Double Exchange I:
A Simple Introduction

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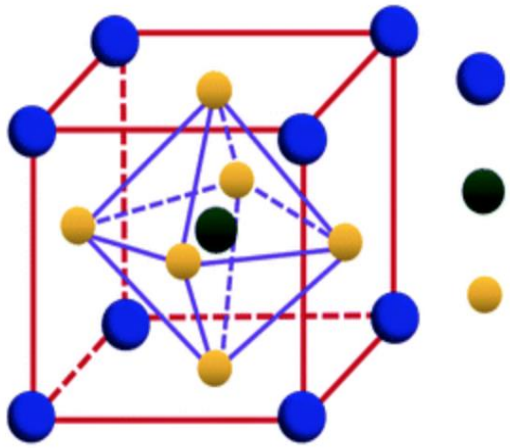
Background: Ferromagnetic compounds of manganese with perovskite structure



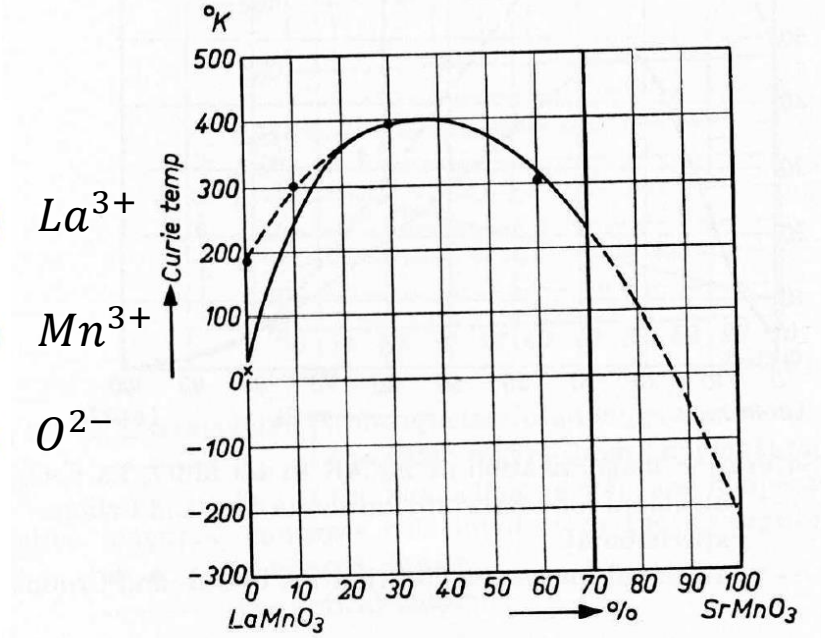
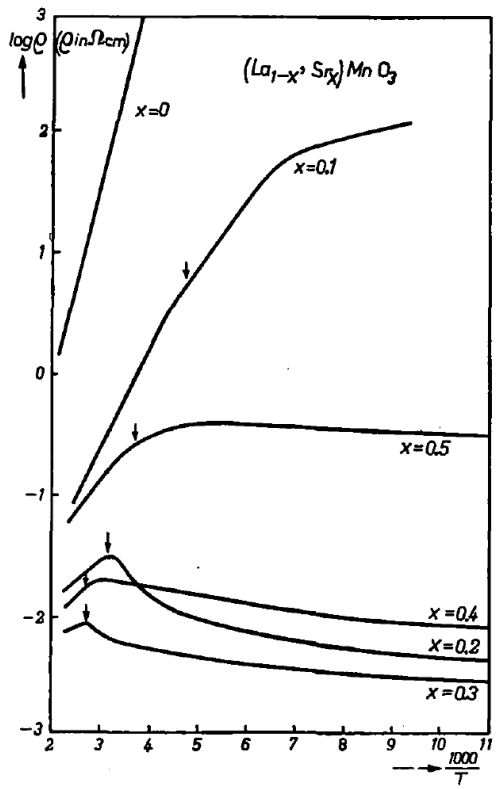
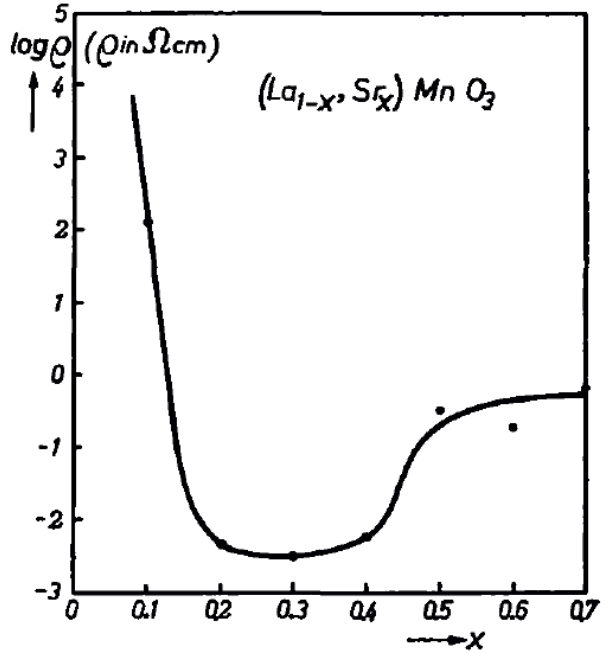


