^{3/2}}\right)-2y^2-2\,\Pi_{+-}(1-y^2)}\end{aligned}$$

$$v^2 \;\sim\; \frac{1}{M^2}\left[2+\frac{5A}{2}\left(\frac{6\pi^2 x}{z^{3/2}}\right)\right](1-y^2)$$

y and Π_{+-} depend on the doping x.

Ferromagnetic Spin Waves: $(\theta = 0)$

$$\mathcal{L}(x) = \pi^- i\partial_t \pi^+ - \frac{1}{2m'}\partial_i \pi^- \partial_i \pi^+ \qquad \longleftarrow \qquad \text{One branch}$$

$$\frac{1}{2m'} \sim \frac{1}{(2M + x)}\left[-2 + \frac{5A}{2}\left(\frac{6\pi^2 x}{z^{3/2}}\right)\right]$$

Antiferromagnetic Spin Waves: $(\theta = \pi)$

$$\mathcal{L}(x) = \partial_t \pi^- \partial_t \pi^+ - v^2 \partial_i \pi^- \partial_i \pi^+ \qquad \longleftarrow \qquad \text{Two branches}$$

$$v^2 \sim \frac{1}{M^2}\left[2 + \frac{5A}{2}\left(\frac{6\pi^2 x}{z^{3/2}}\right)\right]$$

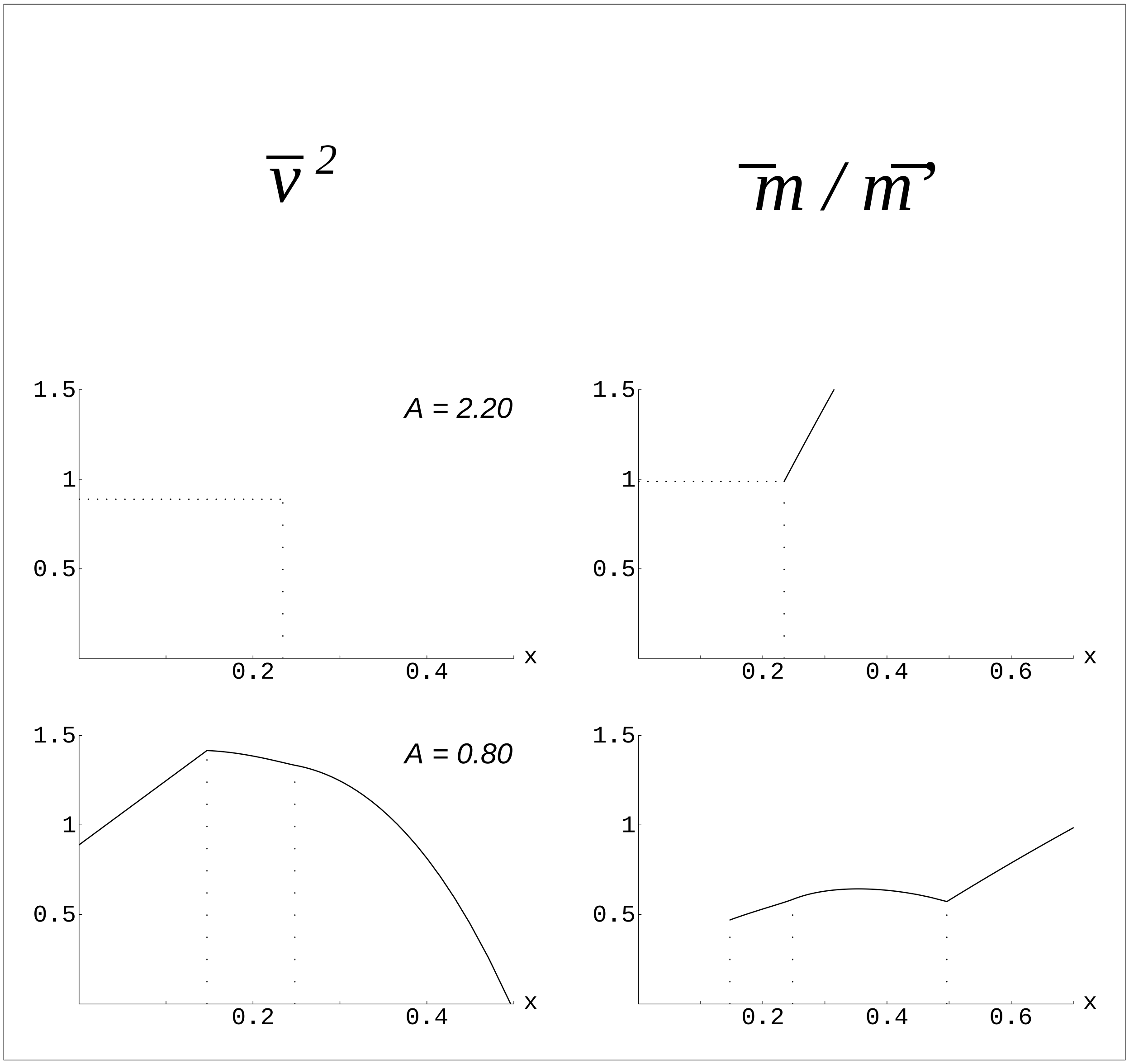

Figure 2: Doping dependence of the velocities and the masses.
$A = 2.20 \longrightarrow F - AF$ phase separation region
$A = 0.80 \longrightarrow$ canted phase
Horizontal dotted lines correspond to the phase separation regions, and the vertical dotted lines correspond to the phase transitions.

Canted Phases vs. Phase Separation

Phase Separation Region guess:

- Two macroscopic F and AF domains.
- The interphase does not modifies qualitatively the properties.

Under such circumstances:

PS: One F and two AF spin wave branches

C: One F and one AF spin wave branches (see [7])

PS: Splitting of the AF branches by a magnetic field

C: No modification of the AF branch by a magnetic field

Different behavior of the mass and velocity with the doping

PS: Phase Separation: in fig. 2 $A = 2.20$

C: Canted Phase: in fig. 2 $A = 0.80$

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