Double Exchange, Magnetism and Transport in Condensed Matter Physics

J.M.B. Lopes dos Santos\textsuperscript{1} V.M. Pereira\textsuperscript{1} E.V. Castro\textsuperscript{1} A.H. Neto\textsuperscript{2}

\textsuperscript{1}Universidade do Porto & \textsuperscript{2}Boston University

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4 Summary
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Heisenberg exchange

- Coulomb exchange between localized states

\[ J_{ij} = V_{ji} \]

- Heisenberg exchange is ferromagnetic (Pauli Principle)

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Anderson exchange

- Hopping between localized states

\[ \text{Anderson exchange is anti-ferromagnetic (Pauli Principle)} \]

\[ -J \mathbf{S}_i \cdot \mathbf{S}_j \quad J < 0 \]
Anderson exchange

- Hopping between localized states

- Anderson exchange is anti-ferromagnetic (Pauli Principle)
  \[-JS_i \cdot S_j \quad J < 0\]
Manganites

- Chemical formula, AMnO$_3$

A = La, Nd, Pr, Ca, Sr, Ba, Pb

- $A^{2+}Mn^{4+}O_3^{2-} \rightarrow Mn$ is $(3d)^3$ ($x = 1$)
- $A^{3+}Mn^{3+}O_3^{2-} \rightarrow Mn$ is $(3d)^4$ ($x = 0$)
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  E.V. Castro (MSc Thesis, UA)
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Double Exchange

\[ \text{Mn}^{4+} \quad O^{2-} \quad \text{Mn}^{3+} \]

\[ \text{Mn}^{3+} \quad O^{-} \quad \text{Mn}^{3+} \]

\[ \text{Mn}^{3+} \quad O^{2-} \quad \text{Mn}^{4+} \]

\[ t_{\text{Mn-O}} \]
Double Exchange Hamiltonian

Ferromagnetic Kondo model

\[ \hat{H}_{FK} = -\sum_{i,j,\sigma} tc_{i\sigma}^{\dagger} c_{j\sigma} - J_H \sum_{i} \sigma \cdot \mathbf{S}_i \]

\[ J_H \gg t, \quad S \gg 1 \quad \text{(classical } \mathbf{S}) \]

In low energy sector, electrons have spin parallel to \( \mathbf{Mn} \) spin.

Double Exchange (DE) Model

\[ \hat{H}_{DE} = -\sum t_{ij} \left[ \{\mathbf{S}\} \right] c_i^{\dagger} c_j t_{ij} \]

\[ t_{ij} = t \langle \theta_i, \varphi_i | \theta_j, \varphi_j \rangle = t \cos \left( \frac{\theta_{ij}}{2} \right) e^{\varphi_{ij}} \]
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Manganites are much more than DE (orbital degeneracy, phonons, charge ordering, inhomegenities).
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Effective Spin Hamiltonian

- $\{S\} \Rightarrow \mathcal{F}_{el}[\{S\}] \Rightarrow \mathcal{E}_{el}[\{S\}] \quad (T \ll T_F)$
- $\mathcal{F}_s(T) = -\beta^{-1} \ln \text{Tr}\{S\} e^{-\beta \mathcal{E}_{el}[\{S\}]}$
- Mean Field Hamiltonian, $\hat{H}_{mf} = -\mathbf{h} \cdot \sum_i S_i$

$$\mathcal{F}_{mf}(\mathcal{M}) = \langle \mathcal{E}_{el} \rangle_{pm} - TS_{pm}(\mathcal{M})$$
Effective Spin Hamiltonian

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Density of States of Disordered Systems.