Fig. 8. Curietemperature of La MnO_3-Sr MnO_3.
• • •: extrapolated paramagnetic Curietemperature
———: ferromagnetic Curietemperatures.



$T = 100K$



1. Standard ceramic technique

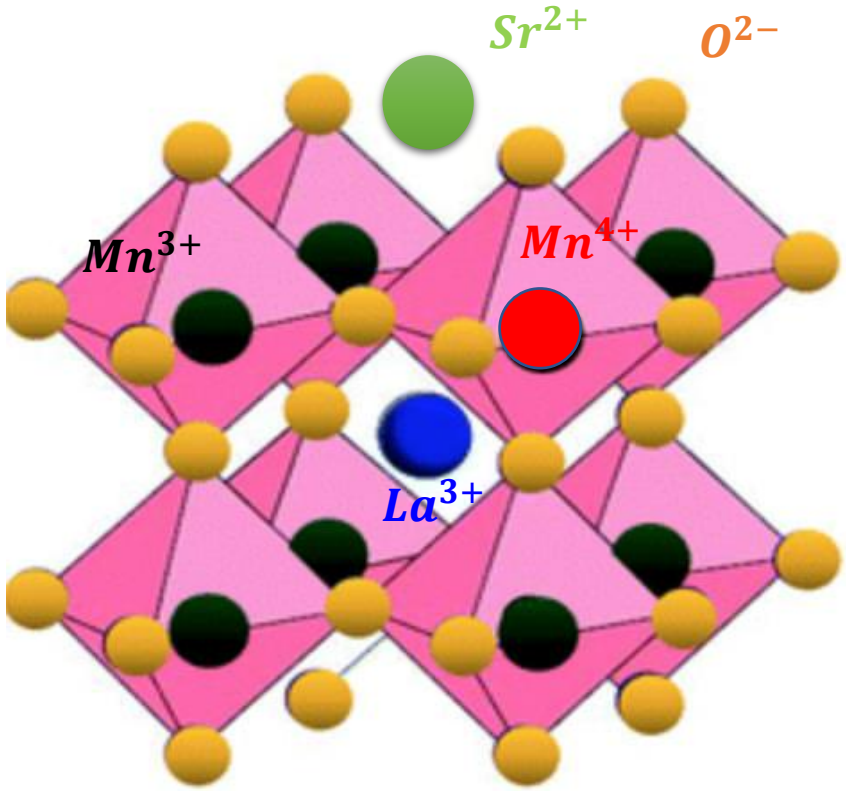
2. $(La^{3+}_{1-x}Me^{2+}_{x})(Mn^{3+}_{1-x}Mn^{4+}_{x})O_3$; Me: large divalent ion like Ca^{2+}, Sr^{2+}, Ba^{2+}, Cd^{2+}, Pb^{2+}