Lanczos Tridiagonalization

\[ |0\rangle \]
\[ b_0 |1\rangle = \hat{H} |0\rangle - a_0 |0\rangle \]
\[ b_1 |2\rangle = \hat{H} |1\rangle - a_1 |1\rangle - b_0^* |0\rangle \]
\[ \vdots \]

\[ \begin{align*}
  a_0 &= \langle 0 | \hat{H} | 0 \rangle \\
  b_0 &= \langle 1 | \hat{H} | 0 \rangle \\
  a_1 &= \langle 1 | \hat{H} | 1 \rangle \\
  b_1 &= \langle 2 | \hat{H} | 1 \rangle
\end{align*} \]
\[ \hat{H} = \sum_{<ij>} t_{ij} c_i^\dagger c_j + \sum_i \epsilon_i c_i^\dagger c_j \]

\[
\Rightarrow \sum_n a_n |n\rangle \langle n| + b_n |n+1\rangle \langle n| + b_n^* |n\rangle \langle n+1| 
\]

\[
G_{00}(\omega) \equiv \langle 0| \frac{1}{\omega - \hat{H}} |0\rangle = \frac{1}{[G_{00}^0]^{-1} - |b_0|^2 G_{11}}
\]
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\]
DOS in PARA and FERRO states.

\[ G_{00}(\omega) = \frac{1}{\omega - a_0 - \frac{|b_0|^2}{\omega - a_1 - \frac{|b_1|^2}{\omega - a_2 - \ldots}}} \]

**Convergence of Coefficients**

**Density of states**
Structure

Eu positions define a cubic lattice

- B₆: 10 Bonding MO (filled).
- Eu²⁺: \( S_{\text{Eu}} = 7/2, a = 4.185 \, \text{Å} \).

EuB₆ is semi-metal,

- Band overlapp at X point.

or a (doped) semiconductor?

- \( \Delta_{\text{ARPES}} \sim 1 \, \text{eV} \).

Crystal Structure

Mandrus et al. (PRB, 2003)
Structure

Eu positions define a cubic lattice

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- $\text{Eu}^{2+}$: $S_{\text{Eu}} = 7/2$, $a = 4.185$ Å.

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Electronic Structure

$\Delta_{\text{ARPES}} \sim 1$ eV.

Massidda et al. (ZPB, 1997)
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ARPES measurement

Denlinger et al. (PRL, 2002)
EuB$_6$ is a ferromagnetic metal.

- $\rho(T = 0) \approx 5\, \mu\Omega\cdot\text{cm}$.
- $T_C \approx 15\, \text{K}$.
- $M_{\text{Sat.}}: 7\, \mu_B /\text{Eu}$

Small carrier density (B$_6$ vacancies)

- $n_e(T > T_C) \approx 0.003$ per unit cell.
- $n_e(T > T_C) \approx 0.009$ per unit cell.

Carrier density highly enhanced below $T_C$

DC resistivity: $\rho(T)$ adm $M$

Paschen et al (PRB, 2000)
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Paschen et al (PRB, 2000)
Blue shift of plasma frequency at $T_C$:

**FM enhances $\omega_P$**

- Broderick et al (PRB 2002)

**Scaling of $\omega_P$ with $M$**

- Broderick et al (PRB 2002)

Plasma frequency scales with the magnetization:

$$\omega_P(T, H) = \omega_P(M)$$
To insulator (upon doping).

Increasing the Ca content:

- $\rho(T)$ evolves to an insulating behavior ($T > T_C$)
- $T_C$ decreases with doping strength $\chi$.
- $n_e$ is (more) enhanced below $T_C$.

A mobility gap?

- $\rho(T)$ scales exponentially $\mathcal{M}(T)$.
- $\omega_P$ also scales exponentially with $\mathcal{M}(T)$.

$\rho(T)$ at 40% doping

Wigger et al. (PRB 2002)
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Peruchi et al. (PRL 2004)
Disorder and localization in the DEM

What can DE model provide?