3, $x = 0,\ 1$: Semiconductor; $0.2 < x < 0.4$: ferromagnetism and good conductivity

4, Correlation between magnetism and conductivity

G.H.Jonker and J.H. Van Santen, Physica 16, 337 (1950)
G.H.Jonker and J.H. Van Santen, Physica 16, 599 (1950)
G.H.Jonker, Physica 22, 707 (1956)

Double Exchange Mechanism: Indirect exchange via conduction electrons



$(La^{3+}_{1-x}Sr^{2+}_{x})(Mn^{3+}_{1-x}Mn^{4+}_{x})O_3$

$Sr^{2+}: [Kr]$

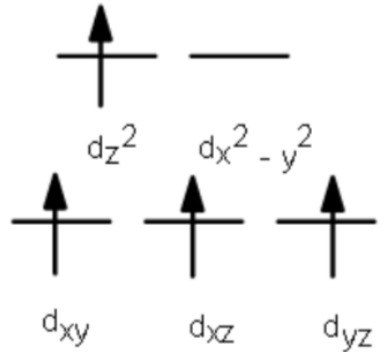
$La^{3+}: [Xe]$

$O^{2-}: [Ne]$

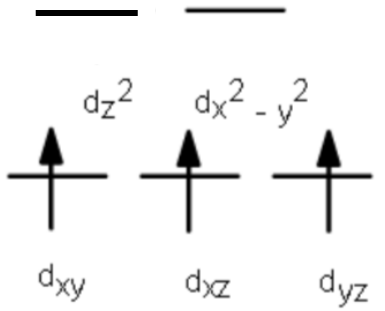
$Mn^{3+}: [Ar]3d^4$

$Mn^{4+}: [Ar]3d^3$

Mn^{3+}



Mn^{4+}



1. **Only Mn ions with incomplete d band**
2. **Both Magnetism and conductivity from Mn ions: their interactions with each other and the crystal field**

Double Exchange Mechanism: Indirect exchange via conduction electrons

$\varphi(r - R_1)$: $\boldsymbol{Mn^{3+}O^{2-}Mn^{4+}}$ $\varphi(r - R_2)$: $\boldsymbol{Mn^{4+}O^{2-}Mn^{3+}}$

Assumptions:

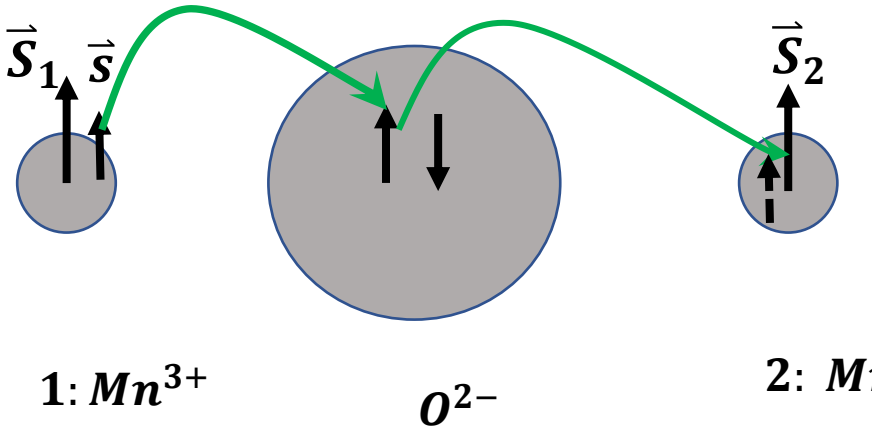
(1) Like free ions, all unpaired spins of incomplete 3d electrons pointing to the same direction;

(2) Exchange between d shells of adjacent atoms is antiferromagnetic and much smaller than double exchange

(3) The spin of an incomplete d shell is strongly coupled to the spin of conduction electrons (b << J)

(4) Conduction electrons do not change their spin orientation when Moving; accordingly they can hop from one ion to the next only if the two ionic spins are not antiparallel

(5) $\vec{s}$ is parallel to $\vec{S}_1$ when in atom 1, while it is parallel to $\vec{S}_2$ when In atom 2 .



$$\Delta H = \begin{bmatrix} -JS & b \\ b & -JS \end{bmatrix}$$

where, J is the exchange integral between $\vec{s}$ **and** $\vec{S}_i, \boldsymbol{i = 1, 2}$;
transfer integral $b = \langle \varphi(r - R_2) | \Delta H | \varphi(r - R_1) \rangle$
$\approx 0.5 - 1\ eV$

C. Zener, Phys.Rev. 82, 403 (1951)
P. W. Anderson and H. Hasegawa, Phys. Rev. 100, 675 (1955)

Double Exchange Mechanism: Indirect exchange via conduction electrons

$$\Delta H: \quad \begin{matrix} & \varphi(r-R_1) & \varphi(r-R_2) \\ \varphi(r-R_1) & \\ \varphi(r-R_2) & \end{matrix} \begin{bmatrix} -JS & b \\ b & -JS \end{bmatrix} \qquad \|\Delta \boldsymbol{H} - \Delta \boldsymbol{E}\| = \mathbf{0}$$

Eigenvalues:

$$\Delta \boldsymbol{E} = -\boldsymbol{JS} \pm \boldsymbol{b}$$

Eigenvectors:

$$\boldsymbol{\varphi}_{\pm} = \frac{\mathbf{1}}{\sqrt{\mathbf{2}}}[\varphi(r-R_1) \pm \varphi(r-R_2)]$$

If $\boldsymbol{kT_C < b}$, $\Delta \boldsymbol{E} = -\boldsymbol{JS} - \boldsymbol{b}$, ferromagnetic !

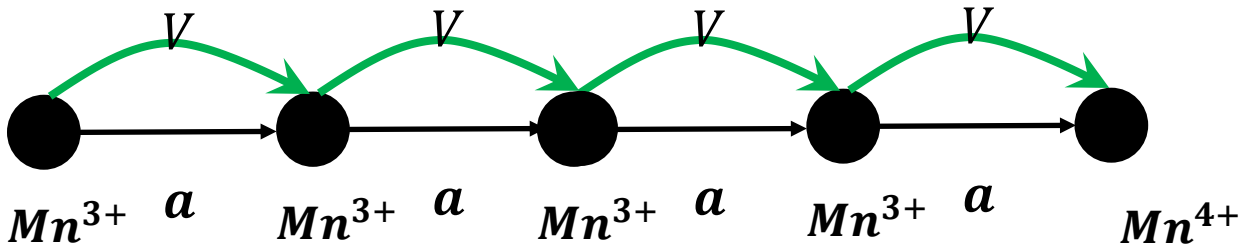
When the hopping is allowed, the ground state energy is lowered (since the conduction electrons are able to participate in the binding)

Double Exchange Mechanism: Conductivity

Hopping rate and average drift velocity of the conduction electron are :

$$\nu = \frac{2b}{h} \quad (1)$$

$$V = a\nu \quad (2)$$



Since the diffusion coefficient D satisfies

$$\vec{J} = -D\nabla(xn) \quad (3)$$

Diffusion electric current $J = -(drift\ current) = -\frac{ex}{a^3}V$ (4)

$$\nabla(xn) = \frac{exn}{a} \quad (5)$$

Hence, $D = \frac{\frac{ex}{a^3}V}{\frac{exn}{a}} = aV$ (6)

Here n is the density of Mn; x is the fraction of Mn ions which have 4+ charge; a is lattice constant

Conductivity $\sigma = xne\mu$ (7), where μ is the electron mobility

Also, **Einstein relation** $\boldsymbol{D = \frac{\mu kT}{e}}$ (8)

Combing (1), (2), (6) , (7) and (8), we have

$$\sigma = \frac{2be^2x}{hakT} \quad (9)$$

If $b \approx kT_C$ (10)

$$\sigma = \frac{2e^2x}{hak}\frac{T_C}{T}. \quad (11)$$

agreeing well with the experimental data in the doping range $0.2 < x < 0.4$

C. Zener, Phys.Rev. 82, 403 (1951)