- \( N(E, \mathcal{M}) \equiv \left\langle N(E, \{\vec{S}_i\}) \right\rangle_{\text{pm}} \)
  (Recursion Method)
- \( \mathcal{M} \) dependent FL, \( E_F(\mathcal{M}) \)
- \( \mathcal{M} \) dependent mobility
  edge, \( E_C(\mathcal{M}) = \left\langle E_C(E, \{\vec{S}_i\}) \right\rangle \)
  (Transfer Matrix)

\[ E_C \lesssim E_F \text{ for } n_e \sim 10^{-3}. \text{ The down shift of } E_C(\mathcal{M}) \text{ enhances } n_e! \]
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Disorder and localization in the DEM

Results for $E_C$

$(\text{Bottom of the band is at -6 in the left axis).}$

$$\Delta(M, n_e) = E_F(M) - E_C(M, n_e).$$

$E_C \lesssim E_F$ for $n_e \sim 10^{-3}$. The down shift of $E_C(M)$ enhances $n_e$!
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\end{align*}
Results for the transport properties - EuB$_6$

- **Carrier density**

- **Plasma frequency**

- Only $E_F$ is tuned for $T > T_C$.

- $\omega_P^2 \propto \langle \mathcal{H} \rangle = t \int_{E_C} E \int_{-\infty}^{\infty} N(\varepsilon, \mathcal{M}) f(\varepsilon) \varepsilon d\varepsilon$.

These (and other) results reproduce the experimental signatures of EuB$_6$!
Doping dilutes magnetic sites and hopping in the lattice: expect mobility edge to move into band.

Proposed Phase diagram

We expect $\text{Eu}_{0.60}\text{Ca}_{0.40}\text{B}_6$ to lie between $x_{\text{MI}}^P$ and $x_{\text{MI}}^F$. Above $T_C$ it has a mobility gap.
Independent Polaron

By creating a ferromagnetic bubble, an electron lowers its energy; but there is a magnetic entropy cost.

\[ \Delta F_{pol}(R, T)/n_e = 4t - 6t \cos(\pi/(R+1)) + TR^3 \log(2S+1) - TS_{cfg} \]

- Minimization gives \( R_{eq}(T) \), and stability temperature, \( T_m \).
- Percolation argument estimates \( T_C \).

Electronic wavefunction of Polaron.

Polarons are seen in Raman scattering at the predicted temperatures. \( T_C \) is depressed relative to mean-field estimate.

J. Lopes dos Santos et. al. Universidade do Porto & Boston University
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Phase separation

At low densities system does not support homogeneous phase!

- Below $T_C(n)$, there are two phases of different densities, $n_+, n_-$
- In GCE (constant $\mu$) transition is first order, $\mathcal{M}(T_C) \neq 0$, $\Delta n \neq 0$,

Phase diagram at low $n_e$.

PS region much larger than polaron region

Where have all the polarons gone?.
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Where have all the polarons gone?.
Electrons are charged!

- Electrostastic energy
  \[ E_{el} = \frac{2}{5} e^2 \pi n^2 R^2 \left( \frac{2 + x - 3x^{1/2}}{x} \right) \]

- Energy of localization
  \[ \frac{E_{loc}}{E_{\infty}(n)} = \left( 1 + \frac{15}{16} \left( \frac{\pi}{6n} \right)^{1/3} \frac{x^{1/3}}{R} \right) \]

- Equilibrium radius \( \sim R_{pol} \)

PS region shrinks to polaron region
Polarons are back!
Coulomb Suppression of Phase Separation

Electrons are charged!

- Electrostatic energy
  \( (x = V_+/V_-) \)
  \[
  \frac{E_{el}}{V} = \frac{2}{5} e^2 \pi n^2 R^2 \frac{2 + x - 3x^{1/2}}{x}
  \]

- Energy of localization
  \[
  \frac{E_{loc}}{E_\infty(n)} = \left(1 + \frac{15}{16} \left(\frac{\pi}{6n}\right)^{1/3} \frac{x^{1/3}}{R}\right)
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Controversy

Does Double Exchange apply when $J \lesssim t$?

- Yes, at very low densities.
- Low energy states have some polarization along local Mn spin direction, even at $M = 0$.
- In weak coupling one recovers $T_{C}^{RKKY}$ from DE picture.

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DE is good starting point for intermediate coupling.

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Summary

- **DE for Double Exchange or Deceptively Easy?**

- The $\text{Eu}_{1-x}\text{Ca}_x\text{B}_6$ seems to be a cleaner (if unexpected) case of a DE system.

- Simple ideas still have (some) room in Condensed Matter Theory.
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